Supporting Information

Predicted Reversal in N-Methylazepine/N-Methyl-7-azanorcaradiene Equilibrium Upon Formation of Their N-Oxides

René Fournier[1], Alexa R. Green[2], Arthur Greenberg[2,*], Edward Lee-Ruff[1,*], Joel F. Liebman[3,*] and Anita Rágyanszki[4,*]

1. Department of Chemistry, York University, Keele Campus, Toronto ON MJ3 1P3 Canada
2. Department of Chemistry, University of New Hampshire, Durham, NH 03824 USA
3. Department of Chemistry and Biochemistry, University of Maryland Baltimore County, Baltimore, MD 21250 USA
4. Department of Physics and Astronomy, York University, Keele Campus, Toronto ON MJ3 1P3 Canada

*E-mail: art.greenberg@unh.edu
leeruff@yorku.ca
jliebman@umbc.edu
a.ragyanszki@utoronto.ca

Cartesian Coordinates (Å) and energies (Hartrees) for all structures calculated using Gaussian 09.

N-methylpyrrole
The number of imaginary frequencies: 0
Total Energy (B3LYP/6-31G*)= -249.47784543
ZPE= -249.367168
Enthalpy= -249.360642
Gibb's Free Energy= -249.396193

C	-0.31737	-1.01923	0.17362
C	1.00946	-1.0133	-0.07679
C	1.4598	0.44188	-0.08284
C	0.36886	1.19813	0.16441
N	-0.76109	0.33469	0.58538
H	-0.95522	-1.87361	0.08373
H	1.62623	-1.86947	-0.25416
H	2.45195	0.79863	-0.26524
H	0.32489	2.26274	0.06655
C	-2.04157	0.72846	-0.0198
H	-2.29179	1.72172	0.28958
H	-1.95658	0.69773	-1.08597
H	-2.80837	0.05254	0.29651

N-methylpyrrole
The number of imaginary frequencies: 0
Total Energy (B3LYP/6-31G**)= -249.48868841
ZPE= -249.37822
Enthalpy= -249.371698
Gibb's Free Energy= -249.407248

C	0.	-0.17376	1.09496
C	0.	-1.46657	0.6966
C	0.	-1.46657	-0.6966
C	0.	-0.17376	-1.09496
N	0.	0.60624	0.
H	0.	0.16939	2.10844
H	0.	-2.32739	1.33212
H	0.	-2.32739	-1.33212
H	0.	0.16939	-2.10844
C	0.	2.07624	0.
H	0.5044	2.43291	-0.87365
H	-1.00881	2.43291	0.
H	0.5044	2.43291	0.87365

N-methylpyrrole
The number of imaginary frequencies: 0
Total Energy (M06/6-311G+**)= -249.34878244
ZPE= -249.239616
Enthalpy= -249.232966
Gibb's Free Energy= -249.269338

C	-0.31737	-1.01923	0.17362
C	1.00946	-1.0133	-0.07679
C	1.4598	0.44188	-0.08284
C	0.36886	1.19813	0.16441
N	-0.76109	0.33469	0.58538
H	-0.95522	-1.87361	0.08373
H	1.62623	-1.86947	-0.25416
H	2.45195	0.79863	-0.26524
H	0.32489	2.26274	0.06655
C	-2.04157	0.72846	-0.0198
H	-2.29179	1.72172	0.28958
H	-1.95658	0.69773	-1.08597
H	-2.80837	0.05254	0.29651

N-Methylpyrrole N-oxide
The number of imaginary frequencies: 0
Total Energy (B3LYP/6-31G*)= -324.56298019
ZPE= -324.449454
Enthalpy= -324.442285
Gibb's Free Energy= -324.479007

C	-0.3294	-1.01791	0.1578
C	1.00468	-1.01444	-0.06029
C	1.45655	0.44566	-0.06634
C	0.35814	1.20372	0.14859
N	-0.75911	0.33403	0.57648
H	-0.97374	-1.86404	0.04035
H	1.62512	-1.87187	-0.21771
H	2.45247	0.80154	-0.22879
H	0.30409	2.26497	0.02323
C	-2.04454	0.72939	-0.01703
H	-2.29215	1.72185	0.29697
H	-1.96841	0.7014	-1.08395
H	-2.80872	0.05267	0.30389
O	-0.87602	0.37583	1.93081

N-Methylpyrrole N-oxide
The number of imaginary frequencies: 0
Total Energy (B3LYP/6-31G**)= -324.57360076
ZPE= -324.46035
Enthalpy= -324.453172
Gibb's Free Energy= -324.489906

C	-0.04298	0.35255	1.15778
C	-0.04298	1.62083	0.7378
C	-0.04298	1.62083	-0.7378
C	-0.04298	0.35255	-1.15778

N	-0.04755	-0.56912	0.
H	-0.10099	-0.10602	2.13324
H	-0.09948	2.50313	1.36302
H	-0.09948	2.50313	-1.36302
H	-0.10099	-0.10602	-2.13324
C	1.16596	-1.45463	0.
H	1.08767	-2.08133	-0.8887
H	2.08944	-0.86521	0.
H	1.08767	-2.08133	0.8887
O	-1.18692	-1.34192	0.

N-methylpyrrole N-oxide

The number of imaginary frequencies: 0

Total Energy (M06/6-311G+**)= -324.43163272

ZPE= -324.31929

Enthalpy= -324.312193

Gibb's Free Energy= -324.348742

C	-0.3294	-1.01791	0.1578
C	1.00468	-1.01444	-0.06029
C	1.45655	0.44566	-0.06634
C	0.35814	1.20372	0.14859
N	-0.75911	0.33403	0.57648
H	-0.97374	-1.86404	0.04035
H	1.62512	-1.87187	-0.21771
H	2.45247	0.80154	-0.22879
H	0.30409	2.26497	0.02323
C	-2.04454	0.72939	-0.01703
H	-2.29215	1.72185	0.29697
H	-1.96841	0.7014	-1.08395
H	-2.80872	0.05267	0.30389
O	-0.87602	0.37583	1.93081

N-methylazepine

The number of imaginary frequencies: 0

Total Energy (B3LYP/6-31G*)= -326.84608435

ZPE= -326.702253

Enthalpy= -326.693875

Gibb's Free Energy= -326.733659

C	0.93863	0.15438	-0.2526
C	2.30347	0.15457	-0.25898
C	3.19274	1.20123	0.04876
C	0.05199	1.2008	0.06344
C	2.91009	2.40177	0.60544
C	0.33949	2.40141	0.61745
H	0.47792	-0.76674	-0.54277
H	2.7617	-0.76642	-0.55344
H	4.22198	1.0244	-0.18427
H	-0.97933	1.02368	-0.15996
H	3.70896	3.11213	0.6512
H	-0.45911	3.11155	0.67068
N	1.62734	2.81624	1.17006
C	1.63404	2.44107	2.59136
H	1.63673	3.32544	3.19368
H	0.76149	1.86222	2.81157
H	2.50877	1.86246	2.8034

N-methylazepine

The number of imaginary frequencies: 0

Total Energy (B3LYP/6-31G**)= -326.85965616

ZPE= -326.716154

Enthalpy= -326.70778

Gibb's Free Energy= -326.747543

C	0.61021	1.77096	0.67637
C	0.61021	1.77096	-0.67637
C	0.61021	0.57868	-1.51904
C	0.61021	0.57868	1.51904
C	0.05418	-0.6014	-1.19368
C	0.05418	-0.6014	1.19368
H	0.69105	2.72773	1.19091
H	0.69105	2.72773	-1.19091
H	1.12518	0.64113	-2.47565
H	1.12518	0.64113	2.47565
H	0.1529	-1.46083	-1.86048
H	0.1529	-1.46083	1.86048
N	-0.68116	-0.8274	0.
C	-1.52746	-2.0092	0.
H	-0.95778	-2.95729	0.
H	-2.17143	-1.99535	0.88425
H	-2.17143	-1.99535	-0.88425

N-methylazepine

The number of imaginary frequencies: 0

Total Energy (M06/6-311G+**)= -326.67492642

ZPE= -326.532731

Enthalpy= -326.524386

Gibb's Free Energy= -326.563984

C	0.62245	1.75336	0.67222
C	0.62245	1.75336	-0.67222
C	0.62245	0.56474	-1.50646
C	0.62245	0.56474	1.50646
C	0.04331	-0.59604	-1.18419
C	0.04331	-0.59604	1.18419
H	0.70572	2.70987	1.18507
H	0.70572	2.70987	-1.18507
H	1.14071	0.61519	-2.46069
H	1.14071	0.61519	2.46069
H	0.11856	-1.45761	-1.85176
H	0.11856	-1.45761	1.85176

N	-0.69474	-0.80586	0.
C	-1.53524	-1.98153	0.
H	-0.95466	-2.92166	0.
H	-2.17953	-1.97387	0.88285
H	-2.17953	-1.97387	-0.88285

N-methylazepine N-oxide

The number of imaginary frequencies: 0

Total Energy (B3LYP/6-31G*)= -401.97429587

ZPE= -401.825754

Enthalpy= -401.817041

Gibb's Free Energy= -401.857431

C	0.82605	0.55465	-0.65489
C	2.17148	0.54639	-0.76242
C	3.08766	1.44622	-0.20978
C	0.02032	1.46506	0.03537
C	2.88442	2.40908	0.72364
C	0.38096	2.42445	0.92372
H	0.31053	-0.22416	-1.17699
H	2.58798	-0.23815	-1.35901
H	4.09119	1.36074	-0.57104
H	-1.02882	1.39218	-0.16184
H	3.7184	3.0554	0.90153
H	-0.40623	3.08073	1.23117
N	1.69221	2.67973	1.54823
C	1.78348	1.84441	2.75439
H	2.70185	2.05143	3.26295
H	0.96013	2.06213	3.40215
H	1.75489	0.81166	2.476
O	1.72659	3.99895	1.87699

N-methylazepine N-oxide

The number of imaginary frequencies: 0

Total Energy (B3LYP/6-31G**)= -401.98779312

ZPE= -401.839695

Enthalpy= -401.830971

Gibb's Free Energy= -401.871365

C	0.75349	1.83108	0.68076
C	0.75349	1.83108	-0.68076
C	0.75349	0.64759	-1.50595
C	0.75349	0.64759	1.50595
C	0.29957	-0.58124	-1.1975
C	0.29957	-0.58124	1.1975
H	0.87786	2.78202	1.19381
H	0.87786	2.78202	-1.19381
H	1.21424	0.74192	-2.48817
H	1.21424	0.74192	2.48817
H	0.42486	-1.46195	-1.81406
H	0.42486	-1.46195	1.81406

N	-0.50404	-0.94862	0.
C	-1.83882	-0.25012	0.
H	-2.35394	-0.60559	-0.89226
H	-2.35394	-0.60559	0.89226
H	-1.73292	0.83728	0.
O	-0.7138	-2.29727	0.

N-methylazepine N-oxide

The number of imaginary frequencies: 0

Total Energy (M06/6-311G+**)= -401.79814103

ZPE= -401.651151

Enthalpy= -401.642487

Gibb's Free Energy= -401.682651

C	0.82605	0.55465	-0.65489
C	2.17148	0.54639	-0.76242
C	3.08766	1.44622	-0.20978
C	0.02032	1.46506	0.03537
C	2.88442	2.40908	0.72364
C	0.38096	2.42445	0.92372
H	0.31053	-0.22416	-1.17699
H	2.58798	-0.23815	-1.35901
H	4.09119	1.36074	-0.57104
H	-1.02882	1.39218	-0.16184
H	3.7184	3.0554	0.90153
H	-0.40623	3.08073	1.23117
N	1.69221	2.67973	1.54823
C	1.78348	1.84441	2.75439
H	2.70185	2.05143	3.26295
H	0.96013	2.06213	3.40215
H	1.75489	0.81166	2.476
O	1.72659	3.99895	1.87699

1,3-Cyclopentadiene

The number of imaginary frequencies: 0

Total Energy (B3LYP/6-31G*)= -194.10105812

ZPE= -194.008165

Enthalpy= -194.003078

Gibb's Free Energy= -194.034762

C	-0.03204	0.83323	-0.57221
C	1.30621	0.8271	-0.35761
C	1.75514	2.2525	0.01266
C	0.56916	3.10434	-0.4754
C	-0.50584	2.29711	-0.64793
H	-0.65144	-0.03154	-0.68801
H	1.94617	-0.02657	-0.43883
H	1.85482	2.33968	1.07444
H	2.68483	2.53007	-0.43847
H	0.5915	4.15886	-0.65532
H	-1.51004	2.62121	-0.82523

1,3-Cyclopentadiene
The number of imaginary frequencies: 0
Total Energy (B3LYP/6-31G**)= -194.11069027
ZPE= -194.017995
Enthalpy= -194.012901
Gibb's Free Energy= -194.044595

C	-0.03204	0.83323	-0.57221
C	1.30621	0.8271	-0.35761
C	1.75514	2.2525	0.01266
C	0.56916	3.10434	-0.4754
C	-0.50584	2.29711	-0.64793
H	-0.65144	-0.03154	-0.68801
H	1.94617	-0.02657	-0.43883
H	1.85482	2.33968	1.07444
H	2.68483	2.53007	-0.43847
H	0.5915	4.15886	-0.65532
H	-1.51004	2.62121	-0.82523

1,3-Cyclopentadiene
The number of imaginary frequencies: 0
Total Energy (M06/6-311G+**)= -193.99039929
ZPE= -193.898575
Enthalpy= -193.893442
Gibb's Free Energy= -193.925181

C	-0.03204	0.83323	-0.57221
C	1.30621	0.8271	-0.35761
C	1.75514	2.2525	0.01266
C	0.56916	3.10434	-0.4754
C	-0.50584	2.29711	-0.64793
H	-0.65144	-0.03154	-0.68801
H	1.94617	-0.02657	-0.43883
H	1.85482	2.33968	1.07444
H	2.68483	2.53007	-0.43847
H	0.5915	4.15886	-0.65532
H	-1.51004	2.62121	-0.82523

1,3,5-Cycloheptatriene
The number of imaginary frequencies: 0
Total Energy (B3LYP/6-31G*)= -271.50958752
ZPE=-271.381192
Enthalpy= -271.374505
Gibb's Free Energy= -271.41033

C	-0.20071	-0.81856	0.32651
C	1.06397	-0.49637	-0.04424
C	1.68974	0.89155	-0.31285
C	-1.34606	0.10738	0.76151
C	1.19882	2.07325	0.5547
C	-1.27725	1.41867	1.06715
C	-0.03587	2.32272	1.05869
H	1.5021	1.14001	-1.33655
H	-0.43367	-1.86275	0.30957
H	1.721	-1.32797	-0.19136
H	2.74077	0.79537	-0.13682
H	-2.31134	-0.34609	0.84812
H	1.9384	2.81469	0.77422
H	-2.19448	1.88081	1.36717
H	-0.16354	3.28474	1.50936

1,3,5-Cycloheptatriene
The number of imaginary frequencies: 0
Total Energy (B3LYP/6-31G**)= -271.52195835
ZPE=-271.393853
Enthalpy= -271.387159
Gibb's Free Energy= -271.422993

C	-0.20071	-0.81856	0.32651
C	1.06397	-0.49637	-0.04424
C	1.68974	0.89155	-0.31285
C	-1.34606	0.10738	0.76151
C	1.19882	2.07325	0.5547
C	-1.27725	1.41867	1.06715
C	-0.03587	2.32272	1.05869
H	1.5021	1.14001	-1.33655
H	-0.43367	-1.86275	0.30957
H	1.721	-1.32797	-0.19136
H	2.74077	0.79537	-0.13682
H	-2.31134	-0.34609	0.84812
H	1.9384	2.81469	0.77422
H	-2.19448	1.88081	1.36717
H	-0.16354	3.28474	1.50936

1,3,5-Cycloheptatriene
The number of imaginary frequencies: 0
Total Energy (M06/6-311G+**)= -271.35461618
ZPE=-271.227611
Enthalpy= -271.22088
Gibb's Free Energy=-271.256734

C	-0.20071	-0.81856	0.32651
C	1.06397	-0.49637	-0.04424
C	1.68974	0.89155	-0.31285
C	-1.34606	0.10738	0.76151
C	1.19882	2.07325	0.5547
C	-1.27725	1.41867	1.06715
C	-0.03587	2.32272	1.05869
H	1.5021	1.14001	-1.33655
H	-0.43367	-1.86275	0.30957
H	1.721	-1.32797	-0.19136
H	2.74077	0.79537	-0.13682
H	-2.31134	-0.34609	0.84812
H	1.9384	2.81469	0.77422

H	-2.19448	1.88081	1.36717
H	-0.16354	3.28474	1.50936

2,4-Cyclopentadienone
The number of imaginary frequencies: 0
Total Energy (B3LYP/6-31G*)= -268.10366059
ZPE=-268.029249
Enthalpy= -268.023604
Gibb's Free Energy= -268.057109

C	-0.01597	0.56911	-0.63699
C	1.53525	0.57813	-0.59521
C	1.96549	1.79004	-0.15552
C	0.72782	2.6481	0.11742
C	-0.48331	1.77579	-0.22148
H	-0.62226	-0.25716	-0.94455
H	2.16679	-0.24094	-0.86942
H	2.9842	2.08978	-0.02407
H	-1.51104	2.06363	-0.14516
O	0.70962	3.83439	0.53688

2,4-Cyclopentadienone
The number of imaginary frequencies: 0
Total Energy (B3LYP/6-31G**)= -268.11018199
ZPE=-268.035857
Enthalpy= -268.030211
Gibb's Free Energy= -268.063716

C	-0.01597	0.56911	-0.63699
C	1.53525	0.57813	-0.59521
C	1.96549	1.79004	-0.15552
C	0.72782	2.6481	0.11742
C	-0.48331	1.77579	-0.22148
H	-0.62226	-0.25716	-0.94455
H	2.16679	-0.24094	-0.86942
H	2.9842	2.08978	-0.02407
H	-1.51104	2.06363	-0.14516
O	0.70962	3.83439	0.53688

2,4-Cyclopentadienone
The number of imaginary frequencies: 0
Total Energy (M06/6-311G+**)=-267.98852408
ZPE=-267.914874
Enthalpy= -267.909179
Gibb's Free Energy= -267.942763

C	-0.01597	0.56911	-0.63699
C	1.53525	0.57813	-0.59521
C	1.96549	1.79004	-0.15552
C	0.72782	2.6481	0.11742
C	-0.48331	1.77579	-0.22148
H	-0.62226	-0.25716	-0.94455
H	2.16679	-0.24094	-0.86942
H	2.9842	2.08978	-0.02407
H	-1.51104	2.06363	-0.14516
O	0.70962	3.83439	0.53688

2,4,6-Cycloheptatrienone
The number of imaginary frequencies: 0
Total Energy (B3LYP/6-31G*)= -345.53739483
ZPE= -345.426757
Enthalpy= -345.41951
Gibb's Free Energy= -345.457457

C	0.4044	-0.40001	-0.15775
C	1.77241	-0.40055	-0.15529
C	2.69105	0.61692	0.1737
C	-0.51461	0.61819	0.16794
C	2.45079	1.88455	0.58091
C	-0.2748	1.88563	0.576
C	1.08787	2.54419	0.79042
H	-0.04191	-1.32554	-0.45626
H	2.21906	-1.32643	-0.4522
H	3.72353	0.34896	0.08952
H	-1.54699	0.35106	0.08004
H	3.3092	2.49215	0.77797
H	-1.13344	2.49392	0.76997
O	1.08765	3.74217	1.17569

2,4,6-Cycloheptatrienone
The number of imaginary frequencies: 0
Total Energy (B3LYP/6-31G**)= -345.54656227
ZPE=-345.436187
Enthalpy=-345.428926
Gibb's Free Energy= -345.466909

C	0.4044	-0.40001	-0.15775
C	1.77241	-0.40055	-0.15529
C	2.69105	0.61692	0.1737
C	-0.51461	0.61819	0.16794
C	2.45079	1.88455	0.58091
C	-0.2748	1.88563	0.576
C	1.08787	2.54419	0.79042
H	-0.04191	-1.32554	-0.45626
H	2.21906	-1.32643	-0.4522
H	3.72353	0.34896	0.08952
H	-1.54699	0.35106	0.08004
H	3.3092	2.49215	0.77797
H	-1.13344	2.49392	0.76997
O	1.08765	3.74217	1.17569

2,4,6-Cycloheptatrienone
The number of imaginary frequencies: 0

Total Energy (M06/6-311G+**)= -345.37465529
ZPE=-345.265377
Enthalpy=-345.257928
Gibb's Free Energy= -345.297053

C	0.4044	-0.40001	-0.15775
C	1.77241	-0.40055	-0.15529
C	2.69105	0.61692	0.1737
C	-0.51461	0.61819	0.16794
C	2.45079	1.88455	0.58091
C	-0.2748	1.88563	0.576
C	1.08787	2.54419	0.79042
H	-0.04191	-1.32554	-0.45626
H	2.21906	-1.32643	-0.4522
H	3.72353	0.34896	0.08952
H	-1.54699	0.35106	0.08004
H	3.3092	2.49215	0.77797
H	-1.13344	2.49392	0.76997
O	1.08765	3.74217	1.17569

2,3-Epoxide N-Methylazepine
The number of imaginary frequencies: 0
Total Energy (B3LYP/6-31G*)= -402.0126142
ZPE= -401.86298
Enthalpy= -401.854323
Gibb's Free Energy= -401.894916

C	-1.97153	-0.86665	0.21864
C	-2.0792	0.477	0.09836
C	-0.81657	1.03296	-0.45425
C	-0.76447	-1.68529	-0.03687
C	0.35442	0.76433	0.37226
C	0.56633	-1.4101	-0.22187
H	-2.85437	-1.44535	0.48705
H	-2.99559	1.0283	0.28163
H	-0.97814	-2.75026	-0.09528
H	1.23067	-2.25728	-0.38004
N	1.2452	-0.18133	-0.21943
C	2.65217	-0.16427	0.16546
H	2.80272	-0.32861	1.24518
H	3.19049	-0.94245	-0.38388
H	3.08022	0.8047	-0.10428
O	0.07826	2.101	-0.03692
H	0.21628	0.62946	1.44876
H	-0.68167	0.83496	-1.51815

2,3-Epoxide N-Methylazepine
The number of imaginary frequencies: 0
Total Energy (B3LYP/6-31G**)= -402.02568814
ZPE= -401.876485
Enthalpy= -401.867821
Gibb's Free Energy= -401.908422

C	0.98337	1.56503	0.95991
C	1.51419	1.48097	-0.29992
C	0.77098	0.59913	-1.22425
C	-0.27211	0.73245	1.52549
C	0.33821	-0.65376	-0.82677
C	-1.08316	-0.29294	0.95543
H	1.45087	2.2507	1.63534
H	2.39553	2.01271	-0.59215
H	-0.54747	0.99384	2.52587
H	-1.84555	-0.69634	1.58863
N	-0.9916	-0.87598	-0.41373
C	-1.31788	-2.30927	-0.40307
H	-0.64737	-2.82283	0.25387
H	-2.32339	-2.44364	-0.06277
H	-1.22039	-2.70462	-1.39256
O	1.10315	-0.57651	-2.16386
H	0.91807	-1.18081	-0.09815
H	0.06457	1.25633	-1.68681

2,3-Epoxide N-Methylazepine
The number of imaginary frequencies: 0
Total Energy (M06/6-311G+**)= -401.83976324
ZPE= -401.691752
Enthalpy= -401.683102
Gibb's Free Energy= -401.72367

C	-1.97153	-0.86665	0.21864
C	-2.0792	0.477	0.09836
C	-0.81657	1.03296	-0.45425
C	-0.76447	-1.68529	-0.03687
C	0.35442	0.76433	0.37226
C	0.56633	-1.4101	-0.22187
H	-2.85437	-1.44535	0.48705
H	-2.99559	1.0283	0.28163
H	-0.97814	-2.75026	-0.09528
H	1.23067	-2.25728	-0.38004
N	1.2452	-0.18133	-0.21943
C	2.65217	-0.16427	0.16546
H	2.80272	-0.32861	1.24518
H	3.19049	-0.94245	-0.38388
H	3.08022	0.8047	-0.10428
O	0.07826	2.101	-0.03692
H	0.21628	0.62946	1.44876
H	-0.68167	0.83496	-1.51815

4,5-Epoxide N-Methylazepine
The number of imaginary frequencies: 0

Total Energy (B3LYP/6-31G*)= -402.04752008
ZPE= -401.897386
Enthalpy= -401.888458
Gibb's Free Energy= -401.930104

C	-1.64868	-0.71215	0.39745
C	-1.655	0.71913	0.35793
C	-0.44281	1.62606	0.11899
C	-0.44434	-1.62081	0.12824
C	0.86032	1.29035	-0.06609
C	0.85605	-1.28843	-0.07968
H	-2.26809	-1.18847	1.12845
H	-0.65255	2.67515	0.10108
H	-0.6576	-2.66917	0.10912
H	1.55506	2.09233	0.07199
H	1.54753	-2.09766	0.02944
N	1.47105	0.0019	-0.46648
C	2.81324	-0.00515	0.133
H	3.34229	-0.87836	-0.18718
H	3.34692	0.86891	-0.177
H	2.72748	-0.01113	1.19955
H	-2.23316	1.23268	1.09746
O	-2.37974	-0.01144	-0.75584

4,5-Epoxide N-Methylazepine
The number of imaginary frequencies: 0
Total Energy (B3LYP/6-31G**)= -402.0607848
ZPE= -401.911089
Enthalpy=-401.902152
Gibb's Free Energy= -401.943808

C	-1.62994	-0.73255	0.39014
C	-1.62993	0.73255	0.39016
C	-0.4817	1.5723	-0.0053
C	-0.48168	-1.57231	-0.00529
C	0.81741	1.23806	-0.12102
C	0.81742	-1.23805	-0.12103
H	-2.3009	-1.21971	1.10274
H	-0.71282	2.61654	-0.20338
H	-0.7128	-2.61655	-0.20337
H	1.52499	2.03453	-0.34095
H	1.52502	-2.03452	-0.34094
N	1.44508	0.00001	-0.0493
C	2.8978	0.	0.11175
H	3.32482	-0.88576	-0.36736
H	3.3248	0.88584	-0.36723
H	3.19608	-0.00007	1.16878
H	-2.30097	1.21969	1.1027
O	-2.35501	-0.00001	-0.63029

4,5-Epoxide N-Methylazepine
The number of imaginary frequencies: 0
Total Energy (M06/6-311G+**)= -401.87335865
ZPE= -401.724678
Enthalpy= -401.715624
Gibb's Free Energy= -401.757962

C	-1.62994	-0.73255	0.39014
C	-1.62993	0.73255	0.39016
C	-0.4817	1.5723	-0.0053
C	-0.48168	-1.57231	-0.00529
C	0.81741	1.23806	-0.12102
C	0.81742	-1.23805	-0.12103
H	-2.3009	-1.21971	1.10274
H	-0.71282	2.61654	-0.20338
H	-0.7128	-2.61655	-0.20337
H	1.52499	2.03453	-0.34095
H	1.52502	-2.03452	-0.34094
N	1.44508	0.00001	-0.0493
C	2.8978	0.	0.11175
H	3.32482	-0.88576	-0.36736
H	3.3248	0.88584	-0.36723
H	3.19608	-0.00007	1.16878
H	-2.30097	1.21969	1.1027
O	-2.35501	-0.00001	-0.63029

N-methylpyrrolidine
The number of imaginary frequencies: 0
Total Energy (B3LYP/6-31G*)= -251.88956837
ZPE= -251.731361
Enthalpy= -251.724164
Gibb's Free Energy=-251.761212

C	-1.15663	-0.45327	0.19297
C	1.15639	-0.45362	0.19329
C	0.77798	1.0303	-0.07053
C	-0.77756	1.03066	-0.07012
H	-2.05637	-0.7771	-0.33946
H	-1.33544	-0.61146	1.26475
H	1.33453	-0.61147	1.26524
H	2.05631	-0.77799	-0.33851
H	1.19788	1.70083	0.6869
H	1.1653	1.36132	-1.04085
H	-1.19669	1.70085	0.68805
H	-1.16528	1.36262	-1.03996
N	-0.00017	-1.27389	-0.20026
C	0.00003	-1.3903	-1.66564
H	0.87482	-1.91947	-1.98127
H	-0.87248	-1.92325	-1.98122
H	-0.0021	-0.41291	-2.10107

N-methylpyrrolidine
The number of imaginary frequencies: 0

Total Energy (B3LYP/6-31G**)= -251.904379
ZPE= -251.746764
Enthalpy= -251.739572
Gibb's Free Energy=-251.776517

C	-0.07138	1.15044	-0.53372
C	-0.07129	-1.15029	-0.53401
C	-1.2628	-0.77695	0.3945
C	-1.26312	0.77669	0.39438
H	0.45507	2.05955	-0.22703
H	-0.43402	1.30923	-1.55803
H	-0.43417	-1.30864	-1.55831
H	0.45527	-2.0595	-0.22783
H	-2.20509	-1.19792	0.02894
H	-1.11008	-1.16732	1.4062
H	-2.20542	1.19716	0.02825
H	-1.11112	1.16732	1.40608
N	0.84465	0.00011	-0.54566
C	1.76509	0.	0.59063
H	2.40898	-0.88422	0.53277
H	2.40905	0.88419	0.53288
H	1.27997	-0.00004	1.58496

N-methylpyrrolidine
The number of imaginary frequencies: 0
Total Energy (M06/6-311G+**)= -251.7568498
ZPE= -251.601035
Enthalpy= -251.593775
Gibb's Free Energy= -251.630876

C	-0.07138	1.15044	-0.53372
C	-0.07129	-1.15029	-0.53401
C	-1.2628	-0.77695	0.3945
C	-1.26312	0.77669	0.39438
H	0.45507	2.05955	-0.22703
H	-0.43402	1.30923	-1.55803
H	-0.43417	-1.30864	-1.55831
H	0.45527	-2.0595	-0.22783
H	-2.20509	-1.19792	0.02894
H	-1.11008	-1.16732	1.4062
H	-2.20542	1.19716	0.02825
H	-1.11112	1.16732	1.40608
N	0.84465	0.00011	-0.54566
C	1.76509	0.	0.59063
H	2.40898	-0.88422	0.53277
H	2.40905	0.88419	0.53288
H	1.27997	-0.00004	1.58496

N-methylpyrrolidine N-oxide
The number of imaginary frequencies: 0
Total Energy (B3LYP/6-31G*)= -327.03549275
ZPE= -326.872485
Enthalpy= -326.864715
Gibb's Free Energy= -326.90296

C	-1.15663	-0.45327	0.19297
C	1.15639	-0.45362	0.19329
C	0.77798	1.0303	-0.07053
C	-0.77756	1.03066	-0.07012
H	-2.05637	-0.7771	-0.33946
H	-1.33544	-0.61146	1.26475
H	1.33453	-0.61147	1.26524
H	2.05631	-0.77799	-0.33851
H	1.19788	1.70083	0.6869
H	1.1653	1.36132	-1.04085
H	-1.19669	1.70085	0.68805
H	-1.16528	1.36262	-1.03996
N	-0.00017	-1.27389	-0.20026
C	0.00003	-1.3903	-1.66564
H	0.87482	-1.91947	-1.98127
H	-0.87248	-1.92325	-1.98122
H	-0.0021	-0.41291	-2.10107
O	-0.00044	-2.50637	0.37472

N-methylpyrrolidine N-oxide
The number of imaginary frequencies: 0
Total Energy (B3LYP/6-31G**)= -327.05036743
ZPE= -326.888069
Enthalpy= -326.880274
Gibb's Free Energy= -326.918536

C	-0.07138	1.15044	-0.53372
C	-0.07129	-1.15029	-0.53401
C	-1.2628	-0.77695	0.3945
C	-1.26312	0.77669	0.39438
H	0.45507	2.05955	-0.22703
H	-0.43402	1.30923	-1.55803
H	-0.43417	-1.30864	-1.55831
H	0.45527	-2.0595	-0.22783
H	-2.20509	-1.19792	0.02894
H	-1.11008	-1.16732	1.4062
H	-2.20542	1.19716	0.02825
H	-1.11112	1.16732	1.40608
N	0.84465	0.00011	-0.54566
C	1.76509	0.	0.59063
H	2.40898	-0.88422	0.53277
H	2.40905	0.88419	0.53288
H	1.27997	-0.00004	1.58496

N-methylpyrrolidine N-oxide
The number of imaginary frequencies: 0

Total Energy (M06/6-311G+**)= -326.90051885
ZPE= -326.739215
Enthalpy= -326.731606
Gibb's Free Energy= -326.769334

C	-0.20642	1.18006	-0.39819
C	-0.20641	-1.17988	-0.39867
C	-1.60313	-0.78221	0.08929
C	-1.60323	0.78213	0.08935
H	0.22053	2.074	0.05958
H	-0.14015	1.27502	-1.4834
H	-0.14032	-1.27427	-1.48394
H	0.22064	-2.07405	0.05855
H	-2.37717	-1.19037	-0.56706
H	-1.80187	-1.16923	1.09398
H	-2.37711	1.1902	-0.56724
H	-1.80238	1.16905	1.094
N	0.71326	0.00002	-0.10279
C	1.10744	-0.00026	1.34796
H	1.72001	-0.88912	1.49744
H	1.72009	0.8885	1.49774
H	0.24363	-0.00033	2.02335
O	1.82397	0.00017	-0.86024

N-methyl-2-pyrroline
The number of imaginary frequencies: 0
Total Energy (B3LYP/6-31G*)= -250.66822024
ZPE= -250.534319
Enthalpy= -250.527508
Gibb's Free Energy= -250.563344

C	-0.02855	-0.57318	-0.15105
C	1.26736	-0.4801	-0.57951
C	1.79391	0.87643	-0.11602
C	0.48097	1.64558	-0.06848
N	-0.40721	0.67078	0.57784
H	-0.67354	-1.41071	-0.31672
H	1.80823	-1.21651	-1.13634
H	2.51541	1.32205	-0.76853
H	0.13582	1.83115	-1.06414
H	2.23671	0.78728	0.85396
H	0.54979	2.5825	0.44371
C	-1.82735	1.03316	0.46483
H	-2.08752	1.13839	-0.56772
H	-2.42756	0.26588	0.90747
H	-2.00069	1.95899	0.97246

N-methyl-2-pyrroline
The number of imaginary frequencies: 0
Total Energy (B3LYP/6-31G**)= -250.68085752
ZPE= -250.547406
Enthalpy= -250.540583
Gibb's Free Energy= -250.576436

C	0.10596	1.1811	-0.02571
C	1.41809	0.82958	0.13671
C	1.51846	-0.66607	-0.15518
C	0.10274	-1.08391	0.21738
N	-0.69193	-0.01873	-0.4077
H	-0.28835	2.16721	0.10471
H	2.22092	1.47863	0.41794
H	2.26785	-1.18171	0.40825
H	-0.01891	-1.03759	1.27943
H	1.71863	-0.8255	-1.19413
H	-0.1541	-2.0704	-0.10785
C	-2.08449	0.00233	0.06267
H	-2.09981	0.10969	1.12716
H	-2.60019	0.82538	-0.38628
H	-2.5671	-0.91275	-0.21051

N-methyl-2-pyrroline
The number of imaginary frequencies: 0
Total Energy (M06/6-311+*G*)= -250.53777695
ZPE= -250.405638
Enthalpy= -250.398822
Gibb's Free Energy= -250.434595

C	-0.02855	-0.57318	-0.15105
C	1.26736	-0.4801	-0.57951
C	1.79391	0.87643	-0.11602
C	0.48097	1.64558	-0.06848
N	-0.40721	0.67078	0.57784
H	-0.67354	-1.41071	-0.31672
H	1.80823	-1.21651	-1.13634
H	2.51541	1.32205	-0.76853
H	0.13582	1.83115	-1.06414
H	2.23671	0.78728	0.85396
H	0.54979	2.5825	0.44371
C	-1.82735	1.03316	0.46483
H	-2.08752	1.13839	-0.56772
H	-2.42756	0.26588	0.90747
H	-2.00069	1.95899	0.97246

N-methyl-2-pyrroline N-oxide
The number of imaginary frequencies: 0
Total Energy (B3LYP/6-31G*)= -325.80112215
ZPE= -325.662988
Enthalpy= -325.655506
Gibb's Free Energy= -325.693031

C	-0.03777	-0.57726	-0.15465
C	1.26273	-0.48143	-0.57967
C	1.79166	0.88052	-0.11066
C	0.47827	1.64772	-0.07115
N	-0.39638	0.66679	0.57367
H	-0.6877	-1.41074	-0.32137
H	1.8054	-1.21671	-1.13624
H	2.51631	1.32576	-0.75993
H	0.13792	1.82472	-1.07001
H	2.23026	0.79201	0.8613
H	0.5341	2.58902	0.43455
C	-1.81636	1.03147	0.46606
H	-2.07939	1.14064	-0.56534
H	-2.4163	0.26345	0.90778
H	-1.98697	1.95575	0.97742
O	-0.09195	0.52844	1.89192

N-methyl-2-pyrroline N-oxide
The number of imaginary frequencies: 0
Total Energy (B3LYP/6-31G**)= -325.81385944
ZPE= -325.676246
Enthalpy= -325.668741
Gibb's Free Energy= -325.706303

C	-0.23379	1.18102	-0.17993
C	-1.52502	0.87048	-0.19439
C	-1.72932	-0.61116	0.01612
C	-0.32087	-1.17138	-0.21707
N	0.61792	0.00123	0.08597
H	0.2688	2.13771	-0.18968
H	-2.33435	1.58937	-0.23912
H	-2.45724	-1.05337	-0.67185
H	-0.19276	-1.46986	-1.26185
H	-2.07849	-0.80218	1.03742
H	-0.00953	-1.96861	0.45469
C	1.84379	-0.04037	-0.77097
H	1.5974	-0.0178	-1.83721
H	2.44721	0.82048	-0.48615
H	2.37766	-0.95301	-0.50559
O	0.98089	0.04214	1.39687

N-methyl-2-pyrroline N-oxide
The number of imaginary frequencies: 0
Total Energy (M06/6-311+*G*)= -325.66847024
ZPE= -325.531815
Enthalpy= -325.524448
Gibb's Free Energy= -325.56161

C	-0.03777	-0.57726	-0.15465
C	1.26273	-0.48143	-0.57967
C	1.79166	0.88052	-0.11066
C	0.47827	1.64772	-0.07115
N	-0.39638	0.66679	0.57367
H	-0.6877	-1.41074	-0.32137
H	1.8054	-1.21671	-1.13624
H	2.51631	1.32576	-0.75993
H	0.13792	1.82472	-1.07001
H	2.23026	0.79201	0.8613
H	0.5341	2.58902	0.43455
C	-1.81636	1.03147	0.46606
H	-2.07939	1.14064	-0.56534
H	-2.4163	0.26345	0.90778
H	-1.98697	1.95575	0.97742
O	-0.09195	0.52844	1.89192

N-methyl-3-pyrroline
The number of imaginary frequencies: 0
Total Energy (B3LYP/6-31G*)= -250.6603928
ZPE= -250.527109
Enthalpy= -250.520299
Gibb's Free Energy= -250.556164

C	1.07009	-1.23529	-0.0877
C	2.59979	-1.2302	0.08945
C	3.00239	0.06358	0.08894
C	1.74564	0.93562	-0.08855
N	0.70686	0.06853	0.48636
H	0.58497	-2.04788	0.41156
H	3.22822	-2.08949	0.19723
H	4.00746	0.41463	0.19625
H	1.56874	1.11503	-1.12846
C	-0.66822	0.49631	0.19132
H	-0.83888	1.46456	0.61354
H	-0.80863	0.53959	-0.86855
H	-1.35805	-0.20383	0.6142
H	0.82239	-1.28338	-1.12752
H	1.80737	1.88035	0.41002

N-methyl-3-pyrroline
The number of imaginary frequencies: 0
Total Energy (B3LYP/6-31G**)= -250.67291059
ZPE= -250.540105
Enthalpy= -250.533291
Gibb's Free Energy= -250.569157

C	0.01026	-0.11685	1.19135
C	0.01026	-1.52903	0.66633
C	0.01026	-1.52903	-0.66633
C	0.01026	-0.11685	-1.19135
N	0.32891	0.68022	0.
H	0.74953	0.05319	1.98809
H	-0.01543	-2.40073	1.31123
H	-0.01543	-2.40073	-1.31123
H	-0.98169	0.1315	-1.62443

C	-0.18554	2.03252	0.
H	0.1764	2.56965	-0.88334
H	-1.29288	2.08671	0.
H	0.1764	2.56965	0.88334
H	-0.98169	0.1315	1.62443
H	0.74953	0.05319	-1.98809

N-methyl-3-pyrroline

The number of imaginary frequencies: 0

Total Energy (M06/6-311+*G*)= -250.53030478

ZPE= -250.398839

Enthalpy= -250.392016

Gibb's Free Energy= -250.427847

C	-0.00138	-0.1147	1.17913
C	-0.00138	-1.51818	0.66335
C	-0.00138	-1.51818	-0.66335
C	-0.00138	-0.1147	-1.17913
N	0.33927	0.66756	0.
H	0.71625	0.05989	1.99335
H	-0.03111	-2.39025	1.3058
H	-0.03111	-2.39025	-1.3058
H	-1.00567	0.14611	-1.5787
C	-0.14704	2.01858	0.
H	0.21801	2.55165	-0.88417
H	-1.25452	2.07526	0.
H	0.21801	2.55165	0.88417
H	-1.00567	0.14611	1.5787
H	0.71625	0.05989	-1.99335

N-methyl-3-pyrroline N-oxide

The number of imaginary frequencies: 0

Total Energy (B3LYP/6-31G*)= -325.80062068

ZPE= -325.662821

Enthalpy= -325.655372

Gibb's Free Energy= -325.692895

C	1.05926	-1.23237	-0.09866
C	2.58767	-1.2308	0.1087
C	2.99275	0.071	0.10821
C	1.73505	0.93937	-0.09948
N	0.711	0.06723	0.47757
H	0.55417	-2.04303	0.38364
H	3.21271	-2.0904	0.23245
H	3.9952	0.42426	0.2315
H	1.56998	1.10051	-1.14432
C	-0.66662	0.4958	0.1958
H	-0.83355	1.46287	0.62216
H	-0.81634	0.54199	-0.86267
H	-1.35271	-0.20552	0.62279
H	0.83169	-1.27213	-1.14343
H	1.7792	1.89382	0.38215
O	0.87454	0.01685	1.82676

N-methyl-3-pyrroline N-oxide

The number of imaginary frequencies: 0

Total Energy (B3LYP/6-31G**)= -325.81340875

ZPE= -325.676093

Enthalpy= -325.668646

Gibb's Free Energy= -325.706136

C	0.22103	0.28223	1.21642
C	0.22103	1.67477	0.66657
C	0.22103	1.67477	-0.66657
C	0.22103	0.28223	-1.21642
N	-0.15212	-0.58721	0.
H	-0.55767	0.06533	1.94953
H	0.20969	2.55257	1.30413
H	0.20969	2.55257	-1.30413
H	1.20189	-0.01004	-1.61561
C	0.60337	-1.88315	0.
H	0.28233	-2.42675	-0.88876
H	1.68864	-1.73164	0.
H	0.28233	-2.42675	0.88876
H	1.20189	-0.01004	1.61561
H	-0.55767	0.06533	-1.94953
O	-1.47766	-0.83814	0.

N-methyl-3-pyrroline N-oxide

The number of imaginary frequencies: 0

Total Energy (M06/6-311+*G*)= -325.6680588

ZPE= -325.53171

Enthalpy= -325.524342

Gibb's Free Energy= -325.561595

C	1.05926	-1.23237	-0.09866
C	2.58767	-1.2308	0.1087
C	2.99275	0.071	0.10821
C	1.73505	0.93937	-0.09948
N	0.711	0.06723	0.47757
H	0.55417	-2.04303	0.38364
H	3.21271	-2.0904	0.23245
H	3.9952	0.42426	0.2315
H	1.56998	1.10051	-1.14432
C	-0.66662	0.4958	0.1958
H	-0.83355	1.46287	0.62216
H	-0.81634	0.54199	-0.86267
H	-1.35271	-0.20552	0.62279
H	0.83169	-1.27213	-1.14343

H	1.7792	1.89382	0.38215
O	0.87454	0.01685	1.82676

N-methylazepane

The number of imaginary frequencies: 0
Total Energy (B3LYP/6-31G*)= -330.51413505
ZPE= -330.297713
Enthalpy= -330.288427
Gibb's Free Energy= -330.330325

C	0.73212	1.51003	-0.4035
C	-0.71609	1.25523	0.03895
C	1.7927	0.77847	0.43621
C	-0.52079	-1.191	0.31221
C	2.04124	-0.69458	0.05474
C	0.80307	-1.48614	-0.4115
N	-1.26022	-0.06586	-0.27351
C	-2.67256	-0.11883	0.08393
H	-3.21445	0.67915	-0.4361
H	-3.10036	-1.07735	-0.22923
H	-2.85932	0.00024	1.1703
H	-0.35545	-1.0579	1.40146
H	-1.16564	-2.07111	0.20855
H	1.02594	-2.55654	-0.31156
H	0.62107	-1.31016	-1.47825
H	2.74655	1.31783	0.37304
H	1.48852	0.83963	1.4906
H	0.89962	2.59119	-0.30925
H	0.83983	1.27152	-1.46966
H	-0.78672	1.46965	1.12797
H	-1.36351	1.98763	-0.46024
H	2.79112	-0.74141	-0.74624
H	2.49617	-1.20044	0.91699

N-methylazepane

The number of imaginary frequencies: 0
Total Energy (B3LYP/6-31G**)= -330.53806647
ZPE= -330.322355
Enthalpy= -330.313145
Gibb's Free Energy= -330.354675

C	0.7311	1.51068	-0.40214
C	-0.71639	1.25629	0.04082
C	1.79174	0.77753	0.43555
C	-0.51944	-1.18994	0.31525
C	2.04163	-0.69371	0.05083
C	0.80285	-1.48699	-0.41006
N	-1.25882	-0.06547	-0.27216
C	-2.67258	-0.12059	0.08033
H	-3.21461	0.67542	-0.44073
H	-3.09839	-1.07873	-0.23368
H	-2.86468	-0.00198	1.16495
H	-0.35201	-1.05591	1.40334
H	-1.16385	-2.06989	0.21472
H	1.02568	-2.55627	-0.30792
H	0.61762	-1.31452	-1.47605
H	2.74434	1.31751	0.37445
H	1.48778	0.83602	1.48928
H	0.8994	2.59073	-0.30712
H	0.83784	1.27383	-1.468
H	-0.78576	1.47129	1.12915
H	-1.36395	1.98832	-0.45733
H	2.78754	-0.73783	-0.75285
H	2.50134	-1.19937	0.90949

N-methylazepane

The number of imaginary frequencies: 0
Total Energy (M06/6-311G+**)= -330.32162526
ZPE= -330.107821
Enthalpy= -330.09853
Gibb's Free Energy= -330.140342

C	1.51265	0.65777	0.68028
C	1.78687	-0.75362	0.1749
C	0.55687	-1.62184	-0.03627
C	0.78962	1.53617	-0.33554
C	-0.53615	-0.9995	-0.90604
C	-0.73095	1.41941	-0.33053
H	0.94042	0.62182	1.62108
H	2.33902	-0.67556	-0.77611
H	0.12066	-1.891	0.93777
H	-0.10723	-0.64267	-1.8541
H	1.18303	1.31841	-1.33996
H	-1.12031	1.98155	-1.19752
H	2.47396	1.12315	0.93659
H	2.46827	-1.2637	0.87008
H	0.86559	-2.57467	-0.49074
H	1.02842	2.59515	-0.16187
H	-1.25018	-1.7895	-1.18581
H	-1.11088	1.94537	0.55708
N	-1.29038	0.07892	-0.30783
C	-2.04279	-0.26955	0.86647
H	-2.8496	0.45522	1.02999
H	-2.51372	-1.25069	0.72696
H	-1.45141	-0.31833	1.80185

N-methylazepane N-oxide

The number of imaginary frequencies: 0
Total Energy (B3LYP/6-31G*)= -405.65530091
ZPE= -405.433782
Enthalpy= -405.424009

Gibb's Free Energy= -405.46685

C	-0.68389	-0.0867	-0.0655
C	0.86341	-0.02909	-0.0243
C	1.52087	1.3621	0.05709
C	-1.21057	0.349	1.28887
C	1.10761	2.30191	1.22874
C	-1.33626	1.86899	1.50908
H	-1.10813	0.4975	-0.85521
H	1.16889	-0.58993	0.83421
H	1.29525	1.88657	-0.84785
H	1.22426	1.8509	2.19201
H	-0.53585	-0.07286	2.00419
H	-1.42434	1.98096	2.56955
H	-0.94122	-1.11544	-0.20832
H	1.22986	-0.48397	-0.92079
H	2.57332	1.18802	0.14045
H	-2.1988	-0.03456	1.43448
H	1.74807	3.15582	1.15428
H	-2.21801	2.2191	1.01425
N	-0.26066	2.75574	1.02141
C	-0.38413	2.94763	-0.43077
H	-1.35701	3.33045	-0.6585
H	0.35913	3.64182	-0.76328
H	-0.2444	2.01031	-0.92755
O	-0.45463	3.92978	1.6799

N-methylazepane N-oxide

The number of imaginary frequencies: 0

Total Energy (B3LYP/6-31G**)= -405.68570133

ZPE= -405.465245

Enthalpy= -405.455415

Gibb's Free Energy= -405.498192

C	-0.87731	1.5007	0.36873
C	0.51088	1.33419	-0.23712
C	-2.00082	0.77897	-0.39556
C	0.32701	-1.17285	-0.5794
C	-2.18916	-0.71157	-0.04683
C	-0.90207	-1.5005	0.25743
N	1.14604	-0.0214	0.04394
C	2.50298	-0.03427	-0.59869
H	3.06617	0.79804	-0.17874
H	2.97609	-0.96957	-0.30406
H	2.43584	0.04876	-1.68895
H	0.10455	-0.91863	-1.62206
H	1.01517	-2.01981	-0.56491
H	-1.11006	-2.57108	0.1513
H	-0.57176	-1.34045	1.28934
H	-2.95098	1.29611	-0.21842
H	-1.80879	0.88583	-1.47256
H	-1.08295	2.57776	0.37236
H	-0.81883	1.18252	1.41452
H	0.49467	1.50062	-1.32195
H	1.20591	2.03715	0.22537
H	-2.84025	-0.79465	0.83193
H	-2.73665	-1.18964	-0.86925
O	1.2963	-0.19264	1.37965

N-methylazepane N-oxide

The number of imaginary frequencies: 0

Total Energy (M06/6-311G+**)= -405.47684909

ZPE= -405.258482

Enthalpy= -405.24872

Gibb's Free Energy= -405.291518

C	-0.68389	-0.0867	-0.0655
C	0.86341	-0.02909	-0.0243
C	1.52087	1.3621	0.05709
C	-1.21057	0.349	1.28887
C	1.10761	2.30191	1.22874
C	-1.33626	1.86899	1.50908
H	-1.10813	0.4975	-0.85521
H	1.16889	-0.58993	0.83421
H	1.29525	1.88657	-0.84785
H	1.22426	1.8509	2.19201
H	-0.53585	-0.07286	2.00419
H	-1.42434	1.98096	2.56955
H	-0.94122	-1.11544	-0.20832
H	1.22986	-0.48397	-0.92079
H	2.57332	1.18802	0.14045
H	-2.1988	-0.03456	1.43448
H	1.74807	3.15582	1.15428
H	-2.21801	2.2191	1.01425
N	-0.26066	2.75574	1.02141
C	-0.38413	2.94763	-0.43077
H	-1.35701	3.33045	-0.6585
H	0.35913	3.64182	-0.76328
H	-0.2444	2.01031	-0.92755
O	-0.45463	3.92978	1.6799

1-methyl-2,3,4,5-tetrahydro-1H-azepine

The number of imaginary frequencies: 0

Total Energy (B3LYP/6-31G*)= -329.29734188

ZPE=-329.104678

Enthalpy= -329.095641

Gibb's Free Energy= -329.137249

C	-1.93668	0.79405	-0.16536
C	-1.91369	-0.66619	0.29955
C	-0.79253	-1.50046	-0.32623
C	-0.69176	1.60985	0.07132

C	0.60281	-1.21219	0.23494
C	0.60875	1.26272	0.01777
H	-2.16893	0.8014	-1.24481
H	-1.81819	-0.70387	1.39418
H	-0.7804	-1.37039	-1.41717
H	0.55268	-1.24755	1.34067
H	-2.78411	1.30138	0.31486
H	-2.88152	-1.12282	0.05332
H	-0.99385	-2.56353	-0.13769
H	-0.86179	2.67477	0.21549
H	1.27277	-2.02244	-0.07532
H	1.32978	2.07134	0.1237
N	1.23158	0.03078	-0.20714
C	2.67576	0.02755	-0.00353
H	3.11431	0.93087	-0.43659
H	2.96525	-0.02091	1.0617
H	3.11702	-0.83567	-0.51311

1-methyl-2,3,4,5-tetrahydro-1H-azepine
The number of imaginary frequencies: 0
Total Energy (B3LYP/6-31G**)= -329.31548004
ZPE=-329.123508
Enthalpy= -329.114461
Gibb's Free Energy= -329.156073

C	-1.93249	0.79521	-0.17278
C	-1.91545	-0.66385	0.29603
C	-0.79336	-1.50269	-0.32111
C	-0.69029	1.61075	0.07493
C	0.60107	-1.21171	0.23984
C	0.60955	1.26312	0.02435
H	-2.15202	0.79989	-1.25399
H	-1.826	-0.69823	1.39045
H	-0.77885	-1.37979	-1.41203
H	0.54996	-1.2447	1.34503
H	-2.78407	1.30421	0.29592
H	-2.88213	-1.11899	0.04648
H	-0.99535	-2.56362	-0.12654
H	-0.86042	2.67389	0.22642
H	1.27056	-2.02283	-0.06704
H	1.33035	2.07028	0.13838
N	1.22934	0.03054	-0.20594
C	2.67513	0.02562	-0.01156
H	3.11207	0.92845	-0.44494
H	2.97241	-0.02535	1.05051
H	3.11319	-0.83562	-0.52531

1-methyl-2,3,4,5-tetrahydro-1H-azepine
The number of imaginary frequencies: 0
Total Energy (M06/6-311G+**)= -329.12249802
ZPE=-328.932494
Enthalpy= -328.923377
Gibb's Free Energy= -328.965286

C	-1.93321	0.77636	-0.14385
C	-1.88554	-0.6686	0.31918
C	-0.78336	-1.47754	-0.34095
C	-0.69705	1.5925	0.05953
C	0.60182	-1.20425	0.21188
C	0.5986	1.25289	-0.00482
H	-2.18579	0.77908	-1.21868
H	-1.7509	-0.70474	1.41034
H	-0.78202	-1.3067	-1.42726
H	0.55727	-1.23898	1.31985
H	-2.7735	1.28283	0.34757
H	-2.85654	-1.13455	0.10971
H	-0.98156	-2.54636	-0.19233
H	-0.86444	2.65919	0.18934
H	1.27299	-2.01417	-0.09815
H	1.31253	2.07096	0.08133
N	1.22736	0.03279	-0.21823
C	2.65472	0.03368	0.02568
H	3.1068	0.94119	-0.38139
H	2.90006	-0.0243	1.10077
H	3.11779	-0.8232	-0.47342

1-methyl-2,3,4,5-tetrahydro-1H-azepine N-oxide
The number of imaginary frequencies: 0
Total Energy (B3LYP/6-31G*)= -404.42502271
ZPE=-404.228193
Enthalpy= -404.218652
Gibb's Free Energy= -404.26106

C	0.49565	0.4599	-0.25257
C	1.9606	0.36039	0.11322
C	2.62584	1.76027	0.11912
C	-0.31101	1.01637	0.91325
C	2.07129	2.81315	1.12848
C	-0.36455	2.31347	1.21761
H	0.40807	1.08914	-1.11355
H	2.05677	-0.11513	1.06691
H	2.5273	2.17619	-0.8618
H	2.12361	2.40779	2.11735
H	0.10558	-0.51126	-0.47523
H	2.46182	-0.22127	-0.63201
H	3.65685	1.60579	0.36006
H	-0.87414	0.33125	1.5119
H	2.7101	3.66688	1.03929
H	-1.22433	2.65914	1.75256
N	0.67244	3.30432	0.89169
C	0.52912	3.73516	-0.50642
H	-0.45373	4.12962	-0.65912

H	1.25453	4.49139	-0.72275
H	0.68223	2.89808	-1.15508
O	0.47962	4.35813	1.72949

1-methyl-2,3,4,5-tetrahydro-1H-azepine N-oxide

The number of imaginary frequencies: 0

Total Energy (B3LYP/6-31G**)= -404.44322686

ZPE=-404.247194

Enthalpy= -404.237619

Gibb's Free Energy= -404.280085

C	1.96356	0.81312	0.33863
C	2.10879	-0.60245	-0.23877
C	0.95175	-1.54601	0.10421
C	0.81163	1.62637	-0.20456
C	-0.39354	-1.20835	-0.53642
C	-0.47022	1.30415	-0.36417
H	1.87606	0.74597	1.43407
H	2.21458	-0.53759	-1.32906
H	0.8498	-1.63399	1.19366
H	-0.30582	-1.05072	-1.61285
H	2.89003	1.36631	0.15354
H	3.04175	-1.03582	0.14115
H	1.20446	-2.55412	-0.24839
H	1.0502	2.64764	-0.4964
H	-1.11915	-2.00795	-0.38101
H	-1.21661	1.9886	-0.74614
N	-1.16189	0.01815	-0.06544
C	-1.45306	-0.0504	1.41038
H	-2.09483	0.80177	1.62617
H	-2.01237	-0.97213	1.57198
H	-0.5458	-0.01981	2.02088
O	-2.35157	0.01453	-0.74067

1-methyl-2,3,4,5-tetrahydro-1H-azepine N-oxide

The number of imaginary frequencies: 0

Total Energy (M06/6-311G+**)= -404.2475018

ZPE=-404.053202

Enthalpy= -404.043727

Gibb's Free Energy=-404.085774

C	1.77906	0.80797	0.47768
C	2.12165	-0.49627	-0.20889
C	0.96929	-1.52143	-0.05614
C	0.75836	1.59069	-0.33779
C	-0.4141	-1.14154	-0.66999
C	-0.54738	1.32049	-0.33598
H	1.399	0.58295	1.45227
H	2.33546	-0.30886	-1.24042
H	0.81786	-1.69384	0.98897
H	-0.28559	-0.92713	-1.71039
H	2.65349	1.41851	0.56438
H	2.98187	-0.91903	0.26673
H	1.2937	-2.41794	-0.54186
H	1.10631	2.40827	-0.93395
H	-1.03706	-2.00156	-0.5389
H	-1.21606	2.1179	-0.5848
N	-1.14134	0.00879	-0.03599
C	-1.20649	-0.18842	1.41927
H	-1.76721	0.60792	1.86236
H	-1.68405	-1.12208	1.63164
H	-0.21563	-0.19464	1.82306
O	-2.39439	0.01988	-0.56451

1-methyl-2,3,4,7-tetrahydro-1H-azepine

The number of imaginary frequencies: 0

Total Energy (B3LYP/6-31G*)= -329.28700224

ZPE=-329.094545

Enthalpy= -329.085733

Gibb's Free Energy= -329.126397

C	0.46295	0.17234	0.24131
C	1.97537	0.39078	0.04423
C	2.50256	1.83166	-0.01181
C	-0.37683	0.88382	1.02888
C	2.13658	2.73783	1.18466
C	-0.37265	2.36391	1.46212
H	2.45636	-0.09513	0.8673
H	2.13696	2.3141	-0.89413
H	2.30148	2.24591	2.12046
H	-0.43758	2.35657	2.53013
H	0.04036	-0.67463	-0.25765
H	2.25285	-0.06973	-0.88088
H	3.56837	1.74437	-0.04804
H	-1.18608	0.31194	1.43255
H	2.76419	3.60186	1.11792
H	-1.23298	2.83435	1.03385
N	0.75876	3.21509	1.05177
C	0.62038	3.49949	-0.38381
H	-0.33935	3.93424	-0.57039
H	1.38631	4.1821	-0.68762
H	0.71346	2.58915	-0.93835

1-methyl-2,3,4,7-tetrahydro-1H-azepine

The number of imaginary frequencies: 0

Total Energy (B3LYP/6-31G**)= -329.30507753

ZPE=-329.113362

Enthalpy= -329.104525
Gibb's Free Energy= -329.145233

C	-1.51433	0.99972	-0.29773
C	-1.85588	-0.45955	0.03708
C	-0.7246	-1.48048	-0.17996
C	-0.38439	1.68338	-0.01036
C	0.52496	-1.30198	0.70533
C	0.87964	1.19436	0.72044
H	-2.16918	-0.50204	1.05931
H	-0.41509	-1.44656	-1.20366
H	0.23039	-1.23137	1.73156
H	0.68845	1.21373	1.77305
H	-2.27829	1.55365	-0.80214
H	-2.65614	-0.75274	-0.60986
H	-1.13997	-2.43881	0.05236
H	-0.37641	2.71001	-0.31182
H	1.1295	-2.17173	0.55372
H	1.66412	1.87817	0.47169
N	1.36727	-0.14493	0.35048
C	1.56196	-0.17639	-1.10623
H	2.22667	0.61105	-1.39432
H	1.98159	-1.11897	-1.38971
H	0.61935	-0.04415	-1.59499

1-methyl-2,3,4,7-tetrahydro-1H-azepine
The number of imaginary frequencies: 0
Total Energy (M06/6-311G+**)= -329.11354081
ZPE=-328.923838
Enthalpy= -328.915004
Gibb's Free Energy= -328.955568

C	0.46295	0.17234	0.24131
C	1.97537	0.39078	0.04423
C	2.50256	1.83166	-0.01181
C	-0.37683	0.88382	1.02888
C	2.13658	2.73783	1.18466
C	-0.37265	2.36391	1.46212
H	2.45636	-0.09513	0.8673
H	2.13696	2.3141	-0.89413
H	2.30148	2.24591	2.12046
H	-0.43758	2.35657	2.53013
H	0.04036	-0.67463	-0.25765
H	2.25285	-0.06973	-0.88088
H	3.56837	1.74437	-0.04804
H	-1.18608	0.31194	1.43255
H	2.76419	3.60186	1.11792
H	-1.23298	2.83435	1.03385
N	0.75876	3.21509	1.05177
C	0.62038	3.49949	-0.38381
H	-0.33935	3.93424	-0.57039
H	1.38631	4.1821	-0.68762
H	0.71346	2.58915	-0.93835

1-methyl-2,3,4,7-tetrahydro-1H-azepine N-oxide
The number of imaginary frequencies: 0
Total Energy (B3LYP/6-31G*)= -404.43129113
ZPE=-404.234067
Enthalpy= -404.224616
Gibb's Free Energy= -404.266611

C	0.45874	0.16613	0.2198
C	1.97398	0.36932	0.06143
C	2.50955	1.80472	0.00757
C	-0.37234	0.87672	1.00869
C	2.14031	2.74606	1.1813
C	-0.34893	2.34664	1.4712
H	2.4313	-0.11719	0.89753
H	2.15919	2.27549	-0.88715
H	2.30708	2.2883	2.13395
H	-0.37312	2.30691	2.54019
H	0.03122	-0.66405	-0.30263
H	2.27038	-0.09692	-0.8549
H	3.57512	1.70908	-0.01004
H	-1.19202	0.30979	1.39806
H	2.77068	3.60456	1.07872
H	-1.22489	2.82669	1.0876
N	0.76135	3.22591	1.04414
C	0.60023	3.53211	-0.38456
H	-0.36828	3.95516	-0.55165
H	1.35178	4.23135	-0.68644
H	0.6999	2.63269	-0.95554
O	0.62535	4.34769	1.80092

1-methyl-2,3,4,7-tetrahydro-1H-azepine N-oxide
The number of imaginary frequencies: 0
Total Energy (B3LYP/6-31G**)= -404.44946699
ZPE=-404.253037
Enthalpy= -404.243554
Gibb's Free Energy= -404.285602

C	1.92307	0.87597	0.11409
C	2.09044	-0.62982	-0.10959
C	0.90465	-1.50203	0.33143
C	0.83399	1.6357	-0.12024
C	-0.4226	-1.28929	-0.42733
C	-0.54165	1.21328	-0.66868
H	2.27679	-0.7957	-1.1501
H	0.72165	-1.33798	1.37282
H	-0.2463	-1.3535	-1.48075

H	-0.45947	1.11461	-1.73094
H	2.78523	1.39413	0.47889
H	2.93107	-0.94405	0.47308
H	1.2025	-2.51523	0.15937
H	0.94975	2.68046	0.07972
H	-1.07357	-2.0774	-0.11109
H	-1.2242	1.99791	-0.41691
N	-1.1286	-0.02679	-0.1228
C	-1.22486	0.09889	1.33866
H	-1.79047	0.97314	1.58497
H	-1.71157	-0.76551	1.73969
H	-0.24261	0.18052	1.75509
O	-2.36594	-0.12909	-0.67789

1-methyl-2,3,4,7-tetrahydro-1H-azepine N-oxide

The number of imaginary frequencies: 0

Total Energy (M06/6-311G+**)= -404.25465228

ZPE=-404.059795

Enthalpy= -404.050431

Gibb's Free Energy=-404.092144

C	0.45874	0.16613	0.2198
C	1.97398	0.36932	0.06143
C	2.50955	1.80472	0.00757
C	-0.37234	0.87672	1.00869
C	2.14031	2.74606	1.1813
C	-0.34893	2.34664	1.4712
H	2.4313	-0.11719	0.89753
H	2.15919	2.27549	-0.88715
H	2.30708	2.2883	2.13395
H	-0.37312	2.30691	2.54019
H	0.03122	-0.66405	-0.30263
H	2.27038	-0.09692	-0.8549
H	3.57512	1.70908	-0.01004
H	-1.19202	0.30979	1.39806
H	2.77068	3.60456	1.07872
H	-1.22489	2.82669	1.0876
N	0.76135	3.22591	1.04414
C	0.60023	3.53211	-0.38456
H	-0.36828	3.95516	-0.55165
H	1.35178	4.23135	-0.68644
H	0.6999	2.63269	-0.95554
O	0.62535	4.34769	1.80092

1-methyl-2,3,6,7-tetrahydro-1H-azepine

The number of imaginary frequencies: 0

Total Energy (B3LYP/6-31G*)= -329.28622475

ZPE=-329.093718

Enthalpy= -329.084945

Gibb's Free Energy= -329.125486

C	0.65622	0.04817	0.22592
C	1.80932	0.47645	-0.33881
C	2.60467	1.76621	-0.02668
C	-0.01152	0.68273	1.44487
C	2.19411	2.5403	1.25704
C	-0.26028	2.20759	1.41592
H	2.46107	2.44806	-0.83869
H	2.22732	1.94966	2.14863
H	0.62496	0.45232	2.27355
H	-0.52473	2.45334	2.42318
H	0.2084	-0.83519	-0.17907
H	2.23622	-0.17011	-1.07679
H	3.63467	1.48634	0.04875
H	-0.97652	0.23944	1.57593
H	2.87517	3.35964	1.3557
H	-1.06514	2.43583	0.74883
N	0.8605	3.06522	1.00312
C	0.85443	3.27624	-0.45164
H	-0.07965	3.7075	-0.74559
H	1.65233	3.93692	-0.71954
H	0.9862	2.33791	-0.9487

1-methyl-2,3,6,7-tetrahydro-1H-azepine

The number of imaginary frequencies: 0

Total Energy (B3LYP/6-31G**)= -329.30420567

ZPE= -329.112519

Enthalpy= -329.103711

Gibb's Free Energy= -329.144319

C	1.99797	-0.4302	-0.07796
C	1.76928	0.8603	-0.34826
C	0.45115	1.58846	-0.22273
C	0.97454	-1.48002	0.30279
C	-0.51524	0.94658	0.79829
C	-0.42038	-1.271	-0.29984
H	-0.03894	1.68785	-1.20393
H	0.0587	0.71542	1.70449
H	0.89381	-1.58222	1.39549
H	-0.97602	-2.21782	-0.25329
H	3.0231	-0.79045	-0.16407
H	2.61791	1.47108	-0.65701
H	0.65873	2.61831	0.10046
H	1.34125	-2.45151	-0.05297
H	-1.27386	1.68024	1.09353
H	-0.29162	-1.03931	-1.37605
N	-1.23345	-0.25848	0.37624
C	-2.43499	0.02608	-0.39246

H	-2.9834	-0.90701	-0.56853
H	-3.09029	0.69863	0.17161
H	-2.23924	0.48507	-1.38242

1-methyl-2,3,6,7-tetrahydro-1H-azepine

The number of imaginary frequencies: 0

Total Energy (M06/6-311G+**)= -329.11349961

ZPE=-328.923679

Enthalpy= -328.914937

Gibb's Free Energy= -328.955271

C	1.98583	-0.41519	-0.07008
C	1.7457	0.86549	-0.34366
C	0.42498	1.56747	-0.23043
C	0.97413	-1.46395	0.2974
C	-0.51329	0.93413	0.79927
C	-0.40349	-1.25533	-0.30763
H	-0.07178	1.63208	-1.21126
H	0.06905	0.7131	1.70383
H	0.88737	-1.5684	1.38944
H	-0.95658	-2.20448	-0.29285
H	3.01627	-0.76022	-0.14325
H	2.59056	1.48325	-0.64527
H	0.61224	2.60884	0.06172
H	1.34832	-2.43297	-0.05422
H	-1.27575	1.66095	1.10211
H	-0.27248	-0.99307	-1.37912
N	-1.21805	-0.26762	0.3788
C	-2.41151	0.01528	-0.38202
H	-2.94669	-0.91825	-0.58815
H	-3.08156	0.66692	0.18734
H	-2.20669	0.49821	-1.35893

1-methyl-2,3,6,7-tetrahydro-1H-azepine N-oxide

The number of imaginary frequencies: 0

Total Energy (B3LYP/6-31G*)= -404.42326899

ZPE=-404.225979

Enthalpy= -404.216486

Gibb's Free Energy= -404.259077

C	0.63577	0.05068	0.19107
C	1.81061	0.46269	-0.32535
C	2.616	1.74208	0.00561
C	-0.01818	0.66913	1.41353
C	2.20367	2.57041	1.26497
C	-0.23454	2.19901	1.44017
H	2.50056	2.40935	-0.82284
H	2.24317	2.03388	2.18989
H	0.61702	0.39986	2.23141
H	-0.43813	2.40267	2.47069
H	0.16758	-0.80395	-0.25087
H	2.25465	-0.192	-1.04585
H	3.63859	1.44571	0.11224
H	-0.99328	0.2458	1.53552
H	2.88742	3.39231	1.308
H	-1.06983	2.46574	0.82695
N	0.86699	3.07773	0.99765
C	0.83582	3.27861	-0.45823
H	-0.1133	3.68284	-0.74226
H	1.61213	3.95846	-0.74117
H	0.98595	2.34076	-0.95097
O	0.65027	4.25335	1.64615

1-methyl-2,3,6,7-tetrahydro-1H-azepine N-oxide

The number of imaginary frequencies: 0

Total Energy (B3LYP/6-31G**)= -404.44160371

ZPE=-404.245096

Enthalpy= -404.23558

Gibb's Free Energy= -404.278124

C	2.00147	0.51596	0.29064
C	1.72629	-0.78975	0.30569
C	0.67339	-1.51602	-0.58728
C	1.07751	1.51412	-0.35375
C	-0.55367	-0.67522	-1.07595
C	-0.41156	1.41351	0.09795
H	0.29215	-2.31051	0.01964
H	-0.3307	0.01214	-1.86508
H	1.14759	1.35966	-1.41022
H	-0.93173	2.05724	-0.58024
H	2.91412	0.85939	0.73113
H	2.29074	-1.39738	0.98178
H	1.15724	-1.90733	-1.45772
H	1.39723	2.50376	-0.10218
H	-1.27141	-1.39032	-1.42004
H	-0.52046	1.75918	1.1047
N	-1.05058	0.07145	0.04715
C	-0.77633	-0.74779	1.23649
H	-1.12619	-0.23751	2.10948
H	-1.28047	-1.68727	1.14643
H	0.2773	-0.9149	1.31926
O	-2.3855	0.31311	-0.04871

1-methyl-2,3,6,7-tetrahydro-1H-azepine N-oxide

The number of imaginary frequencies: 0

Total Energy (M06/6-311G+**)= -404.25593024

ZPE=-404.061382

Enthalpy= -404.05197
Gibb's Free Energy=-404.093798

C	-2.13243	-0.62773	-0.00619
C	-2.1129	0.69917	0.0899
C	-0.89012	1.57286	0.06504
C	-0.93812	-1.53555	-0.02644
C	0.26186	1.00473	-0.74248
C	0.2522	-1.00399	0.73689
H	-0.57255	1.84981	1.08181
H	-0.10086	0.52604	-1.65426
H	-0.61122	-1.78372	-1.04644
H	0.94894	-1.80485	0.99417
H	-3.1038	-1.11763	-0.04322
H	-3.06576	1.22109	0.15518
H	-1.16244	2.52684	-0.4037
H	-1.22239	-2.49315	0.42425
H	0.97609	1.77506	-1.04426
H	-0.06828	-0.49279	1.65335
N	1.10204	-0.06467	-0.08457
C	2.08847	0.57282	0.8329
H	2.6448	-0.23081	1.31627
H	2.76704	1.15301	0.20788
H	1.59677	1.20693	1.57869
O	1.76069	-0.74713	-1.04068

Triplet Oxygen
The number of imaginary frequencies: 0
Total Energy (B3LYP/6-31G*)= -75.06062312
ZPE= -75.060623
Enthalpy= -75.058263
Gibb's Free Energy= -75.075575

O	0.	0.	0.

Triplet Oxygen
The number of imaginary frequencies: 0
Total Energy (B3LYP/6-31G**)= -75.06062312
ZPE= -75.060623
Enthalpy= -75.058263
Gibb's Free Energy= -75.075575

O	0.	0.	0.

Triplet Oxygen
The number of imaginary frequencies: 0
Total Energy (M06/6-311G+**)= -75.05344297
ZPE= -75.053443
Enthalpy= -75.051083
Gibb's Free Energy= -75.068395

O	0.	0.	0.

Singlet Oxygen
The number of imaginary frequencies: 0
Total Energy (B3LYP/6-31G*)= -74.95739789
ZPE= -74.957398
Enthalpy= -74.955037
Gibb's Free Energy= -74.971313

O	0.	0.	0.

Singlet Oxygen
The number of imaginary frequencies: 0
Total Energy (B3LYP/6-31G**)= -74.95739789
ZPE= -74.957398
Enthalpy= -74.955037
Gibb's Free Energy= -74.971313

O	0.	0.	0.

Singlet Oxygen
The number of imaginary frequencies: 0
Total Energy (M06/6-311G+**)= -74.95543188
ZPE= -74.955432
Enthalpy= -74.953071
Gibb's Free Energy= -74.969347

O	0.	0.	0.

7-methyl-7-azanorcaradiene
The number of imaginary frequencies: 0
Total Energy (B3LYP/6-31G*)=-326.83454058
ZPE= -326.689984
Enthalpy=-326.682268
Gibb's Free Energy= -326.720491

C	1.96758	-0.78106	-0.2494
C	1.9667	0.61802	-0.34996
C	0.88802	1.40813	-0.02297
C	-0.41571	0.93722	0.70222
C	-0.35664	-0.57731	0.48024
C	0.86155	-1.41833	0.14091
H	2.85043	-1.33594	-0.48935
H	2.85186	1.09785	-0.71211
H	0.94559	2.44192	-0.29287
H	0.83621	-2.48521	0.21865
H	-0.39413	0.92431	1.77192
H	-0.82068	-1.13466	1.26695
N	-1.35975	0.10157	-0.24957
C	-2.7971	-0.13006	-0.45273
H	-3.23944	0.73849	-0.89414
H	-2.93485	-0.96948	-1.1018
H	-3.26323	-0.3278	0.48988

7-methyl-7-azanorcaradiene
The number of imaginary frequencies: 0
Total Energy (B3LYP/6-31G**)= -326.84784237
ZPE= -326.703582
Enthalpy= -326.695868
Gibb's Free Energy= -326.734078

C	1.86658	-0.72695	-0.30896
C	1.86652	0.72697	-0.30892
C	0.82595	1.43776	0.17935
C	-0.43635	0.77203	0.53789
C	-0.43622	-0.77204	0.53792
C	0.82604	-1.43774	0.17938
H	2.78195	-1.23639	-0.59808
H	2.78187	1.23649	-0.59798
H	0.91474	2.50678	0.35361
H	0.91476	-2.50677	0.35368
H	-1.07173	1.2685	1.2729
H	-1.07168	-1.26843	1.27288
N	-1.12942	0.00003	-0.49691
C	-2.58389	-0.00006	-0.38983
H	-2.97899	0.88754	-0.89449
H	-2.97884	-0.88773	-0.89446
H	-2.95796	-0.00007	0.64929

7-methyl-7-azanorcaradiene
The number of imaginary frequencies: 0
Total Energy (M06/6-311G+**)= -326.6688665
ZPE= -326.525862
Enthalpy= -326.51812
Gibb's Free Energy= -326.556372

C	1.86736	-0.72717	-0.30848
C	1.86727	0.72699	-0.3085
C	0.82599	1.43804	0.17889
C	-0.43647	0.77206	0.53738
C	-0.43635	-0.77192	0.53743
C	0.82597	-1.43801	0.179
H	2.78349	-1.23668	-0.59757
H	2.78347	1.23657	-0.5974
H	0.91428	2.50789	0.35285
H	0.91386	-2.5079	0.35303
H	-1.07253	1.26895	1.27227
H	-1.07282	-1.26867	1.272
N	-1.13026	0.0002	-0.49695
C	-2.58436	-0.00015	-0.38897
H	-2.97867	0.88861	-0.89404
H	-2.97838	-0.88884	-0.89439
H	-2.95739	-0.0004	0.65145

7-methyl-7-azanorcaradiene N-oxide
The number of imaginary frequencies: 0
Total Energy (B3LYP/6-31G*)= -401.97620874
ZPE= -401.828039
Enthalpy=-401.81928
Gibb's Free Energy= -401.859745

C	1.90702	-0.76695	-0.26941
C	1.92231	0.77444	-0.25264
C	0.86515	1.47579	0.22253
C	-0.47927	0.78862	0.52423
C	-0.47307	-0.74424	0.56603
C	0.82831	-1.46426	0.16868
H	2.76561	-1.29679	-0.62576
H	2.78738	1.29707	-0.60395
H	0.96946	2.52581	0.39994
H	0.87985	-2.53127	0.22968
H	-0.99883	1.39917	1.23287
H	-1.02755	-1.30025	1.29287
N	-1.19431	-0.01676	-0.49064
C	-2.6622	-0.01992	-0.41196
H	-3.0487	0.83602	-0.92467
H	-3.0419	-0.91034	-0.86789
H	-2.96445	0.01226	0.61396
O	-0.81195	-0.0583	-1.79513

7-methyl-7-azanorcaradiene N-oxide
The number of imaginary frequencies: 0
Total Energy (B3LYP/6-31G**)= -401.98966351
ZPE= -401.841848
Enthalpy= -401.83308
Gibb's Free Energy= -401.873557

C	1.90489	0.72696	0.28203
C	1.90523	-0.72705	0.28062
C	0.94617	-1.43689	-0.35466
C	-0.25337	-0.76724	-0.84109
C	-0.2525	0.76857	-0.84149
C	0.94613	1.43748	-0.35318
H	2.76352	1.23737	0.70874
H	2.76448	-1.23784	0.70567
H	1.02988	-2.51044	-0.48731
H	1.02931	2.51139	-0.48328
H	-0.87801	-1.28311	-1.56504
H	-0.87785	1.28469	-1.56453
N	-1.06841	-0.00086	0.23813
C	-2.53029	0.00055	0.01848
H	-2.92878	-0.89135	0.50462

H	-2.92741	0.89181	0.50682
H	-2.77843	0.00199	-1.04642
O	-0.71442	-0.00159	1.48871

7-methyl-7-azanorcaradiene N-oxide

The number of imaginary frequencies: 0
Total Energy (M06/6-311G+**)= -401.80644197
ZPE= -401.659005
Enthalpy= -401.650406
Gibb's Free Energy= -401.690561

C	-1.9366	-0.69675	0.32594
C	-1.91983	0.72422	0.30748
C	-0.97434	1.43326	-0.37774
C	0.29984	0.74459	-0.87686
C	0.29666	-0.79492	-0.8178
C	-0.99917	-1.44498	-0.32655
H	-2.72311	-1.19699	0.85135
H	-2.68794	1.25638	0.82873
H	-1.12616	2.47491	-0.56963
H	-1.17031	-2.48784	-0.49408
H	0.79835	1.24075	-1.68322
H	0.73905	-1.36195	-1.61006
N	1.09013	-0.00025	0.11397
C	2.56009	-0.00873	0.1194
H	2.92013	0.87937	0.59538
H	2.90984	-0.86691	0.65429
H	2.92028	-0.04482	-0.88751
O	0.72863	0.04609	1.42422

Pyridine

The number of imaginary frequencies: 0
Total Energy (B3LYP/6-31G**)= -248.29259287
ZPE= -248.203718
Enthalpy= -248.198501
Gibb's Free Energy= -248.231119 C -1.14249 -0.72173 -0.00022

C	-1.19869	0.67323	-0.00012
C	0.0002	1.38545	0.0001
C	1.19888	0.67291	0.00022
C	1.14229	-0.72204	0.00013
N	-0.0002	-1.42093	-0.0001
H	0.00032	2.47233	0.00016
H	-2.05988	-1.30864	-0.00037
H	-2.15775	1.18284	-0.00023
H	2.1581	1.18221	0.00036
H	2.05951	-1.3092	0.00019

Pyridine N-oxide

The number of imaginary frequencies: 0
Total Energy (B3LYP/6-31G**)= -323.45500559
ZPE= -323.361911
Enthalpy= -323.355908
Gibb's Free Energy= -323.390607

C	0.28383	-1.18039	-0.00018
C	-1.09931	-1.19458	-0.00009
C	-1.82222	0.	0.00012
C	-1.09931	1.19458	0.00024
C	0.28383	1.18039	0.00014
N	0.98713	0.	-0.00007
H	-2.90654	0.	0.0002
H	0.91433	-2.05913	-0.00034
H	-1.60303	-2.15629	-0.00019
H	-1.60303	2.15629	0.00041
H	0.91433	2.05913	0.00022
O	2.26163	0.	-0.00015

Trimethylamine

The number of imaginary frequencies: 0
Total Energy (B3LYP/6-31G**)= -174.4861591
ZPE= -174.365595
Enthalpy= -174.359219
Gibb's Free Energy= -174.391860

N	0.	0.	0.37142
C	0.	1.38908	-0.06099
H	-0.88689	1.89889	0.33175
H	0.88689	1.89889	0.33175
H	0.	1.5053	-1.16421
C	-1.20298	-0.69454	-0.06099
H	-1.20104	-1.71751	0.33175
H	-2.08793	-0.18138	0.33175
H	-1.30363	-0.75265	-1.16421
C	1.20298	-0.69454	-0.06099
H	2.08793	-0.18138	0.33175
H	1.20104	-1.71751	0.33175
H	1.30363	-0.75265	-1.16421

Trimethylamine N-oxide

The number of imaginary frequencies: 0
Total Energy (B3LYP/6-31G**)= -249.62754733
ZPE= -249.502133
Enthalpy= -249.495143
Gibb's Free Energy= -249.529500

N	0.	0.	0.08312
C	0.	1.41754	-0.41881

H	-0.88839	1.89255	-0.0028
H	0.88839	1.89255	-0.0028
H	0.	1.4678	-1.51383
C	-1.22763	-0.70877	-0.41881
H	-1.1948	-1.71564	-0.0028
H	-2.08319	-0.1769	-0.0028
H	-1.27115	-0.7339	-1.51383
C	1.22763	-0.70877	-0.41881
H	2.08319	-0.1769	-0.0028
H	1.1948	-1.71564	-0.0028
H	1.27115	-0.7339	-1.51383
O	0.	0.	1.43938

N-methylaziridine
The number of imaginary frequencies: 0
Total Energy (B3LYP/6-31G*)= -173.23135212
ZPE= -173.13292
Enthalpy= -173.127558
Gibb's Free Energy= -173.159205

C	-0.81263	0.01988	-0.00942
C	0.69188	0.01646	0.01901
H	-1.31927	-0.34205	-0.8796
H	-1.36422	-0.28283	0.85604
H	1.30576	-0.2704	-0.80909
H	1.16767	-0.2429	0.94165
N	-0.06563	1.32111	-0.03859
C	-0.13378	2.19462	-1.21895
H	-1.01422	2.80019	-1.16415
H	0.73094	2.82418	-1.24716
H	-0.16768	1.59529	-2.1047

N-methylaziridine N-oxide
The number of imaginary frequencies: 0
Total Energy (B3LYP/6-31G*)= -248.36984065
ZPE= -248.267481
Enthalpy= -248.261373
Gibb's Free Energy= -248.295118

C	0.91154	0.77392	0.11511
C	0.89824	-0.77227	0.10721
H	0.7465	1.28391	1.04117
H	1.58558	1.27929	-0.54457
H	0.78061	-1.29457	1.03364
H	1.59987	-1.28788	-0.51468
N	-0.20087	0.00088	-0.47225
C	-1.55546	0.00289	0.09869
H	-2.07808	0.87829	-0.22604
H	-2.08198	-0.86901	-0.22913
H	-1.49231	0.00086	1.16682
O	-0.38148	0.00368	-1.8202

N-methylaziridine
The number of imaginary frequencies: 0
Total Energy (B3LYP/6-31G**)= -173.23135212
ZPE= -173.13292
Enthalpy= -173.127558
Gibb's Free Energy= -173.159205

C	0.9011	0.74593	0.12103
C	0.90182	-0.74557	0.12108
H	0.65933	1.24157	1.06284
H	1.57628	1.30308	-0.52521
H	0.66068	-1.24143	1.06294
H	1.57806	-1.30166	-0.52499
N	-0.1564	-0.00029	-0.55436
C	-1.45929	-0.00019	0.09732
H	-2.01925	0.88759	-0.21681
H	-2.0191	-0.88812	-0.2166
H	-1.40297	0.00001	1.20182

N-methylaziridine N-oxide
The number of imaginary frequencies: 0
Total Energy (B3LYP/6-31G**)= -248.36984065
ZPE= -248.267481
Enthalpy= -248.261373
Gibb's Free Energy= -248.295118

C	0.91197	0.77358	0.11543
C	0.89812	-0.77261	0.10775
H	0.74695	1.28376	1.04138
H	1.58629	1.27861	-0.54422
H	0.78015	-1.29473	1.03424
H	1.59968	-1.28856	-0.51395
N	-0.20061	0.00085	-0.47201
C	-1.5553	0.00342	0.0987
H	-2.07756	0.87895	-0.22625
H	-2.08207	-0.86834	-0.22908
H	-1.49234	0.00152	1.16684
O	-0.38099	0.0035	-1.81999

N-methylaziridine
The number of imaginary frequencies: 0
Total Energy (M06/6-311G+**)= -173.14757437
ZPE= -173.050266
Enthalpy= -173.044925
Gibb's Free Energy= -173.076507

C	-0.93158	-0.75352	0.1074
C	-0.93188	0.74813	0.12172
H	-0.69467	-1.35042	0.96325

H	-1.68532	-1.25779	-0.46048
H	-0.82027	1.35583	0.99531
H	-1.61782	1.23386	-0.54044
N	0.19908	0.00654	-0.54255
C	1.51627	0.00101	0.11005
H	2.06081	-0.86878	-0.193
H	2.05878	0.87842	-0.1741
H	1.388	-0.01062	1.17227

N-methylaziridine N-oxide

The number of imaginary frequencies: 0

Total Energy (M06/6-311G+**)= -248.28292193

ZPE= -248.181688

Enthalpy= -248.175647

Gibb's Free Energy= -248.209266

C	0.89389	0.78517	0.1286
C	0.91063	-0.76037	0.13715
H	0.78837	1.31758	1.05072
H	1.55257	1.28652	-0.5494
H	0.69589	-1.26128	1.05795
H	1.65022	-1.27839	-0.43692
N	-0.19019	-0.00268	-0.47178
C	-1.55579	-0.0167	0.07213
H	-2.08411	0.84935	-0.26804
H	-2.06334	-0.89781	-0.26095
H	-1.51393	-0.01187	1.1413
O	-0.34374	-0.00959	-1.82307

Cartesian Coordinates (Å) and energies (Hartrees) for all structures calculated using Gaussian 16.

N-methylazepine N-oxide

The number of imaginary frequencies: 0

B3LYP/6-31G**

Enthalpy = -401.987790971

6	1.969668	-0.680418	0.208142
6	1.969400	0.680840	0.208107
6	0.928373	1.505631	-0.354441
6	0.928837	-1.505655	-0.354106
6	-0.368340	1.197552	-0.538867
6	-0.368016	-1.198005	-0.538327
1	2.865300	-1.192417	0.550726
1	2.864894	1.193165	0.550561
1	1.229467	2.487553	-0.714713
1	1.230211	-2.487594	-0.714117
1	-1.084432	1.813237	-1.067255
1	-1.084025	-1.814112	-1.066334
7	-1.072525	-0.000194	-0.007446
8	-2.358751	-0.000265	-0.468970
6	-1.098760	0.000428	1.498914
1	-1.659893	-0.889641	1.780260
1	-0.094888	-0.001947	1.928068
1	-1.655926	0.893004	1.780144

N-methylazepine N-oxide

The number of imaginary frequencies: 0

APFD/aug-cc-pVDZ

Enthalpy = -401.683840334

6	0.267783	-0.765912	-0.850829
6	0.266149	0.768828	-0.851379
1	-1.024147	-2.511770	-0.522626
6	-0.930445	-1.434678	-0.374622
6	-0.930346	1.435990	-0.371472
6	-1.873434	0.725588	0.290486
6	-1.874281	-0.725756	0.287379
1	-1.023187	2.513828	-0.514689
1	-2.730252	1.239817	0.732943
1	-2.732553	-1.240742	0.726194
7	1.044658	-0.001765	0.246063
6	2.499037	0.001073	0.057002
1	2.886681	0.896917	0.558671
1	2.889451	-0.896205	0.554123
1	2.772801	0.004022	-1.007715
1	0.911605	-1.285576	-1.565411
1	0.911128	1.288788	-1.564505
8	0.659887	-0.003440	1.470147

N-methylazepine N-oxide

The number of imaginary frequencies: 0

APFD/aug-cc-pVTZ

Enthalpy = -401.788822197

6	1.936336	-0.677553	0.211900
6	1.936345	0.677535	0.211970
6	0.910417	1.491864	-0.369788
6	0.910389	-1.491833	-0.369887
6	-0.376347	1.175332	-0.561500
6	-0.376385	-1.175288	-0.561548
1	2.827436	-1.187874	0.561969
1	2.827444	1.187808	0.562110
1	1.212970	2.464927	-0.745423
1	1.212936	-2.464858	-0.745620
1	-1.089698	1.768307	-1.115084
1	-1.089730	-1.768214	-1.115195
7	-1.066001	0.000025	0.000727
8	-2.357261	0.000062	-0.397984

6 -1.018836 -0.000100 1.490928
1 -1.558371 -0.890416 1.801015
1 0.004805 0.000220 1.861470
1 -1.559211 0.889686 1.801089

1-methyl-2,3,4,5-tetrahydro-1H-azepine N-oxide
The number of imaginary frequencies: 0
B3LYP/6-31G**
Enthalpy= -404.439377914
6 2.023212 -0.761124 0.181705
6 1.777779 0.725632 0.493583
6 0.968236 1.412198 -0.618470
6 0.889170 -1.523008 -0.448140
6 -0.551882 1.280359 -0.480836
6 -0.405432 -1.224603 -0.528919
1 2.877818 -0.848634 -0.504799
1 2.750829 1.219588 0.596870
1 1.178119 2.488396 -0.631154
1 1.166901 -2.471881 -0.905311
1 -1.034354 1.436125 -1.452725
7 -1.047619 -0.042198 0.106373
8 -0.851457 -0.062281 1.463086
6 -2.530440 -0.120374 -0.136997
1 -2.769823 -0.148817 -1.205644
1 -2.872303 -1.020394 0.371731
1 -2.970022 0.752761 0.341584
1 -1.109400 -1.896943 -1.006396
1 2.327864 -1.292376 1.094489
1 1.233461 0.813478 1.434658
1 1.286555 1.030340 -1.596322
1 -0.944518 1.997513 0.242163

1-methyl-2,3,4,5-tetrahydro-1H-azepine N-oxide
The number of imaginary frequencies: 0
APFD/aug-cc-pVDZ
Enthalpy= -404.123157784
6 1.941457 -0.789644 0.253272
6 1.779678 0.726556 0.468894
6 0.962522 1.389394 -0.641095
6 0.859247 -1.497314 -0.506966
6 -0.548692 1.281066 -0.459394
6 -0.430196 -1.180479 -0.608579
1 2.884612 -0.981306 -0.288916
1 2.784230 1.180227 0.502029
1 1.188853 2.467696 -0.692664
1 1.157943 -2.407691 -1.037976
1 -1.066516 1.463152 -1.415800
7 -1.031542 -0.038921 0.113207
8 -0.752767 -0.110983 1.433507
6 -2.511481 -0.098481 -0.054054
1 -2.808945 -0.080569 -1.114444
1 -2.834200 -1.022026 0.438811
1 -2.921344 0.760541 0.487075
1 -1.134485 -1.782349 -1.184919
1 2.050641 -1.296140 1.229102
1 1.281831 0.907106 1.430062
1 1.253863 0.970370 -1.620094
1 -0.908765 1.994716 0.294767

1-methyl-2,3,4,5-tetrahydro-1H-azepine N-oxide
The number of imaginary frequencies: 0
APFD/aug-cc-pVTZ
Enthalpy= -404.240506936
6 1.978245 -0.771779 0.209821
6 1.777074 0.723720 0.477927
6 0.963680 1.392242 -0.627109
6 0.866795 -1.501145 -0.473464
6 -0.544562 1.273814 -0.456823
6 -0.417313 -1.195643 -0.560395
1 2.869416 -0.906540 -0.414722
1 2.761400 1.195441 0.543579
1 1.183005 2.463067 -0.668433
1 1.147926 -2.429522 -0.963314
1 -1.047170 1.443774 -1.412615
7 -1.037342 -0.040732 0.113352
8 -0.812266 -0.095833 1.449193
6 -2.507697 -0.100082 -0.110604
1 -2.752460 -0.105179 -1.175110
1 -2.855852 -1.004500 0.380636
1 -2.935467 0.765894 0.386018
1 -1.120898 -1.834517 -1.076943
1 2.198355 -1.295440 1.147590
1 1.267225 0.860499 1.430010
1 1.259835 0.983476 -1.598280
1 -0.913122 1.988571 0.278456

1-methyl-2,3,6,7-tetrahydro-1H-azepine N-oxide
The number of imaginary frequencies: 0
B3LYP/6-31G**
Enthalpy= -404.433978813
6 -0.576807 1.842742 0.666223
6 -0.576807 1.842742 -0.666223
6 0.508217 1.117225 -1.423688
6 0.508217 1.117225 1.423688
6 0.508217 -0.419616 -1.292730
6 0.508217 -0.419616 1.292730
1 0.449230 1.341231 -2.493823

1 1.525868 -0.802219 -1.437872
7 -0.065214 -1.005938 -0.000000
8 -1.418000 -0.893579 -0.000000
6 0.277768 -2.475051 -0.000000
1 1.359134 -2.651960 -0.000000
1 -0.190055 -2.900739 0.886380
1 -0.190055 -2.900739 -0.886380
1 1.525868 -0.802219 1.437872
1 -1.366336 2.335326 1.225810
1 -1.366336 2.335326 -1.225810
1 1.485460 1.495474 -1.093683
1 -0.154553 -0.864943 -2.034635
1 0.449230 1.341231 2.493823
1 -0.154553 -0.864943 2.034635
1 1.485460 1.495474 1.093683

1-methyl-2,3,6,7-tetrahydro-1H-azepine N-oxide
The number of imaginary frequencies: 0
APFD/aug-cc-pVDZ
Enthalpy=-404.118296570
6 -0.580349 1.816900 0.667109
6 -0.580349 1.816900 -0.667109
6 0.516659 1.107151 -1.410951
6 0.516659 1.107151 1.410951
6 0.516659 -0.422673 -1.278441
6 0.516659 -0.422673 1.278441
1 0.478492 1.336464 -2.487119
1 1.540076 -0.813529 -1.409237
7 -0.070970 -0.994026 -0.000000
8 -1.403662 -0.848300 -0.000000
6 0.245188 -2.455492 -0.000000
1 1.329340 -2.652048 -0.000000
1 -0.233266 -2.876859 0.890642
1 -0.233266 -2.876859 -0.890642
1 1.540076 -0.813529 1.409237
1 -1.388686 2.290435 1.228873
1 -1.388686 2.290435 -1.228873
1 1.490200 1.493395 -1.057620
1 -0.141820 -0.873389 -2.031483
1 0.478492 1.336464 2.487119
1 -0.141820 -0.873389 2.031483
1 1.490200 1.493395 1.057620

1-methyl-2,3,6,7-tetrahydro-1H-azepine N-oxide
The number of imaginary frequencies: 0
APFD/aug-cc-pVTZ
Enthalpy=-404.236049675
6 -0.574719 1.823334 0.662558
6 -0.574719 1.823334 -0.662558
6 0.510721 1.106581 -1.409081
6 0.510721 1.106581 1.409081
6 0.510721 -0.421084 -1.273461
6 0.510721 -0.421084 1.273461
1 0.463560 1.331838 -2.476481
1 1.528360 -0.803455 -1.394617
7 -0.071517 -0.995877 -0.000000
8 -1.410929 -0.869542 0.000000
6 0.259926 -2.450388 -0.000000
1 1.338205 -2.625857 -0.000000
1 -0.206064 -2.876044 0.884313
1 -0.206064 -2.876044 -0.884313
1 1.528360 -0.803455 1.394617
1 -1.369087 2.304794 1.219809
1 -1.369087 2.304794 -1.219809
1 1.479264 1.487992 -1.065618
1 -0.131227 -0.870277 -2.028562
1 0.463560 1.331838 2.476481
1 -0.131227 -0.870277 2.028562
1 1.479264 1.487992 1.065618

1-methyl-2,3,4,7-tetrahydro-1H-azepine N-oxide
The number of imaginary frequencies: 0
B3LYP/6-31G**
Enthalpy= -404.444680715
6 -1.958168 0.798791 0.156899
6 -1.884165 -0.677640 0.437836
6 -1.005620 -1.427777 -0.577975
6 -0.979128 1.559437 -0.336153
6 0.502697 -1.340071 -0.351742
6 0.427614 1.166537 -0.695513
1 -2.896859 -1.096736 0.403419
1 -1.252424 -2.496320 -0.561356
1 1.032607 -1.620590 -1.270068
7 1.016583 0.015684 0.124606
8 0.769016 0.175018 1.446679
6 2.509277 0.029320 -0.083156
1 2.780036 -0.002802 -1.144270
1 2.871169 0.938979 0.392858
1 2.909483 -0.834453 0.446194
1 0.532992 0.920207 -1.761754
1 -2.901162 1.289462 0.392927
1 -1.489531 -0.825230 1.449740
1 -1.255107 -1.074703 -1.586040
1 0.817881 -1.993295 0.462973
1 -1.176692 2.619443 -0.484723
1 1.084359 2.014525 -0.486750

1-methyl-2,3,4,7-tetrahydro-1H-azepine N-oxide
The number of imaginary frequencies: 0

APFD/aug-cc-pVDZ
Enthalpy= -404.129255205
6 -1.943774 0.792334 0.160870
6 -1.864537 -0.678237 0.440491
6 -0.997440 -1.416429 -0.583048
6 -0.967470 1.553729 -0.340857
6 0.504767 -1.327512 -0.356899
6 0.432762 1.153455 -0.697393
1 -2.882164 -1.102341 0.421575
1 -1.245076 -2.491298 -0.582848
1 1.043561 -1.600439 -1.279999
7 1.007662 0.015371 0.129391
8 0.738792 0.173323 1.430003
6 2.488691 0.030164 -0.062706
1 2.770414 0.012281 -1.127500
1 2.848037 0.938204 0.432983
1 2.887481 -0.844567 0.462825
1 0.536299 0.894306 -1.767247
1 -2.890611 1.288014 0.402619
1 -1.450380 -0.820152 1.453266
1 -1.252459 -1.046847 -1.591906
1 0.822725 -1.990523 0.458506
1 -1.168570 2.619345 -0.492161
1 1.098777 2.004814 -0.498624

1-methyl-2,3,4,7-tetrahydro-1H-azepine N-oxide
The number of imaginary frequencies: 0
APFD/aug-cc-pVTZ
Enthalpy= -404.246538534
6 -1.937752 0.796618 0.159803
6 -1.877343 -0.673056 0.427883
6 -0.995392 -1.413871 -0.575379
6 -0.964637 1.545607 -0.342658
6 0.499574 -1.331134 -0.323577
6 0.426871 1.135744 -0.707140
1 -2.890669 -1.082608 0.379541
1 -1.246806 -2.478591 -0.577394
1 1.044330 -1.624119 -1.225637
7 1.009679 0.016386 0.131013
8 0.760071 0.200090 1.436158
6 2.484110 0.024091 -0.082977
1 2.739314 -0.012614 -1.144578
1 2.855564 0.932333 0.382703
1 2.887891 -0.837101 0.442810
1 0.515419 0.851957 -1.762379
1 -2.869250 1.295662 0.412803
1 -1.503932 -0.830847 1.444706
1 -1.227361 -1.045564 -1.579855
1 0.796683 -1.977416 0.500914
1 -1.153116 2.606147 -0.478459
1 1.091029 1.983349 -0.537259

N-methylazepane N-oxide
The number of imaginary frequencies: 0
B3LYP/6-31G**
Enthalpy = -405.675354659
6 -0.607085 1.792740 0.777922
6 -0.607085 1.792740 -0.777922
6 0.568106 1.038282 -1.419616
6 0.568106 1.038282 1.419616
6 0.568106 -0.490602 -1.278837
6 0.568106 -0.490602 1.278837
1 -0.562496 2.826694 1.142109
1 -0.562496 2.826694 -1.142109
1 0.568826 1.238510 -2.498135
1 1.516849 1.443877 1.051641
1 1.587025 -0.881026 -1.390306
1 -0.069590 -0.940647 2.040868
7 -0.037297 -1.055132 -0.000000
8 -1.387282 -0.860707 -0.000000
6 0.213796 -2.540083 -0.000000
1 1.282444 -2.779776 -0.000000
1 -0.277798 -2.937635 0.886526
1 -0.277798 -2.937635 -0.886526
1 1.587025 -0.881026 1.390306
1 0.568826 1.238510 2.498135
1 -1.540526 1.353638 1.131392
1 -1.540526 1.353638 -1.131392
1 1.516849 1.443877 -1.051641
1 -0.069590 -0.940647 -2.040868

N-methylazepane N-oxide
The number of imaginary frequencies: 0
APFD/aug-cc-pVDZ
Enthalpy = -405.357516692
6 -0.608566 1.775840 0.774611
6 -0.608566 1.775840 -0.774611
6 0.569551 1.031910 -1.406300
6 0.569551 1.031910 1.406300
6 0.569551 -0.490908 -1.264864
6 0.569551 -0.490908 1.264864
1 -0.572153 2.815685 1.142885
1 -0.572153 2.815685 -1.142885
1 0.584187 1.234582 -2.490714
1 1.519222 1.442856 1.026234
1 1.594027 -0.887282 -1.366734
1 -0.065050 -0.946299 2.036392
7 -0.042627 -1.047369 0.000000
8 -1.373301 -0.839667 -0.000000
6 0.200612 -2.520014 0.000000
1 1.273957 -2.766223 0.000000
1 -0.296638 -2.918428 0.890819
1 -0.296638 -2.918428 -0.890819
1 1.594027 -0.887282 1.366734

1 0.584187 1.234582 2.490714
1 -1.543225 1.325445 1.133449
1 -1.543225 1.325445 -1.133449
1 1.519222 1.442856 -1.026234
1 -0.065050 -0.946299 -2.036392

N-methylazepane N-oxide
The number of imaginary frequencies: 0
APFD/aug-cc-pVTZ
Enthalpy = -405.475774305
6 -0.608880 1.778496 0.773162
6 -0.608880 1.778496 -0.773162
6 0.564014 1.032637 -1.404527
6 0.564014 1.032637 1.404527
6 0.564014 -0.487644 -1.261500
6 0.564014 -0.487644 1.261500
1 -0.571183 2.809741 1.137832
1 -0.571183 2.809741 -1.137832
1 0.574914 1.233755 -2.480047
1 1.505771 1.438754 1.027194
1 1.582187 -0.875613 -1.357279
1 -0.058439 -0.939919 2.031967
7 -0.041192 -1.048597 0.000000
8 -1.378162 -0.860724 0.000000
6 0.221575 -2.514703 0.000000
1 1.290643 -2.737348 0.000000
1 -0.262589 -2.919327 0.884357
1 -0.262589 -2.919327 -0.884357
1 1.582187 -0.875613 1.357279
1 0.574914 1.233755 2.480047
1 -1.538770 1.337450 1.128002
1 -1.538770 1.337450 -1.128002
1 1.505771 1.438754 -1.027194
1 -0.058439 -0.939919 -2.031967

N-methylazepine
The number of imaginary frequencies: 0
B3LYP/6-31G**
Enthalpy = -326.859656161
6 -0.609487 -1.771782 0.676167
6 -0.609487 -1.771782 -0.676167
6 -0.609487 -0.579396 -1.518592
6 -0.609487 -0.579396 1.518592
6 -0.053329 0.600352 -1.193902
6 -0.053329 0.600352 1.193902
1 -0.689963 -2.728232 1.190057
1 -0.689963 -2.728232 -1.190057
1 -1.123176 -0.641556 -2.475142
1 -1.123176 -0.641556 2.475142
1 -0.151617 1.457795 -1.862488
1 -0.151617 1.457795 1.862488
7 0.681491 0.827495 0.000000
6 1.523504 2.013041 0.000000
1 0.950836 2.958234 0.000000
1 2.167430 2.002472 0.883203
1 2.167430 2.002472 -0.883203

N-methylazepine
The number of imaginary frequencies: 0
APFD/aug-cc-pVDZ
Enthalpy = -326.594812304
6 -0.634887 -1.747142 0.677373
6 -0.634887 -1.747142 -0.677373
6 -0.634887 -0.554397 -1.512618
6 -0.634887 -0.554397 1.512618
6 -0.050612 0.611857 -1.181001
6 -0.050612 0.611857 1.181001
1 -0.727264 -2.709068 1.193506
1 -0.727264 -2.709068 -1.193506
1 -1.168036 -0.600160 -2.466926
1 -1.168036 -0.600160 2.466926
1 -0.142786 1.489207 -1.836567
1 -0.142786 1.489207 1.836567
7 0.706137 0.791799 0.000000
6 1.580894 1.940897 0.000000
1 1.035579 2.909451 0.000000
1 2.228447 1.909404 0.887501
1 2.228447 1.909404 -0.887501

N-methylazepine
The number of imaginary frequencies: 0
APFD/zug-cc-pVTZ
Enthalpy = -326.682346079
6 -0.621889 -1.751999 0.672556
6 -0.621889 -1.751999 -0.672556
6 -0.621889 -0.563235 -1.506411
6 -0.621889 -0.563235 1.506411
6 -0.045794 0.598633 -1.181834
6 -0.045794 0.598633 1.181834
1 -0.705900 -2.706045 1.185584
1 -0.705900 -2.706045 -1.185584
1 -1.139456 -0.614618 -2.458628
1 -1.139456 -0.614618 2.458628
1 -0.127540 1.459628 -1.844287
1 -0.127540 1.459628 1.844287
7 0.693358 0.805277 0.000000
6 1.539113 1.974540 0.000000
1 0.970210 2.917998 0.000000
1 2.181132 1.959552 0.880610
1 2.181132 1.959552 -0.880610

1-methyl-2,3,4,5-tetrahydro-1H-azepine
The number of imaginary frequencies: 0
B3LYP/6-31G**
Enthalpy= -329.310375943
6 -1.660774 -0.814901 -0.590395
6 -2.050443 0.546084 0.020195
6 -0.847314 1.381365 0.510666
6 -0.607181 -1.584990 0.176633
6 0.455989 1.204551 -0.281741
6 0.652078 -1.179921 0.419891
1 -2.561653 -1.430564 -0.686480
1 -2.731133 0.391165 0.865819
1 -1.121086 2.442831 0.493684
1 -0.875705 -2.567305 0.554317
1 1.085612 2.088935 -0.123744
7 1.244816 0.060230 0.179915
6 2.629155 0.050140 -0.259049
1 3.103870 1.009002 -0.022126
1 3.175884 -0.739000 0.266142
1 2.744132 -0.126581 -1.342437
1 1.333690 -1.868786 0.918603
1 -1.313274 -0.652734 -1.619447
1 -2.618875 1.113319 -0.728478
1 -0.622567 1.139710 1.554890
1 0.258342 1.164435 -1.367346

1-methyl-2,3,4,5-tetrahydro-1H-azepine
The number of imaginary frequencies: 0
APFD/aug-cc-pVTZ
Enthalpy= -329.132074646
6 -1.631766 -0.804752 -0.602114
6 -2.033773 0.543621 0.003461
6 -0.843468 1.355649 0.528558
6 -0.607016 -1.571976 0.188732
6 0.448144 1.201462 -0.268138
6 0.647505 -1.169017 0.426087
1 -2.525747 -1.418677 -0.735123
1 -2.737962 0.385343 0.825777
1 -1.115489 2.414309 0.558836
1 -0.884640 -2.543172 0.580897
1 1.079520 2.078817 -0.097631
7 1.229899 0.055877 0.162681
6 2.603797 0.053700 -0.264817
1 3.076679 1.007055 -0.015750
1 3.148743 -0.740833 0.247504
1 2.717513 -0.108027 -1.347490
1 1.328222 -1.849614 0.932174
1 -1.246927 -0.637754 -1.613791
1 -2.575874 1.121057 -0.753304
1 -0.620765 1.067129 1.559085
1 0.246905 1.181100 -1.350566

1-methyl-2,3,4,5-tetrahydro-1H-azepine
The number of imaginary frequencies: 0
APFD/aug-cc-pVDZ
Enthalpy= -329.040184702
6 -1.633891 -0.805465 -0.607611
6 -2.037924 0.542103 0.004637
6 -0.846602 1.361647 0.525568
6 -0.611450 -1.578749 0.186986
6 0.452563 1.204956 -0.264153
6 0.648827 -1.172085 0.432424
1 -2.534883 -1.422368 -0.753229
1 -2.743157 0.379817 0.837815
1 -1.122150 2.429166 0.544853
1 -0.894314 -2.555576 0.587196
1 1.087822 2.089626 -0.087390
7 1.235104 0.059056 0.173200
6 2.605490 0.049902 -0.272368
1 3.090609 1.009164 -0.028756
1 3.159006 -0.751845 0.239068
1 2.709858 -0.114779 -1.365143
1 1.334187 -1.856290 0.947418
1 -1.238966 -0.631742 -1.624588
1 -2.593302 1.122752 -0.753707
1 -0.621824 1.085202 1.569104
1 0.259301 1.189624 -1.357934

1-methyl-2,3,6,7-tetrahydro-1H-azepine
The number of imaginary frequencies: 0
B3LYP/6-31G**
Enthalpy= -329.298190209
6 -0.117334 -1.817960 0.668012
6 -0.117334 -1.817960 -0.668012
6 -0.795123 -0.702640 -1.426087
6 -0.795123 -0.702640 1.426087
6 -0.117334 0.685480 -1.243606
6 -0.117334 0.685480 1.243606
1 -0.837360 -0.923310 -2.497320
1 -0.887863 1.472632 -1.374158
7 0.631652 0.846287 -0.000000
6 1.381910 2.091312 -0.000000
1 0.743786 2.997527 -0.000000
1 2.024232 2.137182 0.885874
1 2.024232 2.137182 -0.885874
1 -0.887863 1.472632 1.374158
1 0.382770 -2.607309 1.224157
1 0.382770 -2.607309 -1.224157
1 -1.839519 -0.633339 -1.093264
1 0.608080 0.830160 -2.052764
1 -0.837360 -0.923310 2.497320
1 0.608080 0.830160 2.052764

1 -1.839519 -0.633339 1.093264

1-methyl-2,3,6,7-tetrahydro-1H-azepine
The number of imaginary frequencies: 0
APFD/aug-cc-pVDZ
Enthalpy= -329.028619850

6 -0.117214 -1.802277 0.669165
6 -0.117214 -1.802277 -0.669165
6 -0.803991 -0.690553 -1.413492
6 -0.803991 -0.690553 1.413492
6 -0.117214 0.684780 -1.232261
6 -0.117214 0.684780 1.232261
1 -0.871377 -0.908076 -2.490298
1 -0.882342 1.488555 -1.351028
7 0.635103 0.828533 -0.000000
6 1.394302 2.055214 -0.000000
1 0.760324 2.972453 -0.000000
1 2.040767 2.097090 0.890427
1 2.040767 2.097090 -0.890427
1 -0.882342 1.488555 1.351028
1 0.395616 -2.590891 1.227973
1 0.395616 -2.590891 -1.227973
1 -1.846947 -0.621006 -1.054953
1 0.608872 0.830894 -2.049088
1 -0.871377 -0.908076 2.490298
1 0.608872 0.830894 2.049088
1 -1.846947 -0.621006 1.054953

1-methyl-2,3,6,7-tetrahydro-1H-azepine
The number of imaginary frequencies: 0
APFD/aug-cc-pVTZ
Enthalpy= -329.120153118
6 -0.115721 -1.800088 0.664583
6 -0.115721 -1.800088 -0.664583
6 -0.799039 -0.692754 -1.410560
6 -0.799039 -0.692754 1.410560
6 -0.115721 0.681737 -1.231163
6 -0.115721 0.681737 1.231163
1 -0.859878 -0.911409 -2.478286
1 -0.878052 1.475381 -1.347917
7 0.631095 0.832311 0.000000
6 1.384059 2.060551 0.000000
1 0.747002 2.964152 0.000000
1 2.024250 2.104781 0.883534
1 2.024250 2.104781 -0.883534
1 -0.878052 1.475381 1.347917
1 0.392059 -2.582268 1.218953
1 0.392059 -2.582268 -1.218953
1 -1.834151 -0.623112 -1.058122
1 0.604144 0.826434 -2.041318
1 -0.859878 -0.911409 2.478286
1 0.604144 0.826434 2.041318
1 -1.834151 -0.623112 1.058122

1-methyl-2,3,4,7-tetrahydro-1H-azepine
The number of imaginary frequencies: 0
B3LYP/6-31G**
Enthalpy= -329.304274524
6 1.833298 0.796941 -0.311605
6 1.748059 -0.695644 -0.533662
6 0.866298 -1.402891 0.509448
6 0.867290 1.577518 0.179704
6 -0.642176 -1.269839 0.261397
6 -0.555417 1.179060 0.506237
1 2.762488 -1.109411 -0.480336
1 1.104056 -2.473073 0.539757
1 -1.178569 -1.523506 1.199666
7 -1.050247 0.032799 -0.259575
6 -2.492718 0.078889 -0.449834
1 -3.068776 0.001519 0.493455
1 -2.776431 1.012719 -0.945075
1 -2.803289 -0.750401 -1.094210
1 -0.677565 1.037558 1.601189
1 2.790792 1.261848 -0.542959
1 1.384903 -0.914766 -1.547568
1 1.121763 -1.005611 1.498725
1 -0.952149 -2.016047 -0.482058
1 1.091063 2.630467 0.347851
1 -1.194361 2.034910 0.258478

1-methyl-2,3,4,7-tetrahydro-1H-azepine
The number of imaginary frequencies: 0
APFD/aug-cc-pVDZ
Enthalpy= -329.034597535
6 1.823517 0.786564 -0.317485
6 1.719667 -0.698792 -0.545825
6 0.860971 -1.392823 0.515894
6 0.864605 1.570924 0.186838
6 -0.641458 -1.258127 0.275438
6 -0.551759 1.169588 0.508676
1 2.736338 -1.125749 -0.529289
1 1.101803 -2.467998 0.565011
1 -1.185867 -1.494335 1.221682
7 -1.034729 0.032347 -0.259505
6 -2.464660 0.082312 -0.461276
1 -3.049428 0.018332 0.485324
1 -2.744602 1.015251 -0.973467
1 -2.778119 -0.758139 -1.099903
1 -0.676766 1.018477 1.608760
1 2.788360 1.250660 -0.552126
1 1.318455 -0.906143 -1.555104
1 1.129319 -0.974515 1.501246

1 -0.961500 -2.015588 -0.461592
1 1.098782 2.626912 0.365175
1 -1.198967 2.028534 0.267271

1-methyl-2,3,4,7-tetrahydro-1H-azepine
The number of imaginary frequencies: 0
APFD/aug-cc-pVTZ
Enthalpy= -329.126037128
6 1.819980 0.784657 -0.316078
6 1.720924 -0.698150 -0.537649
6 0.855284 -1.387898 0.516836
6 0.866581 1.564342 0.182039
6 -0.641341 -1.259149 0.260372
6 -0.545663 1.165131 0.508275
1 2.730083 -1.119362 -0.509365
1 1.097178 -2.453102 0.572715
1 -1.188598 -1.502230 1.191995
7 -1.036478 0.034366 -0.258923
6 -2.465314 0.086886 -0.452967
1 -3.036045 0.015298 0.490714
1 -2.744277 1.017512 -0.949909
1 -2.779700 -0.741011 -1.091816
1 -0.662443 1.006823 1.598721
1 2.775630 1.244882 -0.553316
1 1.332289 -0.908651 -1.540997
1 1.107009 -0.965185 1.493915
1 -0.947250 -2.003837 -0.481906
1 1.095623 2.613578 0.350556
1 -1.186864 2.019811 0.276185

N-methylazepane
The number of imaginary frequencies: 0
B3LYP/6-31G**
Enthalpy = -330.534354811
6 -0.123724 -1.768559 0.779985
6 -0.123724 -1.768559 -0.779985
6 -0.850466 -0.578342 -1.425059
6 -0.850466 -0.578342 1.425059
6 -0.123724 0.768839 -1.236262
6 -0.123724 0.768839 1.236262
1 -0.594277 -2.690315 1.142355
1 -0.594277 -2.690315 -1.142355
1 -0.951502 -0.757329 -2.502387
1 -1.875529 -0.518078 1.044370
1 -0.851133 1.600321 -1.335329
1 0.595416 0.893796 2.055068
7 0.652331 0.862959 -0.000000
6 1.492463 2.051620 -0.000000
1 0.917986 2.998952 -0.000000
1 2.136105 2.052321 0.885746
1 2.136105 2.052321 -0.885746
1 -0.851133 1.600321 1.335329
1 -0.951502 -0.757329 2.502387
1 0.908855 -1.787038 1.144541
1 0.908855 -1.787038 -1.144541
1 -1.875529 -0.518078 -1.044370
1 0.595416 0.893796 -2.055068

N-methylazepane
The number of imaginary frequencies: 0
APFD/aug-cc-pVDZ
Enthalpy = -330.262189970
6 -0.124173 -1.749599 0.776635
6 -0.124173 -1.749599 -0.776635
6 -0.857783 -0.567553 -1.412621
6 -0.857783 -0.567553 1.412621
6 -0.124173 0.767764 -1.224833
6 -0.124173 0.767764 1.224833
1 -0.586118 -2.681431 1.144048
1 -0.586118 -2.681431 -1.144048
1 -0.976436 -0.744531 -2.494881
1 -1.884294 -0.506792 1.016680
1 -0.844754 1.615359 -1.311636
1 0.595917 0.894194 2.050876
7 0.653599 0.843264 -0.000000
6 1.503736 2.011210 -0.000000
1 0.935913 2.970142 -0.000000
1 2.151151 2.006138 0.890306
1 2.151151 2.006138 -0.890306
1 -0.844754 1.615359 1.311636
1 -0.976436 -0.744531 2.494881
1 0.914548 -1.756732 1.145893
1 0.914548 -1.756732 -1.145893
1 -1.884294 -0.506792 -1.016680
1 0.595917 0.894194 -2.050876

N-methylazepane
The number of imaginary frequencies: 0
APFD/aug-cc-pVTZ
Enthalpy = -330.355334937
6 -0.121742 -1.749206 0.775353
6 -0.121742 -1.749206 -0.775353
6 -0.853859 -0.569530 -1.410241
6 -0.853859 -0.569530 1.410241
6 -0.121742 0.763356 -1.224235
6 -0.121742 0.763356 1.224235
1 -0.578486 -2.673973 1.139279
1 -0.578486 -2.673973 -1.139279
1 -0.970148 -0.746248 -2.483503
1 -1.870596 -0.507585 1.015801
1 -0.838599 1.601933 -1.310440
1 0.593033 0.887046 2.043155
7 0.650728 0.846893 0.000000

6 1.490725 2.019665 0.000000
1 0.915859 2.963631 0.000000
1 2.132120 2.019859 0.883400
1 2.132120 2.019859 -0.883400
1 -0.838599 1.601933 1.310440
1 -0.970148 -0.746248 2.483503
1 0.909085 -1.753690 1.138273
1 0.909085 -1.753690 -1.138273
1 -1.870596 -0.507585 -1.015801
1 0.593033 0.887046 -2.043155

N-Methylpyrrole N-oxide
The number of imaginary frequencies: 0
B3LYP/6-31G**
Enthalpy= -324.573601410
6 1.618482 0.737646 0.097116
6 1.618414 -0.737501 0.098435
6 0.355178 -1.157788 -0.009827
6 0.355196 1.158013 -0.012549
1 2.501313 1.363007 0.116943
1 2.501241 -1.362844 0.118411
1 -0.094951 -2.133540 -0.104607
1 -0.095166 2.133563 -0.108432
7 -0.562707 -0.000157 -0.096040
8 -1.231366 -0.001924 -1.299503
6 -1.552719 0.001445 1.033634
1 -2.170095 0.888862 0.898347
1 -2.170107 -0.886355 0.900952
1 -1.049673 0.002897 2.005836

N-Methylpyrrole N-oxide
The number of imaginary frequencies: 0
APFD/aug-cc-pVDZ
Enthalpy= -324.322161700
6 1.610683 0.736027 0.095017
6 1.610665 -0.736086 0.095032
6 0.345214 -1.151806 -0.017876
6 0.345274 1.151814 -0.017496
1 2.496476 1.368927 0.116952
1 2.496422 -1.369018 0.117473
1 -0.112032 -2.131874 -0.113321
1 -0.111836 2.131884 -0.113512
7 -0.564700 0.000018 -0.102412
8 -1.230268 0.000086 -1.284835
6 -1.525150 -0.000050 1.037748
1 -2.149438 0.892362 0.915318
1 -2.149489 -0.892440 0.915342
1 -0.995171 -0.000046 2.002758

N-Methylpyrrole N-oxide
The number of imaginary frequencies: 0
APFD/aug-cc-pVTZ
Enthalpy= -324.417780070
6 1.602973 0.734263 0.088198
6 1.602915 -0.734116 0.089678
6 0.346661 -1.149278 -0.016996
6 0.346632 1.149492 -0.019776
1 2.481669 1.360937 0.117130
1 2.481615 -1.360728 0.119017
1 -0.106248 -2.121296 -0.109862
1 -0.106523 2.121310 -0.113620
7 -0.561759 -0.000171 -0.104665
8 -1.240514 -0.001994 -1.282137
6 -1.510277 0.001515 1.044399
1 -2.129362 0.887896 0.934686
1 -2.129527 -0.885055 0.937175
1 -0.968622 0.002830 1.992206

N-methyl-2-pyrroline N-oxide
The number of imaginary frequencies: 0
B3LYP/6-31G**
Enthalpy= -325.813525020
6 1.724798 0.621573 0.102158
6 1.525707 -0.878176 0.092168
6 0.240457 -1.196333 0.009033
6 0.351491 1.129373 -0.362271
1 1.988975 0.981248 1.105913
1 -0.268072 -2.148829 -0.029761
1 0.299008 1.241941 -1.443708
7 -0.647327 -0.014763 -0.108996
8 -1.525491 -0.166833 -1.127449
6 -1.401523 0.197798 1.174408
1 -2.060329 1.048181 0.998616
1 -2.003484 -0.695379 1.337294
1 -0.727303 0.375710 2.019018
1 2.339449 -1.592086 0.147047
1 2.526514 0.944681 -0.570564
1 -0.005125 2.037122 0.125734

N-methyl-2-pyrroline N-oxide
The number of imaginary frequencies: 0
APFD/aug-cc-pVDZ
Enthalpy= -325.559554428
6 1.699228 0.626505 0.099662
6 1.519410 -0.869653 0.081635
6 0.234035 -1.192443 -0.005468
6 0.338910 1.105798 -0.400816
1 1.929546 0.986067 1.119459
1 -0.279209 -2.150390 -0.043246
1 0.302095 1.165155 -1.494631
7 -0.648950 -0.016217 -0.112443
8 -1.552804 -0.168406 -1.083635

6 -1.335260 0.208120 1.193122
1 -2.009696 1.058643 1.037583
1 -1.929268 -0.689577 1.398113
1 -0.614306 0.399022 2.003893
1 2.341219 -1.584606 0.139856
1 2.522242 0.966507 -0.548808
1 -0.035484 2.039994 0.035154

N-methyl-2-pyrroline N-oxide
The number of imaginary frequencies: 0
APFD/aug-cc-pVTZ
Enthalpy= -325.657265137
6 1.700621 0.619649 0.098995
6 1.511624 -0.871104 0.073950
6 0.234307 -1.188048 -0.011483
6 0.337682 1.114584 -0.374683
1 1.948166 0.967604 1.108245
1 -0.276017 -2.136720 -0.053793
1 0.296959 1.220866 -1.455370
7 -0.644978 -0.014008 -0.111152
8 -1.543340 -0.154901 -1.096392
6 -1.341990 0.189963 1.188782
1 -2.008656 1.037663 1.049725
1 -1.929672 -0.704090 1.379165
1 -0.626813 0.366110 1.995222
1 2.323617 -1.583048 0.131502
1 2.506973 0.954709 -0.557000
1 -0.026455 2.023903 0.098124

N-methyl-3-pyrroline N-oxide
The number of imaginary frequencies: 0
B3LYP/6-31G**
Enthalpy= -325.814117087
6 1.659112 0.667757 0.078666
6 1.659089 -0.667824 0.078611
6 0.306599 -1.205279 -0.282567
6 0.306694 1.205298 -0.282477
1 0.205106 -1.468262 -1.338934
1 0.204970 1.468429 -1.338757
7 -0.643806 0.000008 -0.112990
8 -1.660544 0.000082 -0.983480
6 -1.186601 -0.000046 1.292211
1 -1.811178 0.888082 1.377663
1 -1.811409 -0.888032 1.377394
1 -0.387746 -0.000248 2.040368
1 2.513539 -1.301454 0.291465
1 2.513650 1.301364 0.291211
1 -0.052479 2.039171 0.326025
1 -0.052812 -2.039200 0.325669

N-methyl-3-pyrroline N-oxide
The number of imaginary frequencies: 0
APFD/aug-cc-pVDZ
Enthalpy= -325.560494446
6 1.645691 0.668572 0.073567
6 1.645454 -0.668675 0.073390
6 0.296916 -1.192751 -0.296104
6 0.297074 1.193022 -0.295011
1 0.199026 -1.441229 -1.363506
1 0.199004 1.442315 -1.362187
7 -0.643142 0.000052 -0.113380
8 -1.670807 0.000594 -0.948348
6 -1.141950 -0.000658 1.295399
1 -1.768933 0.891751 1.398233
1 -1.769241 -0.892986 1.397129
1 -0.315842 -0.001240 2.023173
1 2.503806 -1.307034 0.291256
1 2.504150 1.306504 0.292150
1 -0.071332 2.040938 0.299241
1 -0.071305 -2.041200 0.297504

N-methyl-3-pyrroline N-oxide
The number of imaginary frequencies: 0
APFD/aug-cc-pVTZ
Enthalpy= -325.657786634
6 1.645070 0.663747 0.071136
6 1.644692 -0.663946 0.071139
6 0.296218 -1.193971 -0.276184
6 0.296470 1.194302 -0.274766
1 0.197894 -1.476386 -1.325430
1 0.197546 1.478063 -1.323537
7 -0.637502 0.000082 -0.112470
8 -1.651287 0.000779 -0.974962
6 -1.162751 -0.000816 1.282626
1 -1.783542 0.885363 1.380999
1 -1.784105 -0.886783 1.379457
1 -0.349976 -0.001704 2.011704
1 2.500305 -1.297236 0.266788
1 2.500777 1.296522 0.267837
1 -0.061962 2.016985 0.344062
1 -0.062319 -2.017520 0.341402

N-methylpyrrolidine N-oxide
The number of imaginary frequencies: 0
B3LYP/6-31G**
Enthalpy= -327.050367463
6 1.603663 0.781996 0.090072
6 1.603543 -0.782088 0.090005
6 0.207002 -1.179916 -0.397304
6 0.206897 1.180170 -0.396436
1 1.804230 1.168334 1.093772
1 1.803291 -1.168510 1.093835
1 0.140440 -1.273784 -1.482064

1 0.140075 1.275167 -1.481082
7 -0.712799 0.000065 -0.102554
8 -1.821085 0.000278 -0.863836
6 -1.111849 -0.000465 1.347292
1 -1.725599 0.887101 1.494613
1 -1.724655 -0.888716 1.494402
1 -0.251770 -0.000117 2.025907
1 -0.218069 -2.074408 0.059459
1 2.376478 -1.189930 -0.566460
1 2.376240 1.189714 -0.566904
1 -0.217920 2.074288 0.061322

N-methylpyrrolidine N-oxide
The number of imaginary frequencies: 0
APFD/aug-cc-pVDZ
Enthalpy= -326.793508853
6 1.589304 0.777796 0.086399
6 1.589429 -0.777691 0.086687
6 0.199576 -1.167377 -0.402643
6 0.199576 1.167034 -0.403601
1 1.787755 1.170543 1.095653
1 1.788462 -1.170027 1.095978
1 0.130996 -1.252875 -1.494831
1 0.131267 1.251498 -1.495891
7 -0.711118 -0.000052 -0.102188
8 -1.817101 -0.000383 -0.838490
6 -1.078865 0.000575 1.343453
1 -1.693654 0.893068 1.502963
1 -1.693458 -0.891899 1.503806
1 -0.199700 0.000991 2.007486
1 -0.233713 -2.070548 0.044126
1 2.368126 -1.192045 -0.570014
1 2.368265 1.192085 -0.570035
1 -0.233833 2.070615 0.042220

N-methylpyrrolidine N-oxide
The number of imaginary frequencies: 0
APFD/aug-cc-pVTZ
Enthalpy= -326.893346480
6 1.583689 0.776507 0.082222
6 1.583959 -0.776276 0.082592
6 0.195638 -1.166252 -0.404176
6 0.195629 1.165640 -0.405808
1 1.779868 1.164568 1.083134
1 1.781225 -1.163802 1.083488
1 0.131965 -1.257010 -1.487102
1 0.132421 1.254540 -1.488921
7 -0.707597 -0.000090 -0.099394
8 -1.821665 -0.000610 -0.832887
6 -1.063806 0.000937 1.345564
1 -1.668754 0.887275 1.514681
1 -1.668737 -0.885172 1.515927
1 -0.180650 0.001392 1.988105
1 -0.230929 -2.060249 0.045229
1 2.355238 -1.185419 -0.570063
1 2.355403 1.185689 -0.569891
1 -0.231199 2.060364 0.041897

N-Methylpyrrole
The number of imaginary frequencies: 0
B3LYP/6-31G**
Enthalpy= -249.488688331
6 1.491542 0.711677 0.016064
6 1.491605 -0.711621 0.016055
6 0.175200 -1.119627 -0.014329
6 0.175126 1.119618 -0.014423
1 2.354859 1.362200 0.022539
1 2.354977 -1.362074 0.022380
1 -0.261470 -2.107877 -0.023476
1 -0.261582 2.107854 -0.023313
7 -0.625375 -0.000019 -0.039882
6 -2.073948 -0.000003 0.026688
1 -2.465245 0.883791 -0.482987
1 -2.464783 -0.886868 -0.477929
1 -2.436274 0.002840 1.061627

N-Methylpyrrole
The number of imaginary frequencies: 0
APFD/aug-cc-pVDZ
Enthalpy= -249.288183211
6 1.489036 0.710705 0.015404
6 1.488925 -0.710786 0.015503
6 0.170288 -1.116176 -0.014162
6 0.170438 1.116181 -0.014125
1 2.356556 1.366817 0.022926
1 2.356410 -1.366932 0.022099
1 -0.271895 -2.109242 -0.022631
1 -0.271591 2.109316 -0.023091
7 -0.623432 0.000002 -0.038810
6 -2.062873 0.000080 0.026085
1 -2.457582 0.887737 -0.486729
1 -2.457117 -0.891483 -0.480206
1 -2.425637 0.003751 1.067072

N-Methylpyrrole
The number of imaginary frequencies: 0
APFD/aug-cc-pVTZ
Enthalpy= -249.356058342
6 1.482743 0.707757 0.014014
6 1.482795 -0.707706 0.014044
6 0.170933 -1.111677 -0.012696
6 0.170896 1.111651 -0.012853
1 2.343550 1.357411 0.020707
1 2.343654 -1.357296 0.020302

1 -0.266361 -2.096940 -0.021290
1 -0.266420 2.096907 -0.021004
7 -0.620071 -0.000019 -0.035081
6 -2.057917 0.000016 0.023689
1 -2.446181 0.881288 -0.485809
1 -2.445715 -0.884811 -0.479914
1 -2.418727 0.003332 1.055381

N-methyl-2-pyrroline
The number of imaginary frequencies: 0
B3LYP/6-31G**
Enthalpy= -250.680844113
6 -1.580164 -0.617095 -0.028381
6 -1.374505 0.875399 0.139141
6 -0.078183 1.152311 -0.057952
6 -0.126568 -1.141239 0.048724
1 -2.221183 -1.073692 0.733501
1 0.400225 2.125893 -0.075806
1 0.069547 -1.998032 -0.603363
7 0.703034 0.017737 -0.334592
6 2.082715 -0.009804 0.113135
1 2.605033 -0.853831 -0.348712
1 2.590996 0.907491 -0.198498
1 2.181199 -0.106315 1.209794
1 -2.167178 1.601922 0.257257
1 -2.031563 -0.845992 -1.005419
1 0.111921 -1.439029 1.085388

N-methyl-2-pyrroline
The number of imaginary frequencies: 0
APFD/aug-cc-pVDZ
Enthalpy= -250.474897760
6 -1.568707 -0.618424 -0.041824
6 -1.373422 0.867641 0.143669
6 -0.075428 1.146756 -0.055101
6 -0.122719 -1.129168 0.063129
1 -2.232117 -1.089974 0.700208
1 0.406399 2.126023 -0.067721
1 0.090651 -2.007614 -0.564609
7 0.697385 0.016705 -0.335908
6 2.068680 -0.009515 0.106068
1 2.586282 -0.873344 -0.338055
1 2.588705 0.899868 -0.229335
1 2.166937 -0.082383 1.211143
1 -2.171183 1.598095 0.266286
1 -1.996673 -0.835249 -1.040073
1 0.108883 -1.396092 1.117864

N-methyl-2-pyrroline
The number of imaginary frequencies: 0
APFD/aug-cc-pVTZ
Enthalpy= -250.545365644
6 -1.566783 -0.615622 -0.040830
6 -1.366675 0.867463 0.140258
6 -0.075913 1.142950 -0.054270
6 -0.124034 -1.129298 0.062163
1 -2.223076 -1.076798 0.699968
1 0.401825 2.114080 -0.065610
1 0.085885 -1.996953 -0.565256
7 0.694942 0.016811 -0.330911
6 2.066120 -0.009751 0.104384
1 2.579776 -0.862289 -0.343329
1 2.577202 0.896919 -0.221821
1 2.162310 -0.089243 1.199546
1 -2.156465 1.592280 0.264383
1 -1.994180 -0.832908 -1.028568
1 0.105839 -1.397218 1.106833

N-methyl-3-pyrroline
The number of imaginary frequencies: 0
B3LYP/6-31G**
Enthalpy= -250.672907553
6 1.528447 -0.666301 -0.042760
6 1.528344 0.666445 -0.042837
6 0.117095 1.191194 0.005632
6 0.117228 -1.191234 0.005572
1 -0.027772 1.988358 0.749633
1 -0.027693 -1.988552 0.749369
7 -0.668125 -0.000121 0.352374
6 -2.037816 -0.000011 -0.113710
1 -2.562067 -0.882936 0.267128
1 -2.561699 0.883243 0.266871
1 -2.131388 -0.000136 -1.218156
1 2.398683 1.311000 -0.099085
1 2.398909 -1.310726 -0.098700
1 -0.164736 -1.623648 -0.977650
1 -0.165147 1.623686 -0.977416

N-methyl-3-pyrroline
The number of imaginary frequencies: 0
APFD/aug-cc-pVDZ
Enthalpy= -250.466571606
6 1.521902 -0.667274 -0.035307
6 1.521939 0.667277 -0.035246
6 0.112892 1.181910 -0.002914
6 0.112879 -1.181905 -0.002892
1 -0.043965 1.994056 0.731027
1 -0.043930 -1.994057 0.731061
7 -0.661297 -0.000001 0.350387
6 -2.024341 0.000009 -0.104413
1 -2.550089 -0.887833 0.280100

1 -2.550051 0.887912 0.280008
1 -2.122706 -0.000046 -1.215231
1 2.398626 1.315138 -0.086399
1 2.398551 -1.315206 -0.086377
1 -0.164501 -1.601313 -1.001119
1 -0.164484 1.601249 -1.001150

N-methyl-3-pyrroline
The number of imaginary frequencies: 0
APFD/aug-cc-pVTZ
Enthalpy= -250.536929435
6 1.518221 -0.662893 -0.036200
6 1.518247 0.662871 -0.036217
6 0.114080 1.180486 -0.001852
6 0.114036 -1.180456 -0.001870
1 -0.039768 1.983059 0.728936
1 -0.039806 -1.983093 0.728869
7 -0.660293 -0.000017 0.348406
6 -2.022204 0.000017 -0.104755
1 -2.543078 -0.881206 0.275184
1 -2.543166 0.881056 0.275492
1 -2.113460 0.000194 -1.206318
1 2.388019 1.304497 -0.087063
1 2.387994 -1.304525 -0.086916
1 -0.164467 -1.595390 -0.990852
1 -0.164497 1.595380 -0.990808

N-methylpyrrolidine
The number of imaginary frequencies: 0
B3LYP/6-31G**
Enthalpy= -251.909652936
6 1.497577 -0.778513 -0.057205
6 1.497372 0.778557 -0.058524
6 0.020846 1.157260 0.162650
6 0.020546 -1.157422 0.161652
1 1.855186 -1.162445 -1.016488
1 1.852351 1.160794 -1.019470
1 -0.174773 1.320605 1.242580
1 -0.176284 -1.322363 1.241118
7 -0.713585 0.000201 -0.346134
6 -2.126797 0.000069 -0.023954
1 -2.324282 -0.001009 1.066758
1 -2.607763 0.885506 -0.452595
1 -2.607865 -0.884463 -0.454333
1 -0.279500 2.069013 -0.365571
1 2.140735 1.200005 0.718830
1 2.139154 -1.198258 0.722541
1 -0.279129 -2.068498 -0.368147

N-methylpyrrolidine
The number of imaginary frequencies: 0
APFD/aug-cc-pVDZ
Enthalpy= -251.695112499

6 1.244938 -0.772727 -0.398674
6 1.244436 0.773124 -0.398851
6 0.070332 1.139457 0.542006
6 0.070461 -1.139704 0.541547
1 1.078591 -1.168279 -1.412898
1 1.076987 1.168300 -1.413042
1 0.444189 1.283586 1.570522
1 0.443966 -1.284497 1.570097
7 -0.842947 -0.000173 0.548978
6 -1.734764 -0.000001 -0.598183
1 -2.384292 -0.887405 -0.557362
1 -2.384301 0.887383 -0.557085
1 -1.224334 0.000150 -1.586110
1 -0.457805 2.060597 0.254965
1 2.196103 1.199785 -0.046899
1 2.196639 -1.198606 -0.045870
1 -0.457536 -2.060693 0.253766

N-methylpyrrolidine
The number of imaginary frequencies: 0
APFD/aug-cc-pVTZ
Enthalpy= -251.767456643
6 1.242315 -0.771295 -0.397569
6 1.241516 0.771955 -0.397780
6 0.069801 1.139314 0.541076
6 0.070235 -1.139596 0.540488
1 1.077140 -1.162833 -1.403038
1 1.074833 1.162985 -1.403207
1 0.440998 1.284660 1.560273
1 0.441155 -1.285562 1.559710
7 -0.839682 -0.000299 0.547297
6 -1.732126 -0.000122 -0.597051
1 -2.374768 -0.881005 -0.556023
1 -2.374482 0.880962 -0.555981
1 -1.220270 -0.000179 -1.573315
1 -0.454804 2.050376 0.250511
1 2.185336 1.192933 -0.047769
1 2.186243 -1.191140 -0.046466
1 -0.454047 -2.050634 0.249240

7-methyl-7-azanorcaradiene
The number of imaginary frequencies: 0
B3LYP/6-31G**
Enthalpy=-326.847852849
6 -0.436335 -0.772082 0.538090
6 -0.436471 0.772316 0.537614
1 0.915223 -2.506512 0.354302
6 0.825961 -1.437596 0.179389

6 0.826126 1.437617 0.179439
6 1.866633 0.726845 -0.309153
6 1.866540 -0.726960 -0.309293
1 0.915317 2.506552 0.354254
1 2.781998 1.236432 -0.598102
1 2.781823 -1.236652 -0.598315
7 -1.129485 -0.000070 -0.496887
6 -2.583903 -0.000008 -0.389471
1 -2.978859 0.887802 -0.893875
1 -2.978971 -0.887530 -0.894316
1 -2.957761 -0.000254 0.649659
1 -1.071784 -1.269090 1.272531
1 -1.071898 1.268947 1.272386

7-methyl-7-azanorcaradiene
The number of imaginary frequencies: 0
APFD/aug-cc-pVDZ
Enthalpy=-326.587401162
6 -0.440908 -0.771702 0.540513
6 -0.441103 0.771773 0.540032
1 0.915933 -2.507708 0.378060
6 0.818491 -1.435448 0.187430
6 0.818462 1.435488 0.187555
6 1.854984 0.725602 -0.315009
6 1.854986 -0.725524 -0.315176
1 0.915700 2.507750 0.378255
1 2.774525 1.239771 -0.607674
1 2.774473 -1.239686 -0.608029
7 -1.113813 -0.000122 -0.493746
6 -2.558149 0.000035 -0.400311
1 -2.951795 0.891930 -0.911486
1 -2.951887 -0.892435 -0.910438
1 -2.943607 0.000631 0.641665
1 -1.088457 -1.270433 1.272807
1 -1.088778 1.269698 1.272864

7-methyl-7-azanorcaradiene
The number of imaginary frequencies: 0
APFD/aug-cc-pVTZ
Enthalpy=-326.673466629
6 -0.436903 -0.768745 0.535988
6 -0.437204 0.768606 0.535592
1 0.913056 -2.492779 0.369844
6 0.818727 -1.428362 0.184642
6 0.818439 1.428441 0.184832
6 1.849643 0.723140 -0.312072
6 1.849784 -0.722830 -0.312262
1 0.912374 2.492856 0.370199
1 2.762042 1.233209 -0.600944
1 2.762210 -1.232713 -0.601385
7 -1.114056 -0.000207 -0.491731
6 -2.556809 0.000055 -0.393940
1 -2.948535 0.885330 -0.898164
1 -2.948769 -0.885248 -0.897951
1 -2.928430 0.000200 0.642626
1 -1.079516 -1.263954 1.260498
1 -1.080095 1.262722 1.260705

7-methyl-7-azanorcaradiene N-oxide
The number of imaginary frequencies: 0
B3LYP/6-31G**
Enthalpy=-401.989673111
6 0.254634 -0.764735 -0.841923
6 0.252136 0.771185 -0.840037
1 -1.028447 -2.509205 -0.492686
6 -0.945139 -1.435976 -0.356914
6 -0.946719 1.438057 -0.350508
6 -1.905222 0.725971 0.283316
6 -1.905061 -0.727865 0.278690
1 -1.030156 2.512205 -0.478847
1 -2.764047 1.235150 0.711207
1 -2.764700 -1.239780 0.701733
7 1.068366 -0.002117 0.237861
6 2.529856 0.001846 0.018614
1 2.925968 0.891977 0.509904
1 2.929522 -0.891087 0.502142
1 2.778608 0.006678 -1.046313
1 0.878737 -1.280348 -1.566656
1 0.877476 1.288921 -1.561995
8 0.713946 -0.006324 1.488632

7-methyl-7-azanorcaradiene N-oxide
The number of imaginary frequencies: 0
APFD/aug-cc-pVDZ
Enthalpy=-401.683840334
6 0.267783 -0.765912 -0.850829
6 0.266149 0.768828 -0.851379
1 -1.024147 -2.511770 -0.522626
6 -0.930445 -1.434678 -0.374622
6 -0.930346 1.435990 -0.371472
6 -1.873434 0.725588 0.290486
6 -1.874281 -0.725756 0.287379
1 -1.023187 2.513828 -0.514689
1 -2.730252 1.239817 0.732943
1 -2.732553 -1.240742 0.726194
7 1.044658 -0.001765 0.246063
6 2.499037 0.001073 0.057002
1 2.886681 0.896917 0.558671
1 2.889451 -0.896205 0.554123
1 2.772801 0.004022 -1.007715
1 0.911605 -1.285576 -1.565411
1 0.911128 1.288788 -1.564505
8 0.659887 -0.003440 1.470147

7-methyl-7-azanorcaradiene N-oxide
The number of imaginary frequencies: 0
APFD/aug-cc-pVTZ
Enthalpy=-401.795253802
6 0.263928 -0.763667 -0.830803
6 0.262819 0.766694 -0.829889
1 -1.020975 -2.497238 -0.498128
6 -0.934220 -1.427234 -0.358865
6 -0.934720 1.428339 -0.355848
6 -1.888396 0.722350 0.276093
6 -1.888491 -0.722963 0.273851
1 -1.021181 2.498858 -0.491328
1 -2.745236 1.233196 0.700001
1 -2.745925 -1.234922 0.695253
7 1.051552 -0.001200 0.238865
6 2.499999 0.000973 0.024261
1 2.896081 0.890650 0.510218
1 2.898170 -0.888494 0.509050
1 2.746718 0.001794 -1.038041
1 0.897166 -1.279772 -1.542379
1 0.897013 1.283080 -1.540378
8 0.693974 -0.003214 1.478860

Benzene
The number of imaginary frequencies: 0
B3LYP/6-31G**
Enthalpy= -232.258203982
6 0.814686 -1.134019 -0.000280
6 -0.574873 -1.272443 0.000166
1 2.470537 0.246283 0.000304
6 1.389539 0.138440 0.000083
6 -1.389553 -0.138436 -0.000008
6 -0.814646 1.134003 -0.000131
6 0.574828 1.272409 0.000062
1 -2.470548 -0.246213 0.000090
1 -1.448104 2.016576 -0.000143
1 1.021853 2.262547 0.000193
1 1.448267 -2.016423 -0.000160
1 -1.021898 -2.262492 0.000362

Benzene
The number of imaginary frequencies: 0
APFD/aug-cc-pVDZ
Enthalpy= -232.065334419
6 1.311421 -0.479269 0.000555
6 0.240609 -1.375214 -0.000334
1 1.909110 1.597376 -0.000326
6 1.070691 0.896171 -0.000158
6 -1.070981 -0.895852 0.000030
6 -1.311271 0.479172 0.000275
6 -0.240382 1.375153 -0.000145
1 -1.908984 -1.597560 -0.000090
1 -2.337620 0.855130 0.000015
1 -0.429291 2.451781 -0.000324
1 2.337521 -0.855853 -0.000059
1 0.428743 -2.451840 -0.000558

Benzene
The number of imaginary frequencies: 0
APFD/aug-cc-pVTZ
Enthalpy= -232.124979909
6 0.746072 -1.171792 -0.000259
6 -0.641901 -1.231916 0.000215
1 2.471100 0.107159 0.000252
6 1.387945 0.060138 0.000090
6 -1.387961 -0.060107 -0.000025
6 -0.746027 1.171770 -0.000111
6 0.641863 1.231872 0.000077
1 -2.471107 -0.107112 -0.000005
1 -1.327926 2.086560 -0.000240
1 1.142586 2.193496 0.000142
1 1.328037 -2.086456 -0.000386
1 -1.142632 -2.193439 0.000322

Trimethylamine
The number of imaginary frequencies: 0
B3LYP/6-31G**
Enthalpy= -169.795990862
6 0.955144 -0.570336 0.000000
1 1.975859 -0.187524 0.000000
1 0.766308 -1.179993 0.889170
1 0.766308 -1.179993 -0.889170
7 -0.000000 0.590677 -0.000000
8 -1.154917 0.229348 -0.000000

Trimethylamine
The number of imaginary frequencies: 0
APFD/aug-cc-pVDZ
Enthalpy= -169.665311125
6 0.946529 -0.566157 0.000000
1 1.974762 -0.185648 0.000000
1 0.754389 -1.180394 0.893556
1 0.754389 -1.180394 -0.893556
7 -0.000000 0.584434 0.000000
8 -1.145339 0.231542 -0.000000

Trimethylamine
The number of imaginary frequencies: 0
APFD/aug-cc-pVTZ
Enthalpy= -169.716346849
6 0.945294 -0.566816 -0.000000
1 1.963677 -0.186875 -0.000000
1 0.755055 -1.174879 0.886696

1	0.755055	-1.174879	-0.886696
7	-0.000000	0.579570	0.000000
8	-1.143194	0.235067	0.000000

Propane

The number of imaginary frequencies: 0
Total Energy (B3LYP/6-31G*)= -119.14424274
ZPE= -119.040122
Enthalpy= -119.034676
Gibb's Free Energy= -119.065764

C	1.27719	-0.25986	0.00002
C	0.	0.5865	0.
H	2.1765	0.36717	0.00003
H	1.32187	-0.90744	0.8847
H	1.3219	-0.90745	-0.88465
C	-1.27719	-0.25986	-0.00002
H	-0.00001	1.24736	0.8776
H	0.00001	1.24735	-0.87762
H	-2.1765	0.36717	-0.00004
H	-1.32187	-0.90745	-0.88469
H	-1.3219	-0.90744	0.88467

Propane

The number of imaginary frequencies: 0
Total Energy (B3LYP/6-31G**)= -119.15535976
ZPE= -119.051645
Enthalpy= -119.046182
Gibb's Free Energy= -119.077296

C	1.27719	-0.25986	0.00002
C	0.	0.5865	0.
H	2.1765	0.36717	0.00003
H	1.32187	-0.90744	0.8847
H	1.3219	-0.90745	-0.88465
C	-1.27719	-0.25986	-0.00002
H	-0.00001	1.24736	0.8776
H	0.00001	1.24735	-0.87762
H	-2.1765	0.36717	-0.00004
H	-1.32187	-0.90745	-0.88469
H	-1.3219	-0.90744	0.88467

Propane

The number of imaginary frequencies: 0
Total Energy (M06/6-311G+(d,p))= -119.06693725
ZPE= -118.964632
Enthalpy= -118.959147
Gibb's Free Energy= -118.990276

C	1.27719	-0.25986	0.00002
C	0.	0.5865	0.
H	2.1765	0.36717	0.00003
H	1.32187	-0.90744	0.8847
H	1.3219	-0.90745	-0.88465
C	-1.27719	-0.25986	-0.00002
H	-0.00001	1.24736	0.8776
H	0.00001	1.24735	-0.87762
H	-2.1765	0.36717	-0.00004
H	-1.32187	-0.90745	-0.88469
H	-1.3219	-0.90744	0.88467