

Supporting Information

Computational Study of Selected Amine and Lactam N-Oxides Including Comparisons of N-O Bond Dissociation Enthalpies with Those of Pyridine N-Oxides

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Cartesian Coordinates (Å) and energies (Hartrees) for all structures.

Quinuclidine

The number of imaginary frequencies: 0

Total Energy (B3LYP/6-31G*)= -329.31071302

ZPE= -329.114741

Enthalpy= -329.107259

N	0	0	
1.29386			
C	1.20023	0.69295	
0.79983			
H	1.19626	1.70683	1.2161
H	2.07629	0.18258	1.2161
C	1.25408	0.72404	-
0.76174			
H	1.27808	1.75683	-
1.13422			
H	2.1605	0.22844	-
1.13422			
C	0	0	-
1.29494			
H	0	0	-
2.39115			
C	0	-1.3859	
0.79983			
H	-0.88003	-1.88941	1.2161
H	0.88003	-1.88941	1.2161
C	0.	-1.44808	-
0.76174			
H	0.88241	-1.98527	-
1.13422			
H	-0.88241	-1.98527	-
1.13422			
C	-1.20023	0.69295	
0.79983			
C	-1.25408	0.72404	-
0.76174			

H	-1.27808	1.75683	-
1.13422			
H	-2.1605	0.22844	-
1.13422			
H	-1.19626	1.70683	1.2161
H	-2.07629	0.18258	1.2161

Quinuclidine

The number of imaginary frequencies: 1 (-100.16 cm⁻¹)

Total Energy (M06/6-311G+(d,p))= -329.13823295

ZPE=-328.945118

Enthalpy=-328.938334

N	0.	0.	
1.29386			
C	1.20023	0.69295	
0.79983			
H	1.19626	1.70683	
1.2161			
H	2.07629	0.18258	
1.2161			
C	1.25408	0.72404	-
0.76174			
H	1.27808	1.75683	-
1.13422			
H	2.1605	0.22844	-
1.13422			
C	0.	0.	-
1.29494			
H	0.	0.	-
2.39115			
C	0.	-1.3859	
0.79983			
H	-0.88003	-1.88941	
1.2161			
H	0.88003	-1.88941	
1.2161			
C	0.	-1.44808	-
0.76174			
H	0.88241	-1.98527	-
1.13422			

H	-0.88241	-1.98527	-
1.13422			
C	-1.20023	0.69295	
0.79983			
C	-1.25408	0.72404	-
0.76174			
H	-1.27808	1.75683	-
1.13422			
H	-2.1605	0.22844	-
1.13422			
H	-1.19626	1.70683	
1.2161			
H	-2.07629	0.18258	
1.2161			

Quinuclidinium

The number of imaginary frequencies: 0
 Total Energy (B3LYP/6-31G*)= -
 329.70138418
 ZPE= -329.489673
 Enthalpy= -329.481994

N	0.	0.	
1.23295			
C	-0.68429	1.27048	
0.75301			
H	-1.67443	1.28443	
1.2142			
H	-0.10465	2.10415	
1.15603			
C	-0.73219	1.25406	-
0.79426			
H	-1.77146	1.25419	-
1.13569			
H	-0.26305	2.16015	-
1.18807			
C	0.	0.	-
1.31307			
H	0.	0.	-
2.40598			
C	1.44241	-0.04263	
0.75301			

H	1.87457	-0.96144	
1.15603			
H	1.94956	0.80788	
1.2142			
C	1.45214	0.00706	-
0.79426			
H	1.97189	0.90703	-
1.13569			
H	2.00227	-0.85227	-
1.18807			
C	-0.75812	-1.22785	
0.75301			
C	-0.71995	-1.26112	-
0.79426			
H	-1.73922	-1.30788	-
1.18807			
H	-0.20043	-2.16122	-
1.13569			
H	-1.76992	-1.1427	
1.15603			
H	-0.27514	-2.09231	
1.2142			
H	0.	0.	
2.25686			

Quinuclidinium

The number of imaginary frequencies: 0
 Total Energy (M06/6-311G+(d,p))= -
 329.52003854
 ZPE= -329.31107
 Enthalpy= -329.303622

N	0.	0.	
1.25297			
C	-1.36295	-0.14344	
0.72939			
H	-1.94822	-0.86846	
1.25542			
H	-1.82127	0.81898	
0.82214			
C	-1.26368	-0.61635	-
0.76063			

H	-1.1531	-1.67669	-
0.85204			
H	-2.15885	-0.31144	-
1.26123			
C	0.	0.	-
1.32633			
H	0.	0.	-
2.39633			
C	0.55726	1.25207	
0.72939			
H	1.61989	1.16778	
0.82214			
H	0.222	2.12144	
1.25542			
C	0.09807	1.40255	-
0.76063			
H	-0.8755	1.83695	-
0.85204			
H	0.80971	2.02534	-
1.26123			
C	0.8057	-1.10863	
0.72939			
C	1.16561	-0.7862	-
0.76063			
H	1.34914	-1.7139	-
1.26123			
H	2.0286	-0.16027	-
0.85204			
H	0.20138	-1.98675	
0.82214			
H	1.72622	-1.25298	
1.25542			
H	0.	0.	
2.25297			

2-Quinuclidone

The number of imaginary frequencies: 0
 Total Energy (B3LYP/6-31G*)= -
 403.32618144
 ZPE= -403.150004
 Enthalpy= -403.141759

N	0.48691	-1.06745	-
0.16205			
C	-0.47643	-0.92982	-
1.2825			
H	0.10416	-0.82594	-
2.20483			
H	-1.01409	-1.88145	-
1.35346			
C	-1.45882	0.26756	-
1.09075			
H	-1.45729	0.91808	-
1.9738			
H	-2.4884	-0.08465	-
0.95483			
C	-1.00067	1.04991	
0.15388			
H	-1.60802	1.95146	
0.28997			
C	-0.26567	-1.15544	
1.11669			
H	0.4551	-1.33621	
1.91978			
H	-0.89881	-2.04654	
1.04599			
C	-1.11731	0.12815	
1.38572			
H	-2.16771	-0.1301	
1.56529			
H	-0.76027	0.65226	
2.2809			
C	1.30668	0.132	-
0.09005			
C	0.48355	1.42132	-
0.03363			
H	0.64315	1.99334	-
0.95814			
H	0.86813	2.03991	
0.78643			
O	2.51097	0.09248	-
0.03314			

2-Quinuclidone

The number of imaginary frequencies: 0
 Total Energy (M06/6-311G+(d,p))= -403.15381144
 ZPE= -402.97944
 Enthalpy= -402.971321

N	0.48691	-1.06745	-
0.16205			
C	-0.47643	-0.92982	-
1.2825			
H	0.10416	-0.82594	-
2.20483			
H	-1.01409	-1.88145	-
1.35346			
C	-1.45882	0.26756	-
1.09075			
H	-1.45729	0.91808	-
1.9738			
H	-2.4884	-0.08465	-
0.95483			
C	-1.00067	1.04991	
0.15388			
H	-1.60802	1.95146	
0.28997			
C	-0.26567	-1.15544	
1.11669			
H	0.4551	-1.33621	
1.91978			
H	-0.89881	-2.04654	
1.04599			
C	-1.11731	0.12815	
1.38572			
H	-2.16771	-0.1301	
1.56529			
H	-0.76027	0.65226	
2.2809			
C	1.30668	0.132	-
0.09005			
C	0.48355	1.42132	-
0.03363			
H	0.64315	1.99334	-
0.95814			

H	0.86813	2.03991
0.78643		
O	2.51097	0.09248
0.03314		

Quinuclidine N-oxide

The number of imaginary frequencies: 0
 Total Energy (B3LYP/6-31G*)= -404.45851715
 ZPE= -404.258001
 Enthalpy= -404.249666

N	0.	0.	-
1.01494			
C	0.	1.41894	-
0.47914			
H	0.88088	1.8794	-
0.92876			
H	-0.88088	1.8794	-
0.92876			
C	0.	1.44852	
1.06897			
H	0.87717	1.98524	
1.44451			
H	-0.87717	1.98524	
1.44451			
C	0.	0.	
1.59707			
H	0.	0.	
2.69282			
C	-1.22884	-0.70947	-
0.47914			
H	-1.18717	-1.70256	-
0.92876			
H	-2.06805	-0.17684	-
0.92876			
C	-1.25445	-0.72426	
1.06897			
H	-2.15786	-0.23297	
1.44451			
H	-1.28069	-1.75228	
1.44451			

C	1.22884	-0.70947	-
0.47914			
C	1.25445	-0.72426	
1.06897			
H	2.15786	-0.23297	
1.44451			
H	1.28069	-1.75228	
1.44451			
H	2.06805	-0.17684	-
0.92876			
H	1.18717	-1.70256	-
0.92876			
O	0.	0.	-
2.36102			

Quinuclidine N-oxide

The number of imaginary frequencies: 1 (-111.32 cm⁻¹)

Total Energy (M06/6-311G+(d,p))= -404.28384052

ZPE= -404.085782

Enthalpy= -404.078242

N	0.	0.	1.01487
C	0.	1.41873	
0.47911			
H	-0.88115	1.87886	
0.92935			
H	0.88115	1.87886	
0.92935			
C	0.	1.44783	-
1.06941			
H	-0.88029	1.98289	-
1.44447			
H	0.88029	1.98289	-
1.44447			
C	0.	0.	-
1.59726			
H	0.	0.	-2.693
C	1.22866	-0.70937	
0.47911			

H	1.18657	-1.70253	
0.92935			
H	2.06772	-0.17633	
0.92935			
C	1.25386	-0.72392	-
1.06941			
H	2.15737	-0.22909	-
1.44447			
H	1.27709	-1.7538	-
1.44447			
C	-1.22866	-0.70937	
0.47911			
C	-1.25386	-0.72392	-
1.06941			
H	-2.15737	-0.22909	-
1.44447			
H	-1.27709	-1.7538	-
1.44447			
H	-2.06772	-0.17633	
0.92935			
H	-1.18657	-1.70253	
0.92935			
O	0.	0.	2.36108

3-Quinuclidone

The number of imaginary frequencies: 0

Total Energy (B3LYP/6-31G*)= -403.32323303

ZPE=-403.146709

Enthalpy=-403.138549

N	1.30151	0.00268	
0.07525			
C	0.85968	-0.73053	-
1.15515			
H	1.13165	-0.15168	-
2.01297			
H	1.31582	-1.69604	-
1.22326			
C	-0.65184	-0.89571	-
1.06607			
C	-1.27006	-0.03722	
0.00742			

H	-2.33603	-0.00599	-
0.07998			
C	0.77916	-0.64701	
1.32271			
H	1.11197	-0.11233	
2.18773			
H	1.14509	-1.64872	
1.4097			
C	-0.788	-0.66465	
1.31416			
H	-1.12774	-1.66884	
1.45939			
H	-1.15377	-0.17529	
2.19259			
C	0.78319	1.34823	-
0.19065			
C	-0.72455	1.3881	
0.07461			
H	-1.15776	2.06744	-
0.62947			
H	-0.9451	1.71401	
1.06963			
H	0.98445	1.50441	-
1.22988			
H	1.24379	2.12251	
0.38662			
O	-1.3034	-1.71942	-
1.75928			

2-Quinuclidone N-oxide

The number of imaginary frequencies: 0

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

478.46497585

ZPE= -478.285174

Enthalpy= -478.275977

N	0.48691	-1.06745	-
0.16205			
C	-0.47643	-0.92982	-
1.2825			
H	0.10416	-0.82594	-
2.20483			
H	-1.01409	-1.88145	-
1.35346			

C	-1.45882	0.26756	-
1.09075			
H	-1.45729	0.91808	-
1.9738			
H	-2.4884	-0.08465	-
0.95483			
C	-1.00067	1.04991	
0.15388			
H	-1.60802	1.95146	
0.28997			
C	-0.26567	-1.15544	
1.11669			
H	0.4551	-1.33621	
1.91978			
H	-0.89881	-2.04654	
1.04599			
C	-1.11731	0.12815	
1.38572			
H	-2.16771	-0.1301	
1.56529			
H	-0.76027	0.65226	
2.2809			
C	1.30668	0.132	-
0.09005			
C	0.48355	1.42132	-
0.03363			
H	0.64315	1.99334	-
0.95814			
H	0.86813	2.03991	
0.78643			
O	2.51097	0.09248	-
0.03314			
O	1.25655	-2.1726	-
0.35145			

2-Quinuclidone N-oxide

The number of imaginary frequencies: 0

Total Energy (M06/6-311G+(d,p))= -

478.28851616

ZPE= -478.110506

Enthalpy= -478.10135

N	-0.67054	-0.6227	-
0.00782			
C	-0.15289	-0.66018	
1.36405			
H	-0.82027	-0.01968	
1.90189			
H	-0.12816	-1.6228	
1.83058			
C	1.29808	-0.06695	
1.34959			
H	1.42597	0.53406	
2.22556			
H	2.02114	-0.85565	
1.34356			
C	1.55511	0.66218	-
0.00696			
H	2.49225	1.17852	
0.00083			
C	0.19732	-1.11255	-
1.09119			
H	-0.24096	-0.70818	-
1.97961			
H	0.25144	-2.1784	-
1.16835			
C	1.61915	-0.5732	-
0.90293			
H	2.22711	-1.26633	-
0.35993			
H	2.0442	-0.40605	-
1.87055			
C	-0.82698	0.83476	-
0.16982			
C	0.44957	1.62091	-
0.43374			
H	0.44611	2.51858	
0.14856			
H	0.56724	1.88245	-
1.46459			
O	-1.94144	1.40318	-
0.03392			

O	-1.86211	-1.26911	-
0.11698			

Manxine

The number of imaginary frequencies: 0

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

447.2362167

ZPE= -446.952794

Enthalpy= -446.942197

N	0.	0.	-1.50549
C	1.25569	-0.70402	-1.34554
H	1.93774	-0.43415	-2.17034
C	2.01641	-0.466	-0.02819
H	2.35145	0.5795	-0.00373
H	2.93968	-1.06269	-0.06589
C	1.29336	-0.78848	1.29027
H	2.02423	-0.60433	2.08954
H	1.0809	-1.86591	1.33775
C	0.	0.	1.66239
H	0.	0.	2.7612
C	0.03616	1.51433	1.29027
C	-0.01814	1.43947	-1.34554
H	-0.59289	1.89521	-2.17034
H	1.00902	1.80214	-1.46403
H	1.05619	-1.77491	-1.46403
H	-0.48875	2.0552	2.08954
H	1.07548	1.86904	1.33775
C	-1.23755	-0.73545	-1.34554
H	-1.34485	-1.46106	-2.17034
H	-2.06521	-0.02723	-1.46403
C	-1.41177	-1.51326	-0.02819
H	-2.39016	-2.01449	-0.06589
H	-0.67386	-2.32616	-0.00373
C	-1.32953	-0.72585	1.29027
H	-1.53548	-1.45087	2.08954
H	-2.15637	-0.00313	1.33775

C	-0.60464	1.97926	-0.02819
H	-0.54952	3.07719	-0.06589
H	-1.67759	1.74666	-0.00373

Manxine

The number of imaginary frequencies: 0
 Total Energy (M06/6-311G+(d,p))= -
 447.00374344
 ZPE= -446.724038
 Enthalpy= -446.713442

N	0.	0.	1.50482
C	-0.4002	1.3839	
1.34423			
H	0.02092	1.98758	
2.16679			
C	0.	2.06906	
0.02447			
H	1.09425	2.15665	-
0.00405			
H	-0.37103	3.10387	
0.06145			
C	-0.48207	1.43455	-
1.29097			
H	-0.14496	2.10557	-
2.09283			
H	-1.58005	1.46555	-
1.33254			
C	0.	0.	-
1.66213			
H	0.	0.	-
2.76084			
C	1.48339	-0.29979	-
1.29097			
C	1.39859	-0.34537	
1.34423			
H	1.71084	-1.01191	
2.16679			
H	1.98365	0.57467	
1.46811			
H	-1.4895	1.43056	
1.46811			

H	1.89596	-0.92725	-
2.09283			
H	2.05923	0.63559	-
1.33254			
C	-0.99839	-1.03853	
1.34423			
H	-1.73176	-0.97567	
2.16679			
H	-0.49415	-2.00522	
1.46811			
C	-1.79186	-1.03453	
0.02447			
H	-2.50252	-1.87326	
0.06145			
H	-2.41484	-0.13068	-
0.00405			
C	-1.00133	-1.13476	-
1.29097			
H	-1.751	-1.17832	-
2.09283			
H	-0.47917	-2.10114	-
1.33254			
C	1.79186	-1.03453	
0.02447			
H	2.87355	-1.23061	
0.06145			
H	1.3206	-2.02597	-
0.00405			

Manxinium

The number of imaginary frequencies: 0
 Total Energy (B3LYP/6-31G*)= -
 447.62559456
 ZPE= -447.326046
 Enthalpy= -447.315473

N	0.	0.	-
1.65093			
C	-1.47473	-0.26177	-
1.30701			
H	-1.83856	-0.89169	-
2.12412			

C	-1.77459	-0.96248
0.01522		
H	-1.31743	-1.95812
0.00671		
H	-2.85495	-1.15186 -
0.02916		
C	-1.47847	-0.26269
1.3514		
H	-1.90479	-0.92023
2.11786		
H	-2.05466	0.66906
1.41891		
C	0.	0.
1.73636		
H	0.	0.
2.8323		
C	0.96673	-1.14905
1.3514		
C	0.96407	-1.14627 -
1.30701		
H	1.69151	-1.14639 -
2.12412		
H	0.37656	-2.0671 -
1.38564		
H	-1.97844	0.70744 -
1.38564		
H	1.74934	-1.18948
2.11786		
H	0.44791	-2.11392
1.41891		
C	0.51066	1.40804 -
1.30701		
H	0.14705	2.03808 -
2.12412		
H	1.60188	1.35966 -
1.38564		
C	0.05377	2.01808
0.01522		
H	0.42993	3.04839 -
0.02916		

H	-1.03707	2.11998
0.00671		
C	0.51174	1.41174 1.3514
H	0.15545	2.10971
2.11786		
H	1.60675	1.44486
1.41891		
C	1.72082	-1.0556
0.01522		
H	2.42502	-1.89653 -
0.02916		
H	2.35449	-0.16187
0.00671		
H	0.	0. -
2.67293		

Manxinium

The number of imaginary frequencies: 0
 Total Energy (M06/6-311G+(d,p))= -447.38206771
 ZPE= -447.08768
 Enthalpy= -447.076867

N	0.	0.
1.65086		
C	-1.29674	0.74867
1.3086		
H	-1.42222	1.46482
2.12604		
C	-1.34158	1.51034 -
0.01308		
H	-0.57486	2.29273 -
0.00362		
H	-2.29413	2.05408
0.03174		
C	-1.29978	0.75429 -
1.35076		
H	-1.47507	1.51965 -
2.11567		
H	-2.15928	0.0753 -
1.42147		

C	0.	0.	-
1.73623			
H	0.	0.	-
2.83218			
C	1.30312	0.7485	-
1.35076			
C	1.29674	0.74867	1.3086
H	1.97968	0.49926	
2.12604			
H	1.06111	1.81232	
1.38802			
H	-2.10007	0.01279	
1.38802			
H	2.05359	0.51762	-
2.11567			
H	1.14485	1.83234	-
1.42147			
C	0.	-1.49734	
1.3086			
H	-0.55747	-1.96409	
2.12604			
H	1.03896	-1.82511	
1.38802			
C	-0.6372	-1.91702	-
0.01308			
H	-0.63182	-3.01381	
0.03174			
H	-1.69813	-1.64421	-
0.00362			
C	-0.00334	-1.50278	-
1.35076			
H	-0.57852	-2.03727	-
2.11567			
H	1.01443	-1.90764	-
1.42147			
C	1.97878	0.40668	-
0.01308			
H	2.92595	0.95973	
0.03174			
H	2.27299	-0.64852	-
0.00362			

H	0.	0.
2.67284		

2-Manxinone

The number of imaginary frequencies: 0
 Total Energy (B3LYP/6-31G*)= -
 521.27190837
 ZPE= -521.006569
 Enthalpy= -520.995563

N	0.80394	-1.29291
0.76415		
C	0.89996	-0.16991
1.69203		
H	1.8352	-0.27835
2.20042		
C	1.00103	1.21541
0.98796		
H	1.79145	1.11764
0.27342		
H	1.25941	1.9053
1.76397		
C	-0.18804	1.90255
0.24047		
H	0.23473	2.82474
0.09973		
H	-0.98355	2.07734
0.93438		
C	-0.82696	1.24119
1.02075		
H	-1.31757	2.02932
1.55278		
C	0.18879	0.63804
2.03208		
C	1.47923	-0.89513
0.44837		
H	0.09331	-0.2046
2.39418		
H	-0.32274	0.54399
2.96716		
H	1.01237	1.31503
2.12321		

C	-0.57773	-1.77244	H	1.42802	-0.41175
0.56656			1.85282		
H	-0.78678	-2.38318	H	0.65544	-1.88546
1.41991			2.39353		
H	-0.62918	-2.35256	C	-0.73939	-0.35062
0.33106			1.82445		
C	-1.68719	-0.70787	H	-0.69949	0.03538
0.5735			2.85163		
H	-2.60424	-1.25118	H	-1.56002	-1.08259
0.66695			1.82982		
H	-1.51059	-0.09666	C	-1.19989	0.84575
1.43381			0.91861		
C	-1.92502	0.23826	H	-1.86629	1.40855
0.62781			1.5871		
H	-2.76453	0.82579	C	-0.13642	1.91422
0.31972			0.51782		
H	-2.16073	-0.33476	C	1.44716	0.42717
1.50015			0.63374		
C	0.69288	-0.76784	H	0.2164	-2.56662
1.72002			0.05129		
H	1.32991	-1.0675	H	-0.65989	2.87473
2.52582			0.4237		
H	-0.15299	-1.41986	H	0.58075	2.0371
1.65453			1.33898		
O	2.7229	-0.70318	C	-0.40468	-0.88734
0.44991			1.70976		
2-Manxinone			H	-0.29501	-1.84493
The number of imaginary frequencies: 0			2.23844		
Total Energy (M06/6-311G+(d,p))= -			H	-0.33479	-0.11343
521.03877972			2.4787		
ZPE= -520.776381			C	-1.78115	-0.85433
Enthalpy= -520.765493			1.03562		
N	0.74085	-0.74859	H	-2.53913	-1.00911
0.81454			1.81615		
C	0.89791	-1.73576	H	-1.86929	-1.71978
0.25992			0.36664		
H	1.91683	-2.1362	C	-2.12954	0.42297
0.25716			0.2565		
C	0.60456	-1.09685	H	-3.13662	0.27149
1.62999			0.15405		

H	-2.22359	1.26574	-
0.95605			
C	0.6687	1.71579	-
0.79817			
H	1.37723	2.54008	-
0.91446			
H	-0.00837	1.72584	-
1.65602			
O	2.55853	0.43064	-
0.11424			

Manxine N-oxide

The number of imaginary frequencies: 0
 Total Energy (B3LYP/6-31G*)= -522.37309036
 ZPE= -522.084864
 Enthalpy= -522.073635

N	0.	0.	
1.49873			
C	1.20619	-0.83645	
1.07701			
H	1.23698	-1.56295	
1.88963			
C	1.21855	-1.58537	-
0.25855			
H	0.39192	-2.30539	-
0.26814			
H	2.12555	-2.20497	-
0.21502			
C	1.24463	-0.83686	-
1.60064			
H	1.37697	-1.6098	-
2.36945			
H	2.14476	-0.21025	-1.662
C	0.	0.	-
1.99638			
H	0.	0.	-
3.09454			
C	-1.34706	-0.65945	-
1.60064			

C	-1.32748	-0.62636	
1.07701			
H	-1.97204	-0.28978	
1.88963			
H	-1.19287	-1.70548	
1.19502			
H	2.07343	-0.18031	
1.19502			
H	-2.08261	-0.38759	-
2.36945			
H	-1.25446	-1.75229	-1.662
C	0.1213	1.46281	
1.07701			
H	0.73506	1.85273	
1.88963			
H	-0.88056	1.8858	
1.19502			
C	0.7637	1.84798	-
0.25855			
H	0.84679	2.94326	-
0.21502			
H	1.80057	1.4921	-
0.26814			
C	0.10243	1.49631	-
1.60064			
H	0.70565	1.99739	-
2.36945			
H	-0.8903	1.96254	-1.662
C	-1.98224	-0.26261	-
0.25855			
H	-2.97234	-0.73829	-
0.21502			
H	-2.19248	0.81328	-
0.26814			
O	0.	0.	
2.87272			

Manxine N-oxide

The number of imaginary frequencies: 0
 Total Energy (M06/6-311G+(d,p))= -522.13655167
 ZPE= -521.850767

Enthalpy= -521.839841

N	0.	0.	
1.49875			
C	0.9879	1.08547	1.0765
H	1.7121	1.02149	
1.88921			
C	1.73182	0.99987	-
0.25914			
H	2.33933	0.08721	-0.269
H	2.46379	1.81892	-
0.21541			
C	0.99256	1.12389	-
1.6009			
H	1.77581	1.15458	-
2.37006			
H	0.48846	2.09794	-
1.66155			
C	0.	0.	-
1.99633			
H	0.	0.	-
3.09449			
C	0.47703	-1.42152	-
1.6009			
C	0.44609	-1.39828	
1.0765			
H	0.02859	-1.99347	
1.88921			
H	1.53255	-1.40871	
1.19477			
H	0.4537	2.03158	
1.19477			
H	0.11199	-2.11518	-
2.37006			
H	1.57264	-1.47199	-
1.66155			
C	-1.43399	0.31281	
1.0765			
H	-1.74069	0.97198	
1.88921			

H	-1.98625	-0.62287	
1.19477			
C	-1.73182	0.99987	-
0.25914			
H	-2.80713	1.22424	-
0.21541			
H	-1.24519	1.98232	-0.269
C	-1.46959	0.29764	-
1.6009			
H	-1.8878	0.96061	-
2.37006			
H	-2.0611	-0.62595	-
1.66155			
C	0.	-1.99974	-
0.25914			
H	0.34334	-3.04316	-
0.21541			
H	-1.09414	-2.06953	-0.269
O	0.	0.	
2.87264			

2-Manxixone N-oxide

The number of imaginary frequencies: 0

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

596.38238012

ZPE= -596.113899

Enthalpy= -596.101871

N	0.74085	-0.74859	-
0.81454			
C	0.89791	-1.73576	
0.25992			
H	1.91683	-2.1362	
0.25716			
C	0.60456	-1.09685	
1.62999			
H	1.42802	-0.41175	
1.85282			
H	0.65544	-1.88546	
2.39353			
C	-0.73939	-0.35062	
1.82445			

H	-0.69949	0.03538
2.85163		
H	-1.56002	-1.08259
1.82982		
C	-1.19989	0.84575
0.91861		
H	-1.86629	1.40855
1.5871		
C	-0.13642	1.91422
0.51782		
C	1.44716	0.42717 -
0.63374		
H	0.2164	-2.56662
0.05129		
H	-0.65989	2.87473
0.4237		
H	0.58075	2.0371
1.33898		
C	-0.40468	-0.88734 -
1.70976		
H	-0.29501	-1.84493 -
2.23844		
H	-0.33479	-0.11343 -
2.4787		
C	-1.78115	-0.85433 -
1.03562		
H	-2.53913	-1.00911 -
1.81615		
H	-1.86929	-1.71978 -
0.36664		
C	-2.12954	0.42297 -
0.2565		
H	-3.13662	0.27149
0.15405		
H	-2.22359	1.26574 -
0.95605		
C	0.6687	1.71579 -
0.79817		
H	1.37723	2.54008 -
0.91446		

H	-0.00837	1.72584 -
1.65602		
O	2.55853	0.43064 -
0.11424		
O	1.60399	-1.26199 -
1.73161		

2-Manxinone N-oxide

The number of imaginary frequencies: 0
 Total Energy (M06/6-311G+(d,p))= -596.1437104
 ZPE= -595.878736
 Enthalpy= -595.866701

N	-1.24978	0.5571 -
0.06119		
C	-1.0225	0.60808
1.44275		
H	-1.99614	0.32254
1.84006		
C	0.05112	-0.3461
1.99545		
H	-0.32017	-1.3668
1.87142		
H	0.05636	-0.17325
3.08038		
C	1.53125	-0.29909
1.54263		
H	2.01883	-1.0936
2.12246		
H	1.99359	0.63328
1.89433		
C	1.95887	-0.50255
0.05467		
H	2.98751	-0.87854 0.134
C	1.22857	-1.61459 -
0.74767		
C	-1.13324	-0.89156 -
0.51665		
H	-0.84036	1.65658
1.69348		
H	1.93006	-1.98733 -
1.50431		

H	-2.90544	0.61422	-
0.75916			
H	-1.65387	0.9151	-
1.97202			
C	-1.68767	-1.0849	-
1.07333			
H	-1.94986	-1.47322	-
0.11137			
H	-2.34727	-1.47227	-
1.82151			
C	-0.3001	-1.55212	-
1.39156			
H	-0.19954	-2.61501	-
1.32036			
H	0.03026	-1.25867	-
2.36606			
O	2.99053	0.44946	
1.17046			

4-Manxinone

The number of imaginary frequencies: 0

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

521.25239348

ZPE=-520.988551

Enthalpy=-520.977154

N	0.13307	0.84165	
0.50607			
C	1.36254	1.48787	
0.15671			
H	1.25326	2.5441	
0.02506			
H	2.0895	1.31269	
0.92205			
C	1.79716	0.75911	-
1.05743			
H	1.17199	0.90246	-
1.91388			
H	2.7932	1.04175	-
1.32746			
C	1.69686	-0.65932	-
0.51302			
C	0.63667	-1.70843	-
0.91479			

H	1.01328	-2.62704	-
0.51578			
H	0.60213	-1.73605	-
1.98388			
C	-0.89826	-1.59071	-
0.47035			
H	-1.30093	-2.5581	-
0.68694			
C	-0.95111	1.47758	-
0.19979			
H	-0.7682	2.53162	-
0.22076			
H	-1.89441	1.29298	
0.27033			
C	-1.00267	0.87996	-
1.55531			
H	-1.64869	1.45303	-
2.1871			
H	-0.01717	0.86828	-
1.97191			
C	-1.60079	-0.55925	-
1.44664			
H	-1.54726	-0.96554	-
2.43505			
H	-2.61817	-0.48052	-
1.12472			
C	-1.30617	-1.36232	
1.11913			
H	-2.30158	-1.7457	
1.20327			
H	-0.6146	-1.9441	
1.69199			
C	-1.43609	0.08983	
1.79697			
H	-2.15519	0.64393	
1.23061			
H	-1.77434	-0.03232	
2.80473			
C	-0.16503	0.87779	
1.82821			

H	-0.30211	1.87002
2.20449		
H	0.59122	0.40416
2.41868		
O	2.55263	-1.00715
0.34152		

1-azabicyclo[3.3.2]decane

The number of imaginary frequencies: 0
 Total Energy (B3LYP/6-31G*)= -
 407.93010375
 ZPE= -407.675878
 Enthalpy= -407.666305

N	-0.05842	-1.37398
0.34609		
C	-0.3559	-0.68727
1.60074		
H	-1.3261	-1.05222
1.96471		
H	0.38935	-1.01717
2.33487		
C	-0.37665	0.88213
1.55362		
H	-1.38404	1.24663
1.80098		
H	0.28604	1.27426
2.33829		
C	-1.10299	-1.34353
0.68607		
H	-1.85267	-2.12557
0.48037		
H	-0.63588	-1.60455
1.64365		
C	-1.85207	0.00369
0.81651		
H	-2.52528	-0.05781
1.68409		
H	-2.50623	0.1239
0.05808		
C	-0.96944	1.26364
0.94962		

H	-1.64785	2.12633	-
1.00527			
H	-0.43759	1.24219	-
1.91101			
C	0.05511	1.51573	
0.20652			
H	0.04755	2.60142	
0.39143			
C	1.52958	1.19307	-
0.18258			
H	1.88833	1.99868	-
0.84006			
H	2.14566	1.24727	
0.7286			
C	1.7907	-0.14637	-
0.89417			
H	2.86552	-0.23568	-1.113
H	1.28597	-0.14617	-
1.87016			
C	1.3388	-1.38555	-0.0966
H	1.96294	-1.49142	
0.80121			
H	1.51049	-2.28541	-
0.70523			

1-azabicyclo[3.3.2]decane

The number of imaginary frequencies: 0
 Total Energy (M06/6-311G+(d,p))= -
 407.7174344
 ZPE= -407.466218
 Enthalpy= -407.456724

N	-0.52936	-1.46194
0.32938		
C	-0.4999	-0.61958
1.55951		
H	-1.39445	-0.78368
2.12321		
H	0.35748	-0.97772
2.09012		
C	-0.37276	0.94423
1.43441		

H	-1.32872	1.38712
1.24763		
H	0.00706	1.25658
2.38471		
C	-1.39231	-0.97358 -
0.75987		
H	-2.38026	-1.34752 -
0.58949		
H	-0.99921	-1.36158 -
1.67629		
C	-1.57078	0.55579 -
0.84377		
H	-2.17852	0.7321 -
1.70659		
H	-2.08256	0.83049
0.05486		
C	-0.37379	1.54878 -
0.93761		
H	-0.85206	2.50592 -
0.93125		
H	0.21792	1.44221 -
1.82272		
C	0.53225	1.46668
0.30102		
H	0.87689	2.45012
0.54382		
C	1.80044	0.67089
0.00631		
H	2.42413	1.30108 -
0.59266		
H	2.30039	0.42148
0.91886		
C	1.54487	-0.56127 -
0.84054		
H	2.49826	-0.94095 -
1.14351		
H	0.9731	-0.26693 -
1.69573		
C	0.8403	-1.69016 -
0.14503		

H	1.42899	-1.97921
0.70043		
H	0.78724	-2.48654 -
0.85767		

1-azabicyclo[3.3.2]decanium

The number of imaginary frequencies: 0

Total Energy (B3LYP/6-31G*)= -408.32021719

ZPE= -408.049901

Enthalpy= -408.040259

N	-0.13461	-1.46116
0.25103		
C	-0.45336	-0.75998
1.5659		
H	-1.48185	-1.04842
1.79589		
H	0.19091	-1.24937
2.30072		
C	-0.27534	0.77838
1.60733		
H	-1.21734	1.20183
1.97221		
H	0.47155	1.00497
2.3749		
C	-1.13751	-1.17567 -
0.88011		
H	-1.8914	-1.96441 -
0.81055		
H	-0.59359	-1.31636 -
1.81601		
C	-1.81961	0.18839 -
0.80598		
H	-2.49203	0.22285 -
1.67202		
H	-2.47889	0.20793
0.06955		
C	-0.92954	1.44154 -
0.81253		
H	-1.60744	2.29785 -
0.72944		

H	-0.4409	1.54941	-	C	-0.27496	0.74301	
1.78855				1.58603			
C	0.13278	1.52877		H	-1.07641	1.20627	
0.31927				2.12266			
H	0.17684	2.57926		H	0.62385	0.74792	
0.62952				2.16656			
C	1.56726	1.19241	-	C	-0.86461	-1.25443	-
0.14847				0.94671			
H	1.91299	1.99894	-	H	-1.65843	-1.97118	-
0.80538				0.9787			
H	2.23716	1.20336		H	-0.23727	-1.36177	-
0.72201				1.80684			
C	1.74233	-0.1234	-	C	-1.6354	0.10511	-
0.91218				0.88284			
H	2.80232	-0.25826	-	H	-2.24253	0.15385	-
1.1601				1.76256			
H	1.22535	-0.07998	-	H	-2.2332	0.02185	-
1.87719				0.00068			
C	1.33692	-1.38574	-	C	-0.95169	1.48489	-
0.16662				0.77639			
H	1.90929	-1.51004		H	-1.75491	2.16005	-
0.7576				0.56684			
H	1.50335	-2.26801	-	H	-0.46429	1.76065	-
0.79192				1.68815			
H	-0.2677	-2.45168		C	0.08232	1.58778	
0.47184				0.34036			
				H	0.16837	2.61287	
				0.6348			
				C	1.47794	1.22474	-
				0.1597			
				H	1.74693	1.95704	-
				0.89202			
				H	2.1402	1.27065	
				0.67946			
				C	1.6508	-0.10168	-0.8213
				H	2.67967	-0.15937	-
				1.10942			
				H	1.01956	-0.14949	-
				1.68394			
				C	1.35389	-1.30913	
				0.04248			

1-azabicyclo[3.3.2]decanium
The number of imaginary frequencies: 0
Total Energy (M06/6-311G+(d,p))= -408.09697078
ZPE= -407.830573
Enthalpy= -407.820844

N	-0.07348	-1.5252	0.2807				
C	-0.72639	-0.75417					
1.37326							
H	-1.76988	-0.79575					
1.14025							
H	-0.52932	-1.22082					
2.31576							

H	1.88252	-1.26662
0.9718		
H	1.68862	-2.1465 -
0.53342		
H	-0.14051	-2.4999
0.49394		

1-azabicyclo[3.3.2]decan-9-one

The number of imaginary frequencies: 0
 Total Energy (B3LYP/6-31G*)= -
 481.95525515
 ZPE= -481.719565
 Enthalpy= -481.709548

N	-0.64665	-0.90237 -
0.70347		
C	-1.25312	0.36241 -
0.78479		
C	-0.29365	1.53804 -
0.82058		
H	0.28174	1.60644 -
1.75096		
H	-0.89531	2.44653 -
0.73537		
C	0.66184	-1.1245 -
1.32772		
C	1.91883	-0.76492 -
0.51327		
H	2.00177	-1.46061
0.32708		
H	2.79206	-0.97122 -
1.14713		
C	1.99631	0.69356 -
0.01215		
H	2.43733	1.31653 -
0.80264		
H	2.69952	0.73973
0.83051		
C	0.66862	1.36927
0.40102		
H	0.94065	2.38957
0.70331		

C	-0.03103	0.74623
1.65421		
H	0.54075	1.06507
2.5354		
H	-1.01933	1.21329
1.75497		
C	-0.18143	-0.7973
1.77078		
H	-0.7356	-1.00458
2.69614		
H	0.81079	-1.23395
1.92366		
C	-0.90707	-1.52493
0.6034		
H	-1.98829	-1.49568
0.75107		
H	-0.60778	-2.57875
0.56292		
H	0.71204	-2.18982 -
1.58887		
H	0.66025	-0.58328 -
2.28011		
O	-2.44749	0.50876 -
0.58513		

1-azabicyclo[3.3.2]decan-2-one

The number of imaginary frequencies: 0
 Total Energy (B3LYP/6-31G*)= -
 481.96668910
 ZPE= -481.730531
 Enthalpy= -481.720529

N	0.75111	0.30232
0.97785		
C	-0.37335	-0.1788
1.78213		
H	-0.03898	-1.06612
2.32769		
H	-0.55822	0.58449
2.54416		
C	-1.68016	-0.48331
0.99357		
H	-2.02513	-1.49614
1.2406		

H	-2.47706	0.19596	
1.32084			
C	1.40207	-0.55281	
0.09792			
C	0.6543	-1.82965	-
0.24261			
H	1.3266	-2.48366	-
0.80306			
H	0.30967	-2.37534	
0.64158			
C	-0.56104	-1.42747	-
1.12743			
H	-1.13091	-2.34228	-
1.33273			
H	-0.18075	-1.07842	-
2.09565			
C	-1.5359	-0.3608	-0.5367
H	-2.52639	-0.61541	-
0.93877			
C	-1.3267	1.11496	-
0.99936			
H	-1.60046	1.16847	-
2.0619			
H	-2.08156	1.71604	-
0.47013			
C	0.04918	1.79951	-
0.85661			
H	-0.05811	2.85729	-
1.13317			
H	0.75069	1.36739	-
1.57807			
C	0.7002	1.70442	
0.53332			
H	1.71484	2.10969	
0.49977			
H	0.13635	2.26997	
1.28309			
O	2.40126	-0.20557	-
0.51931			

The number of imaginary frequencies: 0
 Total Energy (B3LYP/6-31G*)= -
 483.07072469
 ZPE= -482.811552
 Enthalpy= -482.801294

N	1.31918	0.03295	
0.05803			
C	0.74654	-0.33449	
1.41918			
H	1.21536	-1.29829	
1.62283			
H	1.23556	0.38861	
2.07258			
C	-0.78765	-0.37766	
1.65538			
H	-1.04452	-1.37771	
2.02746			
H	-1.02292	0.3117	
2.47575			
C	0.94869	-0.99324	-
1.01594			
H	1.81735	-1.65073	-
0.99387			
H	0.95832	-0.46099	-
1.97097			
C	-0.32944	-1.81242	-
0.81966			
H	-0.39466	-2.48664	-
1.68466			
H	-0.18921	-2.47136	
0.04626			
C	-1.67247	-1.07911	-
0.66782			
H	-2.4342	-1.85084	-
0.49923			
H	-1.94853	-0.59577	-
1.61411			
C	-1.74556	-0.04528	
0.49069			
H	-2.75123	-0.12558	
0.92491			

1-azabicyclo[3.3.2]decane N-oxide

C	-1.62585	1.41793
0.01189		
H	-2.54997	1.68447 -
0.51872		
H	-1.57955	2.07481
0.89244		
C	-0.44675	1.72029 -
0.91491		
H	-0.46769	2.78648 -
1.17885		
H	-0.57478	1.18676 -
1.86479		
C	0.94565	1.4495 -
0.35461		
H	1.15461	2.05543
0.53114		
H	1.71384	1.67808 -
1.09519		
O	2.67861	0.03098
0.19946		

1-azabicyclo[3.3.2]decane N-oxide

The number of imaginary frequencies: 0

Total Energy (M06/6-311G+(d,p))= -482.85412341

ZPE= -482.598276

Enthalpy= -482.587988

N	1.30842	0.004
0.08824		
C	0.69696	-0.68948
1.25429		
H	0.76374	-1.72897
1.00956		
H	1.25534	-0.47187
2.14071		
C	-0.78766	-0.31392
1.63571		
H	-1.1482	-1.13891
2.21389		
H	-0.77222	0.58198
2.22055		
C	0.94203	-0.79639 -
1.10794		

H	1.68902	-1.55336 -
1.22584		
H	0.92187	-0.16219 -
1.9695		
C	-0.36228	-1.63425 -
0.89979		
H	-0.47866	-2.24072 -
1.7736		
H	-0.1518	-2.2295 -
0.03592		
C	-1.75366	-1.02055 -
0.63516		
H	-2.36086	-1.85702 -
0.35851		
H	-2.1529	-0.54511 -
1.50663		
C	-1.78244	0.00406
0.49454		
H	-2.77136	0.03805
0.9017		
C	-1.5466	1.41738 -
0.03129		
H	-2.36824	1.65144 -
0.67552		
H	-1.53139	2.07429
0.81318		
C	-0.31223	1.658 -
0.83467		
H	-0.33778	2.68922 -
1.11897		
H	-0.32968	1.03222 -
1.70243		
C	0.99705	1.41943 -
0.11279		
H	1.03225	1.94282
0.8198		
H	1.74757	1.79707 -
0.77537		
O	2.66092	-0.02165
0.22849		

1-azabicyclo[3.3.2]decan-3-one

The number of imaginary frequencies: 0
 Total Energy (B3LYP/6-31G*)= -
 481.94228995
 ZPE=-481.707444
 Enthalpy=-481.697043

N	0.24784	-1.47809	-
0.31408			
C	1.17167	-0.86629	-
1.26571			
H	2.11432	-1.42711	-
1.23859			
H	0.73918	-1.06019	-
2.25151			
C	1.48243	0.65839	-
1.14241			
H	2.45905	0.79972	-
0.66385			
H	1.59402	1.05998	-
2.15674			
C	0.56511	-1.35699	
1.11992			
H	1.22911	-2.18769	
1.39502			
H	-0.36706	-1.5106	
1.66795			
C	1.23323	-0.05509	
1.59846			
H	1.25111	-0.09693	
2.69428			
H	2.28811	-0.07247	
1.29337			
C	0.62108	1.29167	
1.17111			
H	1.29209	2.07446	
1.54082			
H	-0.33953	1.44781	
1.67114			
C	0.45468	1.49011	-
0.36009			
H	0.66203	2.54228	-
0.58139			

C	-1.01375	1.27641	-
0.84073			
H	-1.60925	2.15207	-
0.57353			
H	-1.01842	1.17355	-
1.93246			
C	-1.64919	0.07406	-
0.17194			
C	-1.1787	-1.29218	-
0.63867			
H	-1.29072	-1.40978	-
1.72078			
H	-1.76825	-2.06403	-
0.13861			
O	-2.38626	0.20063	
0.79672			

1-azabicyclo[3.3.2]decan-4-one

The number of imaginary frequencies: 0
 Total Energy (B3LYP/6-31G*)= -
 481.94313071
 ZPE=-481.708072
 Enthalpy=-481.697750

N	-0.0826	-1.58292	
0.37087			
C	-0.29758	-0.71919	
1.60982			
H	-1.10194	-1.13067	
2.18305			
H	0.63033	-0.80009	
2.13646			
C	-0.64134	0.84077	
1.47387			
H	-1.67873	1.0048	
1.26937			
H	-0.38122	1.26562	
2.42084			
C	-1.08122	-1.3715	-
0.68321			
H	-1.9297	-1.98672	-
0.46761			

H	-0.63077	-1.66776	-	N	0.91829	0.62851	-
1.60745				1.05199			
C	-1.6537	0.05566	-	C	-0.43599	0.42223	-
0.78895				1.51024			
H	-2.29464	0.04806	-	H	-0.87374	1.37496	-
1.64572				1.83875			
H	-2.2113	0.21472		H	-0.42279	-0.2177	-
0.11031				2.40303			
C	-0.74324	1.31174	-	C	-1.43948	-0.21465	-
0.91985				0.52415			
H	-1.43988	2.12226	-	C	1.08582	1.66587	-
0.97144				0.03367			
H	-0.12279	1.30884	-	H	1.17969	2.64655	-
1.7916				0.52689			
C	0.11968	1.51996		H	2.04107	1.48595	
0.34057				0.47312			
H	0.23456	2.57344		C	-0.04653	1.78292	
0.48848				1.0095			
C	1.4771	0.93282		H	0.25644	2.53191	
0.21238				1.75346			
C	1.5912	-0.11669	-	H	-0.93502	2.20465	
0.83308				0.51906			
H	2.58411	-0.12069	-	C	-0.45921	0.49092	
1.23183				1.74019			
H	0.89392	0.07704	-	H	-1.28743	0.75039	
1.62122				2.40968			
C	1.29119	-1.44075	-	H	0.35756	0.15303	
0.20806				2.39076			
H	1.99911	-1.60948		C	-0.92299	-0.69416	
0.57634				0.83545			
H	1.39826	-2.18361	-	H	-1.79953	-1.15637	
0.97069				1.30094			
O	2.45266	1.30699		C	0.13885	-1.82149	
0.9137				0.67977			
				H	0.14882	-2.38479	
				1.62213			
				H	-0.2094	-2.52876	-
				0.08682			
				C	1.57648	-1.38693	
				0.36854			

1-azabicyclo[3.3.2]decan-10-one
The number of imaginary frequencies: 0
Total Energy (B3LYP/6-31G*)= -
481.94671758
ZPE=-481.711904
Enthalpy=-481.701618

H	2.21065	-2.28182	
0.29874			
H	1.9744	-0.80884	
1.21283			
C	1.74347	-0.56698	-
0.92313			
H	1.5258	-1.20351	-
1.79129			
H	2.79798	-0.27118	-
1.01586			
O	-2.60439	-0.34506	-
0.85096			

1-azabicyclo[4.3.3]dodecane
The number of imaginary frequencies: 0
Total Energy (B3LYP/6-31G*)= -486.54115606
ZPE= -486.229503
Enthalpy= -486.217542

N	0.40679	-1.27086	-
0.05346			
C	1.83246	-1.13866	-
0.25423			
H	2.39188	-1.84521	
0.38658			
H	2.06027	-1.4182	-
1.29071			
C	2.35452	0.29	-0.01702
H	2.35545	0.52346	
1.05516			
H	3.40984	0.31516	-
0.32642			
C	1.57118	1.36919	-
0.79145			
H	2.27703	2.17634	-
1.03055			
H	1.26307	0.96079	-
1.76375			
C	0.36878	2.07362	-0.116
H	0.21612	2.99005	-
0.70364			

H	0.68691	2.42642	
0.8765			
C	-1.05047	1.43197	
0.02848			
H	-1.69801	2.32043	
0.05674			
C	-0.06841	-1.48695	
1.29817			
H	0.66282	-2.0887	
1.86652			
H	-0.98842	-2.08664	
1.25747			
C	-0.34699	-0.18671	
2.06502			
H	-0.72789	-0.44805	
3.06388			
H	0.59997	0.33816	
2.23842			
C	-1.34869	0.78041	
1.41252			
H	-1.47394	1.61011	
2.12229			
H	-2.33552	0.29767	
1.36407			
C	-1.56258	0.66008	-
1.23628			
H	-2.54507	1.07838	-
1.49246			
H	-0.91708	0.90467	-
2.09112			
C	-1.75255	-0.86685	-
1.18859			
H	-2.38858	-1.13411	-
0.33472			
H	-2.31736	-1.17643	-
2.07995			
C	-0.45636	-1.68445	-
1.13898			
H	-0.71388	-2.76253	-
1.09212			

H	0.08954	-1.53569	-	H	-0.98842	-2.08664	
2.07775				1.25747			
1-azabicyclo[4.3.3]dodecane				C	-0.34699	-0.18671	
The number of imaginary frequencies: 0				2.06502			
Total Energy (M06/6-311G+(d,p))= -				H	-0.72789	-0.44805	
486.28835181				3.06388			
ZPE= -485.980448				H	0.59997	0.33816	
Enthalpy= -485.96858				2.23842			
N	0.40679	-1.27086	-	C	-1.34869	0.78041	
0.05346				1.41252			
C	1.83246	-1.13866	-	H	-1.47394	1.61011	
0.25423				2.12229			
H	2.39188	-1.84521		H	-2.33552	0.29767	
0.38658				1.36407			
H	2.06027	-1.4182	-	C	-1.56258	0.66008	-
1.29071				1.23628			
C	2.35452	0.29	-0.01702	H	-2.54507	1.07838	-
				1.49246			
H	2.35545	0.52346		H	-0.91708	0.90467	-
1.05516				2.09112			
H	3.40984	0.31516	-	C	-1.75255	-0.86685	-
0.32642				1.18859			
C	1.57118	1.36919	-	H	-2.38858	-1.13411	-
0.79145				0.33472			
H	2.27703	2.17634	-	H	-2.31736	-1.17643	-
1.03055				2.07995			
H	1.26307	0.96079	-	C	-0.45636	-1.68445	-
1.76375				1.13898			
C	0.36878	2.07362	-0.116	H	-0.71388	-2.76253	-
				1.09212			
H	0.21612	2.99005	-	H	0.08954	-1.53569	-
0.70364				2.07775			
H	0.68691	2.42642		1-azabicyclo[4.3.3]dodecanium			
0.8765				The number of imaginary frequencies: 0			
C	-1.05047	1.43197		Total Energy (B3LYP/6-31G*)= -			
0.02848				486.92192592			
H	-1.69801	2.32043		ZPE= -486.593438			
0.05674				Enthalpy= -486.581482			
C	-0.06841	-1.48695		C	1.84633	-1.23573	-
1.29817				0.18455			
H	0.66282	-2.0887					
1.86652							

H	1.09012	2.98158	-
0.31585			
C	-0.60595	1.92852	-
0.9109			
H	-0.96681	2.92533	-
1.05601			
H	-0.3363	1.48455	-
1.84635			
C	-1.82119	1.24406	-
0.26227			
H	-2.57472	1.3084	-
1.01921			
H	-2.06182	1.84388	
0.59049			
C	-1.9164	-0.2029	
0.25507			
H	-2.95983	-0.31354	
0.46461			
C	1.56765	-0.73906	
1.12268			
H	2.42599	-0.36278	
1.63899			
H	1.49359	-1.79984	
1.24163			
C	0.34629	-0.02957	
1.81751			
H	0.50713	-0.19674	
2.86207			
H	0.41805	1.00954	
1.57256			
C	-1.15811	-0.45378	
1.60263			
H	-1.69019	0.13306	
2.32193			
H	-1.23925	-1.49861	
1.81862			
C	-1.6368	-1.25653	-
0.78055			
H	-2.27403	-2.07691	-
0.52403			

H	-1.89911	-0.85136	-
1.7355			
C	-0.28628	-1.91709	-
0.83241			
H	-0.12022	-2.32706	
0.14189			
H	-0.42554	-2.68241	-
1.56712			
C	1.03339	-1.27958	-
1.22358			
H	1.65295	-2.14687	-
1.31774			
H	0.94039	-0.7651	-
2.15715			
N	1.79987	-0.4185	-
0.29204			
H	2.73681	-0.65992	-
0.54477			

1-azabicyclo[4.3.3]dodecan-2-one

The number of imaginary frequencies: 0

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

560.58172753

ZPE= -560.287041

Enthalpy= -560.274841

N	0.58545	0.75154	
0.86174			
C	1.71539	0.32954	
0.20676			
C	2.0561	-1.15378	0.2463
H	2.98249	-1.23669	-
0.32614			
H	2.27506	-1.51172	
1.25936			
C	0.93787	-2.02143	-
0.40669			
H	1.43826	-2.8479	-
0.92418			
H	0.33681	-2.49844	
0.37254			
C	0.01111	-1.30791	-
1.43311			

H	-0.19837	-2.04371	-
2.21798			
H	0.58687	-0.52061	-
1.93232			
C	-1.39014	-0.73444	-
0.98023			
H	-2.10244	-1.24003	-
1.64569			
C	-0.00797	2.00809	
0.39372			
C	-0.5696	1.86102	-
1.02942			
H	-1.00334	2.82777	-
1.3215			
H	0.28457	1.70555	-
1.69468			
C	-1.63889	0.77813	-
1.29626			
H	-1.85544	0.8486	-
2.37095			
H	-2.57735	1.06529	-
0.79887			
C	-1.90333	-1.15059	
0.42704			
H	-2.99982	-1.17723	
0.36486			
H	-1.60875	-2.18752	
0.63085			
C	-1.57375	-0.27368	
1.6451			
H	-2.11206	0.67786	
1.55733			
H	-1.98584	-0.75677	
2.54191			
C	-0.09545	0.01835	1.925
H	-0.02803	0.60553	
2.85426			
H	0.44476	-0.91148	
2.11003			
H	0.75997	2.78747	
0.39464			

H	-0.78422	2.30498	
1.10545			
O	2.35009	1.09107	-
0.52255			

1-azabicyclo[4.3.3]dodecan-9-one

The number of imaginary frequencies: 0

Total Energy (B3LYP/6-31G*)= -560.56902632

ZPE= -560.275236

Enthalpy= -560.262784

N	-0.59816	-1.12485	-
0.31735			
C	0.49517	-2.08473	-
0.16122			
H	0.19976	-2.8482	
0.56938			
H	0.56687	-2.60949	-
1.1208			
C	1.89485	-1.55044	
0.20635			
H	1.98959	-1.43017	
1.2928			
H	2.60505	-2.34588	-
0.0588			
C	2.31371	-0.24138	-
0.48085			
H	3.40539	-0.26492	-
0.59565			
H	1.91763	-0.20702	-
1.5042			
C	1.99816	1.07716	
0.25586			
H	2.6395	1.83519	-
0.21491			
H	2.36504	0.9928	
1.28998			
C	0.56934	1.69873	
0.28875			
H	0.79031	2.75564	
0.49801			

C	-1.8688	0.51282	-1.0041
H	-2.90544	0.61422	-
0.75916			
H	-1.65387	0.9151	-
1.97202			
C	-1.68767	-1.0849	-
1.07333			
H	-1.94986	-1.47322	-
0.11137			
H	-2.34727	-1.47227	-
1.82151			
C	-0.3001	-1.55212	-
1.39156			
H	-0.19954	-2.61501	-
1.32036			
H	0.03026	-1.25867	-
2.36606			
O	2.99053	0.44946	
1.17046			

1-azabicyclo[4.3.3]dodecan-4-one

The number of imaginary frequencies: 0

Total Energy (B3LYP/6-31G*)= -560.55977731

ZPE=-560.266952

Enthalpy=-560.254458

N	0.13307	0.84165	
0.50607			
C	1.36254	1.48787	
0.15671			
H	1.25326	2.5441	
0.02506			
H	2.0895	1.31269	
0.92205			
C	1.79716	0.75911	-
1.05743			
H	1.17199	0.90246	-
1.91388			
H	2.7932	1.04175	-
1.32746			
C	1.69686	-0.65932	-
0.51302			

C	0.63667	-1.70843	-
0.91479			
H	1.01328	-2.62704	-
0.51578			
H	0.60213	-1.73605	-
1.98388			
C	-0.89826	-1.59071	-
0.47035			
H	-1.30093	-2.5581	-
0.68694			
C	-0.95111	1.47758	-
0.19979			
H	-0.7682	2.53162	-
0.22076			
H	-1.89441	1.29298	
0.27033			
C	-1.00267	0.87996	-
1.55531			
H	-1.64869	1.45303	-
2.1871			
H	-0.01717	0.86828	-
1.97191			
C	-1.60079	-0.55925	-
1.44664			
H	-1.54726	-0.96554	-
2.43505			
H	-2.61817	-0.48052	-
1.12472			
C	-1.30617	-1.36232	
1.11913			
H	-2.30158	-1.7457	
1.20327			
H	-0.6146	-1.9441	
1.69199			
C	-1.43609	0.08983	
1.79697			
H	-2.15519	0.64393	
1.23061			
H	-1.77434	-0.03232	
2.80473			

C	-0.16503	0.87779
1.82821		
H	-0.30211	1.87002
2.20449		
H	0.59122	0.40416
2.41868		
O	2.55263	-1.00715
0.34152		

1-azabicyclo[4.3.3]dodecan-5-one

The number of imaginary frequencies: 0
 Total Energy (B3LYP/6-31G*)= -
 560.56282261
 ZPE=-560.269812
 Enthalpy=-560.257410

N	-0.01198	-1.25805	0.4156
C	1.36702	-1.73336	
0.42617			
H	1.65876	-2.02261	
1.44535			
H	1.43343	-2.64799	-
0.17885			
C	2.3722	-0.69004	-
0.12563			
H	2.75784	-0.05497	
0.67964			
H	3.23677	-1.20847	-
0.5599			
C	1.72796	0.24115	-
1.17688			
H	2.52596	0.78952	-
1.69202			
H	1.17885	-0.33393	-
1.92661			
C	0.8708	1.29835	-
0.47507			
C	-0.65876	1.42543	-
0.59741			
H	-0.77258	2.43644	-
1.01831			

C	-0.65584	-0.89722	
1.67668			
H	-0.14289	-1.39167	
2.51626			
H	-1.68145	-1.29309	
1.67578			
C	-0.6842	0.61736	
1.94059			
H	-1.24849	0.7942	
2.86749			
H	0.33727	0.96032	
2.1363			
C	-1.28683	1.51033	
0.83599			
H	-1.18007	2.54295	1.182
H	-2.36632	1.32838	
0.74887			
C	-1.41634	0.49669	-
1.58299			
H	-2.28305	1.06541	-
1.94583			
H	-0.79493	0.32416	-
2.47208			
C	-1.95723	-0.84738	-
1.06783			
H	-2.67703	-0.66372	-
0.26036			
H	-2.53501	-1.32594	-
1.87052			
C	-0.89221	-1.83659	-
0.59135			
H	-1.38834	-2.76011	-
0.22984			
H	-0.27628	-2.13072	-
1.44828			
O	1.44775	2.11122	
0.23351			

1-azabicyclo[4.3.3]dodecan-7-one

The number of imaginary frequencies: 0
 Total Energy (B3LYP/6-31G*)= -
 560.56098819

H	2.71297	-0.34968
0.70871		
H	3.39611	-0.94693 -
0.78611		
C	2.0431	0.71928 -
1.06576		
H	2.96196	1.20949 -
1.41454		
H	1.50147	0.45094 -
1.98404		
C	1.26943	1.82383 -
0.30314		
H	1.37461	2.72065 -
0.92942		
H	1.81972	2.05822
0.61971		
C	-0.24974	1.73443
0.05127		
H	-0.55869	2.78788
0.06383		
C	-0.14086	-1.28978
1.46919		
H	0.45044	-2.07235
1.97468		
H	-1.1964	-1.54091
1.63979		
C	0.1571	0.06906
2.11723		
H	-0.12195	0.00635
3.17913		
H	1.23738	0.25451
2.10511		
C	-0.5751	1.27392
1.50428		
H	-0.35586	2.13055
2.15593		
H	-1.65993	1.11761
1.58332		
C	-1.14911	1.11647 -
1.08008		

H	-1.94391	1.82788 -
1.32295		
H	-0.5481	0.98021 -
1.98803		
C	-1.87766	-0.19247 -
0.78832		
C	-1.04706	-1.47945 -
0.80985		
H	-1.70951	-2.31333 -
0.52235		
H	-0.71749	-1.65398 -
1.8422		
O	-3.06889	-0.21502 -
0.53488		

1-azabicyclo[4.3.3]dodecane N-oxide

The number of imaginary frequencies: 0

Total Energy (B3LYP/6-31G*)= -561.66828587

ZPE= -561.35115

Enthalpy= -561.338551

N	0.40679	-1.27086 -
0.05346		
C	1.83246	-1.13866 -
0.25423		
H	2.39188	-1.84521
0.38658		
H	2.06027	-1.4182 -
1.29071		
C	2.35452	0.29 -0.01702
H	2.35545	0.52346
1.05516		
H	3.40984	0.31516 -
0.32642		
C	1.57118	1.36919 -
0.79145		
H	2.27703	2.17634 -
1.03055		
H	1.26307	0.96079 -
1.76375		
C	0.36878	2.07362 -0.116

H	0.21612	2.99005	-
0.70364			
H	0.68691	2.42642	
0.8765			
C	-1.05047	1.43197	
0.02848			
H	-1.69801	2.32043	
0.05674			
C	-0.06841	-1.48695	
1.29817			
H	0.66282	-2.0887	
1.86652			
H	-0.98842	-2.08664	
1.25747			
C	-0.34699	-0.18671	
2.06502			
H	-0.72789	-0.44805	
3.06388			
H	0.59997	0.33816	
2.23842			
C	-1.34869	0.78041	
1.41252			
H	-1.47394	1.61011	
2.12229			
H	-2.33552	0.29767	
1.36407			
C	-1.56258	0.66008	-
1.23628			
H	-2.54507	1.07838	-
1.49246			
H	-0.91708	0.90467	-
2.09112			
C	-1.75255	-0.86685	-
1.18859			
H	-2.38858	-1.13411	-
0.33472			
H	-2.31736	-1.17643	-
2.07995			
C	-0.45636	-1.68445	-
1.13898			

H	-0.71388	-2.76253	-
1.09212			
H	0.08954	-1.53569	-
2.07775			
O	0.6837	-2.59907	
0.04026			

1-azabicyclo[4.3.3]dodecane N-oxide

The number of imaginary frequencies: 0

Total Energy (M06/6-311G+(d,p))= -

561.41002052

ZPE= -561.096465

Enthalpy= -561.083943

N	1.64025	-0.094	-
0.10182			
C	1.38832	1.35137	-
0.27683			
H	2.06804	1.81274	
0.40875			
H	1.6539	1.54597	-
1.29491			
C	0.07516	2.13291	-
0.05455			
H	-0.28101	2.07203	
0.9526			
H	0.37167	3.13415	-0.288
C	-1.06313	1.79787	-
0.99182			
H	-1.57284	2.71605	-
1.19686			
H	-0.64097	1.3921	-
1.88739			
C	-2.19779	0.92599	-
0.42756			
H	-2.88164	0.84903	-
1.24691			
H	-2.61047	1.48898	
0.38338			
C	-2.09264	-0.50782	
0.12336			
H	-3.11678	-0.79179	
0.24746			

C	1.34163	-0.42766	
1.29732			
H	2.07521	0.09758	
1.87254			
H	1.43749	-1.48355	
1.44158			
C	-0.03841	0.07345	
1.86501			
H	0.05557	-0.04769	
2.92396			
H	-0.12176	1.10564	
1.59571			
C	-1.42472	-0.60472	1.537
H	-2.10957	-0.10635	
2.19085			
H	-1.34707	-1.6446	
1.77683			
C	-1.54899	-1.51405	-
0.85273			
H	-2.0587	-2.42716	-
0.62617			
H	-1.79067	-1.1744	-
1.83818			
C	-0.10711	-1.93499	-
0.77061			
H	0.03919	-2.29551	
0.22615			
H	-0.04985	-2.72408	-1.491
C	1.11529	-1.08758	-
1.06823			
H	1.87821	-1.83766	-
1.08361			
H	1.01949	-0.61099	-
2.02142			
O	2.97689	-0.20514	-
0.32685			

Trimethylamine

The number of imaginary frequencies: 0
 Total Energy (B3LYP/6-31G*)= -
 174.47441505
 ZPE= -174.353287

Enthalpy= -174.346933			
N	-0.23715	0.11869	-
0.00005			
C	0.25311	0.81147	-
1.20029			
H	-0.10517	0.30823	-
2.07395			
H	-0.10173	1.82092	-
1.19941			
H	1.32311	0.80955	-
1.20117			
C	0.25035	-1.26812	-
0.00127			
H	-0.10652	-1.7724	
0.87238			
H	-0.10794	-1.77137	-
0.87492			
H	1.32034	-1.27005	-
0.00214			
C	0.25508	0.81006	1.2002
H	-0.09977	1.81951	
1.20109			
H	-0.10179	0.30579	
2.07385			
H	1.32507	0.80813	
1.19933			

Trimethylamine

The number of imaginary frequencies: 0
 Total Energy (B3LYP/6-31G**)= -
 174.359219
 ZPE= -174.365595
 Enthalpy= -174.359219

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

The number of imaginary frequencies: 0
 Total Energy (M06/6-311G+(d,p))= -174.38202143
 ZPE= -174.262877
 Enthalpy= -174.256485

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

The number of imaginary frequencies: 0
 Total Energy (B3PW91/6-31G*)= -174.41045066
 ZPE= -174.289118
 Enthalpy= -174.282761

N	-0.23715	0.11869	-
0.00005			
C	0.25311	0.81147	-
1.20029			
H	-0.10517	0.30823	-
2.07395			
H	-0.10173	1.82092	-
1.19941			
H	1.32311	0.80955	-
1.20117			
C	0.25035	-1.26812	-
0.00127			
H	-0.10652	-1.7724	
0.87238			
H	-0.10794	-1.77137	-
0.87492			
H	1.32034	-1.27005	-
0.00214			
C	0.25508	0.81006	1.2002
H	-0.09977	1.81951	
1.20109			
H	-0.10179	0.30579	
2.07385			
H	1.32507	0.80813	
1.19933			

Trimethylamine

The number of imaginary frequencies: 0

Total Energy (B3PW91/6-31G**)= -174.42143905

ZPE= -174.300694

Enthalpy= -174.294319

N	-0.23715	0.11869	-
0.00005			
C	0.25311	0.81147	-
1.20029			
H	-0.10517	0.30823	-
2.07395			
H	-0.10173	1.82092	-
1.19941			
H	1.32311	0.80955	-
1.20117			
C	0.25035	-1.26812	-
0.00127			
H	-0.10652	-1.7724	
0.87238			
H	-0.10794	-1.77137	-
0.87492			
H	1.32034	-1.27005	-
0.00214			
C	0.25508	0.81006	1.2002
H	-0.09977	1.81951	
1.20109			
H	-0.10179	0.30579	
2.07385			
H	1.32507	0.80813	
1.19933			

Trimethylamine

The number of imaginary frequencies: 0

Total Energy (B3PW91/6-311G+(d,p))= -174.45968937

ZPE= -174.339866

Enthalpy= -174.333441

N	-0.23715	0.11869	-
0.00005			
C	0.25311	0.81147	-
1.20029			

H	-0.10517	0.30823	-
2.07395			
H	-0.10173	1.82092	-
1.19941			
H	1.32311	0.80955	-
1.20117			
C	0.25035	-1.26812	-
0.00127			
H	-0.10652	-1.7724	
0.87238			
H	-0.10794	-1.77137	-
0.87492			
H	1.32034	-1.27005	-
0.00214			
C	0.25508	0.81006	1.2002
H	-0.09977	1.81951	
1.20109			
H	-0.10179	0.30579	
2.07385			
H	1.32507	0.80813	
1.19933			

Trimethylamine

The number of imaginary frequencies: 0

Total Energy (Hartree Fock 6-31G*)= -173.26929918

ZPE= -173.139801

Enthalpy= -173.13364

N	-0.55556	2.19935	-
0.11514			
C	-0.0653	2.89239	
1.08495			
H	-0.42357	3.90063	
1.08595			
H	-0.42016	2.38691	
1.95872			
H	1.0047	2.8941	
1.08374			
C	-0.06334	0.8142	-
0.11652			
H	-0.41821	0.30872	
0.75724			

H	-0.4202	0.30974	-
0.99006			
H	1.00665	0.81591	-
0.11773			
C	-0.06803	2.8938	-
1.31554			
H	-0.42489	2.38934	-
2.18908			
H	-0.42631	3.90203	-
1.31454			
H	1.00197	2.89551	-
1.31676			

Trimethylamine N-oxide

The number of imaginary frequencies: 0
 Total Energy (B3LYP/6-31G*)= -
 249.61561382
 ZPE= -249.489573
 Enthalpy= -249.482621

N	0.	0.
0.08377		
C	0.	1.41754
0.41816		
H	-0.88839	1.89255
0.00215		
H	0.88839	1.89255
0.00215		
H	0.	1.4678
1.51318		
C	-1.22763	-0.70877
0.41816		
H	-1.1948	-1.71564
0.00215		
H	-2.08319	-0.1769
0.00215		
H	-1.27115	-0.7339
1.51318		
C	1.22763	-0.70877
0.41816		
H	2.08319	-0.1769
0.00215		

H	1.1948	-1.71564	-
0.00215			
H	1.27115	-0.7339	-
1.51318			
O	0.	0.	
1.44003			

Trimethylamine N-oxide

The number of imaginary frequencies: 0
 Total Energy (B3LYP/6-31G**)= -
 249.6275473
 ZPE= -249.502133
 Enthalpy= -249.495143

N	0.	0.
0.08312		
C	0.	1.41754
0.41881		
H	-0.88839	1.89255
0.00215		
H	0.88839	1.89255
0.00215		
H	0.	1.4678
1.51383		
C	-1.22763	-0.70877
0.41881		
H	-1.1948	-1.71564
0.00215		
H	-2.08319	-0.1769
0.00215		
H	-1.27115	-0.7339
1.51383		
C	1.22763	-0.70877
0.41881		
H	2.08319	-0.1769
0.00215		
H	1.1948	-1.71564
0.00215		

H	1.27115	-0.7339	-
1.51383			
O	0.	0.	
1.43938			

Trimethylamine N-oxide
The number of imaginary frequencies: 0
Total Energy (M06/6-311G+(d,p))= -249.52070728
ZPE= -249.396733
Enthalpy= -249.389724

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			

Trimethylamine N-oxide
The number of imaginary frequencies: 0

Total Energy (B3PW91/6-31G*)= -249.52323117			
ZPE= -249.396878			
Enthalpy= -249.389954			
N	0.	0.	0.08377
C	0.	1.41754	-0.41816
H	-0.88839	1.89255	-
0.00215			
H	0.88839	1.89255	-
0.00215			
H	0.	1.4678	-
1.51318			
C	-1.22763	-0.70877	-
0.41816			
H	-1.1948	-1.71564	-
0.00215			
H	-2.08319	-0.1769	-
0.00215			
H	-1.27115	-0.7339	-
1.51318			
C	1.22763	-0.70877	-
0.41816			
H	2.08319	-0.1769	-
0.00215			
H	1.1948	-1.71564	-
0.00215			
H	1.27115	-0.7339	-
1.51318			
O	0.	0.	
1.44003			

Trimethylamine N-oxide
The number of imaginary frequencies: 0
Total Energy (B3PW91/6-31G**) = -249.53436118
ZPE= -249.408677
Enthalpy= -249.401712

N	0.	0.	0.08377
C	0.	1.41754	-0.41816
H	-0.88839	1.89255	-
0.00215			

H	0.88839	1.89255	-
0.00215			
H	0.	1.4678	-
1.51318			
C	-1.22763	-0.70877	-
0.41816			
H	-1.1948	-1.71564	-
0.00215			
H	-2.08319	-0.1769	-
0.00215			
H	-1.27115	-0.7339	-
1.51318			
C	1.22763	-0.70877	-
0.41816			
H	2.08319	-0.1769	-
0.00215			
H	1.1948	-1.71564	-
0.00215			
H	1.27115	-0.7339	-
1.51318			
O	0.	0.	
1.44003			

Trimethylamine N-oxide

The number of imaginary frequencies: 0
 Total Energy (B3PW91/6-311G+(d,p))= -
 249.60267295
 ZPE= -249.477639
 Enthalpy= -249.470642

N	0.	0.	
0.08377			
C	0.	1.41754	-
0.41816			
H	-0.88839	1.89255	-
0.00215			
H	0.88839	1.89255	-
0.00215			
H	0.	1.4678	-
1.51318			
C	-1.22763	-0.70877	-
0.41816			

H	-1.1948	-1.71564	-
0.00215			
H	-2.08319	-0.1769	-
0.00215			
H	-1.27115	-0.7339	-
1.51318			
C	1.22763	-0.70877	-
0.41816			
H	2.08319	-0.1769	-
0.00215			
H	1.1948	-1.71564	-
0.00215			
H	1.27115	-0.7339	-
1.51318			
O	0.	0.	
1.44003			

Trimethylamine N-oxide

The number of imaginary frequencies: 0
 Total Energy (Hartree Fock 6-31G*)= -
 248.04640634
 ZPE= -247.910609
 Enthalpy= -247.904082

N	-0.55556	2.19935	-
0.11514			
C	-0.0653	2.89239	
1.08495			
H	-0.42357	3.90063	
1.08595			
H	-0.42016	2.38691	
1.95872			
H	1.0047	2.8941	
1.08374			
C	-0.06334	0.8142	-
0.11652			
H	-0.41821	0.30872	
0.75724			
H	-0.4202	0.30974	-
0.99006			
H	1.00665	0.81591	-
0.11773			

C	-0.06803	2.8938	-
1.31554			
H	-0.42489	2.38934	-
2.18908			
H	-0.42631	3.90203	-
1.31454			
H	1.00197	2.89551	-
1.31676			
O	-1.91555	2.19718	-
0.11359			

Trimethylaminium

The number of imaginary frequencies: 0
 Total Energy (B3LYP/6-31G*)= -174.85106876
 ZPE= -174.714195
 Enthalpy= -174.707684

N	0.	0.00006	
0.42913			
C	0.	1.38592	-
0.06109			
H	-0.87365	1.89038	
0.29551			
H	0.87366	1.89037	
0.2955			
H	0.	1.38576	-
1.13109			
C	-1.20025	-0.69297	-
0.06077			
H	-1.20025	-1.70172	
0.29605			
H	-2.0739	-0.18851	
0.29582			
H	-1.20025	-0.69313	-
1.13077			
C	1.20025	-0.69298	-
0.06077			
H	2.0739	-0.18852	
0.29582			
H	1.20025	-1.70173	
0.29605			

H	1.20025	-0.69314	-
1.13077			
H	0.	0.00022	
1.42913			

Trimethylaminium

The number of imaginary frequencies: 0
 Total Energy (M06/6-311G+(d,p))= -174.74831058
 ZPE= -174.614346
 Enthalpy= -174.607656

N	0.	0.	-0.38
C	0.	1.38593	0.11
H	0.87365	1.89033	-
0.24667			
H	-0.87365	1.89033	-
0.24667			
H	0.	1.38593	1.18
C	1.20025	-0.69296	0.11
H	1.20025	-1.70177	-
0.24667			
H	2.0739	-0.18856	-
0.24667			
H	1.20025	-0.69296	1.18
C	-1.20025	-0.69296	0.11
H	-2.0739	-0.18856	-
0.24667			
H	-1.20025	-1.70177	-
0.24667			
H	-1.20025	-0.69296	1.18
H	0.	0.	-1.38

Methanamine

The number of imaginary frequencies: 0
 Total Energy (B3LYP/6-31G*)= -249.63811327
 ZPE= -249.512681
 Enthalpy= -249.505072

C	1.93077	-0.00053	-
0.19893			

H	2.78142	-0.00087	
0.45015			
H	1.95289	-0.87417	-
0.81633			
H	1.95352	0.87314	-
0.81625			
C	-1.13364	-1.22098	-
0.01552			
H	-1.97665	-1.22922	-
0.67443			
H	-0.52317	-2.07871	-
0.20664			
H	-1.47351	-1.24395	
0.9988			
O	0.73398	-0.00014	
0.58374			
N	-0.34722	0.00029	-
0.24125			
C	-1.13276	1.2221	-
0.01541			
H	-0.52168	2.07941	-
0.20645			
H	-1.97577	1.23101	-
0.67432			
H	-1.47262	1.24522	
0.99891			

Methanamine

The number of imaginary frequencies: 0
 Total Energy (M06/6-311G+(d,p))= -
 249.53609711
 ZPE= -249.412608
 Enthalpy= -249.405058

C	1.9266	0.	-0.19527
H	2.73029	0.	
0.54658			
H	2.00833	-0.89282	-
0.82931			
H	2.00833	0.89282	-
0.82931			
C	-1.13036	-1.20925	-
0.02138			

H	-1.99892	-1.23176	-0.687
H	-0.50884	-2.08505	-
0.22874			
H	-1.47537	-1.2607	
1.02592			
O	0.71379	0.	
0.54702			
N	-0.35518	0.	-
0.29376			
C	-1.13036	1.20925	-
0.02138			
H	-0.50884	2.08505	-
0.22874			
H	-1.99892	1.23176	-0.687
H	-1.47537	1.2607	
1.02592			

Ethanamine

The number of imaginary frequencies: 0
 Total Energy (B3LYP/6-31G*)= -
 249.68300495
 ZPE= -249.55625
 Enthalpy= -249.548583

C	-0.90757	0.75395	-
0.13564			
H	-1.2254	1.71597	-
0.47974			
H	-1.46972	-0.00717	-
0.63522			
H	-1.06855	0.68155	
0.9197			
C	0.90838	-0.70347	
0.04137			
C	2.40657	-0.88841	-
0.26326			
H	0.7474	-0.77587	
1.09671			
H	0.34622	-1.46459	-
0.45821			
H	2.56755	-0.81601	-
1.3186			

H	2.96873	-0.12729
0.23632		
O	0.48361	0.58222 -
0.41851		
N	2.84322	-2.21006
0.20948		
H	3.81607	-2.33015
0.01167		
H	2.69278	-2.27772
1.19579		

Ethanamine

The number of imaginary frequencies: 0
 Total Energy (M06/6-311G+(d,p))= -249.458677
 ZPE= -249.466382
 Enthalpy= -249.458677

C	2.39094	-0.19573
0.01077		
H	3.19214	0.54169 -
0.08895		
H	2.50576	-0.71973
0.97376		
H	2.48809	-0.93913 -
0.79784		
C	0.0434	-0.34752
0.05415		
C	-1.21436	0.51131 -
0.01284		
H	0.03787	-1.09489 -0.761
H	0.06151	-0.90441
1.00469		
H	-1.21426	1.19365
0.84436		
H	-1.16269	1.13654 -
0.9206		
O	1.16821	0.50193 -
0.06356		
N	-2.40165	-0.34534
0.07822		

H	-3.23306	0.23069
0.19166		
H	-2.52928	-0.85084 -
0.79763		

Dimethylaminomethanol

The number of imaginary frequencies: 0
 Total Energy (B3LYP/6-31G*)= -249.68172356
 ZPE= -249.555788
 Enthalpy= -249.548324

C	-0.54804	1.39222	0.0741
H	0.35805	1.92515	-
0.22934			
H	-1.39713	1.85627	-
0.43704			
H	-0.69544	1.53361	
1.16556			
C	-1.6404	-0.75027	-
0.02821			
H	-1.54883	-1.76248	-
0.43514			
H	-1.86998	-0.83816	
1.05329			
H	-2.4971	-0.26403	-
0.50581			
N	-0.43238	0.00604	-
0.32168			
C	0.737	-0.64005	
0.25148			
H	0.73019	-1.68859	-
0.03969			
H	0.73132	-0.59029	
1.35913			
O	1.96162	-0.10356	-
0.22974			
H	2.23116	0.60334	
0.37443			

Dimethylaminomethanol

The number of imaginary frequencies: 0
 Total Energy (M06/6-311G+(d,p))= -249.58819455
 ZPE= -249.464461

Enthalpy= -249.457371
 C -0.54804 1.39222
 0.0741
 H 0.35805 1.92515 -
 0.22934
 H -1.39713 1.85627 -
 0.43704
 H -0.69544 1.53361
 1.16556
 C -1.6404 -0.75027 -
 0.02821
 H -1.54883 -1.76248 -
 0.43514
 H -1.86998 -0.83816
 1.05329
 H -2.4971 -0.26403 -
 0.50581
 N -0.43238 0.00604 -
 0.32168
 C 0.737 -0.64005
 0.25148
 H 0.73019 -1.68859 -
 0.03969
 H 0.73132 -0.59029
 1.35913
 O 1.96162 -0.10356 -
 0.22974
 H 2.23116 0.60334
 0.37443

Trimethylaminomethanol

The number of imaginary frequencies: 0
 Total Energy (B3LYP/6-31G*)= -
 250.00872901
 ZPE= -249.869457
 Enthalpy= -249.861997

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
 H 0.9051 0.
 1.75938

Trimethylaminomethanol

The number of imaginary frequencies: 0
 Total Energy (M06/6-311G+(d,p))= -
 249.90268818
 ZPE= -249.765408
 Enthalpy= -249.758011

N 0.00359 0.00003 -
 0.00407
 C 0.67148 1.25816 -
 0.48684
 H 0.14803 2.1059 -
 0.04552
 H 1.71605 1.2419 -
 0.16952
 H 0.614 1.28728 -
 1.57638
 C -1.45474 -0.01962 -
 0.37823

H	-1.89576	-0.92111
0.04589		
H	-1.92025	0.86836
0.04817		
H	-1.52719	-0.0194
1.46624		
C	0.70582	-1.23898
0.48779		
H	1.74934	-1.19445
0.16968		
H	0.20563	-2.10114
0.04753		
H	0.65008	-1.26848
1.5774		
O	-0.02599	-0.00107
1.42316		
H	0.90752	0.01216
1.71855		

Nitromethane

The number of imaginary frequencies: 0
 Total Energy (B3LYP/6-31G*)= -
 245.00932726
 ZPE= -244.959092
 Enthalpy= -244.953835

N	2.33004	0.25514	0.
0.00158			
O	3.56716	0.28984	
0.00157			
O	1.68144	1.30916	-
0.00157			
C	1.63103	-1.03803	0.
1.00881			
H	1.46273	-1.35249	-
0.50568			
H	2.22932	-1.76688	
0.50311			

Nitromethane

The number of imaginary frequencies: 1 (-
 29.36 cm⁻¹)
 Total Energy (M06/6-311G+(d,p))= -
 244.94960552
 ZPE= -244.900022

Enthalpy= -244.895614

N	0.15385	0.00001	-
0.00178			
O	0.7726	1.07182	-
0.00802			
O	0.77264	-1.07177	-
0.00774			
C	-1.31608	-0.00001	
0.01272			
H	-1.66278	0.00011	
1.02499			
H	-1.67772	0.87357	-
0.48826			
H	-1.67769	-0.87373	-
0.48803			

Methylnitrite

The number of imaginary frequencies: 0
 Total Energy (B3LYP/6-31G*)= -
 245.00795817
 ZPE= -244.959108
 Enthalpy= -244.953786

C	-0.87908	-0.57341	0.011
0.01543			
H	-0.22485	-1.41968	-
0.84215			
H	-0.69587	0.04584	-
0.0026			
H	-1.89542	-0.90773	-
1.2047			
O	-0.64001	0.17681	
1.21414			
N	-0.82548	1.40039	
0.19049			
O	-1.21785	1.9747	

Methylnitrite

The number of imaginary frequencies: 0
 Total Energy (M06/6-311G+(d,p))= -
 244.94401884
 ZPE= -244.895496
 Enthalpy= -244.890279

C	-1.29687	0.42144	0.
H	-2.31666	0.0373	-
0.00035			
H	-1.10955	1.02791	-
0.89114			
H	-1.11006	1.02756	
0.89149			
O	-0.46824	-0.75474	-
0.00001			
N	0.90934	-0.51993	
0.00001			
O	1.21225	0.63201	-
0.00001			

Pyrrolidine

The number of imaginary frequencies: 0
 Total Energy (B3LYP/6-31G*)= -
 212.58201691
 ZPE= -212.451628
 Enthalpy= -212.445712

C	-0.35518	1.14266	
0.75224			
C	1.66599	0.92763	-
0.11519			
C	1.21815	2.35076	-
0.54335			
C	-0.27836	2.31052	-
0.19821			
H	-1.3606	0.83838	
0.95585			
H	0.12138	1.34396	
1.68886			
H	2.00407	0.96391	
0.89935			
H	2.45269	0.54167	-
0.72922			
H	1.82578	3.03812	
0.00731			
H	1.2855	2.59188	-
1.58365			

H	-0.66829	3.25028	
0.13301			
H	-0.82826	1.99974	-
1.06188			
N	0.4318	0.15228	-
0.06269			
H	0.02441	-0.0232	-
0.95893			

Pyrrolidine

The number of imaginary frequencies: 0
 Total Energy (M06/6-311G+(d,p))= -
 212.47328852
 ZPE= -212.344771
 Enthalpy= -212.33877

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

H -0.00003 -1.35474 -
1.21799

Pyrrolidine N-oxide

The number of imaginary frequencies: 0

Total Energy (B3LYP/6-31G*)= -
287.7234805

ZPE= -287.588302

Enthalpy= -287.581788

C -0.00033 1.14666
0.49444

C 0.22374 -1.05371
0.76688

C 0.96197 -0.79536 -
0.52621

C 1.08575 0.74368 -
0.53982

H -0.47516 2.07704
0.26244

H 0.45616 1.22377
1.45911

H 0.81878 -0.84826
1.63211

H -0.13466 -2.05837
0.85127

H 1.89161 -1.30274 -
0.67863

H 0.2804 -1.09447 -
1.29491

H 2.00673 1.16062 -
0.18931

H 0.93355 1.05243 -
1.55294

N -0.85181 -0.02712
0.58429

O -1.56281 -0.24663 -
0.55408

H -1.50044 0.02115
1.34386

Pyrrolidine N-oxide

The number of imaginary frequencies: 0

Total Energy (M06/6-311G+(d,p))= -
287.61263562

ZPE= -287.478669

Enthalpy= -287.472253

C 0.01206 -1.18031
0.52425

C 0.01184 1.18049
0.52397

C -1.21089 0.77991 -
0.31338

C -1.21052 -0.78023 -
0.31346

H 0.54995 -2.05773
0.1677

H -0.22877 -1.28622
1.5907

H -0.22873 1.2867
1.59044

H 0.54951 2.05786 0.167

H -2.12812 1.19622
0.11317

H -1.10535 1.15647 -
1.33143

H -2.12776 -1.19704
0.11264

H -1.1044 -1.15665 -
1.3315

N 0.94195 0.00013
0.34004

O 1.49591 0.00001 -
0.88636

H 1.64784 0.00032
1.10359

Pyrroline

The number of imaginary frequencies: 0

Total Energy (B3LYP/6-31G*)= -
211.37224827
ZPE= -211.266433
Enthalpy= -211.260945

C	-0.49599	1.00851
0.46461		
C	1.66072	0.9327 -
0.09942		
C	1.21845	2.35201 -
0.52028		
C	-0.28937	2.31892 -
0.27064		
H	-1.27831	0.80132
1.16457		
H	2.05448	0.96858
0.89485		
H	2.40803	0.54681 -
0.76087		
H	1.80627	3.01176
0.08312		
H	1.3273	2.62831 -
1.54824		
H	-0.64141	3.22178
0.18302		
H	-0.80971	2.17064 -
1.19377		
N	0.43286	0.14649
0.05661		

Pyrroline

The number of imaginary frequencies: 0
Total Energy (M06/6-311G+(d,p))= -
211.26189917
ZPE= -211.157429
Enthalpy= -211.151965

C	0.79886	-0.91542 -
0.04069		
C	-1.23392	0.0008
0.07707		
C	-0.2629	1.20077 -0.0989

C	1.13211	0.55755
0.07986		
H	1.56696	-1.68896 -
0.09765		
H	-2.03854	-0.01318 -
0.66631		
H	-1.71638	-0.00663
1.06376		
H	-0.35942	1.62428 -
1.10418		
H	-0.45414	2.00652
0.61532		
H	1.86709	0.88284 -
0.66596		
H	1.57371	0.7638
1.06555		
N	-0.43489	-1.23298 -
0.04494		

Methyl Pyrrolidine

The number of imaginary frequencies: 0
Total Energy (B3LYP/6-31G*)= -
251.88956837
ZPE= -251.731361
Enthalpy= -251.724164

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			

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			

Methyl Pyrrolidine

The number of imaginary frequencies: 0
 Total Energy (M06/6-311G+(d,p))= -251.7568498
 ZPE= -251.601035
 Enthalpy= -251.593775

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			

Methyl Pyrrolidine N-oxide

The number of imaginary frequencies: 0
 Total Energy (B3LYP/6-31G*)= -327.03549275
 ZPE= -326.872485
 Enthalpy= -326.864715

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		

Methyl Pyrrolidine N-oxide

The number of imaginary frequencies: 0
 Total Energy (M06/6-311G+(d,p))= -
 326.90051885
 ZPE= -326.739215
 Enthalpy= -326.731606

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		

Methyl Pyrrolidinone

The number of imaginary frequencies: 0
 Total Energy (B3LYP/6-31G*)= -
 325.94471629
 ZPE= -325.804999
 Enthalpy= -325.797138

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	1.19788	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	2.33218	-0.87742 -
0.50154		

Methyl Pyrrolidinone

The number of imaginary frequencies: 0
 Total Energy (M06/6-311G+(d,p))= -
 325.8093828
 ZPE= -325.67156
 Enthalpy= -325.663666

C	-0.50075	-1.34309
0.05295		

C	0.13557	0.87519 -
0.11685		
C	-1.33952	0.80633
0.3062		
C	-1.73765	-0.52461 -
0.31782		
H	-0.49936	-2.3329 -
0.35345		
H	-0.41913	-1.41815
1.11719		
H	-1.40259	0.75096
1.37291		
H	-1.93719	1.6317 -
0.02004		
H	-2.66302	-0.91016
0.05628		
H	-1.81925	-0.4489 -
1.38201		
N	0.57997	-0.4906 -
0.50495		
C	1.91786	-0.84833 -0.012
H	2.64179	-0.17871 -
0.42724		
H	1.93585	-0.77582
1.05539		
H	2.14976	-1.85087 -
0.30534		
O	0.84772	1.91254 -
0.13428		

Methyl Pyrrolidinone N-oxide

The number of imaginary frequencies: 0
 Total Energy (B3LYP/6-31G*)= -
 401.06253971
 ZPE= -400.91912
 Enthalpy= -400.910648

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	1.19788	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	2.33218	-0.87742	-
0.50154			
O	-0.00044	-2.50637	
0.37472			

Methyl Pyrrolidinone N-oxide

The number of imaginary frequencies: 0
 Total Energy (M06/6-311G+(d,p))= -
 400.9215923
 ZPE= -400.780264
 Enthalpy= -400.771751

C	-0.48471	-1.28217	-0.5346
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C	-0.0026	0.99053	-
0.06214			
C	-1.49677	0.84499	-
0.05282			
C	-1.78687	-0.65491	-
0.0592			
H	-0.37844	-1.24163	-
1.62724			
H	-0.30977	-2.29782	-
0.1736			
H	-1.91474	1.37381	
0.80611			
H	-1.86375	1.35238	-
0.95306			
H	-2.01179	-1.00562	
0.94849			
H	-2.61807	-0.91988	-
0.7162			
N	0.55348	-0.40619	
0.06882			
C	1.90545	-0.59017	-
0.47633			
H	2.54161	0.16753	-
0.02093			
H	2.23699	-1.58619	-
0.17945			
H	1.89512	-0.48166	-
1.56483			
O	0.69431	1.94486	-
0.16503			
O	0.52337	-0.49076	
1.42871			

Pyridine

The number of imaginary frequencies: 0
 Total Energy (B3LYP/6-31G*)= -
 248.28497285
 ZPE= -248.195939
 Enthalpy= -248.190725

C	-2.54788	-2.09617	0.
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C	-1.141	-2.09617	0.
C	-0.47431	-0.86957	0.
C	-1.22838	0.30522	-
0.00024			
C	-2.63158	0.20242	-
0.00038			
N	-3.29111	-0.97253	-
0.0002			
H	0.62424	-0.82979	-
0.00095			
H	-3.11342	-3.04499	
0.00012			
H	-0.58627	-3.04307	
0.00026			
H	-0.74435	1.29015	-
0.00034			
H	-3.26493	1.10748	-
0.00046			

Pyridine
The number of imaginary frequencies: 0
Total Energy (B3LYP/6-31G**)= -248.2925931
ZPE= -248.203715
Enthalpy= -248.198499

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
The number of imaginary frequencies: 0
Total Energy (M06/6-311G+(d,p))= -248.15337889
ZPE= -248.06551
Enthalpy= -248.060238

C	-1.14254	-0.72168	-
0.00022			
C	-1.19865	0.67327	-
0.00012			
C	0.00025	1.38544	0.0001
C	1.19889	0.67286	
0.00022			
C	1.14228	-0.72207	
0.00012			
N	-0.00025	-1.42094	-
0.0001			
H	0.00041	2.47232	
0.00016			
H	-2.05996	-1.30855	-
0.00037			

H	-2.15768	1.18294	-
0.00023			
H	2.15812	1.18216	
0.00036			
H	2.05949	-1.30926	
0.00019			

Pyridine

The number of imaginary frequencies: 0
 Total Energy (B3PW91/6-31G*)= -
 248.18841608
 ZPE= -248.099146
 Enthalpy= -248.093923

C	-2.54788	-2.09617	0.
C	-1.141	-2.09617	0.
C	-0.47431	-0.86957	0.
C	-1.22838	0.30522	-
0.00024			
C	-2.63158	0.20242	-
0.00038			
N	-3.29111	-0.97253	-
0.0002			
H	0.62424	-0.82979	-
0.00095			
H	-3.11342	-3.04499	
0.00012			
H	-0.58627	-3.04307	
0.00026			
H	-0.74435	1.29015	-
0.00034			
H	-3.26493	1.10748	-
0.00046			

Pyridine

The number of imaginary frequencies: 0
 Total Energy (B3PW91/6-31G**) = -
 248.19559822
 ZPE= -248.106489
 Enthalpy= -248.101263

C	-2.54788	-2.09617	0.
C	-1.141	-2.09617	0.

C	-0.47431	-0.86957	0.
C	-1.22838	0.30522	-
0.00024			
C	-2.63158	0.20242	-
0.00038			
N	-3.29111	-0.97253	-
0.0002			
H	0.62424	-0.82979	-
0.00095			
H	-3.11342	-3.04499	
0.00012			
H	-0.58627	-3.04307	
0.00026			
H	-0.74435	1.29015	-
0.00034			
H	-3.26493	1.10748	-
0.00046			

Pyridine

The number of imaginary frequencies: 0
 Total Energy (B3PW91/6-311G+(d,p))= -
 248.24903458
 ZPE= -248.160401
 Enthalpy= -248.155163

C	-2.54788	-2.09617	0.
C	-1.141	-2.09617	0.
C	-0.47431	-0.86957	0.
C	-1.22838	0.30522	-
0.00024			
C	-2.63158	0.20242	-
0.00038			
N	-3.29111	-0.97253	-
0.0002			
H	0.62424	-0.82979	-
0.00095			
H	-3.11342	-3.04499	
0.00012			
H	-0.58627	-3.04307	
0.00026			

H	-0.74435	1.29015	-	C	-1.19865	0.67327	-
0.00034				0.00012			
H	-3.26493	1.10748	-	C	0.00025	1.38544	0.0001
0.00046				C	1.19889	0.67286	
				0.00022			
				C	1.14228	-0.72207	
				0.00012			
				N	-0.00025	-1.42094	-
				0.0001			
				H	0.00041	2.47232	
				0.00016			
				H	-2.05996	-1.30855	-
				0.00037			
				H	-2.15768	1.18294	-
				0.00023			
				H	2.15812	1.18216	
				0.00036			
				H	2.05949	-1.30926	
				0.00019			
				O	-0.00048	-2.78094	-
				0.0002			
Pyridine				Pyridine N-oxide			
The number of imaginary frequencies: 0				The number of imaginary frequencies: 0			
Total Energy (Hartree Fock 6-31G*)= -246.69581967				Total Energy (B3LYP/6-31G**) = -323.4550059			
ZPE= -246.60038				ZPE= -323.361915			
Enthalpy= -246.595443				Enthalpy= -323.355913			
C	-2.09349	-0.73061		C	0.28383	-1.18039	-
0.00597				0.00018			
C	-0.68661	-0.73061		C	-1.09931	-1.19458	-
0.00597				0.00009			
C	-0.01992	0.49599		C	-1.82222	0.	
0.00597				0.00012			
C	-0.77399	1.67078		C	-1.09931	1.19458	
0.00573				0.00024			
C	-2.17719	1.56797		C	0.28383	1.18039	
0.00559				0.00014			
N	-2.83672	0.39302		N	0.98713	0.	-
0.00578				0.00007			
H	1.07862	0.53577					
0.00502							
H	-2.65904	-1.67944					
0.00609							
H	-0.13188	-1.67752					
0.00624							
H	-0.28996	2.6557					
0.00563							
H	-2.81054	2.47304					
0.00551							
Pyridine N-oxide							
The number of imaginary frequencies: 0							
Total Energy (B3LYP/6-31G*)= -323.44719083							
ZPE= -323.353921							
Enthalpy= -323.347923							
C	-1.14254	-0.72168	-				
0.00022							

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			

Pyridine N-oxide

The number of imaginary frequencies: 0
 Total Energy (M06/6-311G+(d,p))= -
 323.30740415
 ZPE= -323.215418
 Enthalpy= -323.209346

C	0.28383	-1.18039	-
0.00018			
C	-1.0993	-1.19457	-
0.00009			
C	-1.82223	0.	0.00012
C	-1.0993	1.19457	
0.00024			
C	0.28383	1.18039	
0.00014			
N	0.98715	0.	-0.00007
H	-2.90656	0.	0.0002
H	0.91434	-2.05915	-
0.00034			
H	-1.60306	-2.15628	-
0.00019			
H	-1.60306	2.15628	
0.00041			
H	0.91434	2.05915	
0.00022			
O	2.26164	0.	-0.00015

Pyridine N-oxide

The number of imaginary frequencies: 0
 Total Energy (B3PW91/6-31G*)= -
 323.32403049
 ZPE= -323.23042
 Enthalpy= -323.224425

C	-1.14254	-0.72168	-
0.00022			
C	-1.19865	0.67327	-
0.00012			
C	0.00025	1.38544	0.0001
C	1.19889	0.67286	
0.00022			
C	1.14228	-0.72207	
0.00012			
N	-0.00025	-1.42094	-
0.0001			
H	0.00041	2.47232	
0.00016			
H	-2.05996	-1.30855	-
0.00037			
H	-2.15768	1.18294	-
0.00023			
H	2.15812	1.18216	
0.00036			
H	2.05949	-1.30926	
0.00019			
O	-0.00048	-2.78094	-
0.0002			

Pyridine N-oxide

The number of imaginary frequencies: 0
 Total Energy (B3PW91/6-31G**)= -
 323.33143154
 ZPE= -323.237998
 Enthalpy= -323.231997

C	-1.14254	-0.72168	-
0.00022			
C	-1.19865	0.67327	-
0.00012			
C	0.00025	1.38544	0.0001

C	1.19889	0.67286
0.00022		
C	1.14228	-0.72207
0.00012		
N	-0.00025	-1.42094 -
0.0001		
H	0.00041	2.47232
0.00016		
H	-2.05996	-1.30855 -
0.00037		
H	-2.15768	1.18294 -
0.00023		
H	2.15812	1.18216
0.00036		
H	2.05949	-1.30926
0.00019		
O	-0.00048	-2.78094 -
0.0002		

Pyridine N-oxide

The number of imaginary frequencies: 0
 Total Energy (B3PW91/6-311G+(d,p))= -
 323.40973925
 ZPE= -323.316995
 Enthalpy= -323.310954

C	-1.14254	-0.72168 -
0.00022		
C	-1.19865	0.67327 -
0.00012		
C	0.00025	1.38544 0.0001
C	1.19889	0.67286
0.00022		
C	1.14228	-0.72207
0.00012		
N	-0.00025	-1.42094 -
0.0001		
H	0.00041	2.47232
0.00016		

H	-2.05996	-1.30855 -
0.00037		
H	-2.15768	1.18294 -
0.00023		
H	2.15812	1.18216
0.00036		
H	2.05949	-1.30926
0.00019		
O	-0.00048	-2.78094 -
0.0002		

Pyridine N-oxide

The number of imaginary frequencies: 0
 Total Energy (Hartree Fock 6-31G*)= -
 321.47376757
 ZPE= -321.373766
 Enthalpy= -321.36815

C	-2.16262	0.83539 -
0.00001		
C	-0.76123	0.85701 -
0.0001		
C	-0.09527	2.08267 -
0.0003		
C	-0.84878	3.25654 -
0.0004		
C	-2.24802	3.17597 -
0.0003		
N	-2.86495	1.98161 -
0.00011		
H	0.97402	2.12168 -
0.00036		
H	-2.67825	-0.10217
0.00014		
H	-0.2072	-0.05839 -
0.00002		
H	-0.36294	4.20988 -
0.00054		
H	-2.83061	4.07346 -
0.00038		

O -4.22404 1.93202 -
0.00002

1-aza-1,5-cyclohexadiene
The number of imaginary frequencies: 0
Total Energy (B3LYP/6-31G*)= -
249.45870093
ZPE= -249.347657
Enthalpy= -249.341681

C 0.37908 1.18845 -
0.18375

C -0.93979 1.31014 -
0.04061

C -1.79539 0.11421
0.2909

C -1.13588 -1.1706 -
0.23762

C 0.3445 -1.18968
0.01706

N 1.05209 -0.08239 -
0.00258

H -1.92356 0.06011
1.38332

H 1.08605 1.9818 -
0.38487

H -1.39333 2.29399 -
0.12646

H -1.59346 -2.05336
0.22159

H 0.91659 -2.09979
0.14684

H -2.79905 0.22722 -
0.13304

H -1.32822 -1.25515 -
1.32117

1-aza-1,5-cyclohexadiene
The number of imaginary frequencies: 0
Total Energy (M06/6-311G+(d,p))= -
249.32863153
ZPE= -249.218936

Enthalpy= -249.212941

C -1.30685 0.51792
0.11675

C -0.27511 1.37255
0.04709

C 1.11229 0.84984 -
0.23605

C 1.22763 -0.59801
0.26603

C -0.02081 -1.37997 -
0.08674

N -1.19517 -0.8713 -
0.13781

H 1.31265 0.89812 -
1.31938

H -2.32199 0.85394
0.31067

H -0.43782 2.44245
0.15038

H 2.11889 -1.09531 -
0.13119

H 0.07163 -2.44909 -
0.2945

H 1.87305 1.47698
0.24204

H 1.32686 -0.60202
1.36419

1-aza-1,5-cyclohexadiene N-oxide
The number of imaginary frequencies: 0
Total Energy (B3LYP/6-31G*)= -
324.62216936
ZPE= -324.506535
Enthalpy= -324.499747

C -0.19281 -0.39727
0.27347

C 1.1456 -0.49899
0.07719

C 1.99666 0.77312
0.13746

C	1.21655	1.94232	-
0.47833			
C	-0.18847	2.02146	
0.14144			
N	-0.83095	0.92792	
0.43008			
H	2.21505	0.98053	
1.16419			
H	-0.78986	-1.28358	
0.32721			
H	1.60067	-1.4521	-
0.09428			
H	1.75709	2.84856	-
0.30104			
H	-0.64579	2.97332	
0.31379			
H	2.91098	0.64255	-
0.40279			
H	1.10658	1.79106	-
1.53186			
O	-2.11604	1.00378	
0.86871			

1-aza-1,5-cyclohexadiene N-oxide

The number of imaginary frequencies: 0
 Total Energy (M06/6-311G+(d,p))= -324.48401976
 ZPE= -324.369799
 Enthalpy= -324.362988

C	0.37908	1.18845	-
0.18375			
C	-0.93979	1.31014	-
0.04061			
C	-1.79539	0.11421	
0.2909			
C	-1.13588	-1.1706	-
0.23762			
C	0.3445	-1.18968	
0.01706			

N	1.05209	-0.08239	-
0.00258			
H	-1.92356	0.06011	
1.38332			
H	1.08605	1.9818	-
0.38487			
H	-1.39333	2.29399	-
0.12646			
H	-1.59346	-2.05336	
0.22159			
H	0.91659	-2.09979	
0.14684			
H	-2.79905	0.22722	-
0.13304			
H	-1.32822	-1.25515	-
1.32117			
O	2.3194	-0.01165	
0.14449			

1-aza-1,3-cyclohexadiene

The number of imaginary frequencies: 0
 Total Energy (B3LYP/6-31G*)= -249.45863067
 ZPE= -249.347311
 Enthalpy= -249.341338

C	0.12247	1.41622	
0.05956			
C	1.28988	0.50759	-
0.23369			
C	0.98654	-0.92084	
0.24342			
C	-1.28937	-0.54996	-
0.11523			
C	-1.112	0.89422	
0.11551			
H	1.72373	-1.62288	-
0.15981			
H	1.48855	0.51894	-
1.31824			

H	2.20622	0.8724
0.24574		
H	0.29014	2.48606
0.16604		
H	-2.30108	-0.91108 -
0.32081		
H	-1.99297	1.50892
0.28168		
H	1.07631	-0.96859
1.34059		
N	-0.35371	-1.42388 -
0.09324		

1-aza-1,3-cyclohexadiene

The number of imaginary frequencies: 0
 Total Energy (M06/6-311G+(d,p))= -
 249.32790699
 ZPE= -249.217931
 Enthalpy= -249.211943

C	0.05418	1.40668
0.05834		
C	1.24473	0.55694 -
0.25474		
C	1.02053	-0.85133
0.26701		
C	-1.24639	-0.61173 -
0.12628		
C	-1.14633	0.82804
0.13011		
H	1.8113	-1.52571 -
0.07494		
H	1.39612	0.54363 -
1.34672		
H	2.16095	0.97686
0.17378		
H	0.16962	2.48184
0.1697		
H	-2.23358	-1.01981 -
0.36247		

H	-2.05155	1.3979
0.31667		
H	1.07007	-0.84637
1.36887		
N	-0.26904	-1.42569 -
0.09879		

1-aza-1,3-cyclohexadiene N-oxide

The number of imaginary frequencies: 0
 Total Energy (B3LYP/6-31G*)= -
 324.63277973
 ZPE= -324.516577
 Enthalpy= -324.509843

C	0.6267	1.31775	0.03798
C	1.42079	0.06392 -	
0.21697			
C	0.65931	-1.17255	
0.28757			
C	-1.42639	0.03063 -	
0.04753			
C	-0.75579	1.24484	
0.09511			
H	1.13967	-2.09446 -	
0.05729			
H	1.62495	-0.05519 -	
1.29413			
H	2.39981	0.10172	
0.27882			
H	1.14155	2.26987	
0.12251			
H	-2.50727	-0.04326 -	
0.0897			
H	-1.35127	2.14476	
0.22445			
H	0.67434	-1.17434	
1.39069			
N	-0.71792	-1.15182 -	
0.21393			
O	-1.42449	-2.28268	
0.05349			

1-aza-1,3-cyclohexadiene N-oxide

The number of imaginary frequencies: 0

Total Energy (M06/6-311G+(d,p))= -324.49391803

ZPE= -324.379107

Enthalpy= -324.372359

C	1.82733	0.14558
0.02194		
C	1.14609	-1.17099 -
0.25112		
C	-0.28121	-1.17587
0.29827		
C	-0.36318	1.22259 -
0.05323		
C	1.0764	1.26062
0.08901		
H	-0.89464	-1.97468 -
0.11745		
H	1.13042	-1.35737 -
1.33734		
H	1.69393	-2.0095
0.19419		
H	2.90984	0.18604
0.09445		
H	-0.97065	2.10895 -
0.1874		
H	1.52776	2.2399
0.22214		
H	-0.28773	-1.26345
1.39158		
N	-1.03086	0.08546 -
0.0064		
O	-2.29069	-0.02746 -
0.10557		

1-aza-2,4-cyclohexadiene

The number of imaginary frequencies: 0

Total Energy (B3LYP/6-31G*)= -249.45167887

ZPE= -249.340348

Enthalpy= -249.334173

C	-2.30401	-1.31125
0.62248		
C	-1.05536	-1.80673 -
0.13119		
C	-0.1519	-0.90396 -
0.56671		
C	-0.45591	0.58853 -
0.38571		
C	-1.70425	0.97052 -
0.02491		
N	-2.78378	-0.0306
0.06441		
H	0.7636	-1.22337 -
1.01919		
H	-3.08856	-2.03408
0.53947		
H	-0.89672	-2.85296 -
0.28972		
H	0.30693	1.32027 -
0.55163		
H	-1.91192	2.00101
0.17478		
H	-3.51227	0.31062
0.65844		
H	-2.04402	-1.17826
1.65186		

1-aza-2,4-cyclohexadiene

The number of imaginary frequencies: 0

Total Energy (M06/6-311G+(d,p))= -249.32709401

ZPE= -249.216903

Enthalpy= -249.210703

C	1.39067	0.19943
0.18922		
C	0.43142	1.33873 -
0.08369		
C	-0.89712	1.12767 -
0.05346		

C	-1.43794	-0.21217	
0.11795			
C	-0.58177	-1.25494	
0.00288			
N	0.76669	-1.06151	-0.224
H	-1.58545	1.95708	-
0.20181			
H	2.32173	0.32422	-
0.37781			
H	0.84949	2.32853	-
0.24406			
H	-2.50207	-0.38075	
0.23128			
H	-0.91262	-2.28996	
0.00251			
H	1.35338	-1.87985	-
0.14273			
H	1.67716	0.17896	
1.26318			

1-aza-2,4-cyclohexadiene N-oxide

The number of imaginary frequencies: 0
 Total Energy (B3LYP/6-31G*)= -324.57303945
 ZPE= -324.457626
 Enthalpy= -324.450823

C	-0.28085	-1.18491	-
0.26375			
C	1.22585	-1.16982	
0.04782			
C	1.87146	0.01417	
0.06584			
C	1.05357	1.3002	-
0.11439			
C	-0.29787	1.24445	-
0.02711			
N	-0.96005	-0.02079	
0.34208			
H	2.93331	0.0551	
0.19119			

H	-0.39958	-1.15661	-
1.32677			
H	1.75565	-2.08257	
0.22415			
H	1.54544	2.23312	-
0.29502			
H	-0.88229	2.12337	-
0.20277			
H	-0.72605	-2.07669	
0.12537			
O	-2.25038	-0.0092	-
0.08746			
H	-0.93599	-0.10124	
1.33855			

1-aza-2,4-cyclohexadiene N-oxide

The number of imaginary frequencies: 0
 Total Energy (M06/6-311G+(d,p))= -324.44453052
 ZPE= 324.329983
 Enthalpy= -324.323224

C	-0.24836	-1.20084	-
0.26519			
C	1.22684	-1.15818	
0.03638			
C	1.84678	0.03148	
0.10207			
C	1.07425	1.2597	-
0.11747			
C	-0.26053	1.24207	-
0.05667			
N	-0.97969	-0.00998	
0.31366			
H	2.91511	0.10598	
0.28375			
H	-0.46106	-1.14334	-
1.34039			
H	1.76833	-2.09344	
0.14919			

H	1.59192	2.18676	-
0.34905			
H	-0.95202	2.06128	-
0.20094			
H	-0.76377	-2.07453	
0.13585			
O	-2.27625	0.00994	-
0.05223			
H	-0.86456	-0.09778	
1.34905			

Pyridinium

The number of imaginary frequencies: 0
 Total Energy (B3LYP/6-31G*)= -
 248.65697731
 ZPE= -248.553721
 Enthalpy= -248.548407

C	-0.03244	-0.6621	
1.23589			
C	-0.00269	0.69287	
1.26532			
C	0.00936	1.47622	-
0.05326			
C	-0.01009	0.79169	-
1.21517			
C	-0.04363	-0.74752	-
1.18302			
N	-0.05324	-1.38613	-
0.05082			
H	0.03277	2.54596	-
0.05137			
H	-0.04093	-1.21208	
2.15368			
H	0.01227	1.21173	
2.20098			
H	-0.00229	1.31275	-
2.14969			
H	-0.05917	-1.29655	-
2.10129			

H	-0.07511	-2.38589	-
0.05126			

Pyridinium

The number of imaginary frequencies: 0
 Total Energy (M06/6-311G+(d,p))= -
 248.51713791
 ZPE= -248.415283
 Enthalpy= -248.409911

C	-0.67805	1.18452	0.
C	0.70573	1.2185	0.
C	1.41588	0.01296	0.
C	0.72825	-1.20555	0.
C	-0.65595	-1.19671	0.
N	-1.30935	-0.01185	0.
H	2.50153	0.02298	0.
H	-1.30651	2.06722	0.
H	1.21529	2.17534	0.
H	1.25524	-2.15289	0.
H	-1.26803	-2.09086	0.
H	-2.32731	-0.0212	0.

1-hydroxy-Pyridine

The number of imaginary frequencies: 0
 Total Energy (B3LYP/6-31G*)= -
 323.81123177
 ZPE= -323.70567
 Enthalpy= -323.699038

C	-1.16523	-0.8132	
0.03587			
C	-1.21205	0.72488	-
0.02244			
C	-0.05685	1.42088	-
0.03123			
C	1.26901	0.65134	
0.01742			
C	1.25249	-0.70323	
0.06791			

N	-0.02711	-1.43997	
0.07636			
H	-0.06515	2.49009	-
0.0714			
H	-2.07813	-1.3713	
0.04312			
H	-2.1514	1.23618	-
0.05563			
H	2.19958	1.17946	
0.01156			
H	2.17539	-1.2436	
0.10195			
O	-0.01475	-2.79896	
0.12744			
H	0.77863	-3.1281	-
0.30128			

1-hydroxy-Pyridine

The number of imaginary frequencies: 0
 Total Energy (M06/6-311G+(d,p))= -
 323.66548298
 ZPE= -323.560957
 Enthalpy= -323.554271

C	0.23341	1.19246	-
0.00621			
C	-1.15148	1.2099	
0.00375			
C	-1.85266	0.00002	
0.01094			
C	-1.15151	-1.2099	
0.00332			
C	0.23337	-1.1925	-
0.00605			
N	0.8679	0.00001	
0.00682			
H	-2.93802	0.00004	
0.0132			
H	0.87049	2.06819	-
0.03361			

H	-1.6652	2.16469	-
0.00291			
H	-1.66533	-2.16463	-
0.00298			
H	0.87062	-2.06813	-
0.03229			
O	2.24805	-0.0001	-
0.10418			
H	2.60097	0.00066	
0.80976			

3-cyano-Pyridine

The number of imaginary frequencies: 0
 Total Energy (B3LYP/6-31G*)= -
 340.52598067
 ZPE= -340.438405
 Enthalpy= -340.431459

C	-3.05562	-2.66599	-
0.00376			
C	-1.65433	-2.64359	
0.01081			
C	-0.98909	-1.41677	0.011
0.00339			
C	-1.74292	-0.24238	-
0.00339			
C	-3.14204	-0.32347	-
0.0176			
N	-3.75522	-1.51899	-
0.01742			
H	0.08013	-1.37726	
0.02198			
H	-3.57194	-3.60317	-
0.00399			
H	-1.25726	0.71105	-
0.00357			
H	-3.72602	0.57305	-
0.02868			
C	-0.85613	-3.9605	
0.02645			
N	-0.26184	-4.94099	
0.03809			

3-cyano-Pyridine

The number of imaginary frequencies: 0

Total Energy (M06/6-311G+(d,p))= -340.3605528

ZPE= -340.273929

Enthalpy= -340.266949

C	0.12048	-1.18974	0.
C	-0.59443	0.0218	0.
C	0.12883	1.2242	0.
C	1.5174	1.15859	0.
C	2.1282	-0.0978	0.
N	1.45178	-1.25419	0.
H	-0.39357	2.1756	0.
H	-0.41672	-2.13554	0.
H	2.11898	2.06197	0.
H	3.21325	-0.18147	0.
C	-2.02657	0.01677	0.
N	-3.18969	0.00799	0.

3-cyano-Pyridine N-oxide

The number of imaginary frequencies: 0

Total Energy (B3LYP/6-31G*)= -415.68426162

ZPE= -415.592623

Enthalpy= -415.584834

C	0.06948	-0.91129	0.
C	-0.91135	0.07723	0.
C	-0.55674	1.43507	0.
C	0.80257	1.74355	0.
C	1.75609	0.74304	0.
N	1.40225	-0.58791	0.
H	-1.31838	2.2051	0.
H	-0.13164	-1.97347	0.
H	1.13791	2.77546	0.
H	2.82567	0.90402	0.

O	2.28982	-1.49665	0.
C	-2.28998	-0.32043	0.
N	-3.40976	-0.63222	0.

3-cyano-Pyridine N-oxide

The number of imaginary frequencies: 0

Total Energy (M06/6-311G+(d,p))= -415.51038779

ZPE= -415.419669

Enthalpy= -415.411843

C	0.	0.91394	0.
C	0.90284	-0.14628	0.
C	0.44603	-1.47324	0.
C	-0.93279	-1.6775	0.
C	-1.8075	-0.6074	0.
N	-1.3535	0.69281	0.
H	1.14694	-2.29894	0.
H	0.28128	1.95775	0.
H	-1.3456	-2.68092	0.
H	-2.88622	-0.6866	0.
O	-2.16942	1.66639	0.
C	2.30771	0.14542	0.
N	3.44795	0.37118	0.

4-cyano-Pyridine

The number of imaginary frequencies: 0

Total Energy (B3LYP/6-31G*)= -340.52459398

ZPE= -340.437063

Enthalpy= -340.430124

C	-0.40029	-0.58541	-0.01707
C	1.00108	-0.56384	-0.01753
C	1.66703	0.66249	-0.00048

C	0.9138	1.83722	
0.01661			
C	-0.48544	1.75697	
0.01624			
N	-1.0993	0.56192	-0.0004
H	-0.91715	-1.5222	-
0.03009			
H	1.55521	-1.47908	-
0.03083			
H	1.4	2.79028	0.02988
H	-1.06896	2.65376	
0.02929			
C	3.20602	0.71843	-
0.00052			
N	4.35186	0.76015	-
0.00055			

4-cyano-Pyridine

The number of imaginary frequencies: 0
 Total Energy (M06/6-311G+(d,p))= -
 340.35906587
 ZPE= -340.272444
 Enthalpy= -340.265476

C	-1.50627	1.14355	0.
C	-0.11359	1.20613	0.
C	0.60141	0.	0.
C	-0.11359	-1.20613	0.
C	-1.50627	-1.14355	0.
N	-2.20212	0.	0.
H	-2.0922	2.06068	0.
H	0.40392	2.15925	0.
H	0.40392	-2.15925	0.
H	-2.0922	-2.06068	0.
C	2.03706	0.	0.
N	3.19985	0.	0.

4-cyano-Pyridine N-oxide

The number of imaginary frequencies: 0
 Total Energy (B3LYP/6-31G*)= -
 415.68843336
 ZPE= -415.596614
 Enthalpy= -415.588847

C	-0.40024	-0.58449	-
0.00878			
C	1.00116	-0.56304	-
0.00932			
C	1.66727	0.66251	-
0.0006			
C	0.91391	1.83643	
0.00824			
C	-0.48534	1.75604	
0.00828			
N	-1.1024	0.56179	-
0.00007			
H	-0.91597	-1.52195	-
0.01535			
H	1.55505	-1.47847	-
0.01634			
H	1.39987	2.7897	
0.01492			
H	-1.0678	2.65359	0.015
O	-2.4615	0.51237	
0.00034			
C	3.20624	0.71849	-
0.00069			
N	4.3521	0.76008	-
0.00076			

4-cyano-Pyridine N-oxide

The number of imaginary frequencies: 0
 Total Energy (M06/6-311G+(d,p))= -
 415.51409429
 ZPE= -415.423306
 Enthalpy= -415.415492

C	1.04962	-1.18413
0.00001		
C	-0.32757	-1.20253
0.00001		

C	-1.0566	0.00001	0.
C	-0.32757	1.20254	
0.00001			
C	1.04963	1.18413	
0.00001			
N	1.75342	0.	0.
H	1.67902	-2.06362	0.
H	-0.83939	-2.1586	
0.00001			
H	-0.83938	2.15861	
0.00001			
H	1.67903	2.06361	
0.00001			
O	3.02055	-0.00001	-
0.00002			
C	-2.48419	0.00001	0.
N	-3.64821	-0.00001	-
0.00001			

2-hydroxy-Pyridine

The number of imaginary frequencies: 0
 Total Energy (B3LYP/6-31G*)= -323.51588142
 ZPE= -323.422209
 Enthalpy= -323.41607

C	-1.70067	-0.65433	-
0.00164			
C	-0.29927	-0.63503	-
0.00012			
C	0.36866	0.59034	
0.00169			
C	-0.38269	1.76641	
0.00194			
C	-1.78206	1.68842	
0.00038			
N	-2.39784	0.49424	-
0.00135			

H	1.43801	0.62749	
0.00287			
H	-2.21904	-1.59038	-
0.00303			
H	0.25339	-1.55125	-
0.00035			
H	0.10505	2.71878	
0.00331			
O	-2.55997	2.88832	
0.00062			
H	-2.73308	3.15764	-
0.90442			

2-hydroxy-Pyridine

The number of imaginary frequencies: 0
 Total Energy (M06/6-311G+(d,p))= -323.38753442
 ZPE= -323.294564
 Enthalpy= -323.288361

C	0.99985	-1.22953	-
0.00002			
C	1.81732	-0.10489	
0.00009			
C	1.20135	1.15327	-
0.00008			
C	-0.18351	1.23798	-
0.00002			
C	-0.90375	0.03356	-
0.00003			
N	-0.34147	-1.17223	-
0.00006			
H	1.80054	2.05994	-
0.00002			
H	1.42872	-2.22994	-
0.00004			
H	2.89752	-0.20675	
0.00025			
H	-0.71092	2.18538	
0.00005			

O -2.25708 0.08689
0.00006
H -2.55648 -0.84043
0.00002

2-carboxy-Pyridine

The number of imaginary frequencies: 0
Total Energy (B3LYP/6-31G*)= -
436.85938679
ZPE= -436.755087
Enthalpy= -436.747324

C 1.7186 -1.23797
0.00032
C 2.53278 -0.10114
0.00033
C 1.92424 1.15289
0.00015
C 0.53308 1.21892 -
0.00005
C -0.18796 0.01996 -
0.00008
N 0.38442 -1.19228
0.00013
H 2.52032 2.06116
0.00016
H 2.16171 -2.23235
0.00045
H 3.61395 -0.20322
0.00048
H -0.00286 2.16117 -
0.00018
C -1.68567 0.10587 -
0.00023
O -2.29595 1.15768 -
0.00036
O -2.29682 -1.09449 -
0.00017
H -1.63544 -1.79032 -
0.00013

2-carboxy-Pyridine

The number of imaginary frequencies: 0
Total Energy (M06/6-311G+(d,p))= -
436.70529032
ZPE= -436.601643
Enthalpy= -436.593822

C 1.66966 -1.23606
0.00031
C 2.5029 -0.11529
0.00033
C 1.92164 1.1535
0.00015
C 0.53216 1.25801 -
0.00006
C -0.21239 0.07885 -
0.00007
N 0.33633 -1.14606
0.00012
H 2.54217 2.04515
0.00016
H 2.08563 -2.24104
0.00045
H 3.5813 -0.23965
0.00049
H 0.0157 2.2112 -
0.00021
C -1.7219 0.1194 -
0.00029
O -2.3546 1.15072 -
0.00031
O -2.29271 -1.09554 -
0.00018
H -1.55305 -1.74509 -
0.0001

2-carboxy-Pyridine N-oxide

The number of imaginary frequencies: 0
Total Energy (B3LYP/6-31G*)= -
512.02448163
ZPE= -511.916422
Enthalpy= -511.907975

C	1.66966	-1.23606	
0.00031			
C	2.5029	-0.11529	
0.00033			
C	1.92164	1.1535	
0.00015			
C	0.53216	1.25801	-
0.00006			
C	-0.21239	0.07885	-
0.00007			
N	0.33633	-1.14606	
0.00012			
H	2.54217	2.04515	
0.00016			
H	2.08563	-2.24104	
0.00045			
H	3.5813	-0.23965	
0.00049			
H	0.0157	2.2112	-
0.00021			
C	-1.7219	0.1194	-
0.00029			
O	-2.3546	1.15072	-
0.00031			
O	-2.29271	-1.09554	-
0.00018			
H	-1.55305	-1.74509	-
0.0001			
O	-0.44112	-2.26194	
0.0001			

2-carboxy-Pyridine N-oxide

The number of imaginary frequencies: 0
 Total Energy (M06/6-311G+(d,p))= -511.8594662
 ZPE= -511.752215
 Enthalpy= -511.743647

C	-1.77734	1.02321	0.0003
C	-2.55957	-0.11467	
0.0003			

C	-1.9576	-1.37621	
0.00013			
C	-0.57036	-1.43871	-
0.00004			
C	0.2062	-0.28216	-
0.00005			
N	-0.41282	0.94794	
0.00012			
H	-2.55597	-2.28072	
0.00014			
H	-2.15273	2.03761	
0.00042			
H	-3.63859	-0.00061	
0.00045			
H	-0.02807	-2.37719	-
0.00017			
C	1.71727	-0.41024	-
0.0002			
O	2.21834	-1.515	-
0.00038			
O	2.41535	0.71685	-
0.00026			
H	1.76035	1.48162	-
0.00011			
O	0.26045	2.0602	
0.00011			

2-Pyridone

The number of imaginary frequencies: 0
 Total Energy (B3LYP/6-31G*)= -323.51790653
 ZPE= -323.424021
 Enthalpy= -323.417805

C	-1.8924	0.68529	
0.13687			
C	-0.46108	0.93021	-
0.35424			
C	-0.02365	2.19097	-
0.49075			

C	-0.92536	3.34888	-
0.05024			
C	-2.11117	3.11354	
0.57158			
N	-2.74047	1.77228	
0.67189			
H	0.94411	2.38593	-
0.90345			
H	0.17358	0.10651	-
0.60648			
H	-0.60593	4.35708	-
0.21275			
H	-2.60985	3.94024	
1.03287			
O	-2.37024	-0.47619	
0.05803			
H	-3.58952	1.74449	
0.1443			

2-Pyridone

The number of imaginary frequencies: 0
 Total Energy (M06/6-311G+(d,p))= -
 323.38844194
 ZPE= -323.295431
 Enthalpy= -323.289162

C	-1.06793	0.06468	
0.00025			
C	-0.24816	1.26434	-
0.00034			
C	1.11647	1.20264	
0.00011			
C	1.80662	-0.04718	
0.00008			
C	1.06195	-1.18969	-
0.00016			
N	-0.30094	-1.12399	
0.00007			
H	1.6948	2.12371	
0.00041			

H	-0.78218	2.20802	-
0.0001			
H	2.8886	-0.09729	
0.00004			
H	1.49261	-2.18554	-
0.00043			
O	-2.29317	0.00283	-
0.00003			
H	-0.85557	-1.97241	
0.00023			

Piperidine

The number of imaginary frequencies: 0
 Total Energy (B3LYP/6-31G*)= -
 251.90382822
 ZPE= -251.744054
 Enthalpy= -251.737514

C	0.80382	-0.90026	
0.03176			
C	1.37062	0.53089	-
0.01985			
C	0.84842	1.31759	
1.18814			
C	-0.68376	1.33307	
1.13349			
C	-1.20021	-0.11774	
1.15683			
H	2.43973	0.49715	
0.00788			
H	1.12156	-1.37685	
0.93553			
H	1.16457	-1.4533	-
0.81021			
H	1.17087	0.84406	
2.09185			
H	1.22361	2.31925	
1.15976			
H	-1.0683	1.86694	1.9773
H	-1.00586	1.81248	
0.23275			

H	-0.87764	-0.59622	
2.05788			
H	-2.26948	-0.1124	
1.11767			
H	1.05345	1.00837	-
0.92335			
N	-0.67191	-0.8579	-
0.00685			
H	-0.96641	-0.40343	-
0.84752			

Piperidine

The number of imaginary frequencies: 0
 Total Energy (M06/6-311G+(d,p))= -
 251.7736967
 ZPE= -251.616109
 Enthalpy= -251.609536

C	0.00832	-0.79156	
1.21662			
C	0.00832	0.74696	1.2659
C	-0.63986	1.33068	0.
C	0.00832	0.74696	-
1.2659			
C	0.00832	-0.79156	-
1.21662			
H	-0.51435	1.09782	
2.1661			
H	-1.02808	-1.15594	
1.27119			
H	0.53487	-1.20911	
2.08319			
H	-1.71252	1.08526	0.
H	-0.57077	2.4258	0.
H	-0.51435	1.09782	-
2.1661			
H	1.04647	1.10377	-
1.34443			
H	-1.02808	-1.15594	-
1.27119			

H	0.53487	-1.20911	-
2.08319			
H	1.04647	1.10377	
1.34443			
N	0.60573	-1.35515	0.
H	1.60481	-1.14691	0.

Piperidine

The number of imaginary frequencies: 0
 Total Energy (B3PW91/6-31G*)= -
 251.8164414
 ZPE= -251.656285
 Enthalpy= -251.649749

C	0.80382	-0.90026	
0.03176			
C	1.37062	0.53089	-
0.01985			
C	0.84842	1.31759	
1.18814			
C	-0.68376	1.33307	
1.13349			
C	-1.20021	-0.11774	
1.15683			
H	2.43973	0.49715	
0.00788			
H	1.12156	-1.37685	
0.93553			
H	1.16457	-1.4533	-
0.81021			
H	1.17087	0.84406	
2.09185			
H	1.22361	2.31925	
1.15976			
H	-1.0683	1.86694	1.9773
H	-1.00586	1.81248	
0.23275			
H	-0.87764	-0.59622	
2.05788			

H	-2.26948	-0.1124	
1.11767			
H	1.05345	1.00837	-
0.92335			
N	-0.67191	-0.8579	-
0.00685			
H	-0.96641	-0.40343	-
0.84752			

H	-2.26948	-0.1124	
1.11767			
H	1.05345	1.00837	-
0.92335			
N	-0.67191	-0.8579	-
0.00685			
H	-0.96641	-0.40343	-
0.84752			

Piperidine

The number of imaginary frequencies: 0
 Total Energy (B3PW91/6-31G**) = -251.832313
 ZPE = -251.672731
 Enthalpy = -251.666174

C	0.80382	-0.90026	
0.03176			
C	1.37062	0.53089	-
0.01985			
C	0.84842	1.31759	
1.18814			
C	-0.68376	1.33307	
1.13349			
C	-1.20021	-0.11774	
1.15683			
H	2.43973	0.49715	
0.00788			
H	1.12156	-1.37685	
0.93553			
H	1.16457	-1.4533	-
0.81021			
H	1.17087	0.84406	
2.09185			
H	1.22361	2.31925	
1.15976			
H	-1.0683	1.86694	1.9773
H	-1.00586	1.81248	
0.23275			
H	-0.87764	-0.59622	
2.05788			

Piperidine

The number of imaginary frequencies: 0
 Total Energy (B3PW91/6-311G+(d,p)) = -251.88472135
 ZPE = -251.726148
 Enthalpy = -251.719542

C	0.80382	-0.90026	
0.03176			
C	1.37062	0.53089	-
0.01985			
C	0.84842	1.31759	
1.18814			
C	-0.68376	1.33307	
1.13349			
C	-1.20021	-0.11774	
1.15683			
H	2.43973	0.49715	
0.00788			
H	1.12156	-1.37685	
0.93553			
H	1.16457	-1.4533	-
0.81021			
H	1.17087	0.84406	
2.09185			
H	1.22361	2.31925	
1.15976			
H	-1.0683	1.86694	1.9773
H	-1.00586	1.81248	
0.23275			
H	-0.87764	-0.59622	
2.05788			

H	-2.26948	-0.1124	
1.11767			
H	1.05345	1.00837	-
0.92335			
N	-0.67191	-0.8579	-
0.00685			
H	-0.96641	-0.40343	-
0.84752			

Piperidine N-oxide

The number of imaginary frequencies: 0
 Total Energy (B3LYP/6-31G*)= -
 327.0440554
 ZPE= -326.879636
 Enthalpy= -326.872325

C	0.80347	-0.89926	
0.03148			
C	1.37057	0.53182	-
0.01909			
C	0.84895	1.31772	
1.18899			
C	-0.68267	1.33355	
1.13361			
C	-1.19976	-0.11706	
1.15609			
H	2.43967	0.49773	
0.00868			
H	1.12103	-1.37637	
0.93504			
H	1.16483	-1.45127	-
0.8109			
H	1.17105	0.84358	
2.0925			
H	1.2245	2.31927	
1.16133			
H	-1.06737	1.86712	
1.97753			
H	-1.00423	1.81349	
0.23297			

H	-0.87757	-0.59598	
2.05705			
H	-2.26903	-0.11045	
1.11688			
H	1.05356	1.00998	-
0.92229			
N	-0.67284	-0.85879	-
0.00789			
H	-0.96914	-0.40744	-
0.84961			
O	-1.15312	-2.13083	
0.02136			

Piperidine N-oxide

The number of imaginary frequencies: 0
 Total Energy (M06/6-311G+(d,p))= -
 326.91190613
 ZPE= -326.749232
 Enthalpy= -326.741974

C	0.09165	0.39957	
1.23954			
C	0.09165	-1.13015	
1.26347			
C	0.74857	-1.7078	0.
C	0.09165	-1.13015	-
1.26347			
C	0.09165	0.39957	-
1.23954			
H	0.61246	-1.47217	
2.16602			
H	1.10029	0.82154	
1.22377			
H	-0.44991	0.84998	
2.07398			
H	1.81803	-1.45531	0.
H	0.68088	-2.80185	0.
H	0.61246	-1.47217	-
2.16602			

H	-0.9413	-1.49953	-
1.34587			
H	1.10029	0.82154	-
1.22377			
H	-0.44991	0.84998	-
2.07398			
H	-0.9413	-1.49953	
1.34587			
N	-0.56273	0.96836	0.
H	-1.53432	0.59157	0.
O	-0.54495	2.31266	0.

Piperidine N-oxide

The number of imaginary frequencies: 0
 Total Energy (B3PW91/6-31G*)= -326.92875651
 ZPE= -326.763861
 Enthalpy= -326.756572

C	0.09302	0.39957	
1.23188			
C	0.09302	-1.12482	1.258
C	0.74921	-1.70012	0.
C	0.09302	-1.12482	-1.258
C	0.09302	0.39957	-
1.23188			
H	0.61267	-1.46598	
2.16164			
H	1.10203	0.82206	
1.21291			
H	-0.44526	0.85182	
2.06809			
H	1.81835	-1.44562	0.
H	0.68408	-2.79446	0.
H	0.61267	-1.46598	-
2.16164			
H	-0.93988	-1.49501	-
1.34041			

H	1.10203	0.82206	-
1.21291			
H	-0.44526	0.85182	-
2.06809			
H	-0.93988	-1.49501	
1.34041			
N	-0.56203	0.96462	0.
H	-1.52969	0.57835	0.
O	-0.55316	2.29841	0.

Piperidine N-oxide

The number of imaginary frequencies: 0
 Total Energy (B3PW91/6-31G**)= -326.94396243
 ZPE= -326.779742
 Enthalpy= -326.772426

C	0.80347	-0.89926	
0.03148			
C	1.37057	0.53182	-
0.01909			
C	0.84895	1.31772	
1.18899			
C	-0.68267	1.33355	
1.13361			
C	-1.19976	-0.11706	
1.15609			
H	2.43967	0.49773	
0.00868			
H	1.12103	-1.37637	
0.93504			
H	1.16483	-1.45127	-
0.8109			
H	1.17105	0.84358	
2.0925			
H	1.2245	2.31927	
1.16133			
H	-1.06737	1.86712	
1.97753			

H	-1.00423	1.81349
0.23297		
H	-0.87757	-0.59598
2.05705		
H	-2.26903	-0.11045
1.11688		
H	1.05356	1.00998 -
0.92229		
N	-0.67284	-0.85879 -
0.00789		
H	-0.96914	-0.40744 -
0.84961		
O	-1.15312	-2.13083
0.02136		

Piperidine N-oxide

The number of imaginary frequencies: 0
 Total Energy (B3PW91/6-311G+(d,p))= -
 327.02772616
 ZPE= -326.863969
 Enthalpy= -326.856636

C	0.80347	-0.89926
0.03148		
C	1.37057	0.53182 -
0.01909		
C	0.84895	1.31772
1.18899		
C	-0.68267	1.33355
1.13361		
C	-1.19976	-0.11706
1.15609		
H	2.43967	0.49773
0.00868		
H	1.12103	-1.37637
0.93504		
H	1.16483	-1.45127 -
0.8109		
H	1.17105	0.84358
2.0925		

H	1.2245	2.31927
1.16133		
H	-1.06737	1.86712
1.97753		
H	-1.00423	1.81349
0.23297		
H	-0.87757	-0.59598
2.05705		
H	-2.26903	-0.11045
1.11688		
H	1.05356	1.00998 -
0.92229		
N	-0.67284	-0.85879 -
0.00789		
H	-0.96914	-0.40744 -
0.84961		
O	-1.15312	-2.13083
0.02136		

Piperidinium

The number of imaginary frequencies: 0
 Total Energy (B3LYP/6-31G*)= -
 252.2859402
 ZPE= -252.110728
 Enthalpy= -252.104086

C	0.2563	0.70643	1.21342
C	-0.25474	-0.74618	
1.24371			
C	0.25761	-1.48092	0.
C	-0.25474	-0.74618 -	
1.24371			
C	0.2563	0.70643 -	
1.21342			
H	0.10397	-1.23684	
2.12432			
H	1.32629	0.70745	
1.21061			
H	-0.09987	1.22324	
2.07999			

H	1.3276	-1.48454	0.
H	-0.09992	-2.48943	0.
H	0.10397	-1.23684	-
2.12432			
H	-1.32474	-0.74843	-
1.24647			
H	1.32629	0.70745	-
1.21061			
H	-0.09987	1.22324	-
2.07999			
H	-1.32474	-0.74843	
1.24647			
N	-0.23698	1.38978	0.
H	-1.23696	1.3833	0.
H	0.09254	2.33393	0.

Piperidinium

The number of imaginary frequencies: 0
 Total Energy (M06/6-311G+(d,p))= -252.14582512
 ZPE= -251.973176
 Enthalpy= -251.966535

C	-0.01538	-0.74124	
1.27281			
C	-0.01538	0.78498	
1.26832			
C	-0.67423	1.35037	0.
C	-0.01538	0.78498	-
1.26832			
C	-0.01538	-0.74124	-
1.27281			
H	-0.54349	1.11969	
2.16719			
H	-1.02853	-1.15319	
1.26942			
H	0.5376	-1.16721	
2.11354			
H	-1.74484	1.10712	0.

H	-0.60063	2.44169	0.
H	-0.54349	1.11969	-
2.16719			
H	1.0163	1.15152	-
1.36189			
H	-1.02853	-1.15319	-
1.26942			
H	0.5376	-1.16721	-
2.11354			
H	1.0163	1.15152	
1.36189			
N	0.6456	-1.25965	0.
H	1.63257	-0.97419	0.
H	0.64443	-2.28581	0.

Piperideine

The number of imaginary frequencies: 0
 Total Energy (B3LYP/6-31G*)= -250.68792691
 ZPE= -250.552631
 Enthalpy= -250.546306

C	-2.07985	-1.79356	-0.0563
C	-0.55751	-1.63904	-
0.2454			
C	-0.48945	0.3334	
1.20161			
C	-2.02668	0.37596	
1.1092			
C	-2.53773	-1.05764	
1.20991			
H	-0.01514	-2.40174	-
0.76407			
H	-2.56803	-1.36076	-
0.90439			
H	-2.33982	-2.82885	
0.01785			
H	-0.21326	-0.01662	
2.17429			

H	-0.10058	1.3184
1.04845		
H	-2.40771	0.97091
1.91279		
H	-2.34223	0.79797
0.17795		
H	-2.13427	-1.51611
2.0885		
H	-3.60626	-1.07955
1.26157		
N	0.08263	-0.59333
0.20215		

Piperidine

The number of imaginary frequencies: 0
 Total Energy (M06/6-311G+(d,p))= -250.55535317
 ZPE= -250.421846
 Enthalpy= -250.415526

C	-1.46593	-0.03236	-
0.10309			
C	-0.6106	-1.28267	-
0.05486			
C	1.44143	-0.12494	
0.12621			
C	0.72363	1.15552	-
0.32129			
C	-0.67552	1.21859	
0.30171			
H	-1.15183	-2.23392	-
0.11839			
H	-1.86442	0.07197	-
1.1245			
H	-2.3435	-0.17948	
0.54075			
H	1.78447	-0.02729	
1.1669			
H	2.34748	-0.28683	-
0.47088			

H	1.32103	2.03397	-
0.04786			
H	0.63495	1.15955	-
1.41679			
H	-0.58395	1.25474	
1.39585			
H	-1.20776	2.12749	-
0.00174			
N	0.65507	-1.36073	
0.05494			

Piperidine N-oxide

The number of imaginary frequencies: 0
 Total Energy (B3LYP/6-31G*)= -325.85702784
 ZPE= -325.716731
 Enthalpy= -325.709625

C	-2.08123	-1.79408	-
0.05013			
C	-0.56199	-1.62795	-
0.25884			
C	-0.49373	0.33486	
1.19748			
C	-2.02953	0.37622	
1.10149			
C	-2.53384	-1.05886	
1.21551			
H	-0.02924	-2.37362	-
0.81115			
H	-2.58157	-1.36391	-
0.89245			
H	-2.33254	-2.83136	
0.02599			
H	-0.22584	-0.01254	
2.17342			
H	-0.10293	1.31897	
1.04352			
H	-2.41225	0.97676	
1.9001			
H	-2.3462	0.7904	0.1671

H	-2.12261	-1.51065
2.09395		
H	-3.60186	-1.08654
1.27436		
N	0.0904	-0.5958
0.20607		
O	1.36173	-0.3776
0.22488		

Piperidine N-oxide

The number of imaginary frequencies: 0
 Total Energy (M06/6-311G+(d,p))= -
 325.71737713
 ZPE= -325.578818
 Enthalpy= -325.571733

C	1.1169	1.27399	-
0.10727			
C	-0.38305	1.21071	-
0.07714			
C	-0.41689	-1.23105	
0.09571			
C	1.05279	-1.21775	-
0.31594			
C	1.77604	-0.03767	
0.3384			
H	-0.98671	2.10985	-
0.13628			
H	1.45321	1.52909	-
1.12602			
H	1.44829	2.10752	
0.52648			
H	-0.5494	-1.55471	
1.13348			
H	-1.02854	-1.87903	-
0.53451			
H	1.50858	-2.17376	-
0.03244			
H	1.13117	-1.13916	-
1.40856			

H	1.71378	-0.1312
1.43079		
H	2.83955	-0.0345
0.07564		
N	-1.08114	0.10558
0.00697		
O	-2.35458	0.05469
0.0525		

Benzene

The number of imaginary frequencies: 0
 Total Energy (B3LYP/6-31G*)= -
 232.24865193
 ZPE= -232.147884
 Enthalpy= -232.142551

C	-0.07905	0.01976	0.
C	1.31611	0.01976	0.
C	2.01365	1.22751	0.
C	1.31599	2.43602	-
0.0012			
C	-0.07883	2.43594	-
0.00168			
C	-0.77643	1.22774	-
0.00068			
H	-0.62881	-0.93255	
0.00045			
H	1.86562	-0.93275	
0.00132			
H	3.11333	1.22759	
0.00063			
H	1.86619	3.38817	-
0.00126			
H	-0.62895	3.38823	-
0.00263			
H	-1.87604	1.22792	-
0.00086			

Benzene

The number of imaginary frequencies: 0
 Total Energy (M06/6-311G+(d,p))= -
 232.11261199

ZPE= -232.013098
 Enthalpy= -232.007708
 C 1.06282 -0.9059 -
 0.00001
 C -0.25327 -1.37325 -
 0.00007
 C -1.31599 -0.46745
 0.00006
 C -1.06275 0.90599 -
 0.00001
 C 0.25315 1.37327 -
 0.00006
 C 1.31603 0.46735
 0.00006
 H 1.8897 -1.61101
 0.00007
 H -0.45015 -2.44198 -
 0.00008
 H -2.34004 -0.83108
 0.00015
 H -1.8898 1.61089 -
 0.00001
 H 0.45028 2.44195 -
 0.00002
 H 2.33999 0.83123
 0.00006

Benzene
 The number of imaginary frequencies: 0
 Total Energy (B3PW91/6-31G*)= -
 232.15906676
 ZPE= -232.058021
 Enthalpy= -232.05268
 C -0.07905 0.01976 0.
 C 1.31611 0.01976 0.
 C 2.01365 1.22751 0.
 C 1.31599 2.43602 -
 0.0012
 C -0.07883 2.43594 -
 0.00168

C -0.77643 1.22774 -
 0.00068
 H -0.62881 -0.93255
 0.00045
 H 1.86562 -0.93275
 0.00132
 H 3.11333 1.22759
 0.00063
 H 1.86619 3.38817 -
 0.00126
 H -0.62895 3.38823 -
 0.00263
 H -1.87604 1.22792 -
 0.00086

Benzene
 The number of imaginary frequencies: 0
 Total Energy (B3PW91/6-31G**)= -
 232.16807009
 ZPE= -232.067176
 Enthalpy= -232.061831

C -0.07905 0.01976 0.
 C 1.31611 0.01976 0.
 C 2.01365 1.22751 0.
 C 1.31599 2.43602 -
 0.0012
 C -0.07883 2.43594 -
 0.00168
 C -0.77643 1.22774 -
 0.00068
 H -0.62881 -0.93255
 0.00045
 H 1.86562 -0.93275
 0.00132
 H 3.11333 1.22759
 0.00063
 H 1.86619 3.38817 -
 0.00126

H -0.62895 3.38823 -
0.00263

H -1.87604 1.22792 -
0.00086

Benzene

The number of imaginary frequencies: 0
Total Energy (B3PW91/6-311G+(d,p))= -
232.21577033
ZPE= -232.115389
Enthalpy= -232.110038

C -0.07905 0.01976 0.

C 1.31611 0.01976 0.

C 2.01365 1.22751 0.

C 1.31599 2.43602 -
0.0012

C -0.07883 2.43594 -
0.00168

C -0.77643 1.22774 -
0.00068

H -0.62881 -0.93255
0.00045

H 1.86562 -0.93275
0.00132

H 3.11333 1.22759
0.00063

H 1.86619 3.38817 -
0.00126

H -0.62895 3.38823 -
0.00263

H -1.87604 1.22792 -
0.00086

Phenol

The number of imaginary frequencies: 1 (-
350.23 cm⁻¹)
Total Energy (B3LYP/6-31G*)= -
307.45835198
ZPE= -307.354566
Enthalpy= -307.34847

C 0.49055 -0.07725
0.00017

C 1.89195 -0.07726
0.00056

C 2.59266 1.13639 -
0.00004

C 1.89197 2.35004 -
0.00102

C 0.49057 2.35005 -
0.00141

C -0.21014 1.1364 -
0.00082

H -0.04445 -1.00389
0.00062

H 2.42695 -1.00391
0.00131

H 3.66266 1.13638
0.00026

H -0.04443 3.2767 -
0.00217

H -1.28014 1.13641 -
0.00111

O 2.60697 3.58845 -
0.00163

H 2.76723 3.86499 -
0.90686

Phenol

The number of imaginary frequencies: 1 (-
358.89 cm⁻¹)
Total Energy (M06/6-311G+(d,p))= -
307.32521462
ZPE= -307.222264
Enthalpy= -307.216106

C 0.49055 -0.07725
0.00017

C 1.89195 -0.07726
0.00056

C 2.59266 1.13639 -
0.00004

C	1.89197	2.35004	-
0.00102			
C	0.49057	2.35005	-
0.00141			
C	-0.21014	1.1364	-
0.00082			
H	-0.04445	-1.00389	
0.00062			
H	2.42695	-1.00391	
0.00131			
H	3.66266	1.13638	
0.00026			
H	-0.04443	3.2767	-
0.00217			
H	-1.28014	1.13641	-
0.00111			
O	2.60697	3.58845	-
0.00163			
H	2.76723	3.86499	-
0.90686			

Phenol

The number of imaginary frequencies: 1 (-351.81 cm⁻¹)
 Total Energy (B3PW91/6-31G*)= -307.34118811
 ZPE= -307.237045
 Enthalpy= -307.230945

C	0.49055	-0.07725	
0.00017			
C	1.89195	-0.07726	
0.00056			
C	2.59266	1.13639	-
0.00004			
C	1.89197	2.35004	-
0.00102			
C	0.49057	2.35005	-
0.00141			
C	-0.21014	1.1364	-
0.00082			

H	-0.04445	-1.00389	
0.00062			
H	2.42695	-1.00391	
0.00131			
H	3.66266	1.13638	
0.00026			
H	-0.04443	3.2767	-
0.00217			
H	-1.28014	1.13641	-
0.00111			
O	2.60697	3.58845	-
0.00163			
H	2.76723	3.86499	-
0.90686			

Phenol

The number of imaginary frequencies: 1 (-352.75 cm⁻¹)
 Total Energy (B3PW91/6-31G**)= -307.35457193
 ZPE= -307.250439
 Enthalpy= -307.244334

C	0.49055	-0.07725	
0.00017			
C	1.89195	-0.07726	
0.00056			
C	2.59266	1.13639	-
0.00004			
C	1.89197	2.35004	-
0.00102			
C	0.49057	2.35005	-
0.00141			
C	-0.21014	1.1364	-
0.00082			
H	-0.04445	-1.00389	
0.00062			
H	2.42695	-1.00391	
0.00131			
H	3.66266	1.13638	
0.00026			

H	-0.04443	3.2767	-
0.00217			
H	-1.28014	1.13641	-
0.00111			
O	2.60697	3.58845	-
0.00163			
H	2.76723	3.86499	-
0.90686			

Phenol

The number of imaginary frequencies: 1 (-355.52 cm⁻¹)
 Total Energy (B3PW91/6-311G+(d,p))= -307.42853754
 ZPE= -307.32493
 Enthalpy= -307.318804

C	0.49055	-0.07725	
0.00017			
C	1.89195	-0.07726	
0.00056			
C	2.59266	1.13639	-
0.00004			
C	1.89197	2.35004	-
0.00102			
C	0.49057	2.35005	-
0.00141			
C	-0.21014	1.1364	-
0.00082			
H	-0.04445	-1.00389	
0.00062			
H	2.42695	-1.00391	
0.00131			
H	3.66266	1.13638	
0.00026			
H	-0.04443	3.2767	-
0.00217			
H	-1.28014	1.13641	-
0.00111			
O	2.60697	3.58845	-
0.00163			

H	2.76723	3.86499	-
0.90686			

Phenoxide

The number of imaginary frequencies: 0
 Total Energy (B3LYP/6-31G*)= -306.88416774
 ZPE= -306.793442
 Enthalpy= -306.787254

C	1.04882	-0.56995	
0.00005			
C	2.45022	-0.57002	
0.00054			
C	3.15099	0.64359	0.
C	2.45035	1.85727	-
0.00103			
C	1.04895	1.85735	-
0.00151			
C	0.34819	0.64374	-
0.00097			
H	0.51377	-1.49657	
0.00046			
H	2.98517	-1.4967	
0.00131			
H	4.22099	0.64353	
0.00036			
H	2.9854	2.78389	-
0.00144			
H	0.514	2.78402	-
0.00229			
O	-1.08181	0.64381	-
0.00146			

Phenoxide

The number of imaginary frequencies: 0
 Total Energy (M06/6-311G+(d,p))= -306.76850993
 ZPE= -306.678655
 Enthalpy= -306.672387

C	-0.28635	1.21265	0.
C	1.10202	1.20101	0.

C	1.83103	0.	0.
C	1.10202	-1.20101	0.
C	-0.28635	-1.21265	0.
C	-1.08463	0.	0.
H	-0.83192	2.15714	0.
H	1.64175	2.15246	0.
H	2.92018	0.	0.
H	1.64175	-2.15246	0.
H	-0.83192	-2.15714	0.
O	-2.35078	0.	0.

Phenoxide

The number of imaginary frequencies: 0
 Total Energy (B3PW91/6-31G*)= -306.76798829
 ZPE= -306.676996
 Enthalpy= -306.6708

C	1.04882	-0.56995	0.00005
C	2.45022	-0.57002	0.00054
C	3.15099	0.64359	0.
C	2.45035	1.85727	-0.00103
C	1.04895	1.85735	-0.00151
C	0.34819	0.64374	-0.00097
H	0.51377	-1.49657	0.00046
H	2.98517	-1.4967	0.00131
H	4.22099	0.64353	0.00036
H	2.9854	2.78389	-0.00144

H	0.514	2.78402	-0.00229
O	-1.08181	0.64381	-0.00146

Phenoxide

The number of imaginary frequencies: 0
 Total Energy (B3PW91/6-31G**)= -306.77579656
 ZPE= -306.68491
 Enthalpy= -306.678712

C	1.04882	-0.56995	0.00005
C	2.45022	-0.57002	0.00054
C	3.15099	0.64359	0.
C	2.45035	1.85727	-0.00103
C	1.04895	1.85735	-0.00151
C	0.34819	0.64374	-0.00097
H	0.51377	-1.49657	0.00046
H	2.98517	-1.4967	0.00131
H	4.22099	0.64353	0.00036
H	2.9854	2.78389	-0.00144
H	0.514	2.78402	-0.00229
O	-1.08181	0.64381	-0.00146

Phenoxide

The number of imaginary frequencies: 0
 Total Energy (B3PW91/6-311G+(d,p))= -306.86725975
 ZPE= -306.776989
 Enthalpy= -306.770741

C	1.04882	-0.56995		C	-1.23419	-0.09159
0.00005				1.15888		
C	2.45022	-0.57002		H	2.502	0.47984
0.00054				0.06271		
C	3.15099	0.64359	0.	H	1.20402	-1.44288
				0.90656		
C	2.45035	1.85727	-	H	1.20676	-1.4471
0.00103				0.90191		
C	1.04895	1.85735	-	H	-1.05633	-0.46422
0.00151				0.96539		
C	0.34819	0.64374	-	H	-1.05923	-1.95146
0.00097				0.0635		
H	0.51377	-1.49657		H	1.20627	0.88353
0.00046				2.12527		
H	2.98517	-1.4967		H	1.20976	2.37251
0.00131				1.09867		
H	4.22099	0.64353		H	-1.05671	1.86846
0.00036				2.06229		
H	2.9854	2.78389	-	H	-1.05324	1.86563
0.00144				0.25385		
H	0.514	2.78402	-	H	-0.96818	-0.59731
0.00229				2.12419		
O	-1.08181	0.64381	-	H	-2.35274	-0.05653
0.00146				1.09394		
				H	1.11478	1.01947
				0.96455		

Cyclohexane

The number of imaginary frequencies: 0

Total Energy (B3LYP/6-31G*)= -235.88044327

ZPE= -235.709245

Enthalpy= -235.702607

C	-0.68364	-0.89724	0.
C	0.83147	-0.89724	0.
C	1.3834	0.51383	0.
C	0.83374	1.31837	
1.16066			
C	-0.68139	1.31903	
1.16017			

Cyclohexane

The number of imaginary frequencies: 0

Total Energy (M06/6-311G+(d,p))= -235.74170309

ZPE= -235.572734

Enthalpy= -235.566134

C	1.41187	-0.33689
0.23177		
C	0.41394	-1.39013
0.23177		
C	-0.99755	-1.05372
0.23173		

C	-1.41187	0.33689	-
0.23177			
C	-0.41394	1.39013	
0.23177			
C	0.99755	1.05372	-
0.23173			
H	-1.70942	-1.80653	-
0.12723			
H	0.42879	-1.43952	-
1.33177			
H	0.70921	-2.38334	
0.12701			
H	1.46359	-0.34914	
1.33171			
H	2.41924	-0.57756	-
0.12822			
H	-1.46359	0.34914	-
1.33171			
H	-2.41924	0.57756	
0.12822			
H	-0.70921	2.38334	-
0.12701			
H	-0.42879	1.43952	
1.33177			
H	1.03335	1.09098	-
1.33175			
H	1.70942	1.80653	
0.12723			
H	-1.03335	-1.09098	
1.33175			

Cyclohexane

The number of imaginary frequencies: 0
 Total Energy (B3PW91/6-31G*)= -235.79991158
 ZPE= -235.628375
 Enthalpy= -235.621737

C	-0.68364	-0.89724	0.
C	0.83147	-0.89724	0.

C	1.3834	0.51383	0.
C	0.83374	1.31837	
1.16066			
C	-0.68139	1.31903	
1.16017			
C	-1.23419	-0.09159	
1.15888			
H	2.502	0.47984	
0.06271			
H	1.20402	-1.44288	
0.90656			
H	1.20676	-1.4471	-
0.90191			
H	-1.05633	-0.46422	-
0.96539			
H	-1.05923	-1.95146	
0.0635			
H	1.20627	0.88353	
2.12527			
H	1.20976	2.37251	
1.09867			
H	-1.05671	1.86846	
2.06229			
H	-1.05324	1.86563	
0.25385			
H	-0.96818	-0.59731	
2.12419			
H	-2.35274	-0.05653	
1.09394			
H	1.11478	1.01947	-
0.96455			

Cyclohexane

The number of imaginary frequencies: 0
 Total Energy (B3PW91/6-31G**) = -235.81539469
 ZPE= -235.644589
 Enthalpy= -235.637903

C	-0.52919	-1.36163	
0.22935			

C	-1.44445	-0.22267	-
0.22939			
C	-0.91503	1.13895	
0.2294			
C	0.52919	1.36163	-
0.22934			
C	1.44445	0.22267	0.2294
C	0.91502	-1.13895	-
0.22942			
H	-1.56141	1.94345	-
0.14206			
H	-1.50938	-0.23263	-
1.32715			
H	-2.46417	-0.37997	
0.14279			
H	-0.55257	-1.42175	
1.32714			
H	-0.90269	-2.32375	-
0.14193			
H	0.5526	1.42177	-
1.32713			
H	0.90269	2.32374	
0.14196			
H	2.46417	0.37997	-
0.14278			
H	1.50937	0.2326	
1.32716			
H	0.95559	-1.18907	-
1.3272			
H	1.56141	-1.94346	0.142
H	-0.95563	1.18911	
1.32717			

Cyclohexane

The number of imaginary frequencies: 0
 Total Energy (B3PW91/6-311G+(d,p))= -235.8589444
 ZPE= -235.689291
 Enthalpy= -235.682583

C	0.	-1.45193	0.25667
C	-1.2574	-0.72596	-
0.25667			
C	-1.2574	0.72596	
0.25667			
C	0.	1.45193	-0.25667
C	1.2574	0.72596	
0.25667			
C	1.2574	-0.72596	-
0.25667			
H	-2.13106	1.23037	-0.1
H	-1.2574	-0.72596	-
1.32667			
H	-2.13106	-1.23037	0.1
H	0.	-1.45193	1.32667
H	0.	-2.46073	-0.1
H	0.	1.45193	-1.32667
H	0.	2.46073	0.1
H	2.13106	1.23037	-0.1
H	1.2574	0.72596	
1.32667			
H	1.2574	-0.72596	-
1.32667			
H	2.13106	-1.23037	0.1
H	-1.2574	0.72596	
1.32667			

Cyclohexene

The number of imaginary frequencies: 0
 Total Energy (B3LYP/6-31G*)= -234.64828834
 ZPE= -234.501263
 Enthalpy= -234.494842

C	-1.09705	-2.25773	-
0.09838			
C	0.41779	-2.25199	
0.12713			

C	0.93262	-0.82852	-
0.15134			
C	0.15985	0.21534	
0.68073			
C	-1.11685	-0.013	1.0939
C	-1.74518	-1.41963	
1.01803			
H	1.97685	-0.77566	
0.07599			
H	0.6251	-2.54628	
1.13475			
H	0.90114	-2.92981	-
0.54505			
H	-1.31126	-1.84627	-
1.06259			
H	-1.48166	-3.25488	-
0.0468			
H	0.63273	1.14297	
0.92728			
H	-1.69215	0.79701	
1.49117			
H	-1.57375	-1.91002	
1.95346			
H	-2.79722	-1.34005	
0.83977			
H	0.77709	-0.60796	-
1.18675			

Cyclohexene

The number of imaginary frequencies: 0
 Total Energy (M06/6-311G+(d,p))= -234.51167786
 ZPE= -234.366563
 Enthalpy= -234.360136

C	-0.37174	-0.67134	-
1.19224			
C	0.37174	0.67134	-
1.19224			
C	0.00551	1.50293	
0.04786			

C	-0.00551	0.66851	
1.3061			
C	0.00551	-0.66851	
1.3061			
C	-0.00551	-1.50293	
0.04786			
H	0.70963	2.33869	
0.16382			
H	1.45443	0.48193	-
1.19273			
H	0.15032	1.23633	-
2.10602			
H	-1.45443	-0.48193	-
1.19273			
H	-0.15032	-1.23633	-
2.10602			
H	-0.01996	1.20449	
2.25474			
H	0.01996	-1.20449	
2.25474			
H	0.98274	-1.97072	-
0.09014			
H	-0.70963	-2.33869	
0.16382			
H	-0.98274	1.97072	-
0.09014			

1,3-Cyclohexadiene

The number of imaginary frequencies: 0
 Total Energy (B3LYP/6-31G*)= -233.41893221
 ZPE= -233.296105
 Enthalpy= -233.289987

C	-0.15118	0.13054	
0.24939			
C	1.32754	0.10935	-
0.18631			
C	2.02124	1.27034	-
0.27831			

C	1.35327	2.58323	
0.16487			
C	-0.13997	2.58558	-
0.21611			
C	-0.82738	1.3048	
0.28723			
H	-0.64641	-0.78146	0.51
H	1.80897	-0.82106	-
0.40418			
H	3.03042	1.27026	-
0.63391			
H	1.4551	2.66525	
1.22685			
H	-0.60147	3.44849	
0.2167			
H	-1.83632	1.33633	
0.6421			
H	1.82749	3.41813	-
0.30731			
H	-0.24093	2.6198	-
1.28078			

1,3-Cyclohexadiene

The number of imaginary frequencies: 0
 Total Energy (M06/6-311G+(d,p))= -
 233.28434875
 ZPE= -233.162923
 Enthalpy= -233.15679

C	-0.7637	0.10482	
1.26813			
C	0.7637	-0.10482	
1.26813			
C	1.45068	-0.06654	
0.10016			
C	0.7097	0.3001	-
1.19706			
C	-0.7097	-0.3001	-
1.19706			
C	-1.45068	0.06654	
0.10016			

H	-1.28239	0.26836	
2.18961			
H	1.28239	-0.26836	
2.18961			
H	2.50164	-0.26688	
0.08443			
H	0.65063	1.36689	-
1.25519			
H	-1.2401	0.0774	-
2.04622			
H	-2.50164	0.26688	
0.08443			
H	1.2401	-0.0774	-
2.04622			
H	-0.65063	-1.36689	-
1.25519			

Cyclohexanol

The number of imaginary frequencies: 0
 Total Energy (B3LYP/6-31G*)= -
 311.09023047
 ZPE= -310.914856
 Enthalpy= -310.907074

C	-1.69842	-0.9235	-
0.03227			
C	-0.16061	-0.92136	
0.04987			
C	0.35182	0.53086	
0.04271			
C	-0.22796	1.28577	
1.25332			
C	-1.76576	1.28364	
1.17118			
C	-2.2782	-0.16859	
1.17833			
H	1.4203	0.53234	
0.09979			
H	0.14899	-1.40438	
0.95306			

H	0.24222	-1.44588	-
0.79126			
H	-2.00802	-0.44048	-
0.93546			
H	-2.05446	-1.93251	-
0.0273			
H	0.08164	0.80275	
2.15651			
H	-2.1686	1.80815	
2.01231			
H	-2.07536	1.76666	
0.26799			
H	-1.9686	-0.6516	
2.08152			
H	-3.34667	-0.17007	
1.12126			
H	0.04222	1.01388	-
0.86047			
O	0.24788	2.63427	
1.24667			
H	1.20651	2.6356	
1.29788			

Cyclohexanol

The number of imaginary frequencies: 0
 Total Energy (M06/6-311G+(d,p))= -
 310.9561851
 ZPE= -310.782442
 Enthalpy= -310.774714

C	1.87188	0.015	-0.27822
C	1.14616	1.27958	
0.20746			
C	-0.34037	1.25452	-
0.18469			
C	-1.03808	-0.01488	
0.32185			
C	-0.31932	-1.2696	-
0.17361			
C	1.16738	-1.25843	
0.21595			

H	-0.85392	2.14483	
0.20746			
H	1.23313	1.34863	
1.30195			
H	1.62713	2.17808	-
0.19869			
H	1.89506	0.01191	-
1.37782			
H	2.91685	0.02568	
0.05675			
H	-1.01273	-0.01168	
1.42704			
H	-0.82456	-2.15708	
0.22535			
H	-0.42203	-1.30947	-
1.26703			
H	1.25839	-1.31957	
1.31058			
H	1.66502	-2.14978	-
0.18566			
H	-0.44264	1.28377	-
1.27849			
O	-2.38974	-0.09818	-
0.13038			
H	-2.84767	0.70295	
0.16909			

Cyclohexanol

The number of imaginary frequencies: 0
 Total Energy (B3PW91/6-31G*)= -
 310.98134763
 ZPE= -310.805554
 Enthalpy= -310.797773

C	-1.69842	-0.9235	-
0.03227			
C	-0.16061	-0.92136	
0.04987			
C	0.35182	0.53086	
0.04271			

C	-0.22796	1.28577	C	-1.69842	-0.9235	-
1.25332			0.03227			
C	-1.76576	1.28364	C	-0.16061	-0.92136	
1.17118			0.04987			
C	-2.2782	-0.16859	C	0.35182	0.53086	
1.17833			0.04271			
H	1.4203	0.53234	C	-0.22796	1.28577	
0.09979			1.25332			
H	0.14899	-1.40438	C	-1.76576	1.28364	
0.95306			1.17118			
H	0.24222	-1.44588	C	-2.2782	-0.16859	
0.79126			1.17833			
H	-2.00802	-0.44048	H	1.4203	0.53234	
0.93546			0.09979			
H	-2.05446	-1.93251	H	0.14899	-1.40438	
0.0273			0.95306			
H	0.08164	0.80275	H	0.24222	-1.44588	
2.15651			0.79126			
H	-2.1686	1.80815	H	-2.00802	-0.44048	
2.01231			0.93546			
H	-2.07536	1.76666	H	-2.05446	-1.93251	
0.26799			0.0273			
H	-1.9686	-0.6516	H	0.08164	0.80275	
2.08152			2.15651			
H	-3.34667	-0.17007	H	-2.1686	1.80815	
1.12126			2.01231			
H	0.04222	1.01388	H	-2.07536	1.76666	
0.86047			0.26799			
O	0.24788	2.63427	H	-1.9686	-0.6516	
1.24667			2.08152			
H	1.20651	2.6356	H	-3.34667	-0.17007	
1.29788			1.12126			
			H	0.04222	1.01388	
			0.86047			
			O	0.24788	2.63427	
			1.24667			
			H	1.20651	2.6356	
			1.29788			

Cyclohexanol
The number of imaginary frequencies: 0
Total Energy (B3PW91/6-31G**)= -311.00115199
ZPE= -310.825835
Enthalpy= -310.818032

Cyclohexanol

The number of imaginary frequencies: 0
 Total Energy (B3PW91/6-311G+(d,p))= -
 311.07296237
 ZPE= -310.89868
 Enthalpy= -310.890825

C	-1.69842	-0.9235	-
0.03227			
C	-0.16061	-0.92136	
0.04987			
C	0.35182	0.53086	
0.04271			
C	-0.22796	1.28577	
1.25332			
C	-1.76576	1.28364	
1.17118			
C	-2.2782	-0.16859	
1.17833			
H	1.4203	0.53234	
0.09979			
H	0.14899	-1.40438	
0.95306			
H	0.24222	-1.44588	-
0.79126			
H	-2.00802	-0.44048	-
0.93546			
H	-2.05446	-1.93251	-
0.0273			
H	0.08164	0.80275	
2.15651			
H	-2.1686	1.80815	
2.01231			
H	-2.07536	1.76666	
0.26799			
H	-1.9686	-0.6516	
2.08152			
H	-3.34667	-0.17007	
1.12126			
H	0.04222	1.01388	-
0.86047			

O	0.24788	2.63427
1.24667		
H	1.20651	2.6356
1.29788		

Cyclohexanoxide

The number of imaginary frequencies: 0
 Total Energy (B3LYP/6-31G*)= -
 310.46048432
 ZPE= -310.301528
 Enthalpy= -310.294035

C	-2.17913	-2.26853	-
0.02636			
C	-0.64001	-2.29336	
0.01911			
C	-0.10181	-0.85115	-
0.02535			
C	-0.63853	-0.06539	
1.18548			
C	-2.17766	-0.04057	
1.14002			
C	-2.71585	-1.48278	
1.18448			
H	0.96759	-0.8684	
0.00624			
H	-0.31747	-2.76671	
0.92288			
H	-0.26709	-2.83931	-
0.82218			
H	-2.50167	-1.79518	-
0.93013			
H	-2.55308	-3.27059	
0.00453			
H	-0.31599	-0.53875	
2.08926			
H	-2.55057	0.50538	
1.98131			
H	-2.50019	0.43279	
0.23624			
H	-2.39332	-1.95613	
2.08825			

H	-3.78525	-1.46553	
1.15288			
H	-0.42434	-0.3778	-
0.92912			
O	-0.13877	1.2738	1.1442

H	0.59165	-1.54105	-
2.1635			
H	1.12539	0.78331	
1.29784			
O	-0.57575	2.37751	0.

Cyclohexanoxide

The number of imaginary frequencies: 0
 Total Energy (M06/6-311G+(d,p))= -310.34864084
 ZPE= -310.190974
 Enthalpy= -310.183555

C	0.74639	-1.69549	0.
C	0.08897	-1.13045	
1.27017			
C	0.08897	0.40692	
1.26393			
C	-0.59753	1.06331	0.
C	0.08897	0.40692	-
1.26393			
C	0.08897	-1.13045	-
1.27017			
H	-0.41344	0.80182	
2.15935			
H	-0.95188	-1.49063	
1.31339			
H	0.59165	-1.54105	
2.1635			
H	1.81428	-1.42266	0.
H	0.70757	-2.79762	0.
H	-1.64779	0.56877	0.
H	-0.41344	0.80182	-
2.15935			
H	1.12539	0.78331	-
1.29784			
H	-0.95188	-1.49063	-
1.31339			

Cyclohexanoxide

The number of imaginary frequencies: 0
 Total Energy (B3PW91/6-31G*)= -310.35127286
 ZPE= -310.191988
 Enthalpy= -310.184495

C	-2.17913	-2.26853	-
0.02636			
C	-0.64001	-2.29336	
0.01911			
C	-0.10181	-0.85115	-
0.02535			
C	-0.63853	-0.06539	
1.18548			
C	-2.17766	-0.04057	
1.14002			
C	-2.71585	-1.48278	
1.18448			
H	0.96759	-0.8684	
0.00624			
H	-0.31747	-2.76671	
0.92288			
H	-0.26709	-2.83931	-
0.82218			
H	-2.50167	-1.79518	-
0.93013			
H	-2.55308	-3.27059	
0.00453			
H	-0.31599	-0.53875	
2.08926			
H	-2.55057	0.50538	
1.98131			
H	-2.50019	0.43279	
0.23624			

H	-2.39332	-1.95613	
2.08825			
H	-3.78525	-1.46553	
1.15288			
H	-0.42434	-0.3778	-
0.92912			
O	-0.13877	1.2738	1.1442

H	-2.50019	0.43279	
0.23624			
H	-2.39332	-1.95613	
2.08825			
H	-3.78525	-1.46553	
1.15288			
H	-0.42434	-0.3778	-
0.92912			
O	-0.13877	1.2738	1.1442

Cyclohexanoxide

The number of imaginary frequencies: 0
 Total Energy (B3PW91/6-31G**) = -310.36598991
 ZPE = -310.20731
 Enthalpy = -310.199792

C	-2.17913	-2.26853	-
0.02636			
C	-0.64001	-2.29336	
0.01911			
C	-0.10181	-0.85115	-
0.02535			
C	-0.63853	-0.06539	
1.18548			
C	-2.17766	-0.04057	
1.14002			
C	-2.71585	-1.48278	
1.18448			
H	0.96759	-0.8684	
0.00624			
H	-0.31747	-2.76671	
0.92288			
H	-0.26709	-2.83931	-
0.82218			
H	-2.50167	-1.79518	-
0.93013			
H	-2.55308	-3.27059	
0.00453			
H	-0.31599	-0.53875	
2.08926			
H	-2.55057	0.50538	
1.98131			

Cyclohexanoxide

The number of imaginary frequencies: 0
 Total Energy (B3PW91/6-311G+(d,p)) = -310.46013267
 ZPE = -310.302065
 Enthalpy = -310.294548

C	-2.17913	-2.26853	-
0.02636			
C	-0.64001	-2.29336	
0.01911			
C	-0.10181	-0.85115	-
0.02535			
C	-0.63853	-0.06539	
1.18548			
C	-2.17766	-0.04057	
1.14002			
C	-2.71585	-1.48278	
1.18448			
H	0.96759	-0.8684	
0.00624			
H	-0.31747	-2.76671	
0.92288			
H	-0.26709	-2.83931	-
0.82218			
H	-2.50167	-1.79518	-
0.93013			
H	-2.55308	-3.27059	
0.00453			

H	-0.31599	-0.53875	
2.08926			
H	-2.55057	0.50538	
1.98131			
H	-2.50019	0.43279	
0.23624			
H	-2.39332	-1.95613	
2.08825			
H	-3.78525	-1.46553	
1.15288			
H	-0.42434	-0.3778	-
0.92912			
O	-0.13877	1.2738	1.1442

1,3-Cyclohexadiene-1-ol ion

The number of imaginary frequencies: 0
 Total Energy (B3LYP/6-31G*)= -308.06288455
 ZPE= -307.950009
 Enthalpy= -307.943075

C	-2.39644	-0.99279	-
0.08473			
C	-1.18737	-0.65562	-
0.59663			
C	-0.40603	0.53315	-
0.00229			
C	-1.02541	1.39408	
0.84195			
C	-2.53292	1.23688	
1.10459			
C	-2.91972	-0.25388	
1.15883			
H	-0.77084	-1.22108	-
1.40388			
H	-2.97031	-1.77998	-
0.52735			
H	-2.79622	1.69212	
2.03643			

H	-3.06045	1.71802	
0.30765			
H	-2.48319	-0.70895	
2.02327			
H	-3.98575	-0.32833	
1.21295			
H	0.61999	0.68539	-
0.26497			
O	-0.29137	2.45555	
1.45789			

1,3-Cyclohexadiene-1-ol ion

The number of imaginary frequencies: 0
 Total Energy (M06/6-311G+(d,p))= -307.94858474
 ZPE= -307.836671
 Enthalpy= -307.829759

C	-2.39644	-0.99279	-
0.08473			
C	-1.18737	-0.65562	-
0.59663			
C	-0.40603	0.53315	-
0.00229			
C	-1.02541	1.39408	
0.84195			
C	-2.53292	1.23688	
1.10459			
C	-2.91972	-0.25388	
1.15883			
H	-0.77084	-1.22108	-
1.40388			
H	-2.97031	-1.77998	-
0.52735			
H	-2.79622	1.69212	
2.03643			
H	-3.06045	1.71802	
0.30765			
H	-2.48319	-0.70895	
2.02327			

H	-3.98575	-0.32833
1.21295		
H	0.61999	0.68539 -
0.26497		
O	-0.29137	2.45555
1.45789		

1,5-Cyclohexadiene-1-ol ion

The number of imaginary frequencies: 0
 Total Energy (B3LYP/6-31G*)= -308.04298519
 ZPE= -307.930465
 Enthalpy= -307.92353

C	-2.51853	-0.72365 -
0.12507		
C	-0.99771	-0.63793 -
0.33961		
C	-0.3566	0.52872 -
0.08372		
C	-1.13237	1.71417
0.52438		
C	-2.37016	1.51757
1.04089		
C	-2.93616	0.08918
1.11582		
H	-0.45518	-1.48316 -
0.70859		
H	-2.99914	-0.32717 -
0.99497		
H	-2.81591	-1.74156
0.0175		
H	-2.93799	2.34444
1.41338		
H	-2.54907	-0.37516
1.99868		
H	-4.0048	0.11596
1.16272		
H	0.68325	0.63038 -
0.31455		

O	-0.54097	3.01572
0.55806		

1,5-Cyclohexadiene-1-ol ion

The number of imaginary frequencies: 0
 Total Energy (M06/6-311G+(d,p))= -307.92956598
 ZPE= -307.818063
 Enthalpy= -307.811119

C	-2.51853	-0.72365 -
0.12507		
C	-0.99771	-0.63793 -
0.33961		
C	-0.3566	0.52872 -
0.08372		
C	-1.13237	1.71417
0.52438		
C	-2.37016	1.51757
1.04089		
C	-2.93616	0.08918
1.11582		
H	-0.45518	-1.48316 -
0.70859		
H	-2.99914	-0.32717 -
0.99497		
H	-2.81591	-1.74156
0.0175		
H	-2.93799	2.34444
1.41338		
H	-2.54907	-0.37516
1.99868		
H	-4.0048	0.11596
1.16272		
H	0.68325	0.63038 -
0.31455		
O	-0.54097	3.01572
0.55806		

H₂ Gas

The number of imaginary frequencies: 0
 Total Energy (B3LYP/6-31G*)= -1.17548239

ZPE= -1.165337
Enthalpy= -1.162033

H	0.	0.	0.37139
H	0.	0.	-0.37139

H₂ Gas

The number of imaginary frequencies: 0
Total Energy (M06/6-311G+(d,p))= -
1.17039476
ZPE=-1.160564
Enthalpy=-1.157260

H	0.	0.	0.37139
H	0.	0.	-0.37139

H₂ Gas

The number of imaginary frequencies: 0
Total Energy (B3PW91/6-31G*)= -
1.17456185
ZPE= -1.164426
Enthalpy= -1.161121

H	0.	0.	0.37139
H	0.	0.	-0.37139

H₂ Gas

The number of imaginary frequencies: 0
Total Energy (B3PW91/6-31G**)= -
1.17751625
ZPE= -1.167344
Enthalpy= -1.16404

H	0.	0.	0.37139
H	0.	0.	-0.37139

H₂ Gas

The number of imaginary frequencies: 0
Total Energy (B3PW91/6-311G+(d,p))= -
1.17857658
ZPE= -1.168516
Enthalpy= -1.165212

H	0.	0.	0.37268
H	0.	0.	-0.37268

Triplet Oxygen, ³O

The number of imaginary frequencies: 0
Total Energy (B3LYP/6-31G*)= -
75.06062312
ZPE= -75.060623
Enthalpy= -75.058263
O 0. 0. 0.

Triplet Oxygen, ³O

The number of imaginary frequencies: 0
Total Energy (B3LYP/6-31G**)= -
75.06062143
ZPE= -75.060621
Enthalpy= -75.058261
O 0. 0. 0.

Triplet Oxygen, ³O

The number of imaginary frequencies: 0
Total Energy (M06/6-311G+(d,p))= -
75.05344297
ZPE= -75.053443
Enthalpy= -75.051083
O 0. 0. 0.

Triplet Oxygen, ³O

The number of imaginary frequencies: 0
Total Energy (B3PW91/6-31G*)= -
75.03133311
ZPE= -75.031333
Enthalpy= -75.028973
O 0. 0. 0.

Triplet Oxygen, ³O

The number of imaginary frequencies: 0
Total Energy (B3PW91/6-31G**)= -
75.03133311
ZPE= -75.031333
Enthalpy= -75.028973
O 0. 0. 0.

Triplet Oxygen, ³O

The number of imaginary frequencies: 0
Total Energy (B3PW91/6-311G+(d,p))= -
75.05845466
ZPE= -75.058455
Enthalpy= -75.056094
O 0. 0. 0.

Singlet Oxygen, ¹O

The number of imaginary frequencies: 0

Total Energy (B3LYP/6-31G*)= -
74.95739789
ZPE= -74.957398
Enthalpy= -74.955037
O 0. 0. 0.

Singlet Oxygen, ¹O

The number of imaginary frequencies: 0
Total Energy (M06/6-311G+(d,p))= -
74.95543188
ZPE= -74.955432
Enthalpy= -74.953071
O 0. 0. 0.

Carbon Monoxide

The number of imaginary frequencies: 0
Total Energy (B3LYP/6-31G*)= -
113.30945434
ZPE= -113.304423
Enthalpy= -113.301118

C -0.68024 0.02465
0.12843

O -0.30843 0.55045
1.03916

Carbon Monoxide

The number of imaginary frequencies: 0
Total Energy (M06/6-311G+(d,p))= -
113.28594104
ZPE= -113.280844
Enthalpy= -113.277539

C 0. 0. -0.65026

O 0. 0. 0.48769

Carbon Dioxide

The number of imaginary frequencies: 0
Total Energy (B3LYP/6-31G*)= -
188.58094022
ZPE= -188.569347
Enthalpy= -188.565756
C 1.4248 0.55144 0.3892
O 2.45228 0.9147 1.0184
O 0.39732 0.18818 -0.24

Carbon Dioxide

The number of imaginary frequencies: 0
Total Energy (M06/6-311G+(d,p))= -
188.5592754
ZPE= -188.547202
Enthalpy= -188.543659
C 0. 0. 0.
O 0. 0. 1.16916
O 0. 0. -1.16916

Nitric Oxide

The number of imaginary frequencies: 0
Total Energy (B3LYP/6-31G*)= -
129.8881562
ZPE= -129.88362
Enthalpy= -129.880315

O 1.3391 0.28484 0.

N 0.9396 1.41299 0.

Nitric Oxide

The number of imaginary frequencies: 0
Total Energy (M06/6-311G+(d,p))= -
129.85739211
ZPE= -129.852775
Enthalpy= -129.84947

O 0. 0. 0.54073

N 0. 0. -0.61797

Nitrogen Dioxide

The number of imaginary frequencies: 0
Total Energy (B3LYP/6-31G*)= -
205.07220619
ZPE= -205.06338
Enthalpy= -205.059499

N -0.62902 0.26164 -
0.07844

O -0.27177 -0.91919
0.0199

O -0.27175 0.93721 -
1.05189

Nitrogen Dioxide

The number of imaginary frequencies: 0

Total Energy (M06/6-311G+(d,p))= -
 205.03467527
 ZPE= -205.025534
 Enthalpy= -205.021663

N	0.	0.	0.32802
O	0.	1.10685	-0.14351
O	0.	-1.10685	-0.14351

³O₂, Triplet

The number of imaginary frequencies: 0
 Total Energy (B3LYP/6-31G*)= -
 150.32004208
 ZPE= -150.316263
 Enthalpy= -150.312956

O	-1.80199	0.58416	0.
O	-0.64039	0.58416	0.

³O₂, Triplet

The number of imaginary frequencies: 0
 Total Energy (M06/6-311G+(d,p))= -
 150.29135144
 ZPE= -150.287488
 Enthalpy= -150.284182

O	0.	0.	0.6073
O	0.	0.	-0.6073

¹O₂, Singlet

The number of imaginary frequencies: 0
 Total Energy (B3LYP/6-31G*)= -
 150.25742664
 ZPE= -150.253684
 Enthalpy= -150.250376

O	-0.83169	2.06931	0.
O	0.32991	2.06931	0.

¹O₂, Singlet

The number of imaginary frequencies: 0
 Total Energy (M06/6-311G+(d,p))= -
 150.2320003
 ZPE= -150.228126
 Enthalpy= -150.22482

O	0.	0.	0.608
O	0.	0.	-0.608

Bicyclo[1.1.0]butane

The number of imaginary frequencies: 0
 Total Energy (B3LYP/6-31G*)= -
 155.94803158
 ZPE= -155.861217
 Enthalpy= -155.856544

C	-1.29743	0.01091	0.7812
C	-0.00313	-0.00913	-0.18404

C	-1.03745	-1.13365	-0.20384
---	----------	----------	----------

H	-0.93566	-0.08314	1.78379
---	----------	----------	---------

H	-1.67228	-1.18996	1.06333
---	----------	----------	---------

H	-0.83659	-2.14254	0.09058
---	----------	----------	---------

C	-1.02504	1.13205	-0.22061
---	----------	---------	----------

H	-1.668	1.18268	1.07439
---	--------	---------	---------

H	-0.80332	2.14282	0.05157
---	----------	---------	---------

H	0.85437	0.09034	0.44817
---	---------	---------	---------

Bicyclo[1.1.0]butane

The number of imaginary frequencies: 0
 Total Energy (M06/6-311G+(d,p))= -
 155.87025179
 ZPE= -155.784497
 Enthalpy= -155.779812

C	-0.80733	-0.00656	-0.31956
---	----------	----------	----------

C	0.80733	0.00656	-0.31956
---	---------	---------	----------

C	-0.01329	1.13282	0.31767
---	----------	---------	---------

H	-1.11469	-0.10966	1.33926
---	----------	----------	---------

H	-0.01935	1.18618	1.38632
---	----------	---------	---------

H	-0.01902	2.14275	-
0.03575			
C	0.01329	-1.13282	
0.31767			
H	0.01935	-1.18618	
1.38632			
H	0.01902	-2.14275	-
0.03575			
H	1.11469	0.10966	-
1.33926			

1-cyano-Bicyclo[1.1.0]butane

The number of imaginary frequencies: 0
 Total Energy (B3LYP/6-31G*)= -
 248.19372057
 ZPE= -248.107661
 Enthalpy= -248.101465

C	-1.17456	0.00083	
0.72459			
C	-0.0488	-0.00079	-
0.28293			
C	-1.03706	-1.14061	-
0.22917			
H	-1.08061	0.00069	
1.80143			
H	-1.74718	-1.2416	-
1.05321			
H	-0.67545	-2.08454	0.174
C	-1.03427	1.14166	-
0.22941			
H	-1.74456	1.24418	-
1.0531			
H	-0.67019	2.08473	
0.17352			
C	1.35403	-0.00132	-
0.0764			
N	2.50885	-0.00029	
0.0739			

1-cyano-Bicyclo[1.1.0]butane

The number of imaginary frequencies: 0

Total Energy (M06/6-311G+(d,p))= -
 248.08154884
 ZPE= -247.996309
 Enthalpy= -247.990121

C	-1.14802	0.00005	
0.72613			
C	-0.05352	-0.00003	-
0.2782			
C	-1.0329	-1.13224	-
0.22727			
H	-1.04334	0.00004	
1.80049			

H	-1.75195	-1.21366	-
1.0438			
H	-0.66789	-2.0771	0.1664
C	-1.03276	1.1323	-
0.22729			
H	-1.75181	1.21381	-
1.04381			
H	-0.66762	2.07713	
0.16637			
C	1.34359	-0.00015	-
0.08058			
N	2.48918	0.00003	
0.06821			

Cyclobutane

The number of imaginary frequencies: 1 (-
 136.39 cm⁻¹)
 Total Energy (B3LYP/6-31G*)= -
 157.21183323
 ZPE= -157.100818
 Enthalpy= -157.096326

C	0.43478	0.49407	0.
C	1.97803	0.49407	0.
C	1.97797	2.03726	0.
C	0.43474	2.03726	-
0.00027			
H	-0.01821	0.04096	-
0.90642			

H	-0.01788	0.04111	
0.90664			
H	2.43094	0.04126	-
0.90662			
H	2.43091	0.04102	
0.90653			
H	2.43089	2.49002	-
0.90666			
H	2.43069	2.49039	
0.9065			
H	-0.01796	2.48979	-
0.90724			
H	-0.01853	2.49052	
0.90596			

Cyclobutane

The number of imaginary frequencies: 1 (-169.56 cm⁻¹)

Total Energy (M06/6-311G+(d,p))= -157.11692129

ZPE= -157.007394

Enthalpy= -157.002855

C	-0.07615	1.09848	-
0.00016			
C	1.09849	0.07615	-
0.00005			
C	0.07615	-1.09848	-
0.00007			
C	-1.09848	-0.07615	
0.00028			
H	-0.12071	1.74204	
0.88428			
H	-0.12091	1.74147	-0.885
H	1.74166	0.12083	
0.88465			
H	1.74184	0.1208	-
0.88464			
H	0.12095	-1.74189	
0.88446			
H	0.12067	-1.7416	-
0.88483			

H	-1.74136	-0.12076	
0.88521			
H	-1.74215	-0.12087	-
0.88407			

1-cyano-cyclobutane

The number of imaginary frequencies: 0

Total Energy (B3LYP/6-31G*)= -249.45559746

ZPE= -249.345159

Enthalpy= -249.338545

C	-0.07615	1.09848	-
0.00016			
C	1.09849	0.07615	-
0.00005			
C	0.07615	-1.09848	-
0.00007			
C	-1.09848	-0.07615	
0.00028			
H	-0.12091	1.74147	-0.885
H	1.74166	0.12083	
0.88465			
H	1.74184	0.1208	-
0.88464			
H	0.12095	-1.74189	
0.88446			
H	0.12067	-1.7416	-
0.88483			
H	-1.74136	-0.12076	
0.88521			
H	-1.74215	-0.12087	-
0.88407			
C	-0.13884	2.00382	
1.24405			
N	-0.18606	2.68576	
2.18124			

1-cyano-cyclobutane

The number of imaginary frequencies: 0

Total Energy (M06/6-311G+(d,p))= -249.32981858

ZPE= -249.220632

Enthalpy= -249.214045

C	-0.40578	0.16243	0.
C	0.20369	-0.79289	-
1.04213			
C	-0.07507	-1.89255	0.
C	0.20369	-0.79289	
1.04213			
H	-1.47442	0.10829	0.
H	1.2533	-0.62346	-
1.16275			
H	-0.19232	-0.85683	-
2.0341			
H	0.47817	-2.80841	0.
H	-1.10581	-2.17976	0.
H	1.2533	-0.62346	
1.16275			
H	-0.19232	-0.85683	
2.0341			
C	-0.1018	1.53058	0.
N	0.14765	2.64963	0.

Isobutane

The number of imaginary frequencies: 0
 Total Energy (B3LYP/6-31G*)= -158.45880816
 ZPE= -158.326386
 Enthalpy= -158.319765

C	0.	1.46175	-0.09598
C	0.	0.	0.37309
H	0.	0.	1.47365
H	-0.88629	1.99733	
0.26549			
H	0.88629	1.99733	
0.26549			
H	0.	1.52015	-1.19253
C	1.26592	-0.73088	-
0.09598			

C	-1.26592	-0.73088	-
0.09598			
H	1.28659	-1.76622	
0.26549			
H	1.31649	-0.76007	-
1.19253			
H	2.17288	-0.23111	
0.26549			
H	-1.31649	-0.76007	-
1.19253			
H	-1.28659	-1.76622	
0.26549			
H	-2.17288	-0.23111	
0.26549			

Isobutane

The number of imaginary frequencies: 0
 Total Energy (M06/6-311G+(d,p))= -158.36042407
 ZPE= -158.229965
 Enthalpy= -158.223369

C	-0.8703	1.17835	0.
C	0.31399	0.20152	0.
H	1.24021	0.79595	0.
H	-0.85537	1.82432	
0.88629			
H	-0.85537	1.82432	-
0.88629			
H	-1.82469	0.63522	0.
C	0.31399	-0.66693	-
1.26592			
C	0.31399	-0.66693	
1.26592			
H	1.17741	-1.34303	-
1.28659			
H	-0.59309	-1.28378	-
1.31649			
H	0.34826	-0.0511	-
2.17288			

H	-0.59309	-1.28378
1.31649		
H	1.17741	-1.34303
1.28659		
H	0.34826	-0.0511
2.17288		

2-cyano-isobutane

The number of imaginary frequencies: 0
 Total Energy (B3LYP/6-31G*)= -250.69730861
 ZPE= -250.566261
 Enthalpy= -250.558043

C	0.	1.46175	-0.78112
C	0.	0.	-0.31205
H	-0.88629	1.99733	-
0.41965			
H	0.88629	1.99733	-
0.41965			
H	0.	1.52015	-1.87768
C	1.26591	-0.73088	-
0.78112			
C	-1.26591	-0.73088	-
0.78112			
H	1.28659	-1.76622	-
0.41965			
H	1.31649	-0.76007	-
1.87768			
H	2.17288	-0.23111	-
0.41965			
H	-1.31649	-0.76007	-
1.87768			
H	-1.28659	-1.76622	-
0.41965			
H	-2.17288	-0.23111	-
0.41965			
C	0.	0.	
1.22795			

N	0.	0.
2.38795		

2-cyano-isobutane

The number of imaginary frequencies: 0
 Total Energy (M06/6-311G+(d,p))= -250.56898547
 ZPE= -250.439709
 Enthalpy= -250.431521

C	0.	1.46469	-0.77277
C	0.	0.	-0.27937
H	-0.88699	2.00042	-
0.42021			
H	0.88699	2.00042	-
0.42021			
H	0.	1.48094	-
1.86848			
C	1.26846	-0.73234	-
0.77277			
C	-1.26846	-0.73234	-
0.77277			
H	1.28892	-1.76836	-
0.42021			
H	1.28253	-0.74047	-
1.86848			
H	2.17591	-0.23206	-
0.42021			
H	-1.28253	-0.74047	-
1.86848			
H	-1.28892	-1.76836	-
0.42021			
H	-2.17591	-0.23206	-
0.42021			
C	0.	0.	
1.19869			
N	0.	0.	2.36008

Isobutane Oxide

The number of imaginary frequencies: 0
 Total Energy (B3LYP/6-31G*)= -233.0061692
 ZPE= -232.883092

Enthalpy= -232.875636
 C -0.08465 0.42439
 0.00229
 C 1.45504 0.44006 -
 0.02467
 H -0.45153 1.42951
 0.00782
 H -0.45139 -0.0844 -
 0.86462
 H -0.42081 -0.08284
 0.88241
 C 1.98307 -1.00656 -
 0.03263
 C 1.98287 1.17233
 1.22304
 H 3.05285 -0.99567 -
 0.05136
 H 1.6469 -1.51379
 0.84749
 H 1.61632 -1.51535 -
 0.89954
 H 1.64671 0.6651
 2.10316
 H 3.05265 1.18323
 1.2043
 H 1.61599 2.17746
 1.22856
 O 1.9043 1.11795 -
 1.20091

Isobutane Oxide

The number of imaginary frequencies: 0
 Total Energy (M06/6-311G+(d,p))= -
 232.90163743
 ZPE= -232.780778
 Enthalpy= -232.773277

C -1.48801 0.2227 0.
 C 0.06425 0.05546 0.

H -1.81464 0.76608
 0.89058
 H -1.81464 0.76608 -
 0.89058
 H -1.94366 -0.77347 0.
 C 0.5156 -0.67984 -
 1.27764
 C 0.5156 -0.67984
 1.27764
 H 1.60844 -0.74996 -
 1.30523
 H 0.10776 -1.69648 -
 1.31582
 H 0.1856 -0.13249 -
 2.16599
 H 0.10776 -1.69648
 1.31582
 H 1.60844 -0.74996
 1.30523
 H 0.1856 -0.13249
 2.16599
 O 0.5156 1.36104 0.

Tert-butoxide

The number of imaginary frequencies: 0
 Total Energy (B3LYP/6-31G*)= -
 233.03927664
 ZPE= -232.919
 Enthalpy= -232.911557

C -2.95594 -0.07066
 0.00229
 C -1.41625 -0.05499 -
 0.02467
 H -3.32281 0.93446
 0.00782
 H -3.32268 -0.57945 -
 0.86462
 H -3.2921 -0.57789
 0.88241

C	-0.88822	-1.50161	-
0.03263			
C	-0.88842	0.67728	
1.22304			
H	0.18156	-1.49072	-
0.05136			
H	-1.22438	-2.00884	
0.84749			
H	-1.25496	-2.0104	-
0.89954			
H	-1.22458	0.17005	
2.10316			
H	0.18136	0.68818	
1.2043			
H	-1.2553	1.68241	
1.22856			
O	-0.96699	0.6229	-
1.20091			

Tert-butoxide

The number of imaginary frequencies: 0
 Total Energy (M06/6-311G+(d,p))= -
 232.96980782
 ZPE= -232.850251
 Enthalpy= -232.843033

C	0.	1.46319	-0.43682
C	0.	0.	0.15961
H	-0.88471	1.99423	-
0.05736			
H	0.88471	1.99423	-
0.05736			
H	0.	1.53306	-1.54093
C	1.26716	-0.7316	-
0.43682			
C	-1.26716	-0.7316	-
0.43682			
H	1.2847	-1.7633	-
0.05736			
H	1.32767	-0.76653	-
1.54093			

H	2.16941	-0.23093	-
0.05736			
H	-1.32767	-0.76653	-
1.54093			
H	-1.2847	-1.7633	-
0.05736			
H	-2.16941	-0.23093	-
0.05736			
O	0.	0.	1.484

Tert-butanol

The number of imaginary frequencies: 0
 Total Energy (B3LYP/6-31G*)= -
 233.67097108
 ZPE= -233.53469
 Enthalpy= -233.527061

C	-2.78614	0.77678	
0.00423			
C	-1.24647	0.7924	-0.0232
H	-3.15299	1.78192	
0.00918			
H	-3.15316	0.26742	-
0.86222			
H	-3.12206	0.27017	
0.8848			
C	-0.71848	-0.65424	-
0.03032			
C	-0.71825	1.52551	
1.22385			
H	0.3513	-0.64339	-
0.04937			
H	-1.0544	-1.16086	
0.85025			
H	-1.08549	-1.16361	-
0.89677			
H	-1.05416	1.01889	
2.10442			
H	0.35153	1.53636	
1.2048			

H	-1.08509	2.53065
1.2288		
O	-0.79753	1.46947 -
1.20003		
H	-1.12681	1.01247 -
1.97741		

Tert-butanol

The number of imaginary frequencies: 0
 Total Energy (M06/6-311G+(d,p))= -
 233.57822574
 ZPE= -233.443543
 Enthalpy= -233.435882

C	-0.48647	-0.70717
1.26567		
C	0.00063	0.01449 0.
H	-0.16536	-0.16219
2.1595		
H	-1.58284	-0.77034
1.28057		
H	-0.09595	-1.72997
1.3225		
C	-0.48647	-0.70717 -
1.26567		
C	1.52516	0.14866 0.
H	-0.16536	-0.16219 -
2.1595		
H	-0.09595	-1.72997 -
1.3225		
H	-1.58284	-0.77034 -
1.28057		
H	2.00594	-0.83553 0.
H	1.85667	0.6993 -
0.88647		
H	1.85667	0.6993
0.88647		
O	-0.48647	1.36797 0.
H	-1.45634	1.32533 0.

Dimethyldioxirane

The number of imaginary frequencies: 0
 Total Energy (B3LYP/6-31G*)= -
 268.26893635
 ZPE= -268.180245
 Enthalpy= -268.173668

C	0.	0.	0.09405
O	-0.75265	0.	-1.09014
O	0.75265	0.	-1.09014
C	0.	1.29372	0.87204
H	-0.88605	1.35345	
1.51402			
H	0.88605	1.35345	
1.51402			
H	0.	2.13721	0.17866
C	0.	-1.29372	0.87204
H	0.88605	-1.35345	
1.51402			
H	-0.88605	-1.35345	
1.51402			
H	0.	-2.13721	0.17866

Diemthyldioxirane

The number of imaginary frequencies: 0
 Total Energy (M06/6-311G+(d,p))= -
 268.17073042
 ZPE= -268.083194
 Enthalpy= -268.076595

C	0.	0.	0.09405
O	-0.75265	0.	-1.09014
O	0.75265	0.	-1.09014
C	0.	1.29372	0.87204
H	-0.88605	1.35345	
1.51402			
H	0.88605	1.35345	
1.51402			
H	0.	2.13721	
0.17866			

C	0.	-1.29372
0.87204		
H	0.88605	-1.35345
1.51402		
H	-0.88605	-1.35345
1.51402		
H	0.	-2.13721 0.17866

1-azabicyclo[3.3.1]nonan-2-one

The number of imaginary frequencies: 0
 Total Energy (B3LYP/6-31G*)= -442.65877326
 ZPE= -442.45197
 Enthalpy= -442.443029

C	-0.49637	-1.28822 -
0.57938		
C	-0.35609	1.22423
0.35726		
C	-1.62086	0.84888 -
0.48922		
H	0.00119	-0.79517 -
1.38823		
H	-0.49982	-2.34298 -
0.75929		
H	-1.46437	1.24938 -
1.46902		
H	-2.51443	1.2602 -
0.06822		
C	1.4982	-0.78156
0.27343		
C	1.04761	1.20895 -
0.41451		
H	1.80583	1.4413
0.30382		
H	1.00949	1.96103 -
1.17466		
H	-0.49512	2.21928
0.7253		
C	-0.27607	0.19476
1.4253		

H	0.43419	0.4558	2.1818
H	-1.23488	0.06857	
1.8832			
C	1.45124	-0.1463 -	
1.11957			
H	2.32082	-0.73557 -	
1.32327			
H	2.01282	0.54207 -	
1.71596			
C	-1.83906	-0.69692 -	
0.48923			
H	-2.27832	-1.03664	
0.42539			
H	-2.48041	-0.96277 -	
1.30342			
N	0.18165	-1.01827	
0.72304			
O	2.54604	-1.04261	
0.91953			

1-azabicyclo[3.3.1]nonan-2-one

The number of imaginary frequencies: 0
 Total Energy (M06/6-311G+(d,p))= -442.46542043
 ZPE= -442.260754
 Enthalpy= -442.251891

C	1.47992	1.13475
0.30259		
C	0.06654	-1.51858
0.09096		
C	1.03437	-0.97622 -
0.99587		
H	1.31198	1.97218 -
0.37847		
H	2.1127	1.48961
1.12406		
H	0.46244	-0.40392 -
1.74022		
H	1.48569	-1.80863 -
1.54549		

C	-0.91909	1.04429	C	1.8199	-0.07291	-	
0.01271			0.18609				
C	-1.40185	-1.41106	-	C	-0.76203	-1.18497	
0.3435			0.66379				
H	-1.9993	-2.1865	0.1493	C	-0.00207	-1.5653	-
				0.65429			
H	-1.48843	-1.58693	-	H	2.02216	0.36127	-
1.42171				1.1429			
H	0.31208	-2.56073		H	2.69605	-0.01968	
0.32929				0.42582			
C	0.20236	-0.63269		H	-0.13215	-0.83388	-
1.32386				1.42435			
H	-0.60147	-0.80755		H	-0.37165	-2.50766	-
2.04679				1.0011			
H	1.14083	-0.77841		C	-0.38989	0.89081	-
1.86588				0.63882			
C	-1.9898	-0.02338		C	-2.10937	-0.57304	
0.01336				0.23742			
H	-2.44866	-0.06345		H	-2.85726	-0.58977	
1.00852				1.00245			
H	-2.76771	0.28707	-	H	-2.47067	-1.11804	-
0.68583				0.60954			
C	2.11858	-0.06536	-	H	-0.91426	-2.04993	1.275
0.42347				C	0.07376	-0.11999	
H	2.75523	-0.63713		1.4419			
0.26438				H	-0.58188	0.41577	
H	2.77868	0.29181	-	2.09611			
1.22024				H	0.86954	-0.54064	
N	0.1682	0.73597		2.02042			
0.81707				C	-1.77131	0.88819	-
O	-0.9722	2.04129	-	0.03872			
0.67495				H	-1.70032	1.40413	
				0.89599			
				H	-2.5119	1.3659	-
				0.64553			
				C	1.43965	-1.57586	-
				0.30576			
				H	1.54267	-2.10519	
				0.61841			

1-azabicyclo[3.3.1]nonan-2-one N-oxide
The number of imaginary frequencies: 0
Total Energy (B3LYP/6-31G*)= -517.78066499
ZPE= -517.570525
Enthalpy= -517.56056

H	2.06768	-2.03641	-
1.0395			
N	0.67578	0.69627	
0.38612			
O	-0.16179	1.01346	-
1.87028			
O	1.13924	1.89388	
0.83393			

1-azabicyclo[3.3.1]nonan-2-one N-oxide

The number of imaginary frequencies: 0
 Total Energy (M06/6-311G+(d,p))= -517.5822033
 ZPE= -517.374803
 Enthalpy= -517.364771

C	-1.54201	-1.00243	-0.1217
C	-0.0647	1.58133	
0.50268			
C	-1.07029	1.45316	-
0.69354			
H	-1.40068	-1.63532	-
0.99732			
H	-2.11124	-1.5535	
0.62939			
H	-0.52328	1.20489	-
1.61085			
H	-1.54772	2.42095	-0.881
C	0.90566	-0.73077	-
0.56889			
C	1.41296	1.64627	
0.03022			
H	2.02105	2.18527	
0.76515			
H	1.48025	2.20418	-
0.91013			
H	-0.30152	2.48045	
1.08175			
C	-0.19775	0.3506	
1.40313			

H	0.63236	0.2215
2.09731		
H	-1.12641	0.3022
1.97627		
C	2.00555	0.21376
0.15333		
H	2.4325	-0.14896
0.78555		
H	2.78694	0.18609
0.9149		
C	-2.15185	0.37882
0.45584		
H	-2.80987	0.70143
0.3603		
H	-2.786	0.29039
1.34461		
N	-0.17465	-0.84878
0.48961		
O	0.79199	-1.30301
1.62165		
O	0.29435	-1.97981
1.10659		

1-aza-2-adamantanone

The number of imaginary frequencies: 0
 Total Energy (B3LYP/6-31G*)= -480.75695031
 ZPE= -480.543716
 Enthalpy= -480.53497

C	-0.6513	-0.25597	-
0.01662			
H	0.41848	-0.26424	-
0.03661			
H	-0.9986	0.75597	-
0.03286			
C	-1.15275	-0.95091	
1.25587			
H	-0.79286	-0.43121	
2.11917			

C	-1.20094	-1.00657	-
1.23708			
H	-0.86636	-0.52267	-
2.13083			
C	-0.71689	-2.45467	-
1.22808			
H	0.35164	-2.48423	-
1.27557			
H	-1.12553	-2.96348	-
2.07603			
C	-0.61547	-2.42209	
1.28233			
H	-0.94244	-2.91128	
2.17602			
H	0.45402	-2.42786	
1.24982			
C	-1.19071	-3.14143	
0.06084			
H	-0.89325	-4.16811	
0.01238			
C	-2.68548	-3.00313	
0.25131			
C	-2.72471	-0.92451	
1.23932			
H	-3.06625	0.08879	
1.20103			
H	-3.09797	-1.39303	
2.12593			
C	-2.73613	-1.01635	-
1.19312			
H	-3.0999	-0.01061	-
1.22577			
H	-3.10361	-1.55895	-
2.03896			
N	-3.21549	-1.66257	
0.04943			
O	-3.40757	-3.96161	
0.63011			

1-aza-2-adamantanone

The number of imaginary frequencies: 1 (-15.00 cm⁻¹)

Total Energy (M06/6-311G+(d,p))= -480.54649801

ZPE= -480.33593

Enthalpy= -480.327979

C	2.00481	0.00013	-
0.04122			
H	2.67887	0.00047	
0.82639			
H	2.63927	-0.00004	-
0.93848			
C	1.11021	1.25758	-
0.02471			
H	1.72717	2.16493	-
0.06729			
C	1.11045	-1.25744	-
0.02404			
H	1.72752	-2.16474	-
0.06615			
C	0.2477	-1.26374	
1.25372			
H	0.88008	-1.26535	
2.15186			
H	-0.37137	-2.16957	
1.29419			
C	0.24749	1.26438	
1.25307			
H	-0.37169	2.17016	
1.29311			
H	0.87992	1.26657	
2.15117			
C	-0.65208	0.00028	
1.26354			
H	-1.326	0.00044	
2.12563			
C	-1.4899	-0.00011	-
0.01355			

C	0.16561	1.21374	-
1.24339			
H	0.73161	1.20954	-
2.18355			
H	-0.49161	2.09166	-
1.26358			
C	0.16581	-1.2144	-
1.24274			
H	0.7318	-1.21063	-
2.18291			
H	-0.49122	-2.09247	-
1.26242			
N	-0.69008	-0.00042	-
1.23426			
O	-2.69679	-0.00007	-
0.04028			

1-aza-2-adamantanone N-oxide

The number of imaginary frequencies: 0
 Total Energy (B3LYP/6-31G*)= -
 555.89761117
 ZPE= -555.680574
 Enthalpy= -555.670963

C	1.92654	-0.91079	
0.05192			
H	2.90664	-0.48151	
0.0573			
H	2.00627	-1.97736	
0.08316			
C	1.18071	-0.489	-
1.22029			
H	1.71273	-0.83763	-
2.0807			
C	1.13648	-0.41925	
1.27139			
H	1.63833	-0.71952	
2.16743			
C	1.02728	1.11812	
1.23801			

H	2.00369	1.55546	
1.25384			
H	0.47476	1.45332	
2.0908			
C	1.07764	1.05448	-
1.27331			
H	0.56135	1.34726	-
2.16361			
H	2.05585	1.48808	-
1.27262			
C	0.29382	1.52986	-
0.04413			
H	0.17657	2.59319	-
0.06599			
C	-1.05166	0.82736	-
0.07366			
C	-0.24342	-1.11093	-
1.19633			
H	-0.1666	-2.17752	-
1.15915			
H	-0.76856	-0.82057	-
2.08222			
C	-0.28367	-1.03432	
1.23486			
H	-0.21067	-2.10136	
1.26666			
H	-0.83664	-0.68728	
2.08261			
N	-0.98597	-0.62979	-
0.0068			
O	-2.14002	1.45544	-
0.00612			
O	-2.23926	-1.15783	-
0.00146			

1-aza-2-adamantanone N-oxide

The number of imaginary frequencies: 0
 Total Energy (M06/6-311G+(d,p))= -
 555.68378514
 ZPE= -555.468781
 Enthalpy= -555.459194

C	1.9256	-0.93904	0.0004
H	2.94464	-0.53161	
0.00035			
H	2.0157	-2.03288	
0.00072			
C	1.16406	-0.46823	-
1.25524			
H	1.67592	-0.81714	-
2.16103			
C	1.16386	-0.4675	
1.25566			
H	1.6756	-0.81587	
2.16173			
C	1.07179	1.06953	1.2666
H	2.0725	1.51978	
1.27521			
H	0.55193	1.41737	
2.16774			
C	1.07204	1.06882	-
1.26708			
H	0.55238	1.41614	-
2.16856			
H	2.07277	1.51903	-
1.27579			
C	0.3158	1.54057	-
0.00047			
H	0.18723	2.62743	-
0.00074			
C	-1.07154	0.92176	-
0.0004			
C	-0.25347	-1.05592	-
1.24346			
H	-0.26869	-2.14847	-
1.21878			
H	-0.86894	-0.72495	-
2.08433			
C	-0.25363	-1.05515	
1.24399			

H	-0.26901	-2.1477
1.21991		
H	-0.86942	-0.72356
2.08437		
N	-1.04552	-0.64681
0.00006		
O	-2.12403	1.48192
0.00011		
O	-2.2461	-1.1968
0.00006		

Acetone

The number of imaginary frequencies: 0
 Total Energy (B3LYP/6-31G*)= -
 193.15569459
 ZPE= -193.071622
 Enthalpy= -193.065254

C	0.	0.	0.15196
O	0.	0.	1.41036
C	0.	-1.33368	-0.61804
H	-0.5044	-1.20574	-
1.55298			
H	1.00881	-1.64256	-
0.79637			
H	-0.5044	-2.07939	-
0.03977			
C	0.	1.33368	-0.61804
H	0.5044	1.20574	-
1.55298			
H	-1.00881	1.64256	-
0.79637			
H	0.5044	2.07939	-
0.03977			

Acetone

The number of imaginary frequencies: 0
 Total Energy (M06/6-311G+(d,p))= -
 193.07885176
 ZPE= -192.996166
 Enthalpy= -192.990644

C	0.	0.	0.15196
O	0.	0.	1.41036
C	0.	-1.33368	-0.61804
H	-0.5044	-1.20574	-
1.55298			
H	1.00881	-1.64256	-
0.79637			
H	-0.5044	-2.07939	-
0.03977			
C	0.	1.33368	-0.61804
H	0.5044	1.20574	-
1.55298			
H	-1.00881	1.64256	-
0.79637			
H	0.5044	2.07939	-
0.03977			

Hydrogen Peroxide

The number of imaginary frequencies: 1 (-261.15 cm⁻¹)
 Total Energy (B3LYP/6-31G*)= -151.53208497
 ZPE= -151.506399
 Enthalpy= -151.502562

O	-0.64299	-0.14886	0.
H	-1.15889	0.66074	0.
O	0.64299	0.14886	0.
H	1.15889	-0.66074	0.

Hydrogen Peroxide

The number of imaginary frequencies: 1 (-377.89 cm⁻¹)
 Total Energy (M06/6-311G+(d,p))= -151.52110268
 ZPE= -151.494886
 Enthalpy= -151.491055

O	-0.64299	-0.14886	0.
H	-1.15889	0.66074	0.
O	0.64299	0.14886	0.

H	1.15889	-0.66074	0.
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Methylacetate

The number of imaginary frequencies: 0
 Total Energy (B3LYP/6-31G*)= -268.38848966
 ZPE= -268.298165
 Enthalpy= -268.291067

C	0.27318	0.83923	
0.15226			
O	1.49767	0.86066	
0.44164			
C	-0.45023	-0.50727	-
0.03539			
H	-1.47835	-0.40142	
0.24149			
H	-0.38598	-0.80684	-
1.06059			
H	0.011	-1.24911	
0.58254			
O	-0.44654	2.0652	-
0.00234			
C	-0.37666	2.49027	-
1.36591			
H	-0.9152	3.4076	-
1.48159			
H	0.6465	2.64024	-
1.64077			
H	-0.80901	1.74102	-
1.9956			

Methylacetate

The number of imaginary frequencies: 0
 Total Energy (M06/6-311G+(d,p))= -268.30586312
 ZPE= -268.216855
 Enthalpy= -268.209704

C	-0.46052	0.17822	-
0.00005			

O	-0.28541	1.37656	-
0.00001			
C	-1.80139	-0.51814	
0.00003			
H	-1.89229	-1.16153	-
0.88128			
H	-1.89317	-1.15942	
0.88279			
H	-2.5971	0.2274	-
0.00121			
O	0.5495	-0.72391	-
0.00009			
C	1.87184	-0.16319	
0.00006			
H	2.55177	-1.01579	
0.00065			
H	2.02949	0.45296	-
0.88939			
H	2.02897	0.45383	
0.88898			

Water

The number of imaginary frequencies: 0
 Total Energy (B3LYP/6-31G*)= -
 76.40895332
 ZPE= -76.387785
 Enthalpy= -76.384006

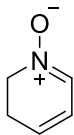
O	-0.00008	-0.8136	0.
H	0.95992	-0.81336	0.
H	-0.3203	0.09142	0.

Water

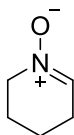
The number of imaginary frequencies: 0
 Total Energy (M06/6-311G+(d,p))= -
 76.41784139
 ZPE= -76.396247
 Enthalpy= -76.392466

O	0.	0.	0.11972
H	0.	0.76156	-0.47888
H	0.	-0.76156	-0.47888

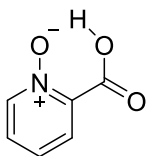
Table 3 Structures



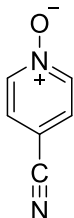
1-Aza-1,3-cyclohexadiene N-oxide



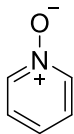
1-Azacyclohexene N-oxide



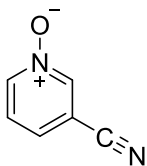
2-Carboxypyridine N-oxide



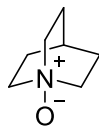
4-Cyanopyridine N-oxide



Pyridine N-oxide (PNO)

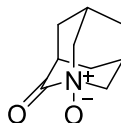


3-Cyanopyridine N-oxide



1-Azabicyclo[2.2.2]octane N-oxide

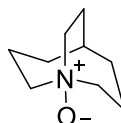
(Quinuclidine-N-oxide)



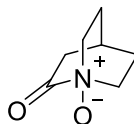
1-Azaadamantane-2-one N-oxide



Trimethylamine N-oxide (TMAO)

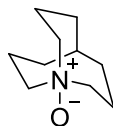


1-Azabicyclo[3.3.2]decane N-oxide



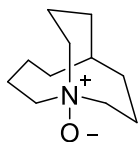
1-Azabicyclo[2.2.2]octan-2-one N-oxide

(2-Quinuclidinone N-oxide)

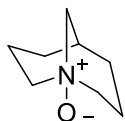


1-Azabicyclo[3.3.3]undecane N-oxide

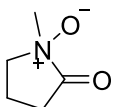
(Manxine N-oxide)



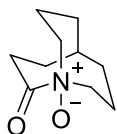
1-Azabicyclo[4.3.3]dodecane N-oxide



1-Azabicyclo[3.3.1]nonan-2-one N-oxide



N-Methyl-2-pyrrolidinone N-oxide



1-Azabicyclo[3.3.3]undecane-2-one N-oxide

(2-Manxinone N-oxide)