Supplemental Information for

ELECTROSPRAY IONIZATION (ESI) FRAGMENTATIONS AND DIMETHYLDIOXIRANE REACTIVITIES OF THREE DIVERSE LACTAMS HAVING FULL, HALF, AND ZERO RESONANCE ENERGIES

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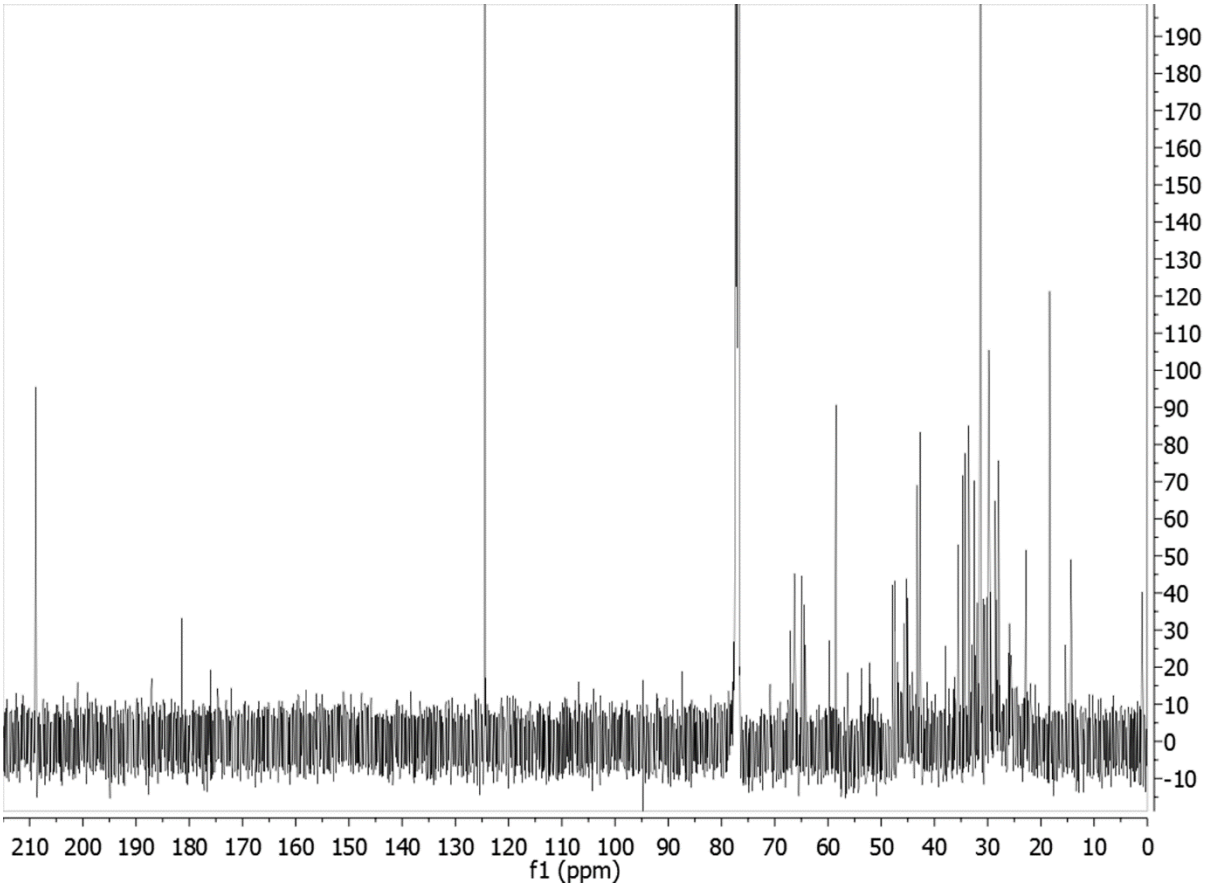
S1. NMR Spectra: Low temperature reaction with DMDO



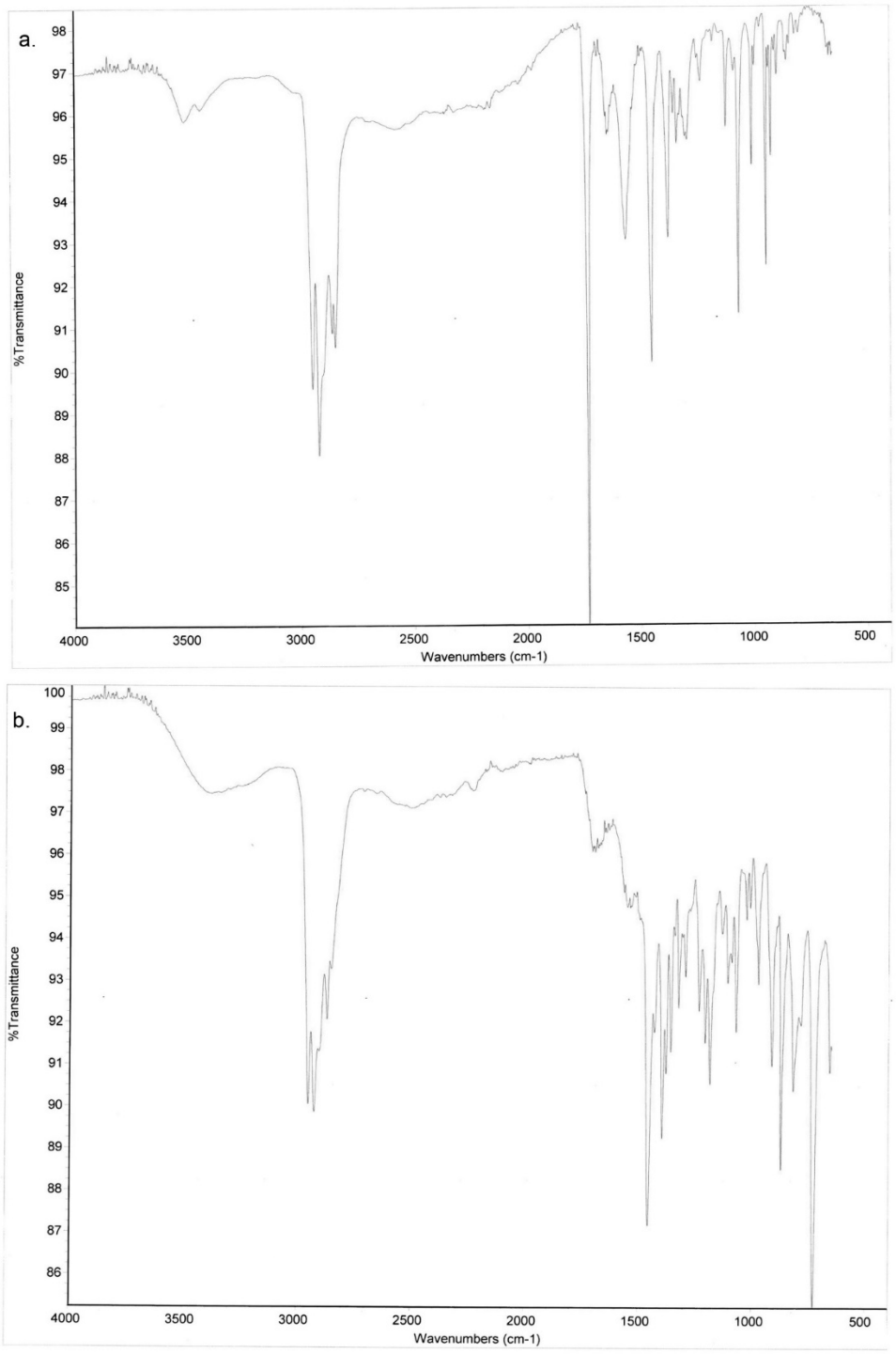
^{13}C-NMR spectrum derived from mixing DMDO/$CDCl_3$ and Kirby lactam/$CDCl_3$ pre-cooled and monitoring at -50 ^{o}C.

A low-temperature NMR study of the reaction between DMDO and Kirby lactam (slight excess) was performed by mixing $CDCl_3$ solutions pre-cooled in dry ice acetone in an NMR tube and immediately placing it in the instrument probe pre-cooled to -50 ^{o}C. The resulting ^{13}C-NMR spectrum is shown above. Residual acetone is observed at 206 ppm and 31 ppm. Particularly intriguing were very small resonances at 87.4, 94.7 and 106.9 ppm. DMDO exhibits peaks at 102.3 and 22.7 ppm in acetone[1,2] and 101.2 and 22.8 ppm in $CDCl_3$.[3] It is possible that the 106.9 ppm shift corresponds to either a hydrate or to 3,3,6,6-tetramethyl-1,2,4,5-tetraoxane (107.48 ppm).[4] The shifts at 87.4 and 94.7 are intriguing due to the low-field predicted values for the N-oxide **8** or possibly even a species such as **24** derived extrusion of CO from **8**. Allowing the

solution to warm to ambient temperature provided the same NMR spectrum that arises from mixing at ambient temperature.

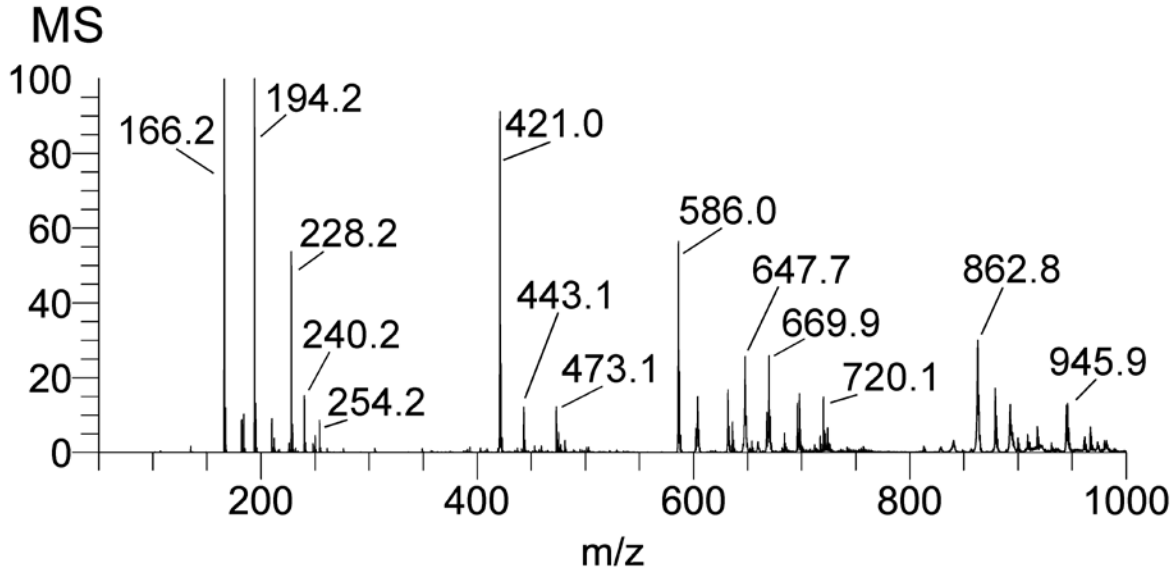
1. Murray, R.W.; Jeyaraman, R.; Pilley, M.K., *J. Org. Chem.* **1987**, *52*, 746.
2. Adam, W.; Chan, Y.Y.; Cremer, D.; Gauss, J.; Scheutzuw, D.; Schindler, M., *J. Org. Chem.* **1987**, *52*, 2800.
3. Gibert, M.; Ferrer, M.; Sánchez-Baeza, F.; Messeguer, A., *Tetrahedron* **1997**, *53*, 8643.
4. Dong, Y.; Vennerstrom, J.L., *J. Heterocycl. Chem.* **2001**, *38*, 463.

S2. IR spectra/discussion of the Kirby lactam before and after oxidation.

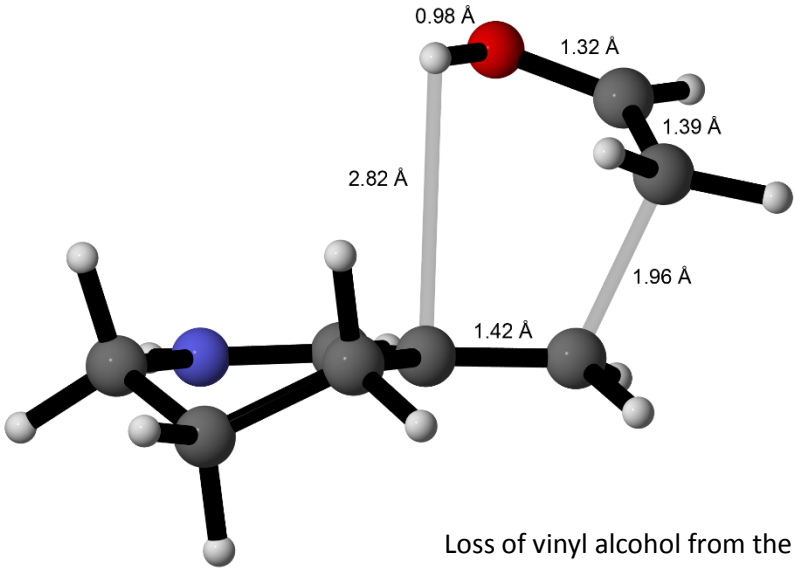


a. and b. compare the infrared spectra obtained for Kirby lactam (dried) and for the TLC R_f 0.75 fraction.

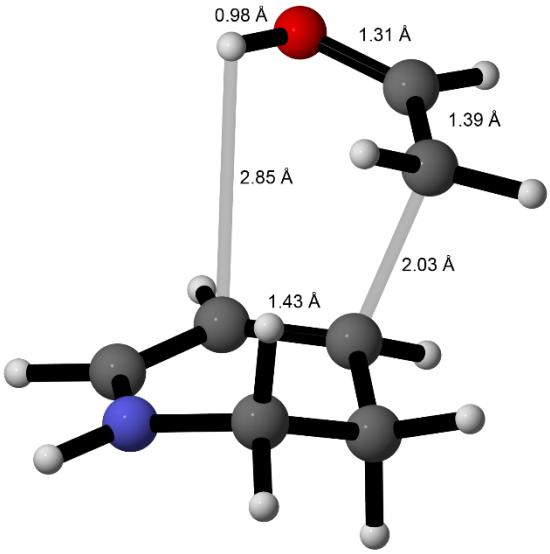
S3. ESI/MS spectra of Rf 0.75 material



S4. Transition State Structures for the McLafferty rearrangement of 1-Azabicyclo[3.3.1] nonan-2-one and 1-Azabicyclo[2.2.2]octan-2-one.



Loss of vinyl alcohol from the 3.3.1 system



Loss of vinyl alcohol from the 2.2.2 system

S5. Ground State Cartesian Coordinates and Energies (0 imaginary modes)

O-Protonated 2-Pyrrollidinone, C1, B3LYP/6-31G*

Energy = -286.979445 au

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.787541	0.009102	0.003611
2	6	0	0.068396	1.228624	0.121822
3	6	0	1.488765	0.681736	-0.160111
4	6	0	1.386822	-0.840949	0.092456
5	7	0	-0.077190	-1.087409	-0.023622
6	1	0	-0.050892	1.626723	1.138890
7	1	0	-0.266461	2.008455	-0.567966
8	1	0	1.762124	0.870168	-1.201277
9	1	0	2.244864	1.144654	0.475131
10	1	0	1.708755	-1.140376	1.094364
11	1	0	1.914453	-1.445697	-0.647267
12	8	0	-2.084958	0.105933	-0.040832
13	1	0	-2.563422	-0.744743	-0.091398
14	1	0	-0.468080	-2.025859	-0.055126

Zero-point correction=	0.122256 (Hartree/Particle)
Thermal correction to Energy=	0.127874
Thermal correction to Enthalpy=	0.128818
Thermal correction to Gibbs Free Energy=	0.093274
Sum of electronic and zero-point Energies=	-286.857189
Sum of electronic and thermal Energies=	-286.851571
Sum of electronic and thermal Enthalpies=	-286.850627
Sum of electronic and thermal Free Energies=	-286.886172

N-Protonated 2-Pyrrollidinone, C1, B3LYP/6-31G*

Energy = -286.964311 au

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.968068	0.118069	0.009813
2	6	0	-0.016195	1.273217	0.139720
3	6	0	1.378015	0.748684	-0.237836
4	6	0	1.387861	-0.723104	0.210352

5	7	0	-0.011822	-1.200374	-0.092807
6	1	0	-0.062550	1.606600	1.186891
7	1	0	-0.378131	2.103706	-0.473823
8	1	0	1.539654	0.822158	-1.318585
9	1	0	2.177560	1.307454	0.252198
10	1	0	1.532673	-0.822405	1.288577
11	1	0	2.115442	-1.346978	-0.310116
12	1	0	-0.364760	-1.927852	0.539347
13	1	0	-0.100025	-1.572233	-1.047061
14	8	0	-2.133348	-0.033629	-0.025010

Zero-point correction=	0.122051 (Hartree/Particle)
Thermal correction to Energy=	0.127821
Thermal correction to Enthalpy=	0.128766
Thermal correction to Gibbs Free Energy=	0.092746
Sum of electronic and zero-point Energies=	-286.842260
Sum of electronic and thermal Energies=	-286.836490
Sum of electronic and thermal Enthalpies=	-286.835546
Sum of electronic and thermal Free Energies=	-286.871566

Initial Acylium Ion from 2-Pyrrolidinone, C1, B3LYP/6-31G*

Energy = -286.906211 au

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.611588	-0.416113	-0.195052
2	1	0	-3.298016	0.118061	0.328435
3	1	0	-2.949601	-1.368066	-0.286769
4	6	0	-1.285376	-0.341420	0.385582
5	1	0	-0.782538	-1.310475	0.264234
6	1	0	-1.276724	-0.110886	1.464021
7	6	0	-0.507986	0.742823	-0.382509
8	1	0	-1.017385	1.709486	-0.310484
9	1	0	-0.439894	0.488690	-1.443192
10	6	0	0.933967	1.025626	0.200082
11	1	0	0.901277	1.239722	1.280475
12	1	0	1.415170	1.877802	-0.305701
13	6	0	1.820658	-0.083307	0.032297
14	8	0	2.495156	-0.974235	-0.129795

Zero-point correction=	0.117212 (Hartree/Particle)
Thermal correction to Energy=	0.124841
Thermal correction to Enthalpy=	0.125785

Thermal correction to Gibbs Free Energy=	0.084791
Sum of electronic and zero-point Energies=	-286.788999
Sum of electronic and thermal Energies=	-286.781371
Sum of electronic and thermal Enthalpies=	-286.780426
Sum of electronic and thermal Free Energies=	-286.821421

Crotti Proposed Acylium Ion Product from 2-Pyrrolidinone, C1, B3LYP/6-31G*

Energy = -230.323087 au

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.002140	-0.532102	-0.234104
2	1	0	2.830950	-1.033791	0.257084
3	1	0	1.974470	-0.584112	-1.319997
4	6	0	1.099920	0.131795	0.488769
5	1	0	1.130842	0.176870	1.573040
6	6	0	-0.047401	0.911300	-0.167802
7	1	0	-0.273798	1.870276	0.323889
8	1	0	0.115954	1.105243	-1.238970
9	6	0	-1.229291	0.082022	-0.071961
10	8	0	-2.091328	-0.636573	0.039442

Zero-point correction=	0.077129 (Hartree/Particle)
Thermal correction to Energy=	0.082655
Thermal correction to Enthalpy=	0.083599
Thermal correction to Gibbs Free Energy=	0.048339
Sum of electronic and zero-point Energies=	-230.245958
Sum of electronic and thermal Energies=	-230.240432
Sum of electronic and thermal Enthalpies=	-230.239488
Sum of electronic and thermal Free Energies=	-230.274748

Ammonia, C3v, B3LYP/6-31G*

Energy = -56.547948 au

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.000000	0.000000	0.119364
2	1	0	0.000000	0.938690	-0.278517
3	1	0	-0.812929	-0.469345	-0.278517
4	1	0	0.812929	-0.469345	-0.278517

Zero-point correction=	0.033850 (Hartree/Particle)
Thermal correction to Energy=	0.036711
Thermal correction to Enthalpy=	0.037655
Thermal correction to Gibbs Free Energy=	0.015807
Sum of electronic and zero-point Energies=	-56.514098
Sum of electronic and thermal Energies=	-56.511237
Sum of electronic and thermal Enthalpies=	-56.510293
Sum of electronic and thermal Free Energies=	-56.532141

O-Protonated, N-Ethyl-2-pyrrollidinone, C1, B3LYP/6-31G*

Energy = -365.621559 au

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.553140	0.814290	-0.035378
2	7	0	0.270958	-0.160083	-0.287638
3	6	0	-0.422415	-1.473971	-0.323412
4	6	0	-1.800735	-1.175509	0.303630
5	6	0	-1.968372	0.355414	0.157226
6	1	0	-0.480493	-1.798447	-1.367970
7	1	0	0.161563	-2.207189	0.236485
8	1	0	-1.800872	-1.450928	1.361204
9	1	0	-2.600860	-1.729700	-0.188712
10	1	0	-2.435849	0.833735	1.024225
11	1	0	-2.552538	0.639201	-0.729266
12	8	0	-0.117083	2.052436	-0.004669
13	1	0	-0.830754	2.685918	0.190907
14	6	0	1.717396	-0.019302	-0.571621
15	1	0	1.927851	-0.679706	-1.418183
16	1	0	1.887442	1.009707	-0.893816
17	6	0	2.581155	-0.372512	0.640300
18	1	0	3.634348	-0.271564	0.362168
19	1	0	2.421883	-1.403353	0.971219
20	1	0	2.384898	0.302959	1.478085

Zero-point correction=	0.178038 (Hartree/Particle)
Thermal correction to Energy=	0.186618
Thermal correction to Enthalpy=	0.187562
Thermal correction to Gibbs Free Energy=	0.144515
Sum of electronic and zero-point Energies=	-365.443521
Sum of electronic and thermal Energies=	-365.434941

Sum of electronic and thermal Enthalpies=	-365.433997
Sum of electronic and thermal Free Energies=	-365.477044

N-Protonated, N-Ethyl-2-pyrrolidinone, C1, B3LYP/6-31G*

Energy = -365.601497 au

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.386780	0.986681	0.002499
2	7	0	-0.247981	-0.462824	-0.224832
3	6	0	0.862818	-1.418587	0.136807
4	6	0	2.146929	-0.678608	-0.258980
5	6	0	1.874095	0.783911	0.124052
6	1	0	-0.424359	-0.528376	-1.236377
7	1	0	0.799133	-1.578449	1.216962
8	1	0	0.708045	-2.369595	-0.375538
9	1	0	2.329397	-0.772456	-1.334854
10	1	0	3.014117	-1.093032	0.258570
11	1	0	2.391712	1.528059	-0.488827
12	1	0	2.141230	0.995557	1.169035
13	8	0	-0.320699	1.931141	0.064364
14	6	0	-1.578743	-0.678139	0.485234
15	1	0	-1.680490	-1.760875	0.598755
16	1	0	-1.471925	-0.233384	1.477802
17	6	0	-2.747127	-0.086500	-0.290182
18	1	0	-3.670691	-0.307727	0.253107
19	1	0	-2.838891	-0.538935	-1.284928
20	1	0	-2.664331	0.997296	-0.391382

Zero-point correction=	0.177782 (Hartree/Particle)
Thermal correction to Energy=	0.186264
Thermal correction to Enthalpy=	0.187208
Thermal correction to Gibbs Free Energy=	0.144501
Sum of electronic and zero-point Energies=	-365.423715
Sum of electronic and thermal Energies=	-365.415233
Sum of electronic and thermal Enthalpies=	-365.414289
Sum of electronic and thermal Free Energies=	-365.456996

Ethylene, D2h, B3LYP/6-31G*

Energy = -78.589474 au

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.665462	0.000000
2	1	0	0.923583	1.239567	0.000000
3	1	0	-0.923585	1.239564	0.000000
4	6	0	0.000000	-0.665462	0.000000
5	1	0	-0.923583	-1.239567	0.000000
6	1	0	0.923585	-1.239564	0.000000

Zero-point correction=	0.050224 (Hartree/Particle)
Thermal correction to Energy=	0.053283
Thermal correction to Enthalpy=	0.054227
Thermal correction to Gibbs Free Energy=	0.028690
Sum of electronic and zero-point Energies=	-78.537234
Sum of electronic and thermal Energies=	-78.534176
Sum of electronic and thermal Enthalpies=	-78.533231
Sum of electronic and thermal Free Energies=	-78.558768

Ketene from Acylium Ion Rearrangement of 2-Pyrrolidinone, C1, B3LYP/6-31G*

Energy = -286.935615 au

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.486120	0.167947	-0.712140
2	1	0	1.024854	-0.356959	-1.551878
3	1	0	2.402907	0.653906	-1.052023
4	6	0	0.498952	1.136624	-0.037531
5	1	0	0.113080	1.798255	-0.820408
6	1	0	1.031916	1.781985	0.668249
7	6	0	-0.607357	0.415051	0.721287
8	1	0	-0.682108	0.510516	1.801421
9	6	0	-1.690423	-0.079442	0.123226
10	8	0	-2.613482	-0.545712	-0.403089
11	7	0	1.870269	-0.911153	0.285631
12	1	0	0.984997	-1.197323	0.751725
13	1	0	2.506534	-0.559147	1.010804
14	1	0	2.310045	-1.728546	-0.151652

Zero-point correction=	0.120726 (Hartree/Particle)

Thermal correction to Energy=	0.127659
Thermal correction to Enthalpy=	0.128603
Thermal correction to Gibbs Free Energy=	0.089661
Sum of electronic and zero-point Energies=	-286.814889
Sum of electronic and thermal Energies=	-286.807956
Sum of electronic and thermal Enthalpies=	-286.807012
Sum of electronic and thermal Free Energies=	-286.845954

Proposed Cyclopropyl Acylium Ion from Fragmentation of 2-Pyrrolidinone, C1, B3LYP/6-31G*

Energy = -230.329592 au

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.982136	1.262307	-1.125439
2	6	0	-1.325417	0.734217	-0.240601
3	6	0	-1.325423	-0.734210	-0.240610
4	6	0	-0.229309	-0.000007	0.611297
5	1	0	-2.026567	1.278150	0.385801
6	1	0	-0.982149	-1.262294	-1.125455
7	1	0	-2.026577	-1.278144	0.385787
8	1	0	-0.308756	-0.000014	1.697758
9	6	0	1.077226	-0.000003	0.151361
10	8	0	2.142965	0.000002	-0.238391

Zero-point correction=	0.078898 (Hartree/Particle)
Thermal correction to Energy=	0.083799
Thermal correction to Enthalpy=	0.084743
Thermal correction to Gibbs Free Energy=	0.051171
Sum of electronic and zero-point Energies=	-230.250694
Sum of electronic and thermal Energies=	-230.245792
Sum of electronic and thermal Enthalpies=	-230.244848
Sum of electronic and thermal Free Energies=	-230.278421

N-Protonated, 1-Azabicyclo[3.3.1]nonan-2-one, C1, B3LYP/6-31G*

Energy = -443.024044 au

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.967729	-1.209895	1.597282
2	7	0	0.433478	-0.724872	0.866789

3	6	0	-1.174535	-1.126216	-1.007861
4	6	0	-1.181500	1.048251	0.339293
5	6	0	-2.024181	0.038165	-0.472017
6	6	0	-0.486337	0.306330	1.484504
7	6	0	-0.349646	-1.787277	0.093647
8	1	0	-0.506876	-0.786170	-1.810494
9	1	0	-2.823863	-0.354377	0.169425
10	1	0	-1.193722	-0.230276	2.122747
11	1	0	-0.977515	-2.290158	0.835183
12	1	0	-1.812493	-1.895332	-1.455184
13	1	0	-1.859964	1.775735	0.795825
14	1	0	-2.515884	0.551724	-1.304322
15	1	0	0.122352	0.956859	2.117501
16	1	0	0.387790	-2.494315	-0.290988
17	6	0	1.530982	-0.081572	-0.069815
18	6	0	-0.135520	1.806443	-0.534503
19	1	0	-0.368033	1.662313	-1.594056
20	1	0	-0.200572	2.882181	-0.352281
21	6	0	1.335977	1.387453	-0.283082
22	1	0	1.995842	1.685373	-1.101841
23	1	0	1.720904	1.882090	0.621411
24	8	0	2.367314	-0.826387	-0.464840

Zero-point correction=	0.215805 (Hartree/Particle)
Thermal correction to Energy=	0.224290
Thermal correction to Enthalpy=	0.225235
Thermal correction to Gibbs Free Energy=	0.182912
Sum of electronic and zero-point Energies=	-442.808239
Sum of electronic and thermal Energies=	-442.799754
Sum of electronic and thermal Enthalpies=	-442.798809
Sum of electronic and thermal Free Energies=	-442.841132

Initial Acylium Ion from 1-Azabicyclo[3.3.1]nonan-2-one, C1, B3LYP/6-31G*

Energy = -442.952566 au

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.801525	-1.534999	0.077403
2	6	0	-2.389114	0.225599	-0.753320
3	6	0	-0.339360	0.894206	0.656189
4	6	0	-1.802567	1.225909	0.258680
5	6	0	-0.259329	-0.601811	1.050220
6	6	0	-2.194335	-1.223134	-0.275027

7	1	0	-1.921054	0.351942	-1.740466
8	1	0	-2.402058	1.198886	1.177509
9	1	0	-0.817153	-0.734763	1.985754
10	1	0	-2.802569	-1.402504	0.621633
11	1	0	-3.455925	0.434341	-0.893786
12	1	0	-0.072999	1.501283	1.534316
13	1	0	-1.870335	2.252010	-0.121960
14	1	0	0.775684	-0.902547	1.295677
15	1	0	-2.525307	-1.939413	-1.032672
16	1	0	-0.230117	-1.599532	-0.763756
17	6	0	0.627000	1.274203	-0.471650
18	1	0	0.429634	0.726011	-1.397898
19	1	0	0.546189	2.339806	-0.708303
20	6	0	2.150263	1.096353	-0.089771
21	1	0	2.802679	1.646026	-0.787923
22	1	0	2.354502	1.464115	0.927950
23	6	0	2.621589	-0.255104	-0.145764
24	8	0	3.039329	-1.301000	-0.251905

Zero-point correction=	0.210098 (Hartree/Particle)
Thermal correction to Energy=	0.220200
Thermal correction to Enthalpy=	0.221144
Thermal correction to Gibbs Free Energy=	0.174258
Sum of electronic and zero-point Energies=	-442.742468
Sum of electronic and thermal Energies=	-442.732365
Sum of electronic and thermal Enthalpies=	-442.731421
Sum of electronic and thermal Free Energies=	-442.778307

Aldehyde from Acylium Ion Rearrangement of 1-Azabicyclo[3.3.1]nonan-2-one, C1, B3LYP/6-31G*

Energy = -443.019906 au

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.226885	-1.391482	0.412647
2	6	0	-2.181668	0.545030	-0.813688
3	6	0	-0.160374	0.803658	0.701649
4	6	0	-1.542443	1.373965	0.309040
5	6	0	-0.238203	-0.683179	0.852989
6	6	0	-2.388839	-0.900031	-0.366526
7	1	0	-1.553992	0.566351	-1.711378
8	1	0	-2.198911	1.376977	1.187868

9	1	0	0.502070	-1.217007	1.436112
10	1	0	-3.263990	-1.006046	0.284847
11	1	0	-3.152628	0.960768	-1.097987
12	1	0	0.127821	1.179607	1.694303
13	1	0	-1.430438	2.416347	-0.002570
14	1	0	-2.516020	-1.581386	-1.212658
15	1	0	-1.207901	-2.392380	0.599970
16	6	0	0.951956	1.261059	-0.294688
17	1	0	0.691623	0.919429	-1.301976
18	1	0	0.898287	2.354234	-0.303201
19	6	0	2.401248	0.859262	0.004295
20	1	0	3.082684	1.456187	-0.617708
21	1	0	2.696517	1.094487	1.039804
22	6	0	2.711903	-0.593669	-0.254332
23	8	0	1.851297	-1.438510	-0.429550
24	1	0	3.781222	-0.875680	-0.279977

Zero-point correction=	0.212485 (Hartree/Particle)
Thermal correction to Energy=	0.222382
Thermal correction to Enthalpy=	0.223326
Thermal correction to Gibbs Free Energy=	0.177128
Sum of electronic and zero-point Energies=	-442.807421
Sum of electronic and thermal Energies=	-442.797524
Sum of electronic and thermal Enthalpies=	-442.796580
Sum of electronic and thermal Free Energies=	-442.842777

Product from loss of vinyl alcohol from 1-Azabicyclo[3.3.1]nonan-2-one, C1, B3LYP/6-31G*

Energy = -289.162174 au

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.928521	1.274582	0.022600
2	1	0	-1.368541	2.190964	-0.021815
3	6	0	0.371224	1.210271	-0.034289
4	1	0	0.905877	2.150722	-0.148219
5	6	0	1.093900	-0.032359	0.047181
6	6	0	2.438230	0.029559	-0.075024
7	1	0	3.052781	-0.865716	-0.041408
8	1	0	2.961193	0.973104	-0.208785
9	6	0	0.286535	-1.295955	0.265872
10	1	0	0.194990	-1.478318	1.345205
11	1	0	0.814593	-2.155953	-0.155172
12	6	0	-1.822997	0.096312	0.138907

13	1	0	-2.117138	0.013192	1.191873
14	1	0	-2.719435	0.319305	-0.445221
15	6	0	-1.111288	-1.160869	-0.360717
16	1	0	-1.031411	-1.121246	-1.453181
17	1	0	-1.726898	-2.029885	-0.113057

Zero-point correction=	0.151526 (Hartree/Particle)
Thermal correction to Energy=	0.157953
Thermal correction to Enthalpy=	0.158897
Thermal correction to Gibbs Free Energy=	0.121471
Sum of electronic and zero-point Energies=	-289.010648
Sum of electronic and thermal Energies=	-289.004222
Sum of electronic and thermal Enthalpies=	-289.003278
Sum of electronic and thermal Free Energies=	-289.040704

Vinyl Alcohol, Cs, B3LYP/6-31G*

Energy = -153.802228 au

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.239221	-0.073357	0.000000
2	1	0	1.427443	-1.142054	0.000000
3	1	0	2.086789	0.601519	0.000000
4	6	0	0.000000	0.414028	0.000000
5	1	0	-0.195978	1.486169	0.000000
6	8	0	-1.106593	-0.393462	0.000000
7	1	0	-1.900834	0.158034	0.000000

Zero-point correction=	0.055136 (Hartree/Particle)
Thermal correction to Energy=	0.059051
Thermal correction to Enthalpy=	0.059995
Thermal correction to Gibbs Free Energy=	0.030424
Sum of electronic and zero-point Energies=	-153.747092
Sum of electronic and thermal Energies=	-153.743177
Sum of electronic and thermal Enthalpies=	-153.742233
Sum of electronic and thermal Free Energies=	-153.771804

N-Protonated 2-quinuclidone, C1, B3LYP/6-31G*

Energy = -403.705855 au

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.408909	-1.047907	-1.256017
2	1	0	-0.977475	-1.980345	-1.224098
3	1	0	0.276642	-1.092432	-2.105260
4	6	0	-1.306578	0.215363	-1.259505
5	1	0	-2.360063	-0.076880	-1.280498
6	1	0	-1.117838	0.801570	-2.163591
7	6	0	-1.018620	1.059719	0.000025
8	1	0	-1.647851	1.953000	0.000044
9	7	0	0.451567	-1.028887	-0.000036
10	1	0	1.103422	-1.821431	-0.000059
11	6	0	-0.408560	-1.047732	1.256201
12	1	0	-0.977424	-1.979992	1.224353
13	1	0	0.277209	-1.092534	2.105251
14	6	0	-1.305847	0.215819	1.260030
15	1	0	-2.359397	-0.076121	1.281955
16	1	0	-1.116222	0.802265	2.163779
17	6	0	0.466136	1.477507	-0.000469
18	1	0	0.734739	2.080673	0.876820
19	1	0	0.734313	2.079969	-0.878378
20	6	0	1.338458	0.252631	-0.000193
21	8	0	2.516563	0.106508	-0.000062

Zero-point correction=	0.186884 (Hartree/Particle)
Thermal correction to Energy=	0.194535
Thermal correction to Enthalpy=	0.195479
Thermal correction to Gibbs Free Energy=	0.154638
Sum of electronic and zero-point Energies=	-403.518971
Sum of electronic and thermal Energies=	-403.511320
Sum of electronic and thermal Enthalpies=	-403.510376
Sum of electronic and thermal Free Energies=	-403.551218

Initial Acylium Ion from 2-quinuclidone, C1, B3LYP/6-31G*

Energy = -403.642961 au

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.240782	0.661715	-0.453547
2	6	0	0.127884	0.998315	0.871566
3	6	0	1.087080	-1.335933	0.553203
4	6	0	-0.195379	-0.503028	0.765539

5	6	0	1.974522	-0.765244	-0.571907
6	6	0	1.052363	1.479053	-0.269684
7	1	0	0.633534	1.149495	1.832817
8	1	0	1.637173	-1.297656	1.501897
9	1	0	1.508678	-0.946589	-1.554392
10	1	0	0.499755	1.498621	-1.223329
11	1	0	-0.788551	1.607633	0.913029
12	1	0	0.844773	-2.391384	0.373341
13	1	0	-0.721871	-0.851342	1.659903
14	1	0	2.926568	-1.303081	-0.595033
15	1	0	1.357416	2.512465	-0.082970
16	1	0	2.940479	0.853769	0.258533
17	6	0	-1.171258	-0.810686	-0.462097
18	1	0	-1.403694	-1.884787	-0.533181
19	1	0	-0.732173	-0.486516	-1.417657
20	6	0	-2.414949	-0.129039	-0.325564
21	8	0	-3.393643	0.413343	-0.165557

Zero-point correction=	0.181966 (Hartree/Particle)
Thermal correction to Energy=	0.190804
Thermal correction to Enthalpy=	0.191748
Thermal correction to Gibbs Free Energy=	0.148052
Sum of electronic and zero-point Energies=	-403.460995
Sum of electronic and thermal Energies=	-403.452157
Sum of electronic and thermal Enthalpies=	-403.451213
Sum of electronic and thermal Free Energies=	-403.494910

Aldehyde from Acylium Ion Rearrangement of 2-Quinuclidone, C1, B3LYP/6-31G*

Energy = -403.700221 au

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.305673	0.269297	-1.228720
2	1	0	0.602932	-0.205532	-1.920985
3	1	0	2.207503	0.536952	-1.785194
4	6	0	0.707408	1.482007	-0.516895
5	1	0	0.276281	2.145466	-1.273230
6	1	0	1.521929	2.041641	-0.041165
7	6	0	-0.343206	1.131573	0.562130
8	1	0	-0.499465	2.047909	1.139942
9	6	0	0.252091	0.087123	1.536157
10	1	0	-0.515381	-0.463988	2.091753

11	1	0	0.859104	0.581483	2.313511
12	6	0	1.160543	-0.909479	0.913834
13	1	0	1.469246	-1.779755	1.490320
14	7	0	1.684888	-0.778039	-0.255419
15	6	0	-1.740524	0.746745	0.025194
16	1	0	-2.049925	1.445255	-0.766237
17	1	0	-2.493866	0.890151	0.816588
18	6	0	-1.948610	-0.657727	-0.488563
19	1	0	-2.955962	-0.863098	-0.900848
20	8	0	-1.110278	-1.539332	-0.450587
21	1	0	2.305363	-1.512796	-0.590647

Zero-point correction=	0.183630 (Hartree/Particle)
Thermal correction to Energy=	0.192415
Thermal correction to Enthalpy=	0.193359
Thermal correction to Gibbs Free Energy=	0.149504
Sum of electronic and zero-point Energies=	-403.516591
Sum of electronic and thermal Energies=	-403.507806
Sum of electronic and thermal Enthalpies=	-403.506862
Sum of electronic and thermal Free Energies=	-403.550717

Product from loss of vinyl alcohol from 2-Quinuclidone, C1, B3LYP/6-31G*

Energy = -249.841564 au

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.171466	0.731718	0.246688
2	6	0	-1.215928	-0.728497	-0.215133
3	6	0	0.081078	-1.438904	0.039429
4	7	0	0.136720	1.343784	-0.088498
5	1	0	0.175248	2.347678	-0.245745
6	6	0	1.243834	0.656065	-0.082083
7	1	0	2.167043	1.200604	-0.266165
8	6	0	1.252374	-0.763702	0.126080
9	1	0	2.207553	-1.261670	0.244305
10	1	0	0.075868	-2.525510	0.079631
11	1	0	-1.953322	1.329158	-0.224677
12	1	0	-1.288511	0.807580	1.334858
13	1	0	-2.040088	-1.234862	0.298092
14	1	0	-1.440179	-0.809543	-1.290707

Zero-point correction=	0.123143 (Hartree/Particle)

Thermal correction to Energy=	0.128392
Thermal correction to Enthalpy=	0.129336
Thermal correction to Gibbs Free Energy=	0.094790
Sum of electronic and zero-point Energies=	-249.718420
Sum of electronic and thermal Energies=	-249.713171
Sum of electronic and thermal Enthalpies=	-249.712227
Sum of electronic and thermal Free Energies=	-249.746774

N-Protonated Kirby Lactam, Cs, B3LYP/6-31G*

Energy = -599.093924 au

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.950147	1.278161	-0.166661
2	6	0	-1.218501	-0.000002	-0.736077
3	6	0	0.950149	-1.278161	-0.166661
4	6	0	-0.347724	-1.267134	-1.005021
5	6	0	1.764111	0.000002	-0.474550
6	6	0	-0.347726	1.267134	-1.005020
7	1	0	-0.098813	-1.276633	-2.072812
8	1	0	2.053909	0.000002	-1.532260
9	1	0	-0.098814	1.276634	-2.072811
10	1	0	-0.937265	-2.172430	-0.811203
11	1	0	2.696357	0.000004	0.106184
12	1	0	-0.937270	2.172428	-0.811202
13	6	0	0.559614	1.257798	1.319944
14	1	0	-0.070527	2.108572	1.597233
15	1	0	1.430064	1.231931	1.982734
16	6	0	0.559613	-1.257798	1.319943
17	1	0	1.430062	-1.231933	1.982736
18	1	0	-0.070529	-2.108571	1.597230
19	6	0	-1.549661	0.000000	0.733003
20	7	0	-0.249353	0.000000	1.598491
21	1	0	-0.579945	0.000000	2.570584
22	8	0	-2.580366	0.000002	1.327883
23	6	0	-2.505998	-0.000007	-1.565784
24	1	0	-3.113967	0.884935	-1.356191
25	1	0	-3.113957	-0.884957	-1.356189
26	1	0	-2.253867	-0.000007	-2.630614
27	6	0	1.772080	2.544358	-0.447381
28	1	0	1.201181	3.452650	-0.223703
29	1	0	2.059476	2.582409	-1.503073

30	1	0	2.691222	2.563397	0.148721
31	6	0	1.772090	-2.544353	-0.447376
32	1	0	1.201191	-3.452648	-0.223706
33	1	0	2.691223	-2.563389	0.148737
34	1	0	2.059498	-2.582400	-1.503064

Zero-point correction=	0.304298 (Hartree/Particle)
Thermal correction to Energy=	0.317143
Thermal correction to Enthalpy=	0.318088
Thermal correction to Gibbs Free Energy=	0.267490
Sum of electronic and zero-point Energies=	-598.789626
Sum of electronic and thermal Energies=	-598.776781
Sum of electronic and thermal Enthalpies=	-598.775836
Sum of electronic and thermal Free Energies=	-598.826434

Acylium ion prior to loss of CO from protonated Kirby lactam, C1, B3LYP/6-31G*

Energy = -599.001601 au

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.843345	1.254120	0.109621
2	6	0	1.530499	0.069976	0.203919
3	6	0	-0.724612	-1.244839	0.383582
4	6	0	0.817271	-1.350860	0.408923
5	6	0	-1.138276	0.076695	1.056234
6	6	0	0.607574	1.152233	-0.501053
7	1	0	-0.646790	0.188194	2.031001
8	1	0	1.173119	-1.723200	1.374567
9	1	0	-2.212937	0.065643	1.270256
10	1	0	1.123839	2.114102	-0.425819
11	6	0	-1.879315	1.138043	-1.062338
12	1	0	-1.471007	1.625787	-1.960012
13	1	0	-2.780987	1.697455	-0.793155
14	6	0	-1.265322	-1.236977	-1.103590
15	1	0	-1.681715	-2.220167	-1.344426
16	1	0	-0.434081	-1.088194	-1.809140
17	6	0	2.587531	-0.167381	-0.725221
18	7	0	-2.275573	-0.233980	-1.379626
19	1	0	-3.156708	-0.475412	-0.938173
20	8	0	3.405170	-0.361261	-1.486230
21	6	0	2.189483	0.605647	1.516204
22	1	0	1.386753	0.797055	2.229759

23	1	0	2.726244	1.541671	1.340400
24	1	0	2.870890	-0.130469	1.950430
25	6	0	-0.998512	2.609604	0.816680
26	1	0	-0.900643	3.441181	0.108838
27	1	0	-0.248410	2.749295	1.604405
28	1	0	-1.986275	2.685449	1.283628
29	6	0	-1.288261	-2.454799	1.149155
30	1	0	-0.926213	-3.401215	0.730542
31	1	0	-2.382261	-2.462488	1.084600
32	1	0	-1.017796	-2.425372	2.210932
33	1	0	0.537301	0.914387	-1.566715
34	1	0	1.147032	-2.074520	-0.347385

Zero-point correction=	0.300624 (Hartree/Particle)
Thermal correction to Energy=	0.314816
Thermal correction to Enthalpy=	0.315760
Thermal correction to Gibbs Free Energy=	0.261622
Sum of electronic and zero-point Energies=	-598.700977
Sum of electronic and thermal Energies=	-598.686785
Sum of electronic and thermal Enthalpies=	-598.685841
Sum of electronic and thermal Free Energies=	-598.739979

Carbon Monoxide Loss from Protonated Kirby Lactam, C1, B3LYP/6-31G*

Energy = -485.765444 au

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.283187	-0.646808	1.304595
2	6	0	-0.003346	1.360388	0.000000
3	6	0	0.283187	-0.646808	-1.304595
4	6	0	0.724015	0.832365	-1.248720
5	6	0	0.742109	-1.367876	0.000000
6	6	0	0.724015	0.832365	1.248720
7	1	0	1.805422	0.956788	-1.146037
8	1	0	1.836128	-1.442294	0.000000
9	1	0	1.805422	0.956788	1.146037
10	1	0	0.414307	1.362970	-2.156990
11	1	0	0.360113	-2.396952	0.000000
12	1	0	0.414307	1.362970	2.156990
13	6	0	-1.235466	-0.429999	1.231522
14	1	0	-1.612710	0.127192	2.093112
15	1	0	-1.840243	-1.328176	1.090610
16	6	0	-1.235466	-0.429999	-1.231522

17	1	0	-1.840243	-1.328176	-1.090610
18	1	0	-1.612710	0.127192	-2.093112
19	7	0	-1.340911	0.444242	0.000000
20	1	0	-2.187079	1.018370	0.000000
21	6	0	-0.374521	2.831479	0.000000
22	1	0	-0.944289	3.111607	0.893171
23	1	0	-0.944289	3.111607	-0.893171
24	1	0	0.543976	3.428024	0.000000
25	6	0	0.724015	-1.391048	2.563133
26	1	0	0.388828	-0.874209	3.469507
27	1	0	1.815689	-1.463580	2.603662
28	1	0	0.322381	-2.410044	2.584499
29	6	0	0.724015	-1.391048	-2.563133
30	1	0	0.388828	-0.874209	-3.469507
31	1	0	0.322381	-2.410044	-2.584499
32	1	0	1.815689	-1.463580	-2.603662

Zero-point correction=	0.294938 (Hartree/Particle)
Thermal correction to Energy=	0.305932
Thermal correction to Enthalpy=	0.306876
Thermal correction to Gibbs Free Energy=	0.260305
Sum of electronic and zero-point Energies=	-485.470506
Sum of electronic and thermal Energies=	-485.459513
Sum of electronic and thermal Enthalpies=	-485.458569
Sum of electronic and thermal Free Energies=	-485.505140

Carbon Monoxide, Civ, B3LYP/6-31G*

Energy = -113.309455 au

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	-0.650301
2	8	0	0.000000	0.000000	0.487726

Zero-point correction=	0.004932 (Hartree/Particle)
Thermal correction to Energy=	0.007292
Thermal correction to Enthalpy=	0.008237
Thermal correction to Gibbs Free Energy=	-0.014207
Sum of electronic and zero-point Energies=	-113.304523
Sum of electronic and thermal Energies=	-113.302162
Sum of electronic and thermal Enthalpies=	-113.301218
Sum of electronic and thermal Free Energies=	-113.323661

N-methyl-2-pyrrolidinone, C1, B3LYP/6-31G*

Energy = -325.944716 au

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.188052	0.870978	-0.003359
2	7	0	-0.555592	-0.452844	-0.046663
3	6	0	0.551634	-1.380593	0.126640
4	6	0	1.792763	-0.516415	-0.189055
5	6	0	1.335995	0.915428	0.133638
6	1	0	0.575484	-1.775558	1.155522
7	1	0	0.450583	-2.237618	-0.550653
8	1	0	2.035964	-0.601718	-1.253463
9	1	0	2.670380	-0.835328	0.379615
10	1	0	1.756746	1.682377	-0.521380
11	1	0	1.572233	1.203503	1.166261
12	6	0	-1.937043	-0.876148	-0.013965
13	1	0	-2.149637	-1.580678	-0.827908
14	1	0	-2.558192	0.014157	-0.131401
15	1	0	-2.184195	-1.364077	0.939663
16	8	0	-0.951501	1.823169	-0.044126

Zero-point correction=	0.136980 (Hartree/Particle)
Thermal correction to Energy=	0.143995
Thermal correction to Enthalpy=	0.144940
Thermal correction to Gibbs Free Energy=	0.106023
Sum of electronic and zero-point Energies=	-325.807736
Sum of electronic and thermal Energies=	-325.800721
Sum of electronic and thermal Enthalpies=	-325.799777
Sum of electronic and thermal Free Energies=	-325.838694

N-methyl-2-pyrrolidinone, C1, B3LYP/6-31+G**

Energy = -325.96988462 au

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.182923	0.869715	-0.004835
2	7	0	-0.558982	-0.448769	-0.055022
3	6	0	0.546215	-1.382238	0.127692
4	6	0	1.793116	-0.524875	-0.182664

5	6	0	1.339065	0.911833	0.127298
6	1	0	.559493	-1.770460	1.158872
7	1	0	0.443287	-2.239915	-0.547117
8	1	0	2.046203	-0.618191	-1.243711
9	1	0	2.663408	-0.842422	0.397037
10	1	0	1.757976	1.671136	-0.536824
11	1	0	1.575488	1.211174	1.156083
12	6	0	-1.942527	-0.872940	-0.013864
13	1	0	-2.149349	-1.595206	-0.812108
14	1	0	-2.570547	0.009160	-0.150807
15	1	0	-2.186490	-1.339310	0.950629
16	8	0	-0.943034	1.830806	-0.038582

Zero-point correction=	0.133752 (Hartree/Particle)
Thermal correction to Energy=	0.140898
Thermal correction to Enthalpy=	0.141842
Thermal correction to Gibbs Free Energy=	0.102656
Sum of electronic and zero-point Energies=	-325.836133
Sum of electronic and thermal Energies=	-325.828986
Sum of electronic and thermal Enthalpies=	-325.828042
Sum of electronic and thermal Free Energies=	-325.867229

N-methyl-2-pyrrolidinone N-oxide, C1, B3LYP/6-31G*

Energy = -401.062540 au

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.030960	0.984789	-0.075418
2	6	0	0.517135	-1.314347	-0.505894
3	6	0	1.813270	-0.624640	-0.048265
4	6	0	1.482261	0.880041	-0.085074
5	1	0	0.368477	-2.308349	-0.080223
6	1	0	0.421982	-1.348447	-1.598504
7	1	0	2.651710	-0.886538	-0.699471
8	1	0	2.043790	-0.936124	0.970122
9	1	0	1.827147	1.361548	-1.008838
10	1	0	1.907121	1.440725	0.750708
11	6	0	-1.920777	-0.662979	-0.438899
12	1	0	-1.943086	-0.696204	-1.532499
13	1	0	-2.531817	0.158828	-0.068076
14	1	0	-2.251572	-1.608624	-0.007616
15	8	0	-0.755993	1.934812	-0.196655
16	7	0	-0.546818	-0.424101	0.045313

17	8	0	-0.472957	-0.407973	1.431469

Zero-point correction=	0.140607 (Hartree/Particle)
Thermal correction to Energy=	0.148258
Thermal correction to Enthalpy=	0.149203
Thermal correction to Gibbs Free Energy=	0.109155
Sum of electronic and zero-point Energies=	-400.921932
Sum of electronic and thermal Energies=	-400.914281
Sum of electronic and thermal Enthalpies=	-400.913337
Sum of electronic and thermal Free Energies=	-400.953385

N-methyl-2-pyrrolidinone N-oxide, C1, B3LYP/6-31+G**

Energy = -401.09501837 au

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.001648	0.990298	-0.061352
2	6	0	0.492781	-1.299606	-0.531635
3	6	0	1.806927	-0.653127	-0.064864
4	6	0	1.506989	0.859090	-0.053748
5	1	0	0.327871	-2.306796	-0.146416
6	1	0	0.387529	-1.285919	-1.623617
7	1	0	2.631280	-0.911080	-0.734503
8	1	0	2.045423	-1.001022	0.940136
9	1	0	1.872840	1.371045	-0.951672
10	1	0	1.921671	1.381469	0.811236
11	6	0	-1.925133	-0.598632	-0.478233
12	1	0	-2.549952	0.179352	-0.043201
13	1	0	-2.264066	-1.582351	-0.152848
14	8	0	-0.705077	1.957153	-0.171935
15	7	0	-0.557969	-0.410294	0.059742
16	8	0	-0.523499	-0.487092	1.445783
17	1	0	-1.917694	-0.521262	-1.569099

Zero-point correction=	0.137312 (Hartree/Particle)
Thermal correction to Energy=	0.145117
Thermal correction to Enthalpy=	0.146061
Thermal correction to Gibbs Free Energy=	0.105695
Sum of electronic and zero-point Energies=	-400.957706
Sum of electronic and thermal Energies=	-400.949902
Sum of electronic and thermal Enthalpies=	-400.948958
Sum of electronic and thermal Free Energies=	-400.989324

1-Azabicyclo[3.3.1]nonan-2-one, C1, B3LYP/6-31G*

Energy = -442.663033 au

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.456061	2.180685	0.535557
2	6	0	-0.912215	1.288456	0.200041
3	7	0	0.300623	-0.689212	0.899923
4	6	0	-1.370998	-1.042470	-0.859951
5	6	0	-0.644875	-1.676925	0.345573
6	6	0	-1.913267	0.373241	-0.553985
7	6	0	-0.404396	0.494074	1.411720
8	1	0	-0.653818	-0.994323	-1.688960
9	1	0	-1.345513	-1.961368	1.138958
10	1	0	-2.814432	0.283437	0.069905
11	1	0	-1.227011	0.152521	2.049113
12	1	0	-2.191032	-1.689471	-1.196086
13	1	0	-0.083569	-2.563085	0.046867
14	1	0	-2.231679	0.853826	-1.488101
15	1	0	0.265132	1.081782	2.046785
16	6	0	1.388058	-0.420154	0.062315
17	8	0	1.974517	-1.296918	-0.554822
18	6	0	0.332617	1.727766	-0.635702
19	1	0	0.446214	2.816701	-0.599218
20	1	0	0.188597	1.468201	-1.691332
21	6	0	1.652278	1.065638	-0.138117
22	1	0	1.982784	1.541116	0.793037
23	1	0	2.456681	1.172056	-0.868771

Zero-point correction=	0.202857 (Hartree/Particle)
Thermal correction to Energy=	0.210894
Thermal correction to Enthalpy=	0.211838
Thermal correction to Gibbs Free Energy=	0.170566
Sum of electronic and zero-point Energies=	-442.460176
Sum of electronic and thermal Energies=	-442.452139
Sum of electronic and thermal Enthalpies=	-442.451195
Sum of electronic and thermal Free Energies=	-442.492467

1-Azabicyclo[3.3.1]nonan-2-one, C1, B3LYP/6-31+G**

Energy = -442.69466863 au

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	1	0	-1.459808	2.176464	0.543391
2	6	0	-0.916451	1.285957	0.203466
3	7	0	0.303939	-0.689796	0.890327
4	6	0	-1.378727	-1.045262	-0.858672
5	6	0	-0.642163	-1.681876	0.340401
6	6	0	-1.920205	0.370676	-0.547984
7	6	0	-0.402639	0.490093	1.411727
8	1	0	-0.672268	-0.997750	-1.696338
9	1	0	-1.336319	-1.966622	1.138731
10	1	0	-2.818260	0.280098	0.079589
11	1	0	-1.221823	0.142800	2.049362
12	1	0	-2.201545	-1.693074	-1.184549
13	1	0	-0.084346	-2.568375	0.036776
14	1	0	-2.242502	0.852148	-1.479680
15	1	0	0.266780	1.076528	2.047006
16	6	0	1.392614	-0.414175	0.062080
17	8	0	1.993826	-1.289901	-0.549991
18	6	0	0.325361	1.728878	-0.635267
19	1	0	0.436114	2.817619	-0.597986
20	1	0	0.180066	1.469882	-1.690448
21	6	0	1.649415	1.071071	-0.141368
22	1	0	1.981337	1.545676	0.789190
23	1	0	2.451161	1.180205	-0.873701

Zero-point correction=	0.198137 (Hartree/Particle)
Thermal correction to Energy=	0.206365
Thermal correction to Enthalpy=	0.207309
Thermal correction to Gibbs Free Energy=	0.165725
Sum of electronic and zero-point Energies=	-442.496531
Sum of electronic and thermal Energies=	-442.488304
Sum of electronic and thermal Enthalpies=	-442.487360
Sum of electronic and thermal Free Energies=	-442.528943

1-Azabicyclo[3.3.1]nonan-2-one N-oxide, C1, B3LYP/6-31G*

Energy = -517.785053 au

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-2.292658	0.893851	1.301935
2	6	0	-1.507109	0.558704	0.614460

3	6	0	-1.032603	-1.311805	-1.096529
4	6	0	0.192571	-1.715069	-0.264507
5	6	0	-2.098836	-0.563446	-0.272381
6	6	0	-0.369386	-0.041318	1.439231
7	1	0	-0.697477	-0.690358	-1.936010
8	1	0	-0.022208	-2.477983	0.488619
9	1	0	-2.608141	-1.278596	0.388253
10	1	0	-0.671467	-0.907452	2.032967
11	1	0	-1.469701	-2.212134	-1.543980
12	1	0	1.028225	-2.047460	-0.879831
13	1	0	-2.866533	-0.153781	-0.940323
14	1	0	0.120586	0.664369	2.109881
15	6	0	1.161242	0.548855	-0.458319
16	8	0	1.841220	0.253512	-1.402935
17	6	0	-0.969905	1.797069	-0.175888
18	1	0	-1.386439	2.720776	0.238878
19	1	0	-1.303351	1.748516	-1.219129
20	6	0	0.580720	1.903841	-0.146893
21	1	0	0.926250	2.236410	0.837354
22	1	0	0.951700	2.613002	-0.890220
23	7	0	0.716930	-0.535712	0.516480
24	8	0	1.850347	-0.806032	1.223085

Zero-point correction=	0.205805 (Hartree/Particle)
Thermal correction to Energy=	0.214977
Thermal correction to Enthalpy=	0.215921
Thermal correction to Gibbs Free Energy=	0.172265
Sum of electronic and zero-point Energies=	-517.579248
Sum of electronic and thermal Energies=	-517.570076
Sum of electronic and thermal Enthalpies=	-517.569132
Sum of electronic and thermal Free Energies=	-517.612788

1-Azabicyclo[3.3.1]nonan-2-one N-oxide, C1, B3LYP/6-31+G**

Energy = -517.82678158 au

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-2.301619	0.816888	1.330629
2	6	0	-1.516508	0.513606	0.628647
3	6	0	-1.009892	-1.302503	-1.122263
4	6	0	0.225555	-1.701064	-0.302572
5	6	0	-2.090240	-0.603656	-0.274739
6	6	0	-0.359337	-0.071551	1.439638

7	1	0	-0.696569	-0.654433	-1.949535
8	1	0	0.020564	-2.481301	0.434648
9	1	0	-2.574756	-1.345988	0.373676
10	1	0	-0.641367	-0.952908	2.019742
11	1	0	-1.423459	-2.203684	-1.588397
12	1	0	1.062268	-2.013787	-0.926815
13	1	0	-2.873515	-0.198834	-0.926441
14	1	0	0.109629	0.635800	2.123525
15	6	0	1.149360	0.591091	-0.454027
16	8	0	1.854229	0.330347	-1.389368
17	6	0	-1.019644	1.777014	-0.145646
18	1	0	-1.452822	2.682920	0.289332
19	1	0	-1.363418	1.738482	-1.185429
20	6	0	0.527078	1.922545	-0.130325
21	1	0	0.873070	2.254202	0.854122
22	1	0	0.874044	2.647073	-0.869610
23	7	0	0.736605	-0.531603	0.507564
24	8	0	1.869957	-0.824861	1.218784

Zero-point correction=	0.201236 (Hartree/Particle)
Thermal correction to Energy=	0.210591
Thermal correction to Enthalpy=	0.211535
Thermal correction to Gibbs Free Energy=	0.167603
Sum of electronic and zero-point Energies=	-517.625546
Sum of electronic and thermal Energies=	-517.616191
Sum of electronic and thermal Enthalpies=	-517.615247
Sum of electronic and thermal Free Energies=	-517.659179

Kirby Lactam, Cs, B3LYP/6-31G*

Energy = -598.706499 au

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.203340	0.000003	-0.700112
2	6	0	-0.945358	1.274755	-0.145597
3	6	0	-0.945353	-1.274757	-0.145595
4	6	0	-1.762955	-0.000004	-0.454551
5	6	0	0.339644	-1.257580	-1.000447
6	6	0	0.339640	1.257581	-1.000449
7	1	0	-2.068936	-0.000006	-1.511480
8	1	0	0.086445	-1.264039	-2.070853
9	1	0	0.086443	1.264039	-2.070855

10	1	0	-2.687818	-0.000007	0.141274
11	1	0	0.928664	-2.165992	-0.809606
12	1	0	0.928655	2.165996	-0.809606
13	6	0	-0.507706	-1.211285	1.336423
14	1	0	0.095041	-2.090359	1.598431
15	1	0	-1.381397	-1.208604	2.001549
16	6	0	1.485983	0.000002	0.809863
17	6	0	-0.507709	1.211285	1.336421
18	1	0	0.095037	2.090359	1.598427
19	1	0	-1.381399	1.208603	2.001549
20	7	0	0.287452	0.000002	1.638696
21	8	0	2.591813	0.000000	1.295782
22	6	0	2.498171	0.000009	-1.511727
23	1	0	3.105136	-0.882217	-1.284580
24	1	0	3.105120	0.882248	-1.284585
25	1	0	2.274980	0.000005	-2.585574
26	6	0	-1.768790	2.538116	-0.415083
27	1	0	-2.677380	2.557911	0.199614
28	1	0	-2.076937	2.590312	-1.466680
29	1	0	-1.192435	3.444410	-0.190704
30	6	0	-1.768774	-2.538125	-0.415088
31	1	0	-2.677370	-2.557930	0.199599
32	1	0	-1.192413	-3.444414	-0.190705
33	1	0	-2.076910	-2.590323	-1.466688

Zero-point correction=	0.290046 (Hartree/Particle)
Thermal correction to Energy=	0.302716
Thermal correction to Enthalpy=	0.303660
Thermal correction to Gibbs Free Energy=	0.253055
Sum of electronic and zero-point Energies=	-598.416452
Sum of electronic and thermal Energies=	-598.403783
Sum of electronic and thermal Enthalpies=	-598.402839
Sum of electronic and thermal Free Energies=	-598.453443

Kirby Lactam, Cs, B3LYP/6-31+G**

Energy = -598.74928892 au

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.205329	-0.000001	-0.699632
2	6	0	-0.945151	1.275349	-0.145861
3	6	0	-0.945153	-1.275347	-0.145858
4	6	0	-1.762369	0.000000	-0.455349

5	6	0	0.341248	-1.258641	-0.998594
6	6	0	0.341251	1.258638	-0.998597
7	1	0	-2.066665	-0.000001	-1.512256
8	1	0	0.090014	-1.264515	-2.068875
9	1	0	0.090020	1.264512	-2.068879
10	1	0	-2.686548	0.000000	0.140458
11	1	0	0.930166	-2.165982	-0.805964
12	1	0	0.930170	2.165979	-0.805966
13	6	0	-0.508792	-1.213307	1.336880
14	1	0	0.092967	-2.092026	1.599799
15	1	0	-1.382092	-1.208346	2.001355
16	6	0	1.484939	-0.000001	0.811357
17	6	0	-0.508789	1.213310	1.336876
18	1	0	0.092973	2.092028	1.599792
19	1	0	-1.382088	1.208355	2.001353
20	7	0	0.286831	0.000001	1.637517
21	8	0	2.591170	-0.000002	1.301464
22	6	0	2.496894	0.000001	-1.517021
23	1	0	3.105019	-0.881928	-1.294871
24	1	0	3.105000	0.881947	-1.294890
25	1	0	2.264134	-0.000012	-2.588289
26	6	0	-1.768765	2.538991	-0.416392
27	1	0	-2.677515	2.558240	0.196996
28	1	0	-2.075343	2.590119	-1.467936
29	1	0	-1.192907	3.444838	-0.191849
30	6	0	-1.768763	-2.538992	-0.416393
31	1	0	-2.677519	-2.558246	0.196987
32	1	0	-1.192904	-3.444837	-0.191846
33	1	0	-2.075332	-2.590121	-1.467939

Zero-point correction=	0.283399 (Hartree/Particle)
Thermal correction to Energy=	0.296307
Thermal correction to Enthalpy=	0.297251
Thermal correction to Gibbs Free Energy=	0.246306
Sum of electronic and zero-point Energies=	-598.465890
Sum of electronic and thermal Energies=	-598.452982
Sum of electronic and thermal Enthalpies=	-598.452038
Sum of electronic and thermal Free Energies=	-598.502983

Kirby Lactam N-oxide, Cs, B3LYP/6-31G*

Energy = -673.845536 au

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z

1	6	0	-0.962602	-0.000010	-1.126490
2	6	0	1.032835	-1.273918	-0.159855
3	6	0	1.032793	1.273942	-0.159828
4	6	0	1.894786	0.000032	-0.306227
5	6	0	-0.064090	1.259508	-1.245000
6	6	0	-0.064061	-1.259487	-1.245022
7	1	0	2.393034	0.000056	-1.285617
8	1	0	0.391698	1.269499	-2.244668
9	1	0	0.391719	-1.269455	-2.244693
10	1	0	2.687541	0.000049	0.454855
11	1	0	-0.682200	2.164208	-1.167379
12	1	0	-0.682135	-2.164212	-1.167404
13	6	0	0.346284	1.240553	1.215371
14	1	0	-0.335731	2.080886	1.375244
15	1	0	1.056977	1.218717	2.046254
16	6	0	-1.572803	-0.000016	0.272846
17	6	0	0.346327	-1.240565	1.215345
18	1	0	-0.335655	-2.080924	1.375214
19	1	0	1.057021	-1.218709	2.046228
20	7	0	-0.512044	-0.000026	1.427578
21	8	0	-2.729722	-0.000008	0.562886
22	6	0	-2.071122	-0.000049	-2.183821
23	1	0	-2.709996	0.882885	-2.084583
24	1	0	-2.709944	-0.883017	-2.084528
25	1	0	-1.632954	-0.000073	-3.188429
26	6	0	1.894520	-2.538961	-0.272646
27	1	0	2.670275	-2.559007	0.501911
28	1	0	2.393217	-2.585012	-1.248078
29	1	0	1.286378	-3.444904	-0.163169
30	6	0	1.894399	2.539041	-0.272636
31	1	0	2.670197	2.559152	0.501876
32	1	0	1.286195	3.444941	-0.163130
33	1	0	2.393038	2.585139	-1.248097
34	8	0	-1.051272	-0.000049	2.637481

Zero-point correction=	0.293877 (Hartree/Particle)
Thermal correction to Energy=	0.307464
Thermal correction to Enthalpy=	0.308408
Thermal correction to Gibbs Free Energy=	0.256360
Sum of electronic and zero-point Energies=	-673.551660
Sum of electronic and thermal Energies=	-673.538073
Sum of electronic and thermal Enthalpies=	-673.537128
Sum of electronic and thermal Free Energies=	-673.589177

Kirby Lactam N-oxide, Cs, B3LYP/6-31+G**

Energy = -673.89833408 au

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.964522	-0.000064	-1.125556
2	6	0	1.032522	-1.273282	-0.161857
3	6	0	1.032410	1.273347	-0.161879
4	6	0	1.894796	0.000074	-0.310345
5	6	0	-0.066467	1.260145	-1.244607
6	6	0	-0.066370	-1.260186	-1.244579
7	1	0	2.389491	0.000092	-1.290823
8	1	0	0.386922	1.268990	-2.244628
9	1	0	0.387010	-1.269026	-2.244603
10	1	0	2.688194	0.000127	0.449161
11	1	0	-0.684323	2.164072	-1.165118
12	1	0	-0.684141	-2.164169	-1.165055
13	6	0	0.348711	1.241495	1.215522
14	1	0	-0.329233	2.084833	1.374327
15	1	0	1.063124	1.220310	2.042591
16	6	0	-1.574149	-0.000044	0.274460
17	6	0	0.348819	-1.241449	1.215542
18	1	0	-0.329045	-2.084845	1.374372
19	1	0	1.063230	-1.220175	2.042612
20	7	0	-0.508344	-0.000017	1.423886
21	8	0	-2.730886	-0.000017	0.565144
22	6	0	-2.071326	-0.000154	-2.185037
23	1	0	-2.710123	0.882433	-2.089722
24	1	0	-2.710018	-0.882810	-2.089636
25	1	0	-1.626568	-0.000182	-3.186041
26	6	0	1.893329	-2.539630	-0.273110
27	1	0	2.669843	-2.558645	0.499784
28	1	0	2.389995	-2.586535	-1.248807
29	1	0	1.285067	-3.444508	-0.161822
30	6	0	1.893069	2.539795	-0.273199
31	1	0	2.669618	2.558953	0.499656
32	1	0	1.284695	3.444600	-0.161927
33	1	0	2.389683	2.586732	-1.248923
34	8	0	-1.049108	-0.000035	2.646764

Zero-point correction=	0.287381 (Hartree/Particle)
Thermal correction to Energy=	0.301222
Thermal correction to Enthalpy=	0.302166
Thermal correction to Gibbs Free Energy=	0.249708

Sum of electronic and zero-point Energies=	-673.610953
Sum of electronic and thermal Energies=	-673.597113
Sum of electronic and thermal Enthalpies=	-673.596168
Sum of electronic and thermal Free Energies=	-673.648626

Kirby Lactam Hydrate, C1, B3LYP/6-31G*

Energy = -675.135530 au

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.906584	-0.020290	0.925232
2	6	0	-1.161126	-1.260103	0.088293
3	6	0	-1.126208	1.284435	0.086328
4	6	0	-1.996384	0.023937	0.291494
5	6	0	0.035251	1.247739	1.105443
6	6	0	0.000454	-1.262430	1.106833
7	1	0	-2.433065	0.030538	1.301882
8	1	0	-0.367387	1.260691	2.128926
9	1	0	-0.402583	-1.263348	2.130471
10	1	0	-2.839312	0.034929	-0.416201
11	1	0	0.656437	2.144638	0.992197
12	1	0	0.595349	-2.176810	0.994254
13	6	0	-0.508623	1.211878	-1.331720
14	1	0	0.117126	2.086099	-1.527597
15	1	0	-1.299568	1.190469	-2.092827
16	6	0	1.423498	-0.011896	-0.547257
17	6	0	-0.533359	-1.197924	-1.323433
18	1	0	0.072198	-2.090212	-1.507365
19	1	0	-1.316379	-1.165240	-2.092047
20	7	0	0.313930	-0.002505	-1.505029
21	8	0	2.186059	1.143691	-0.846007
22	1	0	2.972496	1.098405	-0.279757
23	8	0	2.213151	-1.159891	-0.746733
24	1	0	2.424773	-1.152815	-1.697539
25	6	0	-1.956441	2.561194	0.248702
26	1	0	-2.399366	2.619165	1.251070
27	1	0	-2.776452	2.598031	-0.479897
28	1	0	-1.338912	3.456607	0.103780
29	6	0	2.055942	-0.042906	1.941522
30	1	0	1.657522	-0.074697	2.962858
31	1	0	2.679635	0.858321	1.872761
32	1	0	2.696476	-0.918582	1.797494
33	6	0	-2.028160	-2.513249	0.240469

34	1	0	-2.477427	-2.562717	1.240372
35	1	0	-1.436008	-3.425632	0.095100
36	1	0	-2.845317	-2.523032	-0.492239

Zero-point correction=	0.317824 (Hartree/Particle)
Thermal correction to Energy=	0.331636
Thermal correction to Enthalpy=	0.332580
Thermal correction to Gibbs Free Energy=	0.280598
Sum of electronic and zero-point Energies=	-674.817706
Sum of electronic and thermal Energies=	-674.803893
Sum of electronic and thermal Enthalpies=	-674.802949
Sum of electronic and thermal Free Energies=	-674.854932

Kirby Lactam Hydrate N-oxide, C1, B3LYP/6-31G*

Energy = -750.303271 au

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.628190	-0.000017	1.274957
2	6	0	1.221347	1.270182	0.035989
3	6	0	1.221337	-1.270184	0.035967
4	6	0	2.098391	-0.000006	0.076704
5	6	0	0.272123	-1.258533	1.258925
6	6	0	0.272109	1.258504	1.258942
7	1	0	2.710515	-0.000017	0.989173
8	1	0	0.869679	-1.278080	2.180515
9	1	0	0.869654	1.278053	2.180537
10	1	0	2.795646	-0.000008	-0.773914
11	1	0	-0.352587	-2.158295	1.257334
12	1	0	-0.352604	2.158263	1.257341
13	6	0	0.370585	-1.226111	-1.246971
14	1	0	-0.303830	-2.078501	-1.322579
15	1	0	0.978385	-1.179017	-2.155330
16	6	0	-1.459967	-0.000004	-0.015152
17	6	0	0.370589	1.226144	-1.246945
18	1	0	-0.303830	2.078535	-1.322513
19	1	0	0.978372	1.179072	-2.155315
20	7	0	-0.499173	0.000017	-1.270008
21	8	0	-2.211980	-1.151126	-0.166165
22	1	0	-2.423551	-1.126683	-1.133927
23	8	0	-2.211966	1.151137	-0.166126
24	1	0	-2.423559	1.126727	-1.133881
25	8	0	-1.343799	0.000029	-2.354512

26	6	0	-1.557640	-0.000024	2.497435
27	1	0	-0.966352	0.000032	3.420849
28	1	0	-2.200075	-0.885811	2.498291
29	1	0	-2.200148	0.885710	2.498228
30	6	0	2.085306	-2.537400	0.028451
31	1	0	2.702039	-2.589718	0.933438
32	1	0	2.759153	-2.555309	-0.837009
33	1	0	1.465038	-3.440943	-0.007069
34	6	0	2.085328	2.537387	0.028498
35	1	0	2.702050	2.589688	0.933492
36	1	0	1.465080	3.440943	-0.007033
37	1	0	2.759188	2.555283	-0.836954

Zero-point correction=	0.323026 (Hartree/Particle)
Thermal correction to Energy=	0.337237
Thermal correction to Enthalpy=	0.338181
Thermal correction to Gibbs Free Energy=	0.285316
Sum of electronic and zero-point Energies=	-749.980245
Sum of electronic and thermal Energies=	-749.966034
Sum of electronic and thermal Enthalpies=	-749.965090
Sum of electronic and thermal Free Energies=	-750.017955

Dimethyldioxirane, C2v, B3LYP/6-31G*

Energy = -268.268936 au

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.094059	0.000005	0.000004
2	8	0	-1.090156	-0.000041	0.752675
3	8	0	-1.090149	-0.000072	-0.752679
4	6	0	0.872019	1.293854	-0.000007
5	1	0	0.178447	2.137173	-0.000063
6	1	0	1.513950	1.353483	-0.886068
7	1	0	1.513866	1.353538	0.886111
8	6	0	0.872156	-1.293764	0.000009
9	1	0	1.514124	-1.353316	0.886047
10	1	0	1.513975	-1.353392	-0.886133
11	1	0	0.178673	-2.137157	0.000100

Zero-point correction=	0.086951 (Hartree/Particle)
Thermal correction to Energy=	0.092658
Thermal correction to Enthalpy=	0.093602
Thermal correction to Gibbs Free Energy=	0.058619

Sum of electronic and zero-point Energies= -268.181985
Sum of electronic and thermal Energies= -268.176279
Sum of electronic and thermal Enthalpies= -268.175335
Sum of electronic and thermal Free Energies= -268.210317

Dimethyldioxirane, C2v, B3LYP/6-31+G**

Energy = -268.28833682 au

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.095709	0.000003	-0.000004
2	8	0	-1.091219	0.000004	0.753859
3	8	0	-1.091221	-0.000086	-0.753857
4	6	0	0.872421	1.293436	-0.000024
5	1	0	0.180445	2.137337	-0.000388
6	1	0	1.513872	1.349913	-0.885796
7	1	0	1.513298	1.350232	0.886145
8	6	0	0.872521	-1.293370	0.000024
9	1	0	1.513924	-1.349822	0.885832
10	1	0	1.513452	-1.350095	-0.886109
11	1	0	0.180611	-2.137326	0.000328

Zero-point correction= 0.084830 (Hartree/Particle)
Thermal correction to Energy= 0.090624
Thermal correction to Enthalpy= 0.091568
Thermal correction to Gibbs Free Energy= 0.056429
Sum of electronic and zero-point Energies= -268.203507
Sum of electronic and thermal Energies= -268.197713
Sum of electronic and thermal Enthalpies= -268.196769
Sum of electronic and thermal Free Energies= -268.231908

Acetone, C2v, B3LYP/6-31G*

Energy = -193.155695 au

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.185314	-0.000012
2	8	0	0.000000	1.400985	0.000002
3	6	0	-1.293096	-0.614796	0.000001
4	1	0	-1.341438	-1.267325	-0.880974

5	1	0	-2.148532	0.063549	0.000019
6	1	0	-1.341400	-1.267328	0.880976
7	6	0	1.293096	-0.614796	0.000001
8	1	0	1.341438	-1.267325	-0.880974
9	1	0	1.341400	-1.267328	0.880976
10	1	0	2.148532	0.063549	0.000019

Zero-point correction=	0.082425 (Hartree/Particle)
Thermal correction to Energy=	0.087900
Thermal correction to Enthalpy=	0.088844
Thermal correction to Gibbs Free Energy=	0.053752
Sum of electronic and zero-point Energies=	-193.073270
Sum of electronic and thermal Energies=	-193.067795
Sum of electronic and thermal Enthalpies=	-193.066851
Sum of electronic and thermal Free Energies=	-193.101942

Acetone, C2v, B3LYP/6-31+G**

Energy = -193.17450920 au

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.181691	0.000000
2	8	0	0.000000	1.400679	0.000000
3	6	0	1.293264	-0.613644	-0.001738
4	1	0	1.382165	-1.180944	0.932994
5	1	0	2.146431	0.059456	-0.099180
6	1	0	1.298419	-1.344433	-0.818828
7	6	0	-1.293264	-0.613644	0.001738
8	1	0	-1.298419	-1.344432	0.818828
9	1	0	-1.382165	-1.180945	-0.932994
10	1	0	-2.146431	0.059455	0.099180

Zero-point correction=	0.080533 (Hartree/Particle)
Thermal correction to Energy=	0.086023
Thermal correction to Enthalpy=	0.086967
Thermal correction to Gibbs Free Energy=	0.052187
Sum of electronic and zero-point Energies=	-193.093976
Sum of electronic and thermal Energies=	-193.088486
Sum of electronic and thermal Enthalpies=	-193.087542
Sum of electronic and thermal Free Energies=	-193.122322

Water, C2v, B3LYP/6-31G*

Energy = -76.408953 au

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.000000	0.761579	-0.478976
2	8	0	0.000000	0.000000	0.119744
3	1	0	0.000000	-0.761579	-0.478976

Zero-point correction=	0.020749 (Hartree/Particle)
Thermal correction to Energy=	0.023584
Thermal correction to Enthalpy=	0.024528
Thermal correction to Gibbs Free Energy=	0.003082
Sum of electronic and zero-point Energies=	-76.388204
Sum of electronic and thermal Energies=	-76.385370
Sum of electronic and thermal Enthalpies=	-76.384425
Sum of electronic and thermal Free Energies=	-76.405872

S3. Transition State Cartesian Coordinates and Energies (1 imaginary mode)

Transition State for the Loss of Ethylene from N-Ethyl-2-pyrrolidinone, C1, B3LYP/6-31G*

Energy = -365.539827 au

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.248486	0.817806	-0.289178
2	8	0	0.691308	1.605219	-0.473698
3	1	0	0.292544	-0.654780	-1.614251
4	6	0	1.935068	-1.168924	0.414046
5	1	0	1.973806	-1.930811	-0.360129
6	1	0	1.343227	-1.411910	1.292730
7	6	0	2.709821	-0.003194	0.346600
8	1	0	3.519622	0.003896	-0.386287
9	1	0	2.938511	0.480440	1.299897
10	1	0	1.913049	0.794033	-0.120292
11	7	0	-0.210242	-0.480597	-0.748293
12	6	0	-1.476540	-1.202722	-0.474927
13	1	0	-1.276549	-2.243974	-0.212457
14	1	0	-2.096539	-1.185918	-1.378597
15	6	0	-1.525743	1.040254	0.482932
16	1	0	-2.178119	1.664285	-0.143239
17	1	0	-1.341873	1.596569	1.405295
18	6	0	-2.092410	-0.381517	0.678663
19	1	0	-3.182923	-0.411091	0.652733
20	1	0	-1.773786	-0.788530	1.643414

Zero-point correction=	0.170568 (Hartree/Particle)
Thermal correction to Energy=	0.178943
Thermal correction to Enthalpy=	0.179888
Thermal correction to Gibbs Free Energy=	0.137608
Sum of electronic and zero-point Energies=	-365.369259
Sum of electronic and thermal Energies=	-365.360884
Sum of electronic and thermal Enthalpies=	-365.359940
Sum of electronic and thermal Free Energies=	-365.402220

Transition state for the transfer of hydride to form the ketene in 2-pyrrolidinone rearrangement, C1, B3LYP/6-31G*

Energy = -286.919612 au

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.890187	0.392994	-0.080393
2	1	0	2.353566	0.665429	0.870835
3	1	0	2.547878	0.717503	-0.889794
4	6	0	0.488344	1.056171	-0.204889
5	1	0	0.486913	2.074738	0.187761
6	1	0	0.176975	1.096611	-1.253307
7	6	0	-0.462071	0.123607	0.598363
8	1	0	-0.487453	0.278093	1.683501
9	1	0	0.285063	-0.914059	0.382132
10	7	0	1.670523	-1.069997	-0.082635
11	1	0	1.718194	-1.488864	-1.011896
12	1	0	2.296900	-1.584443	0.534619
13	6	0	-1.735356	-0.069927	0.114583
14	8	0	-2.769790	-0.296512	-0.311424

Zero-point correction=	0.115595 (Hartree/Particle)
Thermal correction to Energy=	0.121780
Thermal correction to Enthalpy=	0.122724
Thermal correction to Gibbs Free Energy=	0.085613
Sum of electronic and zero-point Energies=	-286.804017
Sum of electronic and thermal Energies=	-286.797832
Sum of electronic and thermal Enthalpies=	-286.796888
Sum of electronic and thermal Free Energies=	-286.833999

Transition state for the loss of ammonia from ketene in the 2-pyrrolidinone rearrangement, C1, B3LYP/6-31G*

Energy = -286.856960

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.112997	1.654538	-0.034131
2	1	0	0.343680	2.459099	0.665813
3	1	0	-0.508974	2.021088	-0.853680
4	6	0	1.271072	0.872105	-0.478384
5	1	0	2.219561	0.948672	0.036129
6	1	0	1.278325	0.422634	-1.463821
7	1	0	1.178497	-2.064622	-0.276207
8	1	0	2.759633	-1.618355	-0.360190
9	1	0	1.964271	-1.559268	1.077482
10	7	0	1.862717	-1.394734	0.075635

11	6	0	-0.515099	0.465382	0.690632
12	1	0	-0.232125	0.234128	1.711243
13	6	0	-1.472692	-0.279416	0.126994
14	8	0	-2.302444	-0.919487	-0.362109

Zero-point correction=	0.114117 (Hartree/Particle)
Thermal correction to Energy=	0.122238
Thermal correction to Enthalpy=	0.123182
Thermal correction to Gibbs Free Energy=	0.081204
Sum of electronic and zero-point Energies=	-286.742843
Sum of electronic and thermal Energies=	-286.734722
Sum of electronic and thermal Enthalpies=	-286.733778
Sum of electronic and thermal Free Energies=	-286.775756

Transition state for the McLafferty Rearrangement in 1-Azabicyclo[3.3.1]nonan-2-one fragmentation, C1, B3LYP/6-31G*

Energy = -442.967383 au

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.828888	-0.502403	-0.217257
2	1	0	3.569842	-0.951996	0.438782
3	8	0	2.070406	-1.410554	-0.794379
4	6	0	2.578810	0.861171	-0.248752
5	1	0	2.068887	1.282098	-1.113482
6	1	0	3.348459	1.500088	0.175185
7	6	0	1.091625	0.971487	1.027865
8	1	0	1.199069	2.052356	1.102221
9	1	0	1.498590	0.457120	1.895368
10	6	0	-0.123773	0.477243	0.479484
11	1	0	1.405779	-0.999433	-1.378294
12	6	0	-0.950716	1.286056	-0.504101
13	1	0	-0.618561	1.110968	-1.540336
14	1	0	-0.812711	2.357611	-0.320947
15	6	0	-0.606442	-0.760634	0.890854
16	1	0	-0.055418	-1.360512	1.610859
17	6	0	-2.442936	0.926940	-0.381459
18	1	0	-2.827486	1.295357	0.576237
19	1	0	-3.020848	1.411891	-1.173337
20	6	0	-2.660835	-0.586624	-0.460597
21	1	0	-2.466070	-0.960520	-1.474749
22	1	0	-3.690703	-0.849656	-0.205020
23	1	0	-2.064978	-2.166533	0.861919

24	7	0	-1.769263	-1.276260	0.483486

Zero-point correction=	0.209656 (Hartree/Particle)
Thermal correction to Energy=	0.219903
Thermal correction to Enthalpy=	0.220847
Thermal correction to Gibbs Free Energy=	0.173781
Sum of electronic and zero-point Energies=	-442.757727
Sum of electronic and thermal Energies=	-442.747481
Sum of electronic and thermal Enthalpies=	-442.746537
Sum of electronic and thermal Free Energies=	-442.793602

Transition state for the McLafferty Rearrangement in 2- Quinuclidone fragmentation, C1, B3LYP/6-31G*

Energy = -403.644201 au

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.962928	-0.728205	-0.678508
2	1	0	2.931731	-1.224982	-0.768668
3	1	0	1.429886	-0.877153	-1.627190
4	6	0	1.170344	-1.310815	0.499486
5	1	0	1.809450	-1.345216	1.393810
6	1	0	0.896051	-2.345184	0.276980
7	6	0	-0.031496	-0.456957	0.882748
8	1	0	-0.551977	-0.810791	1.768963
9	7	0	2.186946	0.705661	-0.471455
10	1	0	3.002948	1.140118	-0.881565
11	6	0	1.291019	1.460765	0.170560
12	1	0	1.520033	2.521616	0.224724
13	6	0	0.157219	0.953999	0.786219
14	1	0	-0.491350	1.640574	1.317270
15	6	0	-1.441775	-1.087654	-0.427975
16	1	0	-1.517520	-2.147284	-0.202666
17	1	0	-0.906840	-0.843801	-1.341750
18	6	0	-2.531292	-0.306694	-0.077787
19	8	0	-2.700821	0.948338	-0.423604
20	1	0	-3.279723	-0.629698	0.641978
21	1	0	-2.006429	1.248840	-1.041326

Zero-point correction=	0.181226 (Hartree/Particle)
Thermal correction to Energy=	0.190247

Thermal correction to Enthalpy=	0.191191
Thermal correction to Gibbs Free Energy=	0.147021
Sum of electronic and zero-point Energies=	-403.462975
Sum of electronic and thermal Energies=	-403.453954
Sum of electronic and thermal Enthalpies=	-403.453010
Sum of electronic and thermal Free Energies=	-403.497180

Transition state for the oxidation of N-methyl-2-pyrrolidinone by DMDO, C1, B3LYP/6-31G*

Energy = -594.176275 au

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.938818	0.742089	-0.238780
2	6	0	-1.312987	0.051552	0.976031
3	8	0	-1.001894	0.444412	2.073049
4	6	0	2.081629	-0.379250	-0.136602
5	8	0	0.476752	-0.230921	-0.611469
6	8	0	2.151787	-1.242435	-1.075712
7	6	0	-2.150344	-1.150589	0.579674
8	1	0	-1.723428	-2.058637	1.012834
9	1	0	-3.145100	-1.015363	1.023007
10	6	0	-1.828968	0.308985	-1.330793
11	1	0	-1.292015	0.401761	-2.275785
12	1	0	-2.714372	0.961574	-1.344884
13	6	0	-2.179749	-1.143505	-0.959010
14	1	0	-3.149985	-1.437730	-1.367087
15	1	0	-1.409210	-1.806217	-1.353631
16	6	0	-0.557110	2.146523	-0.150795
17	1	0	0.028054	2.283520	0.757942
18	1	0	-1.452243	2.779081	-0.106406
19	1	0	0.040052	2.398982	-1.027561
20	6	0	2.078235	-0.868792	1.307082
21	1	0	3.112920	-1.031522	1.635849
22	1	0	1.546112	-1.821646	1.359364
23	1	0	1.610088	-0.150127	1.987552
24	6	0	2.752017	0.974122	-0.360626
25	1	0	3.834866	0.858913	-0.224449
26	1	0	2.407067	1.738209	0.344959
27	1	0	2.569421	1.301844	-1.386956

Zero-point correction=	0.224127 (Hartree/Particle)
Thermal correction to Energy=	0.237591
Thermal correction to Enthalpy=	0.238535

Thermal correction to Gibbs Free Energy=	0.184374
Sum of electronic and zero-point Energies=	-593.952148
Sum of electronic and thermal Energies=	-593.938684
Sum of electronic and thermal Enthalpies=	-593.937740
Sum of electronic and thermal Free Energies=	-593.991901

Transition state for the oxidation of N-methyl-2-pyrrolidinone by DMDO, C1, B3LYP/6-31+G**

Energy = -594.22229521 au

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.921631	0.725631	-0.256777
2	6	0	-1.323002	0.073629	0.971014
3	8	0	-1.017244	0.492983	2.061855
4	6	0	2.076759	-0.376318	-0.123282
5	8	0	0.501761	-0.250872	-0.633927
6	8	0	2.195332	-1.242540	-1.067085
7	6	0	-2.171814	-1.126876	0.604373
8	1	0	-1.747133	-2.027699	1.053903
9	1	0	-3.160423	-0.974103	1.054268
10	6	0	-1.821467	0.281326	-1.341030
11	1	0	-1.282941	0.337743	-2.287811
12	1	0	-2.689758	0.955374	-1.369804
13	6	0	-2.211102	-1.151569	-0.934603
14	1	0	-3.193533	-1.422300	-1.328238
15	1	0	-1.468368	-1.849277	-1.322660
16	6	0	-0.545223	2.136081	-0.199129
17	1	0	0.063384	2.296435	0.689311
18	1	0	0.023700	2.379273	-1.096477
19	6	0	2.059640	-0.879665	1.314795
20	1	0	3.092326	-1.055549	1.639629
21	1	0	1.518675	-1.827224	1.359308
22	1	0	1.601010	-0.160698	2.000828
23	6	0	2.750692	0.977936	-0.325818
24	1	0	3.829731	0.853754	-0.175956
25	1	0	2.399629	1.732449	0.385928
26	1	0	2.584150	1.318443	-1.350044
27	1	0	-1.444728	2.760130	-0.139408

Zero-point correction=	0.218843 (Hartree/Particle)
Thermal correction to Energy=	0.232540
Thermal correction to Enthalpy=	0.233484

Thermal correction to Gibbs Free Energy=	0.178813
Sum of electronic and zero-point Energies=	-594.003452
Sum of electronic and thermal Energies=	-593.989756
Sum of electronic and thermal Enthalpies=	-593.988811
Sum of electronic and thermal Free Energies=	-594.043483

Transition state for the oxidation of 1-Azabicyclo[3.3.1]nonan-2-one by DMDO, C1, B3LYP/6-31G*

Energy = -710.900287 au

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.296142	-0.251240	-0.147759
2	6	0	0.390518	0.916409	0.716912
3	8	0	-0.130308	0.908791	1.807612
4	6	0	1.094663	-0.144608	-1.391035
5	1	0	0.674254	0.664483	-1.988600
6	1	0	0.939515	-1.071071	-1.947403
7	6	0	0.591673	-1.515120	0.572357
8	1	0	0.333712	-2.321642	-0.117814
9	1	0	-0.072016	-1.566868	1.434800
10	6	0	2.557030	0.074255	-0.987236
11	1	0	3.165356	0.140320	-1.896657
12	6	0	3.017754	-1.170268	-0.188356
13	1	0	3.063381	-2.019141	-0.884197
14	1	0	4.036502	-1.020851	0.189432
15	6	0	2.075910	-1.527922	0.981024
16	1	0	2.215547	-0.821197	1.809186
17	1	0	2.328854	-2.517636	1.378520
18	6	0	1.273045	2.011947	0.167687
19	1	0	1.351276	2.792518	0.927174
20	1	0	0.801171	2.453763	-0.717916
21	6	0	2.663892	1.420286	-0.200974
22	1	0	3.208976	2.163206	-0.791626
23	1	0	3.240603	1.273230	0.719483
24	8	0	-1.300233	-0.344258	-0.793878
25	8	0	-3.211636	-0.530231	-1.422653
26	6	0	-2.851390	-0.110844	-0.267948
27	6	0	-3.018526	1.379056	0.029405
28	1	0	-2.733081	1.953403	-0.855996
29	1	0	-2.430670	1.701978	0.895078
30	1	0	-4.075730	1.582250	0.243379
31	6	0	-3.060797	-1.024530	0.938041

32	1	0	-2.830373	-2.053999	0.652034
33	1	0	-4.112948	-0.980377	1.247931
34	1	0	-2.442544	-0.720076	1.789592

Zero-point correction=	0.289751 (Hartree/Particle)
Thermal correction to Energy=	0.304595
Thermal correction to Enthalpy=	0.305539
Thermal correction to Gibbs Free Energy=	0.248489
Sum of electronic and zero-point Energies=	-710.610537
Sum of electronic and thermal Energies=	-710.595692
Sum of electronic and thermal Enthalpies=	-710.594748
Sum of electronic and thermal Free Energies=	-710.651798

Transition state for the oxidation of 1-Azabicyclo[3.3.1]nonan-2-one by DMDO, C1, B3LYP/6-31+G**

Energy = -710.95411021 au

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.286124	-0.202627	-0.137545
2	6	0	0.454224	0.997966	0.669568
3	8	0	-0.050723	1.066130	1.767523
4	6	0	1.091502	-0.204578	-1.383507
5	1	0	0.721490	0.594975	-2.025044
6	1	0	0.886942	-1.147873	-1.892977
7	6	0	0.505942	-1.449362	0.640677
8	1	0	0.204390	-2.271708	-0.012173
9	1	0	-0.153893	-1.426609	1.506816
10	6	0	2.562975	-0.048053	-0.983147
11	1	0	3.172683	-0.061040	-1.893598
12	6	0	2.953356	-1.276490	-0.125159
13	1	0	2.957742	-2.156960	-0.781546
14	1	0	3.976294	-1.164306	0.252839
15	6	0	1.988677	-1.530526	1.053440
16	1	0	2.168920	-0.803229	1.854386
17	1	0	2.179372	-2.517268	1.489658
18	6	0	1.388545	2.015423	0.064127
19	1	0	1.508945	2.830119	0.780017
20	1	0	0.940154	2.430260	-0.845569
21	6	0	2.745000	1.327864	-0.266282
22	1	0	3.331647	2.006920	-0.892131
23	1	0	3.310801	1.196834	0.662810
24	8	0	-1.318534	-0.173502	-0.822692

25	8	0	-3.214194	-0.260234	-1.487568
26	6	0	-2.848136	-0.093191	-0.260661
27	6	0	-3.063917	1.286510	0.354120
28	1	0	-2.806508	2.051900	-0.381932
29	1	0	-2.476089	1.429729	1.265631
30	1	0	-4.125547	1.394871	0.606905
31	6	0	-3.064514	-1.257749	0.703926
32	1	0	-2.773799	-2.191754	0.217725
33	1	0	-4.131210	-1.315413	0.951037
34	1	0	-2.509520	-1.127100	1.639250

Zero-point correction=	0.282941 (Hartree/Particle)
Thermal correction to Energy=	0.298125
Thermal correction to Enthalpy=	0.299069
Thermal correction to Gibbs Free Energy=	0.240752
Sum of electronic and zero-point Energies=	-710.671170
Sum of electronic and thermal Energies=	-710.655986
Sum of electronic and thermal Enthalpies=	-710.655041
Sum of electronic and thermal Free Energies=	-710.713359

Transition state for the oxidation of Kirby Lactam by DMDO, C1, B3LYP/6-31G*

Energy = -866.952475 au

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.325833	-0.286438	-0.000037
2	6	0	0.243631	-0.901776	-1.228272
3	1	0	-0.258609	-0.439068	-2.083555
4	1	0	-0.046565	-1.955228	-1.204065
5	6	0	0.243574	-0.901797	1.228214
6	6	0	-0.062545	1.173577	-0.000010
7	8	0	-0.953018	1.977880	0.000012
8	6	0	1.773194	-0.706151	1.276231
9	6	0	1.773254	-0.706139	-1.276213
10	6	0	1.435717	1.486837	0.000012
11	8	0	-1.972220	-0.886472	-0.000082
12	8	0	-3.862587	-1.531864	-0.000095
13	6	0	-3.479823	-0.302853	-0.000016
14	1	0	-0.258710	-0.439109	2.083482
15	1	0	-0.046614	-1.955250	1.203970
16	6	0	2.047470	0.812437	1.260233
17	1	0	1.639035	1.279982	2.166548
18	1	0	3.129066	1.004215	1.263471
19	6	0	1.666008	2.999229	0.000026

20	1	0	1.219924	3.466981	-0.883041
21	1	0	2.740552	3.213826	0.000057
22	1	0	1.219875	3.466972	0.883073
23	6	0	2.047532	0.812447	-1.260183
24	1	0	3.129129	1.004224	-1.263366
25	1	0	1.639145	1.280001	-2.166515
26	6	0	2.343489	-1.357016	-2.541548
27	1	0	2.140281	-2.434188	-2.557648
28	1	0	3.430015	-1.219955	-2.593371
29	1	0	1.906347	-0.918403	-3.446586
30	6	0	2.378999	-1.335042	0.000019
31	1	0	2.199371	-2.419170	0.000009
32	1	0	3.468902	-1.194121	0.000046
33	6	0	2.343372	-1.357042	2.541583
34	1	0	2.140151	-2.434212	2.557667
35	1	0	1.906198	-0.918428	3.446605
36	1	0	3.429898	-1.219994	2.593451
37	6	0	-3.681198	0.496696	1.288195
38	1	0	-3.416898	-0.135988	2.140041
39	1	0	-4.740787	0.768625	1.380269
40	1	0	-3.088469	1.415987	1.304733
41	6	0	-3.681251	0.496877	-1.288105
42	1	0	-3.417006	-0.135694	-2.140051
43	1	0	-3.088509	1.416159	-1.304548
44	1	0	-4.740841	0.768835	-1.380085

Zero-point correction=	0.377778 (Hartree/Particle)
Thermal correction to Energy=	0.397136
Thermal correction to Enthalpy=	0.398080
Thermal correction to Gibbs Free Energy=	0.332526
Sum of electronic and zero-point Energies=	-866.574697
Sum of electronic and thermal Energies=	-866.555339
Sum of electronic and thermal Enthalpies=	-866.554395
Sum of electronic and thermal Free Energies=	-866.619949

Transition state for the oxidation of Kirby Lactam by DMDO, C1, B3LYP/6-31+G**

Energy = -867.01674912 au

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.326198	-0.285155	-0.000050
2	6	0	0.243335	-0.902925	-1.229307
3	1	0	-0.255746	-0.441862	-2.086927

4	1	0	-0.045105	-1.956632	-1.204991
5	6	0	0.243259	-0.902967	1.229220
6	6	0	-0.060365	1.174136	-0.000007
7	8	0	-0.954017	1.976341	0.000020
8	6	0	1.773792	-0.706951	1.276064
9	6	0	1.773871	-0.706917	-1.276051
10	6	0	1.438248	1.487216	0.000027
11	8	0	-1.991086	-0.899957	-0.000122
12	8	0	-3.877608	-1.526798	-0.000136
13	6	0	-3.464863	-0.294798	-0.000021
14	1	0	-0.255878	-0.441939	2.086825
15	1	0	-0.045173	-1.956675	1.204845
16	6	0	2.048186	0.811445	1.260916
17	1	0	1.639309	1.278628	2.166513
18	1	0	3.129222	1.002880	1.263837
19	6	0	1.674782	2.998800	0.000056
20	1	0	1.232625	3.469495	-0.882651
21	1	0	2.750420	3.204657	0.000093
22	1	0	1.232568	3.469471	0.882746
23	6	0	2.048266	0.811478	-1.260840
24	1	0	3.129303	1.002912	-1.263687
25	1	0	1.639449	1.278684	-2.166452
26	6	0	2.342941	-1.358538	-2.542159
27	1	0	2.140021	-2.435119	-2.557688
28	1	0	3.428849	-1.221228	-2.593997
29	1	0	1.905728	-0.920196	-3.446563
30	6	0	2.379577	-1.336124	0.000016
31	1	0	2.199080	-2.419460	-0.000004
32	1	0	3.468825	-1.194522	0.000052
33	6	0	2.342785	-1.358609	2.542188
34	1	0	2.139854	-2.435188	2.557678
35	1	0	1.905524	-0.920283	3.446577
36	1	0	3.428692	-1.221309	2.594090
37	6	0	-3.676579	0.502693	1.286771
38	1	0	-3.413142	-0.125550	2.141429
39	1	0	-4.738426	0.764699	1.368356
40	1	0	-3.091243	1.426220	1.301387
41	6	0	-3.676661	0.502956	-1.286635
42	1	0	-3.413287	-0.125117	-2.141437
43	1	0	-3.091319	1.426480	-1.301107
44	1	0	-4.738512	0.764984	-1.368092

Zero-point correction=	0.369052 (Hartree/Particle)
Thermal correction to Energy=	0.388771
Thermal correction to Enthalpy=	0.389715
Thermal correction to Gibbs Free Energy=	0.323386

Sum of electronic and zero-point Energies=	-866.647697
Sum of electronic and thermal Energies=	-866.627978
Sum of electronic and thermal Enthalpies=	-866.627034
Sum of electronic and thermal Free Energies=	-866.693363

Transition state for the oxidation of the hydrate of Kirby Lactam by DMDO, C1, B3LYP/6-31G*

Energy = -943.403671 au

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.329810	-0.075065	0.000031
2	6	0	0.033084	-0.820325	-1.218510
3	1	0	-0.332262	-0.261405	-2.080522
4	1	0	-0.476850	-1.789372	-1.187044
5	6	0	0.033141	-0.820294	1.218573
6	6	0	0.254418	1.330980	0.000001
7	6	0	1.571763	-0.997609	1.273218
8	6	0	1.571702	-0.997641	-1.273223
9	6	0	1.799263	1.213050	-0.000036
10	8	0	-2.102509	0.528067	0.000082
11	8	0	-3.967480	1.023488	0.000132
12	6	0	-3.435872	-0.180239	0.000018
13	1	0	-0.332166	-0.261351	2.080586
14	1	0	-0.476797	-1.789341	1.187157
15	6	0	2.212584	0.410476	1.256986
16	1	0	1.927890	0.963056	2.159098
17	1	0	3.306700	0.311305	1.268790
18	6	0	2.439386	2.607476	-0.000069
19	1	0	2.139538	3.175257	-0.885753
20	1	0	3.532411	2.517496	-0.000097
21	1	0	2.139585	3.175276	0.885619
22	6	0	2.212523	0.410445	-1.257059
23	1	0	3.306638	0.311273	-1.268914
24	1	0	1.927786	0.963000	-2.159171
25	6	0	1.958569	-1.767394	-2.540354
26	1	0	1.498989	-2.763476	-2.558379
27	1	0	3.045543	-1.900398	-2.595504
28	1	0	1.640851	-1.231767	-3.442950
29	6	0	2.006710	-1.757179	-0.000004
30	1	0	1.571646	-2.767772	0.000019
31	1	0	3.098340	-1.884242	-0.000028
32	6	0	1.958691	-1.767329	2.540349
33	1	0	1.499110	-2.763409	2.558424

34	1	0	1.641018	-1.231677	3.442947
35	1	0	3.045668	-1.900333	2.595450
36	6	0	-3.609674	-0.994821	-1.282646
37	1	0	-3.401918	-0.355710	-2.144735
38	1	0	-4.647069	-1.342344	-1.352906
39	1	0	-2.956897	-1.875867	-1.312349
40	6	0	-3.609661	-0.995064	1.282530
41	1	0	-3.401853	-0.356126	2.144734
42	1	0	-2.956913	-1.876138	1.312040
43	1	0	-4.647065	-1.342565	1.352755
44	8	0	-0.180534	1.962283	1.159714
45	1	0	-1.157007	1.873075	1.147950
46	8	0	-0.180596	1.962257	-1.159703
47	1	0	-1.157068	1.873042	-1.147879

Zero-point correction=	0.406154 (Hartree/Particle)
Thermal correction to Energy=	0.426300
Thermal correction to Enthalpy=	0.427245
Thermal correction to Gibbs Free Energy=	0.360329
Sum of electronic and zero-point Energies=	-942.997517
Sum of electronic and thermal Energies=	-942.977371
Sum of electronic and thermal Enthalpies=	-942.976427
Sum of electronic and thermal Free Energies=	-943.043343