

Understanding the Mechanism of the Chiral Phosphoric Acid-Catalyzed Aza-Cope Rearrangement

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Full list of authors in the Gaussian 09 reference

Gaussian 09, Revision E.01,

M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2013.

Energy profile of enantiodetermining step

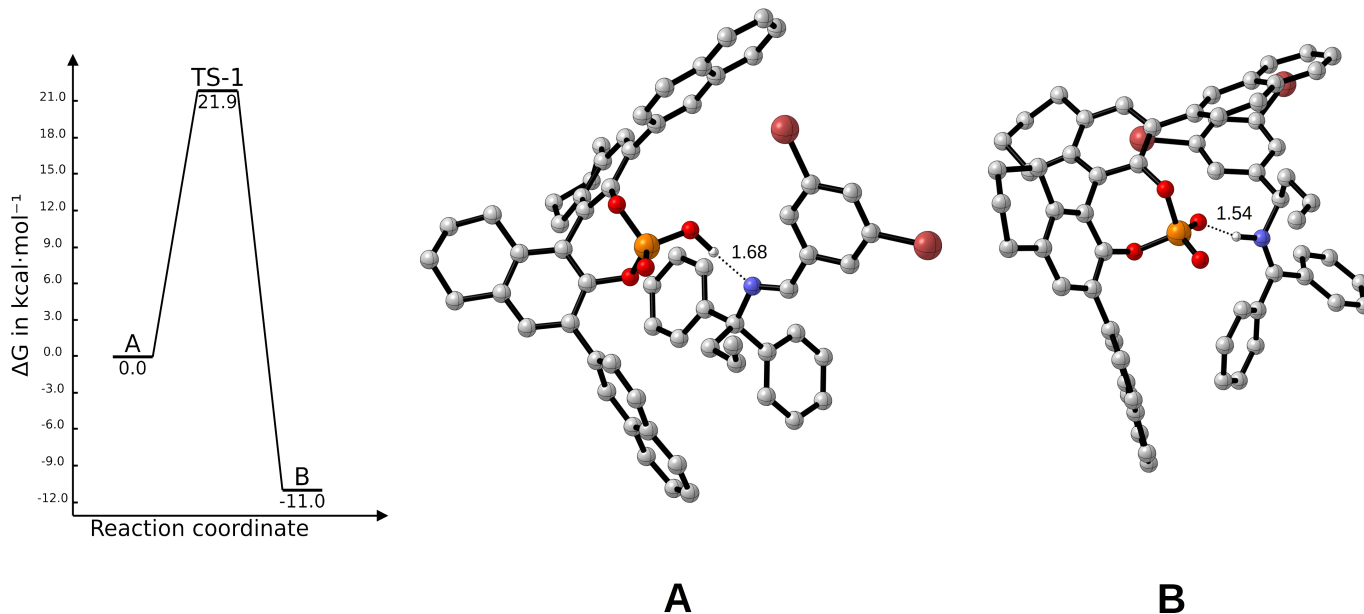


Figure S1. Energy profile of the enantiodetermining step and optimized structures of intermediates **A** and **B** obtained with M06-2X/6-31G*, single point with M06-2X/def2-TZVPP in dibutylether (SMD), and thermal corrections with M06-2X/6-31G*.

TS Structures of Model System

TS-A

M06-2X/def2-TZVPP-SMD(toluene) Energy = -1741.55089552

Number of Imaginary Frequencies = 1

Lowest Frequency = 346.9523i

M06-2X/6-31G* Geometry

C	-0.814589	-0.784308	2.046099
C	-1.244589	-0.781914	0.281399
C	-1.524506	0.353582	2.490199
H	0.268410	-0.677792	1.979299
H	-1.137975	-1.748413	2.430899
C	-1.104725	1.642788	2.087399
H	-2.529304	0.227667	2.892299
N	-0.803207	0.461292	-0.155101
C	-0.492172	-1.957203	-0.324901
C	-2.749386	-0.987236	0.112499
C	-1.433224	1.589983	0.359999
C	-1.003843	2.916589	-0.201301
H	-2.518122	1.486467	0.316099
H	0.232092	0.524708	-0.326101
H	-0.021227	1.791704	2.092699
H	-1.690537	2.482679	2.457999

C	4.089128	-1.921236	-0.613201
C	3.096130	-2.086550	0.271299
C	4.879110	-0.735924	-0.941101
C	4.871793	0.462176	-0.350001
O	2.537117	-1.169759	1.107399
O	4.100587	0.826464	0.722299
P	2.510793	0.446841	0.763299
O	1.906390	0.627532	-0.602701
O	1.890784	1.091732	1.951499
C	-3.581377	-1.563848	1.070899
C	-4.930474	-1.787068	0.797899
C	-5.464279	-1.434876	-0.435901
C	-4.638488	-0.863364	-1.402401
C	-3.292491	-0.648844	-1.133501
H	-3.191373	-1.851143	2.042599
H	-5.561768	-2.236378	1.557999
H	-6.515377	-1.605292	-0.645501
H	-2.644097	-0.210835	-1.887701
H	-5.042292	-0.587270	-2.371401
C	-0.699553	-3.243806	0.185399
C	-0.091037	-4.345797	-0.400401
C	0.725161	-4.179785	-1.518701
C	0.929742	-2.905382	-2.032901
C	0.325326	-1.795191	-1.444901
H	0.524311	-0.810088	-1.848701
H	-1.361651	-3.394516	1.033399
H	-0.262922	-5.335700	0.010399
H	1.197974	-5.040378	-1.981801
H	1.573440	-2.758373	-2.894001
C	0.305350	3.385809	-0.076001
C	0.652432	4.608314	-0.641601
C	-0.297079	5.368800	-1.320701
C	-1.604972	4.906081	-1.436501
C	-1.956854	3.682375	-0.875501
H	-2.976149	3.314560	-0.967901
H	1.046858	2.799720	0.457999
H	-2.350381	5.494770	-1.961801
H	2.633545	-3.060157	0.403799
H	4.346241	-2.821432	-1.163401
H	5.526881	1.264685	-0.671501
H	5.577912	-0.843614	-1.764701
H	1.672327	4.966629	-0.547701
H	-0.018493	6.323404	-1.756401

TS-A-2

M06-2X/def2-TZVPP-SMD(toluene) Energy = -1741.55086987

Number of Imaginary Frequencies = 1

Lowest Frequency = 353.9001i

M06-2X/6-31G* Geometry

C	-0.723987	-0.802013	2.054598
C	-1.164087	-0.828522	0.266098
C	-1.518408	0.275771	2.487398
H	0.346409	-0.616692	1.975898
H	-0.972368	-1.789218	2.435998
C	-1.201134	1.593777	2.068098
H	-2.508304	0.076152	2.896998
N	-0.830012	0.442085	-0.168402
C	-2.651880	-1.151551	0.124398
C	-0.337065	-1.947906	-0.345302
C	-1.537133	1.523071	0.360498
C	-1.200259	2.872777	-0.209702
H	-2.612829	1.345350	0.319298
H	0.183185	0.609604	-0.391802

H	-0.131639	1.823898	2.078898
H	-1.846150	2.386965	2.444098
C	4.134132	-1.790318	-0.499402
C	3.119135	-1.934438	0.362998
C	4.906509	-0.604703	-0.864602
C	4.855585	0.619896	-0.334002
O	2.516117	-0.991550	1.137898
O	4.051777	1.015480	0.702298
P	2.468285	0.612349	0.730698
O	1.878683	0.733338	-0.647802
O	1.819872	1.287736	1.887098
C	0.427931	-1.733391	-1.493602
C	1.085952	-2.800378	-2.102802
C	0.986377	-4.084980	-1.583102
C	0.222381	-4.304295	-0.437402
C	-0.439139	-3.245008	0.170198
H	0.538712	-0.739289	-1.907902
H	1.687348	-2.611466	-2.986002
H	1.499593	-4.912270	-2.063502
H	-1.060036	-3.439720	1.039998
H	0.131401	-5.302997	-0.022102
C	-3.419168	-1.801266	1.090098
C	-4.750661	-2.128892	0.837098
C	-5.332367	-1.809804	-0.384002
C	-4.571480	-1.165489	-1.357702
C	-3.242386	-0.846563	-1.108702
H	-2.644896	-0.350951	-1.869102
H	-2.992162	-2.065258	2.052498
H	-5.330551	-2.633804	1.603198
H	-6.370063	-2.061524	-0.577902
H	-5.012585	-0.913397	-2.317002
C	0.088130	3.405003	-0.122402
C	0.354606	4.650008	-0.682902
C	-0.654808	5.370588	-1.318002
C	-1.941598	4.845063	-1.394502
C	-2.213073	3.598258	-0.839002
H	-3.215665	3.181638	-0.900902
H	0.874041	2.851318	0.383398
H	-2.733209	5.402747	-1.885002
H	2.668054	-2.909747	0.523198
H	4.421150	-2.709813	-1.001002
H	5.497469	1.422708	-0.680602
H	5.626311	-0.734189	-1.666802
H	1.357698	5.058627	-0.618002
H	-0.439327	6.343292	-1.749402

TS-B

M06-2X/def2-TZVPP-SMD(toluene) Energy = -1741.54997807

Number of Imaginary Frequencies = 1

Lowest Frequency = 412.8436i

M06-2X/6-31G* Geometry

C	-0.742298	-0.890501	1.906997
C	-1.392999	-0.705101	0.191797
C	-1.192899	0.305599	2.497497
H	0.318302	-0.935700	1.651397
H	-1.163098	-1.824901	2.271297
C	-0.643401	1.541199	2.080797
H	-2.134099	0.311298	3.046597
N	-0.862800	0.506499	-0.218103
C	-0.795497	-1.903801	-0.521203
C	-2.914699	-0.739603	0.198597
C	-1.276801	1.665099	0.419297
C	-0.732102	2.961699	-0.106303

H	-2.358901	1.702798	0.552097
H	0.183000	0.460800	-0.278803
H	0.425399	1.539700	1.861497
H	-1.007701	2.436399	2.581497
C	4.377402	-0.984096	1.963297
C	4.676201	0.146404	1.303997
C	3.452903	-2.067897	1.635497
C	2.868503	-2.284597	0.453697
O	4.176400	0.650504	0.144097
O	3.068702	-1.498597	-0.648003
P	2.777701	0.120602	-0.532003
O	1.672801	0.314101	0.486597
O	2.638700	0.682702	-1.893503
C	-3.696598	-1.212003	1.251597
C	-5.085698	-1.261305	1.136397
C	-5.708098	-0.835305	-0.030703
C	-4.933599	-0.364504	-1.089703
C	-3.549499	-0.323303	-0.979003
H	-3.236398	-1.553703	2.173397
H	-5.677598	-1.633005	1.966897
H	-6.789298	-0.870206	-0.117303
H	-2.942499	0.035697	-1.805303
H	-5.407999	-0.031205	-2.007303
C	-1.201896	-3.191101	-0.150403
C	-0.662495	-4.307901	-0.773703
C	0.288005	-4.153100	-1.783803
C	0.681103	-2.876699	-2.168203
C	0.139302	-1.752700	-1.546403
H	0.466902	-0.773100	-1.881403
H	-1.953496	-3.319302	0.624497
H	-0.985294	-5.299901	-0.473603
H	0.714805	-5.025499	-2.268603
H	1.427403	-2.734899	-2.942603
C	-1.405503	4.137699	0.234797
C	-0.938104	5.370799	-0.204203
C	0.209096	5.434500	-0.992303
C	0.877597	4.263101	-1.338203
C	0.416998	3.024900	-0.898803
H	0.965199	2.134801	-1.195803
H	-2.304603	4.084398	0.845997
H	1.768997	4.298602	-1.956103
H	5.439200	0.810205	1.698097
H	4.936302	-1.109996	2.885797
H	2.197604	-3.119998	0.265397
H	3.243203	-2.785297	2.423097
H	-1.470805	6.277799	0.063697
H	0.577195	6.395101	-1.339103

TS-B-2

M06-2X/def2-TZVPP-SMD(toluene) Energy = -1741.54997703

Number of Imaginary Frequencies = 1

Lowest Frequency = 412.7971i

M06-2X/6-31G* Geometry

C	-0.742215	-0.890588	1.906994
C	-1.392911	-0.705275	0.191894
C	-1.192890	0.305421	2.497494
H	0.318385	-0.935610	1.651394
H	-1.162934	-1.824980	2.271294
C	-0.643565	1.541109	2.080794
H	-2.134090	0.311140	3.046694
N	-0.862986	0.506414	-0.218106
C	-2.914611	-0.740044	0.198694
C	-0.795335	-1.903887	-0.521106

C	-1.277162	1.664923	0.419294
C	-0.732635	2.961611	-0.106306
H	-2.359261	1.702445	0.552294
H	0.182813	0.460993	-0.278906
H	0.425235	1.539688	1.861394
H	-1.007846	2.436317	2.581394
C	4.378284	-0.983494	1.962894
C	4.676707	0.147200	1.303494
C	3.453761	-2.067275	1.635394
C	2.869257	-2.284163	0.453794
O	4.176117	0.651411	0.143894
O	3.069273	-1.498167	-0.648006
P	2.777606	0.120839	-0.532006
O	1.672710	0.313862	0.486694
O	2.638118	0.682942	-1.893506
C	-1.201562	-3.191279	-0.150306
C	-0.661985	-4.307990	-0.773606
C	0.288518	-4.153110	-1.783706
C	0.681545	-2.876618	-2.168006
C	0.139568	-1.752707	-1.546406
H	-1.953164	-3.319464	0.624594
H	-0.984705	-5.299983	-0.473506
H	0.715401	-5.025418	-2.268506
H	0.467088	-0.773113	-1.881306
H	1.427748	-2.734733	-2.942506
C	-3.696521	-1.212328	1.251794
C	-5.085522	-1.261799	1.136494
C	-5.708013	-0.836087	-0.030706
C	-4.933604	-0.365402	-1.089806
C	-3.549503	-0.324031	-0.979006
H	-2.942396	0.034957	-1.805406
H	-3.236228	-1.553737	2.173594
H	-5.677430	-1.633387	1.966994
H	-6.789214	-0.871264	-0.117306
H	-5.407997	-0.032393	-2.007406
C	-1.406511	4.137425	0.234494
C	-0.939286	5.370716	-0.204506
C	0.208115	5.434592	-0.992306
C	0.877091	4.263378	-1.337806
C	0.416666	3.025088	-0.898406
H	0.965148	2.135076	-1.195206
H	-2.305812	4.083944	0.845394
H	1.768592	4.298960	-1.955406
H	5.439720	0.810985	1.697294
H	4.937681	-1.109305	2.885094
H	2.198240	-3.119549	0.265694
H	3.244347	-2.784670	2.423194
H	-1.472367	6.277627	0.063194
H	0.576035	6.395284	-1.339006

TS-A-3

M06-2X/def2-TZVPP-SMD(toluene) Energy = -1741.54921887

Number of Imaginary Frequencies = 1

Lowest Frequency = 365.2891i

M06-2X/6-31G* Geometry

C	-0.397616	-0.868998	1.955606
C	-1.070017	-0.938995	0.236106
C	-1.244612	0.106106	2.512106
H	0.623685	-0.562603	1.736106
H	-0.476421	-1.881098	2.344406
C	-1.139306	1.453405	2.079906
H	-2.141813	-0.208790	3.044606
N	-0.956911	0.365104	-0.209094

C	-0.198721	-1.940899	-0.504894
C	-2.511319	-1.445989	0.289706
C	-1.708706	1.348208	0.434706
C	-1.619600	2.732307	-0.145394
H	-2.750008	1.040712	0.542706
H	-0.008809	0.658300	-0.563694
H	-0.112504	1.806000	1.941906
H	-1.810303	2.166908	2.556606
C	4.803081	-1.390221	0.011306
C	3.473481	-1.532215	0.001006
C	5.482586	-0.249824	0.620106
C	5.006692	0.998378	0.581906
O	2.630585	-0.681112	0.659606
O	3.908194	1.356783	-0.152194
P	2.390792	0.896489	0.232206
O	1.586092	0.974393	-1.035094
O	1.859794	1.551092	1.463306
C	-3.054522	-2.190086	1.336106
C	-4.357224	-2.680781	1.256906
C	-5.134023	-2.432577	0.131506
C	-4.597820	-1.693880	-0.921494
C	-3.297018	-1.211685	-0.846094
H	-2.471923	-2.401489	2.227106
H	-4.761227	-3.257079	2.083306
H	-6.149125	-2.811773	0.073306
H	-2.874315	-0.641587	-1.668994
H	-5.192719	-1.494777	-1.807394
C	-0.065027	-3.242100	-0.010294
C	0.639769	-4.204503	-0.722894
C	1.208770	-3.883505	-1.953994
C	1.073276	-2.593305	-2.454794
C	0.373580	-1.623302	-1.739494
H	0.295485	-0.622701	-2.144494
H	-0.532928	-3.519498	0.929906
H	0.734464	-5.207903	-0.320294
H	1.753367	-4.635408	-2.516594
H	1.515477	-2.327207	-3.409394
C	-0.401297	3.408802	-0.243494
C	-0.368292	4.680702	-0.805794
C	-1.539389	5.285807	-1.257494
C	-2.754992	4.616412	-1.147494
C	-2.793798	3.341612	-0.590394
H	-3.740400	2.812517	-0.507794
H	0.512301	2.945598	0.119206
H	-3.671490	5.083416	-1.494294
H	2.965677	-2.378213	-0.454094
H	5.398578	-2.176624	-0.442894
H	5.503796	1.838776	1.056706
H	6.427286	-0.412529	1.130606
H	0.580411	5.201197	-0.887294
H	-1.504985	6.280307	-1.691494

TS-A-4

M06-2X/def2-TZVPP-SMD(toluene) Energy = -1741.54921754

Number of Imaginary Frequencies = 1

Lowest Frequency = 365.6470i

M06-2X/6-31G* Geometry

C	-0.397188	-0.869008	1.955896
C	-1.069587	-0.939213	0.236096
C	-1.244594	0.105786	2.512296
H	0.624010	-0.562202	1.736396
H	-0.475581	-1.881109	2.344596
C	-1.139803	1.453087	2.080096

H	-2.141592	-0.209520	3.044696
N	-0.957096	0.364888	-0.208904
C	-0.197781	-1.940607	-0.504904
C	-2.510684	-1.446822	0.289796
C	-1.709202	1.347783	0.434796
C	-1.620611	2.731883	-0.145204
H	-2.750400	1.039876	0.542996
H	-0.009298	0.658494	-0.564004
H	-0.113105	1.806093	1.941996
H	-1.811008	2.166382	2.556796
C	5.482208	-0.248570	0.620496
C	5.006200	0.999527	0.581996
C	4.803116	-1.389174	0.011696
C	3.473517	-1.531383	0.000996
O	3.907798	1.357420	-0.152604
O	2.630311	-0.680388	0.659396
P	2.390401	0.897210	0.231996
O	1.585600	0.975205	-1.035204
O	1.859596	1.551707	1.463296
C	-3.053379	-2.191626	1.335896
C	-4.355776	-2.682935	1.256796
C	-5.132877	-2.434740	0.131596
C	-4.597282	-1.695336	-0.921304
C	-3.296585	-1.212528	-0.845804
H	-2.470577	-2.403122	2.226796
H	-4.759472	-3.259737	2.082996
H	-6.147875	-2.814446	0.073296
H	-2.874289	-0.641925	-1.668604
H	-5.192283	-1.496240	-1.807004
C	-0.063272	-3.241806	-0.010404
C	0.641934	-4.203702	-0.723204
C	1.210332	-3.882498	-1.954504
C	1.074024	-2.592299	-2.455304
C	0.373917	-1.622803	-1.739704
H	0.295211	-0.622204	-2.144804
H	-0.530570	-3.519409	0.930096
H	0.737341	-5.207101	-0.320604
H	1.755137	-4.634094	-2.517204
H	1.515822	-2.325996	-3.410004
C	-0.402616	3.408892	-0.243204
C	-0.370124	4.680892	-0.805604
C	-1.541528	5.285384	-1.257404
C	-2.756724	4.615376	-1.147404
C	-2.795015	3.340676	-0.590404
H	-3.741312	2.811169	-0.507804
H	0.511287	2.946098	0.119496
H	-3.673427	5.081970	-1.494304
H	5.502894	1.840031	1.056796
H	6.426809	-0.411063	1.131296
H	2.966022	-2.377486	-0.454304
H	5.398921	-2.175470	-0.442404
H	0.578372	5.201798	-0.887004
H	-1.507535	6.279884	-1.691404

TS-A-5

M06-2X/def2-TZVPP-SMD(toluene) Energy = -1741.54921710

Number of Imaginary Frequencies = 1

Lowest Frequency = 365.5523i

M06-2X/6-31G* Geometry

C	-0.397502	-0.869096	1.955786
C	-1.070003	-0.938995	0.236086
C	-1.244401	0.106006	2.512286
H	0.623798	-0.562698	1.736186

H	-0.476304	-1.881196	2.344486
C	-1.139098	1.453305	2.080086
H	-2.141601	-0.208893	3.044786
N	-0.957000	0.365005	-0.208914
C	-2.511303	-1.445992	0.289786
C	-0.198704	-1.940796	-0.504914
C	-1.708698	1.348206	0.434886
C	-1.619596	2.732306	-0.145114
H	-2.749999	1.040808	0.542986
H	-0.009100	0.658303	-0.564014
H	-0.112298	1.805904	1.941986
H	-1.809997	2.166807	2.556886
C	5.482199	-0.249807	0.620786
C	5.006401	0.998394	0.582086
C	4.803097	-1.390305	0.011886
C	3.473496	-1.532403	0.000786
O	3.908202	1.356296	-0.152814
O	2.630098	-0.681301	0.658886
P	2.390701	0.896599	0.231886
O	1.585801	0.975000	-1.035214
O	1.860302	1.551000	1.463286
C	-0.064907	-3.242097	-0.010514
C	0.639892	-4.204298	-0.723214
C	1.208892	-3.883199	-1.954314
C	1.073395	-2.592899	-2.455014
C	0.373596	-1.623097	-1.739514
H	-0.532607	-3.519596	0.929786
H	0.734790	-5.207798	-0.320714
H	1.753491	-4.635000	-2.517014
H	0.295498	-0.622397	-2.144514
H	1.515695	-2.326599	-3.409514
C	-3.297103	-1.211391	-0.845814
C	-4.598004	-1.693588	-0.921214
C	-5.134005	-2.432688	0.131586
C	-4.357006	-2.681289	1.256786
C	-3.054305	-2.190491	1.335986
H	-2.471605	-2.402192	2.226886
H	-2.874602	-0.641092	-1.668714
H	-5.193004	-1.494387	-1.807014
H	-6.149106	-2.811986	0.073386
H	-4.760907	-3.257788	2.083086
C	-0.401295	3.409004	-0.242914
C	-0.368392	4.680904	-0.805414
C	-1.539491	5.285706	-1.257414
C	-2.754993	4.616108	-1.147714
C	-2.793695	3.341408	-0.590614
H	-3.740196	2.812110	-0.508214
H	0.512304	2.946102	0.120086
H	-3.671392	5.082910	-1.494914
H	5.503102	1.838893	1.056986
H	6.426698	-0.412408	1.131886
H	2.965995	-2.378402	-0.454614
H	5.398795	-2.176806	-0.442014
H	0.580208	5.201602	-0.886514
H	-1.505190	6.280306	-1.691514

TS-A-6

M06-2X/def2-TZVPP-SMD(toluene) Energy = -1741.54921576

Number of Imaginary Frequencies = 1

Lowest Frequency = 365.4323i

M06-2X/6-31G* Geometry

C	-0.397508	-0.869101	1.955804
C	-1.069908	-0.938992	0.236104

C	-1.244496	0.105910	2.512304
H	0.623896	-0.562613	1.736204
H	-0.476120	-1.881200	2.344404
C	-1.139280	1.453208	2.080104
H	-2.141600	-0.209079	3.044804
N	-0.956993	0.365006	-0.208896
C	-2.511215	-1.446175	0.289804
C	-0.198521	-1.940803	-0.504896
C	-1.708781	1.348115	0.434904
C	-1.619764	2.732214	-0.145096
H	-2.750085	1.040628	0.543004
H	-0.009089	0.658395	-0.563996
H	-0.112475	1.805896	1.942104
H	-1.810171	2.166717	2.556904
C	5.482300	-0.249472	0.620804
C	5.006315	0.998734	0.582104
C	4.803286	-1.389964	0.011804
C	3.473684	-1.532147	0.000704
O	3.908119	1.356547	-0.152696
O	2.630195	-0.681237	0.658804
P	2.390614	0.896666	0.231804
O	1.585715	0.974975	-1.035196
O	1.860122	1.550972	1.463304
C	-0.064636	-3.242005	-0.010496
C	0.640252	-4.204213	-0.723196
C	1.209156	-3.883020	-1.954296
C	1.073471	-2.592818	-2.454996
C	0.373683	-1.623010	-1.739596
H	-0.532240	-3.519599	0.929804
H	0.735240	-5.207714	-0.320696
H	1.753847	-4.634827	-2.516996
H	0.295395	-0.622309	-2.144496
H	1.515675	-2.326524	-3.409596
C	-3.297012	-1.211665	-0.845796
C	-4.597818	-1.693950	-0.921296
C	-5.133827	-2.433043	0.131604
C	-4.356830	-2.681553	1.256804
C	-3.054124	-2.190668	1.336004
H	-2.471426	-2.402375	2.226904
H	-2.874605	-0.641171	-1.668596
H	-5.192815	-1.494642	-1.806996
H	-6.148931	-2.812431	0.073304
H	-4.760637	-3.258148	2.083004
C	-0.401556	3.408999	-0.242996
C	-0.368740	4.680899	-0.805396
C	-1.539933	5.285713	-1.257396
C	-2.755341	4.616028	-1.147596
C	-2.793957	3.341228	-0.590596
H	-3.740463	2.811940	-0.508096
H	0.512139	2.946088	0.119904
H	-3.671836	5.082739	-1.494696
H	5.502925	1.839228	1.057004
H	6.426798	-0.411983	1.131904
H	2.966274	-2.378241	-0.454696
H	5.399177	-2.176371	-0.441996
H	0.579866	5.201588	-0.886696
H	-1.505621	6.280213	-1.691496

TS-A-7

M06-2X/def2-TZVPP-SMD(toluene) Energy = -1741.54921539

Number of Imaginary Frequencies = 1

Lowest Frequency = 365.5663i

M06-2X/6-31G* Geometry

C	-0.397407	-0.868912	1.955798
C	-1.069807	-0.939111	0.236098
C	-1.244805	0.105890	2.512198
H	0.623794	-0.562215	1.736298
H	-0.475910	-1.881012	2.344498
C	-1.139801	1.453190	2.079898
H	-2.141905	-0.209308	3.044498
N	-0.957004	0.364889	-0.209002
C	-2.511009	-1.446507	0.289698
C	-0.198210	-1.940813	-0.504802
C	-1.709102	1.347891	0.434598
C	-1.620198	2.731991	-0.145302
H	-2.750302	1.040194	0.542598
H	-0.009203	0.658287	-0.564102
H	-0.113101	1.806087	1.941998
H	-1.811000	2.166491	2.556598
C	5.482394	-0.248227	0.621198
C	5.005998	0.999674	0.582298
C	4.803992	-1.389025	0.012098
C	3.474491	-1.531722	0.000598
O	3.907798	1.357077	-0.152902
O	2.630393	-0.681120	0.658398
P	2.390497	0.896681	0.231598
O	1.585497	0.974983	-1.035402
O	1.859699	1.550782	1.463198
C	0.373891	-1.623114	-1.739502
C	1.073889	-2.592816	-2.454902
C	1.209885	-3.883016	-1.954002
C	0.640985	-4.204115	-0.722802
C	-0.064013	-3.242013	-0.010202
H	0.295394	-0.622514	-2.144602
H	1.515989	-2.326617	-3.409502
H	1.754684	-4.634818	-2.516602
H	-0.531614	-3.519512	0.930098
H	0.736182	-5.207515	-0.320202
C	-3.053810	-2.191206	1.335898
C	-4.356312	-2.682302	1.256698
C	-5.133411	-2.433901	0.131498
C	-4.597609	-1.694602	-0.921302
C	-3.296908	-1.212105	-0.845902
H	-2.874507	-0.641606	-1.668702
H	-2.471011	-2.402807	2.226698
H	-4.760113	-3.259001	2.082898
H	-6.148412	-2.813498	0.073198
H	-5.192609	-1.495500	-1.807102
C	-2.794597	3.341094	-0.590302
C	-2.756094	4.615994	-1.147102
C	-1.540792	5.285791	-1.257002
C	-0.369393	4.680988	-0.805402
C	-0.402097	3.408888	-0.243302
H	0.511702	2.945886	0.119298
H	-3.740998	2.811796	-0.507702
H	0.579108	5.201685	-0.886802
H	5.502100	1.840473	1.057398
H	6.426794	-0.410429	1.132598
H	2.967489	-2.378021	-0.454902
H	5.400290	-2.175227	-0.441602
H	-3.672692	5.082796	-1.493802
H	-1.506589	6.280390	-1.690802

TS-A-8

M06-2X/def2-TZVPP-SMD(toluene) Energy = -1741.54921311

Number of Imaginary Frequencies = 1

Lowest Frequency = 365.5090i

M06-2X/6-31G* Geometry

C	-0.397394	-0.869103	1.955809
C	-1.069894	-0.939107	0.236109
C	-1.244500	0.105892	2.512209
H	0.623904	-0.562597	1.736209
H	-0.476088	-1.881203	2.344409
C	-1.139309	1.453192	2.080109
H	-2.141598	-0.209114	3.044809
N	-0.957002	0.364994	-0.208891
C	-0.198488	-1.940802	-0.504891
C	-2.511191	-1.446216	0.289709
C	-1.708808	1.348089	0.434909
C	-1.619817	2.732190	-0.145091
H	-2.750106	1.040582	0.543009
H	-0.009104	0.658400	-0.563991
H	-0.112511	1.805899	1.942109
H	-1.810313	2.166688	2.556909
C	4.803309	-1.389871	0.011909
C	3.473710	-1.532079	0.000709
C	5.482302	-0.249266	0.620909
C	5.006294	0.998831	0.582109
O	2.630205	-0.681184	0.658809
O	3.908092	1.356624	-0.152791
P	2.390595	0.896714	0.231809
O	1.585694	0.975109	-1.035291
O	1.860091	1.551011	1.463309
C	-3.054086	-2.190819	1.335909
C	-4.356783	-2.681628	1.256809
C	-5.133784	-2.433232	0.131609
C	-4.597889	-1.694029	-0.921291
C	-3.296992	-1.211721	-0.845791
H	-2.471385	-2.402416	2.226809
H	-4.760579	-3.258330	2.083009
H	-6.148782	-2.812539	0.073309
H	-2.874596	-0.641218	-1.668591
H	-5.192790	-1.494733	-1.806991
C	-0.064479	-3.242101	-0.010491
C	0.640427	-4.204196	-0.723191
C	1.209325	-3.882993	-1.954291
C	1.073617	-2.592794	-2.454991
C	0.373711	-1.622998	-1.739591
H	0.295404	-0.622399	-2.144491
H	-0.532178	-3.519604	0.929809
H	0.735333	-5.207696	-0.320591
H	1.754029	-4.634789	-2.516991
H	1.515815	-2.326491	-3.409591
C	-2.794120	3.341182	-0.590491
C	-2.755528	4.615982	-1.147591
C	-1.540132	5.285690	-1.257291
C	-0.368829	4.680897	-0.805491
C	-0.401621	3.408997	-0.242991
H	0.512082	2.946003	0.119809
H	-3.740517	2.811876	-0.507991
H	0.579668	5.201603	-0.886791
H	2.966415	-2.378182	-0.454591
H	5.399214	-2.176267	-0.441891
H	5.502889	1.839334	1.057009
H	6.426803	-0.411760	1.132009
H	-3.672031	5.082677	-1.494591
H	-1.505839	6.280190	-1.691391

TS-A-9

M06-2X/def2-TZVPP-SMD(toluene) Energy = -1741.54921306

Number of Imaginary Frequencies = 1

Lowest Frequency = 365.4511i

M06-2X/6-31G* Geometry

C	-0.397397	-0.869103	1.955798
C	-1.069897	-0.939102	0.236098
C	-1.244496	0.105898	2.512298
H	0.623904	-0.562604	1.736198
H	-0.476098	-1.881203	2.344498
C	-1.139295	1.453198	2.079998
H	-2.141596	-0.209101	3.044798
N	-0.956996	0.364998	-0.208902
C	-2.511197	-1.446201	0.289698
C	-0.198498	-1.940803	-0.504902
C	-1.708795	1.348098	0.434898
C	-1.619893	2.732198	-0.145102
H	-2.750095	1.040499	0.542998
H	-0.009095	0.658397	-0.564002
H	-0.112594	1.805897	1.941998
H	-1.810294	2.166698	2.556798
C	5.482304	-0.249308	0.620798
C	5.006305	0.998792	0.582098
C	4.803303	-1.389808	0.011798
C	3.473703	-1.532107	0.000698
O	3.908105	1.356693	-0.152702
O	2.630204	-0.681106	0.658898
P	2.390605	0.896694	0.231898
O	1.585705	0.974995	-1.035202
O	1.860006	1.550995	1.463398
C	-0.064499	-3.242003	-0.010502
C	0.640400	-4.204204	-0.723202
C	1.209301	-3.883004	-1.954302
C	1.073602	-2.592704	-2.455002
C	0.373703	-1.623004	-1.739602
H	-0.532199	-3.519603	0.929798
H	0.735399	-5.207604	-0.320702
H	1.754000	-4.634805	-2.517002
H	0.295504	-0.622304	-2.144502
H	1.515802	-2.326505	-3.409602
C	-3.296997	-1.211700	-0.845802
C	-4.597797	-1.693999	-0.921302
C	-5.133698	-2.433199	0.131598
C	-4.356698	-2.681699	1.256798
C	-3.054098	-2.190800	1.335998
H	-2.471398	-2.402401	2.226898
H	-2.874596	-0.641301	-1.668602
H	-5.192797	-1.494798	-1.807002
H	-6.148798	-2.812598	0.073298
H	-4.760599	-3.258299	2.082998
C	-0.401693	3.408997	-0.243002
C	-0.368892	4.680897	-0.805502
C	-1.540091	5.285598	-1.257402
C	-2.755492	4.615899	-1.147602
C	-2.794093	3.341199	-0.590502
H	-3.740493	2.811900	-0.508102
H	0.512007	2.945996	0.119798
H	-3.671991	5.082600	-1.494702
H	5.502906	1.839292	1.057098
H	6.426804	-0.411809	1.131798
H	2.966302	-2.378106	-0.454702
H	5.399202	-2.176208	-0.442202
H	0.579709	5.201596	-0.886802
H	-1.505790	6.280198	-1.691502

TS-A-10

M06-2X/def2-TZVPP-SMD(toluene) Energy = -1741.54921158

Number of Imaginary Frequencies = 1

Lowest Frequency = 365.5191i

M06-2X/6-31G* Geometry

C	-0.397320	-0.869001	1.955800
C	-1.069721	-0.939092	0.236100
C	-1.244507	0.105811	2.512300
H	0.623984	-0.562415	1.736200
H	-0.475834	-1.881100	2.344500
C	-1.139489	1.453209	2.080100
H	-2.141611	-0.209277	3.044800
N	-0.957003	0.364907	-0.208900
C	-2.510928	-1.446472	0.289800
C	-0.198235	-1.940704	-0.504900
C	-1.708990	1.347917	0.434900
C	-1.620171	2.732016	-0.145100
H	-2.750194	1.040231	0.543000
H	-0.009199	0.658394	-0.564000
H	-0.112784	1.805995	1.942000
H	-1.810479	2.166518	2.556800
C	5.482188	-0.248981	0.620800
C	5.006205	0.999126	0.582100
C	4.803273	-1.389571	0.011900
C	3.473671	-1.531853	0.000800
O	3.908010	1.356941	-0.152800
O	2.630183	-0.680842	0.658900
P	2.390504	0.896961	0.231800
O	1.585605	0.975172	-1.035300
O	1.859913	1.551369	1.463300
C	0.373770	-1.622911	-1.739600
C	1.073757	-2.592521	-2.455100
C	1.209739	-3.882823	-1.954400
C	0.641035	-4.204015	-0.723200
C	-0.063952	-3.241905	-0.010400
H	0.295283	-0.622310	-2.144600
H	1.515760	-2.326227	-3.409700
H	1.754529	-4.634530	-2.517100
H	-0.531556	-3.519499	0.929900
H	0.736221	-5.207416	-0.320600
C	-3.053738	-2.191165	1.336000
C	-4.356345	-2.682247	1.256800
C	-5.133341	-2.433837	0.131600
C	-4.597531	-1.694644	-0.921300
C	-3.296825	-1.212061	-0.845800
H	-2.874417	-0.641567	-1.668600
H	-2.471041	-2.402673	2.226900
H	-4.760152	-3.258842	2.083000
H	-6.148446	-2.813323	0.073300
H	-5.192629	-1.495436	-1.807000
C	-0.402062	3.408899	-0.243100
C	-0.369445	4.680899	-0.805500
C	-1.540737	5.285515	-1.257300
C	-2.756046	4.615731	-1.147500
C	-2.794463	3.340932	-0.590400
H	-3.740870	2.811545	-0.507900
H	0.511732	2.946087	0.119700
H	-3.672639	5.082344	-1.494500
H	5.502817	1.839719	1.057000
H	6.426686	-0.411493	1.131900
H	2.966259	-2.377946	-0.454500
H	5.399162	-2.175979	-0.442000

H	0.579062	5.201686	-0.886900
H	-1.506623	6.280114	-1.691400

TS-B-3

M06-2X/def2-TZVPP-SMD(toluene) Energy = -1741.54915460

Number of Imaginary Frequencies = 1

Lowest Frequency = 417.9933i

M06-2X/6-31G* Geometry

C	-1.302093	-0.553104	1.975506
C	-1.840194	-0.225104	0.262906
C	-1.028295	0.749697	2.442906
H	-0.431692	-1.167603	1.743706
H	-2.129193	-1.094804	2.429706
C	0.073205	1.460498	1.919706
H	-1.802395	1.301796	2.974806
N	-0.761094	0.464997	-0.273394
C	-3.134494	0.575894	0.250706
C	-2.016292	-1.626804	-0.294094
C	-0.461496	1.721897	0.216006
C	0.688403	2.436499	-0.434694
H	-1.341996	2.356396	0.324906
H	0.100506	-0.131002	-0.308694
H	0.977305	0.880999	1.718506
H	0.243203	2.459898	2.314806
C	4.199906	-0.098797	1.776406
C	3.901206	0.494202	0.617006
C	4.279708	-1.536997	2.025106
C	3.870009	-2.581198	1.287906
O	3.624806	-0.185098	-0.537494
O	3.215609	-2.616698	0.095906
P	2.427808	-1.320799	-0.529094
O	1.387607	-0.877900	0.479006
O	2.036908	-1.603400	-1.928594
C	-3.134791	-2.372706	0.093106
C	-3.311190	-3.671306	-0.368194
C	-2.371589	-4.240405	-1.225594
C	-1.263290	-3.498504	-1.619994
C	-1.080791	-2.195903	-1.162194
H	-3.878192	-1.932806	0.752806
H	-4.184889	-4.236807	-0.059594
H	-2.507088	-5.255605	-1.585594
H	-0.199692	-1.663902	-1.505894
H	-0.518889	-3.920603	-2.287294
C	-3.992895	0.714693	1.340306
C	-5.189695	1.419792	1.215506
C	-5.539296	1.997392	0.000806
C	-4.689296	1.859693	-1.095194
C	-3.501195	1.149694	-0.973494
H	-2.840795	1.032795	-1.828094
H	-3.747494	0.266494	2.298106
H	-5.845596	1.515391	2.075006
H	-6.468797	2.549591	-0.094194
H	-4.953296	2.302992	-2.050094
C	0.970802	3.748199	-0.037494
C	2.045201	4.435700	-0.585794
C	2.852702	3.816001	-1.540094
C	2.564703	2.519001	-1.951094
C	1.481604	1.829600	-1.409094
H	1.273705	0.826399	-1.769394
H	0.342801	4.232998	0.707206
H	3.185404	2.019702	-2.687694
H	3.872804	1.574302	0.492006
H	4.435906	0.553903	2.611506

H	4.067910	-3.591197	1.632506
H	4.765708	-1.823897	2.952906
H	2.253700	5.452901	-0.269394
H	3.698801	4.347702	-1.964094

TS-C

M06-2X/def2-TZVPP-SMD(toluene) Energy = -1741.54847089

Number of Imaginary Frequencies = 1

Lowest Frequency = 408.5775i

M06-2X/6-31G* Geometry

C	-1.404698	-0.755502	2.082200
C	-1.778399	-0.552002	0.322400
C	-1.614700	0.554098	2.567800
H	-0.356198	-1.044101	2.030200
H	-2.072597	-1.544703	2.418400
C	-0.677501	1.547599	2.225300
H	-2.598900	0.843497	2.935400
N	-0.883600	0.432699	-0.088900
C	-1.497097	-1.920902	-0.285500
C	-3.239199	-0.130604	0.180000
C	-0.990401	1.696698	0.457600
C	-0.054002	2.748900	-0.068200
H	-2.018202	2.059397	0.460100
H	0.060401	0.141500	-0.461400
H	0.361199	1.213600	2.204200
H	-0.846202	2.554199	2.603400
C	5.430403	-1.820494	0.357800
C	4.233004	-2.325096	0.672300
C	5.610702	-0.703594	-0.565600
C	4.769100	0.332505	-0.621000
O	3.068503	-1.942897	0.066600
O	3.742600	0.494704	0.272500
P	2.401301	-0.447998	0.222100
O	1.600801	-0.200899	-1.020300
O	1.724701	-0.302798	1.551500
C	-4.244699	-0.540505	1.056300
C	-5.575599	-0.205207	0.818400
C	-5.922800	0.539793	-0.304200
C	-4.928900	0.942394	-1.192500
C	-3.600200	0.605795	-0.954600
H	-4.004398	-1.136205	1.931000
H	-6.341799	-0.532508	1.514200
H	-6.960100	0.800892	-0.487700
H	-2.825000	0.906296	-1.654800
H	-5.186601	1.515594	-2.077700
C	-2.449396	-2.556603	-1.088000
C	-2.161295	-3.781203	-1.685200
C	-0.923394	-4.384701	-1.489900
C	0.023805	-3.762900	-0.681100
C	-0.264396	-2.547001	-0.074500
H	0.479003	-2.097800	0.573100
H	-3.417097	-2.098704	-1.260200
H	-2.909994	-4.258604	-2.309500
H	-0.698893	-5.335401	-1.963500
H	0.998706	-4.211099	-0.520400
C	1.314398	2.750701	0.205200
C	2.129997	3.732402	-0.347100
C	1.587395	4.722801	-1.162100
C	0.219695	4.734000	-1.423600
C	-0.597904	3.751499	-0.874300
H	-1.666004	3.754998	-1.080000
H	1.748899	1.997302	0.853200
H	-0.211306	5.505999	-2.053200

H	4.105904	-3.143896	1.374700
H	6.304703	-2.277193	0.812000
H	4.876499	1.155105	-1.321800
H	6.465402	-0.702593	-1.235500
H	3.193997	3.715303	-0.133700
H	2.227894	5.488102	-1.589500

TS-D

M06-2X/def2-TZVPP-SMD(toluene) Energy = -1741.54843171

Number of Imaginary Frequencies = 1

Lowest Frequency = 342.0687i

M06-2X/6-31G* Geometry

C	-1.114506	-0.795093	1.871999
C	-1.614204	-0.503489	0.178499
C	-1.204697	0.498908	2.438799
H	-0.106609	-1.194400	1.720399
H	-1.805812	-1.547688	2.247899
C	-0.319290	1.516301	2.018299
H	-2.108295	0.790314	2.973999
N	-0.773597	0.521805	-0.273801
C	-1.372414	-1.857491	-0.471401
C	-3.084001	-0.093779	0.116299
C	-0.892388	1.757605	0.354599
C	-0.090580	2.907600	-0.187901
H	-1.937586	2.044213	0.469999
H	0.218801	0.234698	-0.367601
H	0.707008	1.207994	1.808799
H	-0.421683	2.488802	2.496399
C	4.552096	-0.449733	-1.377301
C	3.767188	-1.534227	-1.440601
C	4.899202	0.404765	-0.243501
C	4.598301	0.228067	1.046999
O	3.037584	-2.132522	-0.458401
O	3.881393	-0.809628	1.570099
P	2.483390	-1.300118	0.856899
O	1.795699	-0.060913	0.326999
O	1.780683	-2.247213	1.746299
C	-3.995902	-0.235873	1.160899
C	-5.334100	0.119737	0.989399
C	-5.775196	0.624140	-0.227801
C	-4.871495	0.764833	-1.279901
C	-3.540798	0.403524	-1.111101
H	-3.682705	-0.639975	2.118099
H	-6.028301	-0.000958	1.814999
H	-6.815694	0.903547	-0.358901
H	-2.835097	0.507319	-1.930201
H	-5.204493	1.153736	-2.237001
C	-2.363121	-2.840984	-0.382601
C	-2.150330	-4.109386	-0.910601
C	-0.941632	-4.415594	-1.529201
C	0.047775	-3.442201	-1.619201
C	-0.164416	-2.169600	-1.099801
H	0.636289	-1.444305	-1.179601
H	-3.310319	-2.616278	0.098099
H	-2.931435	-4.859080	-0.833301
H	-0.769839	-5.408995	-1.931401
H	1.004773	-3.668108	-2.077901
C	-0.753572	4.123104	-0.374201
C	-0.072164	5.230700	-0.869401
C	1.280735	5.127990	-1.178901
C	1.944927	3.917786	-0.987901
C	1.272119	2.806790	-0.489001
H	1.805512	1.872186	-0.328501

H	-1.812171	4.200712	-0.137701
H	3.001426	3.833578	-1.223201
H	3.667685	-2.077227	-2.375901
H	5.018798	-0.185536	-2.321401
H	4.943606	0.915064	1.813399
H	5.504108	1.277460	-0.469701
H	-0.598657	6.168803	-1.014101
H	1.816941	5.989086	-1.565401

TS-D-2

M06-2X/def2-TZVPP-SMD(toluene) Energy = -1741.54843135

Number of Imaginary Frequencies = 1

Lowest Frequency = 342.1177i

M06-2X/6-31G* Geometry

C	-1.114501	-0.794998	1.871993
C	-1.614101	-0.503499	0.178493
C	-1.204704	0.499002	2.438793
H	-0.106600	-1.194395	1.720493
H	-1.805799	-1.547600	2.247993
C	-0.319306	1.516404	2.018393
H	-2.108304	0.790400	2.973993
N	-0.773604	0.521803	-0.273707
C	-1.372298	-1.857398	-0.471407
C	-3.084002	-0.093803	0.116293
C	-0.892407	1.757603	0.354593
C	-0.090610	2.907705	-0.187907
H	-1.937608	2.044200	0.469893
H	0.218897	0.234806	-0.367507
H	0.706995	1.208107	1.808793
H	-0.421709	2.488904	2.496393
C	4.551499	-0.449284	-1.377507
C	3.766501	-1.533686	-1.440907
C	4.899197	0.404517	-0.243407
C	4.598497	0.227416	1.047193
O	3.037503	-2.132388	-0.458607
O	3.881100	-0.809885	1.570293
P	2.483301	-1.300289	0.856893
O	1.795598	-0.060891	0.327093
O	1.780503	-2.247391	1.746093
C	-3.995802	-0.235805	1.160793
C	-5.334003	0.119692	0.989293
C	-5.775204	0.623991	-0.228007
C	-4.871404	0.764593	-1.280107
C	-3.540703	0.403296	-1.111207
H	-3.682701	-0.639704	2.118093
H	-6.028302	-0.000810	1.814893
H	-6.815605	0.903388	-0.359207
H	-2.835004	0.506998	-1.930407
H	-5.204405	1.153392	-2.237307
C	-2.362795	-2.841101	-0.382307
C	-2.149892	-4.109500	-0.910207
C	-0.941292	-4.415597	-1.529107
C	0.047906	-3.441895	-1.619507
C	-0.164297	-2.169395	-1.100107
H	0.636201	-1.443893	-1.180107
H	-3.309896	-2.616503	0.098693
H	-2.930790	-4.859402	-0.832607
H	-0.769489	-5.408997	-1.931207
H	1.004807	-3.667793	-2.078407
C	-0.753513	4.123203	-0.374007
C	-0.072115	5.230805	-0.869107
C	1.280785	5.128008	-1.178707
C	1.944988	3.917910	-0.987807

C	1.272091	2.806808	-0.489007
H	1.805493	1.872209	-0.328607
H	-1.812113	4.200900	-0.137407
H	3.001388	3.833612	-1.223207
H	3.666403	-2.076286	-2.376507
H	5.017698	-0.184583	-2.321607
H	4.944395	0.914017	1.813693
H	5.504494	1.277019	-0.469407
H	-0.598518	6.169003	-1.013707
H	1.817083	5.989209	-1.565207

TS-D-3

M06-2X/def2-TZVPP-SMD(toluene) Energy = -1741.54843036

Number of Imaginary Frequencies = 1

Lowest Frequency = 341.8238i

M06-2X/6-31G* Geometry

C	-1.114401	-0.795192	1.871803
C	-1.614199	-0.503488	0.178503
C	-1.204390	0.498809	2.438803
H	-0.106405	-1.194500	1.720203
H	-1.805608	-1.547786	2.247703
C	-0.319082	1.516201	2.018403
H	-2.107988	0.790116	2.974103
N	-0.773590	0.521805	-0.273797
C	-3.083995	-0.093576	0.116503
C	-1.372610	-1.857390	-0.471597
C	-0.892180	1.757606	0.354703
C	-0.090370	2.907600	-0.187897
H	-1.937378	2.044215	0.470203
H	0.218807	0.234697	-0.367797
H	0.707215	1.207793	1.808803
H	-0.421374	2.488602	2.496503
C	4.551502	-0.449139	-1.377497
C	3.766593	-1.533633	-1.440997
C	4.899209	0.404558	-0.243297
C	4.598607	0.227360	1.047303
O	3.037488	-2.132427	-0.458697
O	3.881299	-0.810134	1.570303
P	2.483395	-1.300422	0.856903
O	1.795605	-0.061116	0.327403
O	1.780687	-2.247816	1.746103
C	-2.363418	-2.840782	-0.383097
C	-2.150729	-4.109083	-0.911197
C	-0.941931	-4.415393	-1.529697
C	0.047677	-3.442102	-1.619297
C	-0.164413	-2.169600	-1.099797
H	-3.310716	-2.615974	0.097503
H	-2.931935	-4.858677	-0.834097
H	-0.770240	-5.408795	-1.931897
H	0.636293	-1.444407	-1.179297
H	1.004675	-3.668110	-2.077897
C	-3.995697	-0.235668	1.161103
C	-5.333994	0.119943	0.989803
C	-5.775189	0.624447	-0.227297
C	-4.871588	0.765239	-1.279497
C	-3.540891	0.403828	-1.110797
H	-2.835290	0.507722	-1.929997
H	-3.682500	-0.639971	2.118303
H	-6.028095	-0.000751	1.815503
H	-6.815587	0.904056	-0.358197
H	-5.204685	1.154342	-2.236497
C	-0.753360	4.123005	-0.374597
C	-0.071951	5.230499	-0.869797

C	1.281048	5.127788	-1.178997
C	1.945238	3.917783	-0.987597
C	1.272329	2.806788	-0.488697
H	1.805821	1.872284	-0.327897
H	-1.812060	4.200614	-0.138197
H	3.001737	3.833574	-1.222697
H	3.666488	-2.076032	-2.376597
H	5.017704	-0.184343	-2.321597
H	4.944513	0.913858	1.813803
H	5.504516	1.277153	-0.469197
H	-0.598443	6.168604	-1.014797
H	1.817255	5.988884	-1.565597

TS-D-4

M06-2X/def2-TZVPP-SMD(toluene) Energy = -1741.54842920

Number of Imaginary Frequencies = 1

Lowest Frequency = 341.9388i

M06-2X/6-31G* Geometry

C	-1.114500	-0.795096	1.871898
C	-1.614199	-0.503495	0.178398
C	-1.204597	0.498904	2.438798
H	-0.106501	-1.194398	1.720298
H	-1.805702	-1.547694	2.247798
C	-0.319295	1.516402	2.018298
H	-2.108297	0.790306	2.973898
N	-0.773597	0.521803	-0.273802
C	-3.083999	-0.093692	0.116398
C	-1.372402	-1.857395	-0.471502
C	-0.892295	1.757604	0.354598
C	-0.090492	2.907702	-0.187902
H	-1.937494	2.044306	0.469998
H	0.218902	0.234801	-0.367702
H	0.707104	1.208000	1.808798
H	-0.421693	2.488803	2.496398
C	4.899103	0.404491	-0.243502
C	4.598402	0.227592	1.047098
C	4.551601	-0.449508	-1.377402
C	3.766698	-1.534007	-1.440802
O	3.881200	-0.809807	1.570298
O	3.037597	-2.132505	-0.458402
P	2.483299	-1.300304	0.856998
O	1.795602	-0.061002	0.327098
O	1.780597	-2.247402	1.746298
C	-2.363105	-2.840893	-0.382702
C	-2.150307	-4.109294	-0.910702
C	-0.941608	-4.415496	-1.529402
C	0.047794	-3.441998	-1.619402
C	-0.164403	-2.169498	-1.099902
H	-3.310304	-2.616191	0.098098
H	-2.931309	-4.858992	-0.833402
H	-0.769910	-5.408897	-1.931502
H	0.636199	-1.444200	-1.179702
H	1.004794	-3.668001	-2.078102
C	-3.995799	-0.235790	1.160898
C	-5.333998	0.119713	0.989498
C	-5.775197	0.624214	-0.227702
C	-4.871497	0.764912	-1.279802
C	-3.540797	0.403709	-1.111002
H	-2.835197	0.507508	-1.930202
H	-3.682600	-0.639990	2.118198
H	-6.028298	-0.000985	1.815098
H	-6.815696	0.903617	-0.358702
H	-5.204596	1.153913	-2.236902

C	-0.753389	4.123103	-0.374202
C	-0.071887	5.230702	-0.869302
C	1.281013	5.127899	-1.178902
C	1.945110	3.917697	-0.987802
C	1.272208	2.806799	-0.489002
H	1.805606	1.872098	-0.328502
H	-1.811989	4.200806	-0.137702
H	3.001610	3.833495	-1.223202
H	4.944104	0.914391	1.813498
H	5.504304	1.277190	-0.469502
H	3.666797	-2.076706	-2.376302
H	5.017901	-0.185009	-2.321602
H	-0.598285	6.168803	-1.014102
H	1.817315	5.988998	-1.565402

TS-D-5

M06-2X/def2-TZVPP-SMD(toluene) Energy = -1741.54842725

Number of Imaginary Frequencies = 1

Lowest Frequency = 341.8081i

M06-2X/6-31G* Geometry

C	-1.114405	-0.795091	1.871896
C	-1.614102	-0.503486	0.178496
C	-1.204592	0.498910	2.438796
H	-0.106409	-1.194401	1.720296
H	-1.805713	-1.547784	2.247796
C	-0.319281	1.516401	2.018396
H	-2.108289	0.790219	2.973996
N	-0.773591	0.521905	-0.273804
C	-3.083998	-0.093771	0.116396
C	-1.372316	-1.857388	-0.471504
C	-0.892279	1.757607	0.354696
C	-0.090567	2.907698	-0.187904
H	-1.937576	2.044217	0.469996
H	0.218906	0.234795	-0.367604
H	0.707016	1.207990	1.808896
H	-0.421771	2.488802	2.496496
C	4.551499	-0.449149	-1.377404
C	3.766588	-1.533641	-1.440904
C	4.899107	0.404547	-0.243304
C	4.598406	0.227450	1.047296
O	3.037381	-2.132334	-0.458704
O	3.881195	-0.810042	1.570296
P	2.483290	-1.300328	0.856896
O	1.795603	-0.060921	0.327296
O	1.780480	-2.247621	1.745996
C	-2.362826	-2.840978	-0.382604
C	-2.149939	-4.109380	-0.910604
C	-0.941342	-4.415493	-1.529404
C	0.047968	-3.441903	-1.619504
C	-0.164319	-2.169401	-1.100104
H	-3.310024	-2.616368	0.098296
H	-2.930947	-4.859172	-0.833104
H	-0.769552	-5.408795	-1.931604
H	0.636288	-1.443909	-1.180004
H	1.004866	-3.667713	-2.078304
C	-3.995799	-0.235961	1.160896
C	-5.333995	0.119552	0.989496
C	-5.775190	0.623957	-0.227704
C	-4.871489	0.764748	-1.279904
C	-3.540793	0.403534	-1.111104
H	-2.835091	0.507427	-1.930204
H	-3.682603	-0.640065	2.118196
H	-6.028197	-0.001140	1.815096

H	-6.815687	0.903368	-0.358804
H	-5.204585	1.153751	-2.236904
C	-0.753554	4.123105	-0.374204
C	-0.072143	5.230798	-0.869304
C	1.280756	5.127984	-1.178804
C	1.945044	3.917877	-0.987704
C	1.272132	2.806884	-0.488804
H	1.805623	1.872279	-0.328304
H	-1.812153	4.200816	-0.137704
H	3.001443	3.833667	-1.223004
H	3.666482	-2.076140	-2.376604
H	5.017801	-0.184454	-2.321504
H	4.944313	0.913947	1.813796
H	5.504416	1.277141	-0.469204
H	-0.598533	6.168804	-1.014204
H	1.817065	5.989179	-1.565304

TS-D-6

M06-2X/def2-TZVPP-SMD(toluene) Energy = -1741.54842702

Number of Imaginary Frequencies = 1

Lowest Frequency = 341.9868i

M06-2X/6-31G* Geometry

C	-1.114395	-0.795195	1.871909
C	-1.614195	-0.503595	0.178409
C	-1.204596	0.498805	2.438709
H	-0.106395	-1.194494	1.720209
H	-1.805694	-1.547796	2.247709
C	-0.319297	1.516306	2.018309
H	-2.108196	0.790104	2.974009
N	-0.773596	0.521805	-0.273791
C	-1.372394	-1.857495	-0.471491
C	-3.083995	-0.093896	0.116409
C	-0.892397	1.757505	0.354609
C	-0.090798	2.907706	-0.187991
H	-1.937597	2.044104	0.470009
H	0.218804	0.234806	-0.367791
H	0.707104	1.207906	1.808709
H	-0.421697	2.488705	2.496409
C	4.552105	-0.449491	-1.377191
C	3.767306	-1.533992	-1.440591
C	4.899304	0.404809	-0.243391
C	4.598304	0.228109	1.047209
O	3.037706	-2.132392	-0.458491
O	3.881305	-0.809491	1.570209
P	2.483505	-1.300092	0.856909
O	1.795805	-0.060793	0.326909
O	1.780706	-2.247193	1.746209
C	-3.995795	-0.235897	1.161009
C	-5.333996	0.119602	0.989609
C	-5.775196	0.623902	-0.227591
C	-4.871596	0.764602	-1.279791
C	-3.540896	0.403403	-1.111091
H	-3.682595	-0.639997	2.118309
H	-6.028195	-0.000999	1.815209
H	-6.815696	0.903401	-0.358591
H	-2.835296	0.507104	-1.930191
H	-5.204696	1.153502	-2.236891
C	-2.363093	-2.840996	-0.382791
C	-2.150193	-4.109396	-0.910791
C	-0.941492	-4.415695	-1.529291
C	0.047907	-3.442194	-1.619191
C	-0.164294	-2.169694	-1.099791
H	0.636406	-1.444294	-1.179491

H	-3.310294	-2.616297	0.097909
H	-2.931292	-4.859096	-0.833491
H	-0.769692	-5.409095	-1.931391
H	1.004907	-3.668093	-2.077791
C	-0.753798	4.123005	-0.374191
C	-0.072499	5.230706	-0.869391
C	1.280401	5.128007	-1.178991
C	1.944702	3.918007	-0.987891
C	1.271903	2.806907	-0.489091
H	1.805503	1.872307	-0.328591
H	-1.812398	4.200604	-0.137691
H	3.001202	3.833808	-1.223291
H	3.667706	-2.076992	-2.375991
H	5.018805	-0.185191	-2.321291
H	4.943704	0.915009	1.813609
H	5.504304	1.277610	-0.469491
H	-0.599000	6.168805	-1.014191
H	1.816600	5.989207	-1.565491

TS-E

M06-2X/def2-TZVPP-SMD(toluene) Energy = -1741.54837894

Number of Imaginary Frequencies = 1

Lowest Frequency = 370.8370i

M06-2X/6-31G* Geometry

C	-0.425799	-0.957004	1.901501
C	-0.924800	-1.114702	0.178001
C	-1.498196	-0.223400	2.458601
H	0.504703	-0.408108	1.749801
H	-0.280103	-1.976305	2.253601
C	-1.692390	1.121401	2.074801
H	-2.316898	-0.751496	2.946301
N	-1.140694	0.201999	-0.230199
C	0.285398	-1.773107	-0.460899
C	-2.173503	-1.981397	0.057601
C	-2.177691	0.901403	0.372801
C	-2.467586	2.285204	-0.132499
H	-3.088294	0.304207	0.427601
H	-0.257992	0.754595	-0.255199
H	-0.785188	1.710797	1.927501
H	-2.521588	1.655705	2.534401
C	4.958703	-0.560626	0.257901
C	3.892302	-0.797722	1.036501
C	5.205207	0.495473	-0.720699
C	4.312811	1.343876	-1.237599
O	2.727504	-0.111917	1.153801
O	2.975211	1.332782	-0.939699
P	2.512211	1.455784	0.643901
O	1.006511	1.567890	0.579801
O	3.376915	2.384080	1.392201
C	-2.824703	-1.966694	-1.182699
C	-3.945807	-2.756289	-1.404299
C	-4.429710	-3.586387	-0.394099
C	-3.782510	-3.616990	0.835001
C	-2.661807	-2.817295	1.060401
H	-2.440501	-1.324296	-1.969999
H	-4.440406	-2.726587	-2.369999
H	-5.303913	-4.205884	-0.566999
H	-2.171607	-2.866897	2.027601
H	-4.146213	-4.262289	1.628301
C	1.152601	-1.068411	-1.296299
C	2.291398	-1.686415	-1.804899
C	2.564192	-3.016016	-1.503299
C	1.689989	-3.731413	-0.687799

C	0.558692	-3.113308	-0.169499
H	-0.119710	-3.679505	0.463701
H	0.980505	-0.028610	-1.546399
H	2.975500	-1.107418	-2.417499
H	3.458490	-3.491020	-1.893899
H	1.889385	-4.771814	-0.450799
C	-1.454482	3.224300	-0.351199
C	-1.787076	4.489902	-0.823199
C	-3.116575	4.830507	-1.066999
C	-4.124779	3.898911	-0.838199
C	-3.799484	2.629210	-0.370499
H	-4.584787	1.897413	-0.196699
H	-0.416183	2.969996	-0.144999
H	-5.162478	4.156716	-1.024899
H	3.883198	-1.670922	1.682201
H	5.764200	-1.277430	0.386901
H	4.583814	2.106875	-1.960399
H	6.227507	0.601968	-1.070399
H	-0.999473	5.216498	-0.994999
H	-3.365771	5.822308	-1.431299

TS-B-4

M06-2X/def2-TZVPP-SMD(toluene) Energy = -1741.54835408

Number of Imaginary Frequencies = 1

Lowest Frequency = 354.5951i

M06-2X/6-31G* Geometry

C	-0.755596	-0.841804	1.567900
C	-1.630197	-0.340606	0.099000
C	-0.507399	0.396696	2.212800
H	0.119404	-1.304803	1.111700
H	-1.414295	-1.548306	2.069000
C	0.410500	1.302598	1.644800
H	-1.210199	0.758795	2.962800
N	-0.750499	0.561396	-0.523700
C	-2.952399	0.325192	0.465100
C	-1.826395	-1.651306	-0.653000
C	-0.467101	1.744096	0.147700
C	0.406797	2.752498	-0.541000
H	-1.377102	2.212795	0.520100
H	0.088902	0.116797	-0.922800
H	1.306000	0.860500	1.201000
H	0.561298	2.247298	2.164300
C	4.188901	0.343605	1.432600
C	4.510602	-0.026195	0.188100
C	3.453803	-0.433396	2.429300
C	2.784105	-1.592098	2.312900
O	4.190504	-1.218995	-0.390200
O	2.553606	-2.359598	1.218800
P	2.638705	-1.769898	-0.329000
O	1.736603	-0.553900	-0.351500
O	2.464807	-2.897698	-1.260600
C	-3.070294	-2.291209	-0.649000
C	-3.231491	-3.514909	-1.293700
C	-2.155790	-4.120107	-1.936600
C	-0.913491	-3.490905	-1.937000
C	-0.751594	-2.264104	-1.305000
H	-3.921395	-1.840010	-0.150300
H	-4.204891	-3.995711	-1.286200
H	-2.283889	-5.080307	-2.426800
H	0.236305	-1.820802	-1.314500
H	-0.045691	-3.945103	-2.404200
C	-3.608198	0.140990	1.681500
C	-4.855899	0.719688	1.910700

C	-5.463201	1.489987	0.925500
C	-4.818701	1.673188	-0.296500
C	-3.577800	1.090890	-0.526700
H	-3.077000	1.224391	-1.481500
H	-3.164797	-0.470409	2.461100
H	-5.350599	0.562987	2.864000
H	-6.433202	1.941985	1.105700
H	-5.285302	2.267087	-1.076100
C	1.659598	2.424900	-1.069100
C	2.413496	3.409202	-1.699900
C	1.937593	4.715401	-1.799200
C	0.695793	5.043298	-1.263100
C	-0.065805	4.063497	-0.633500
H	-1.038406	4.316595	-0.218200
H	2.039899	1.409301	-0.978100
H	0.318191	6.058298	-1.334800
H	5.097701	0.611907	-0.466400
H	4.548200	1.318206	1.748600
H	2.349206	-2.050199	3.197100
H	3.472202	-0.034296	3.439500
H	3.383996	3.152003	-2.113000
H	2.535192	5.476702	-2.290800

TS-B-5

M06-2X/def2-TZVPP-SMD(toluene) Energy = -1741.54835326

Number of Imaginary Frequencies = 1

Lowest Frequency = 354.6140i

M06-2X/6-31G* Geometry

C	-0.755997	-0.841699	1.568100
C	-1.630397	-0.340599	0.099100
C	-0.507697	0.396802	2.212900
H	0.119004	-1.304898	1.112000
H	-1.414896	-1.548099	2.069200
C	0.410403	1.302502	1.644900
H	-1.210497	0.759101	2.962800
N	-0.750497	0.561201	-0.523600
C	-2.952497	0.325501	0.465000
C	-1.826796	-1.651199	-0.652800
C	-0.467097	1.744002	0.147700
C	0.407003	2.752202	-0.541000
H	-1.376997	2.212901	0.520000
H	0.088803	0.116502	-0.922600
H	1.305903	0.860202	1.201300
H	0.561303	2.247202	2.164300
C	3.455103	-0.432198	2.428400
C	2.785204	-1.590798	2.313200
C	4.189903	0.344003	1.430800
C	4.510903	-0.026697	0.186400
O	2.554304	-2.359098	1.219700
O	4.190304	-1.219697	-0.391000
P	2.638404	-1.770398	-0.328500
O	1.736403	-0.554398	-0.351100
O	2.463904	-2.898798	-1.259300
C	-0.752096	-2.264499	-1.304400
C	-0.914096	-3.491299	-1.936300
C	-2.156496	-4.120099	-1.936200
C	-3.232296	-3.514599	-1.293700
C	-3.070996	-2.290799	-0.649000
H	0.236004	-1.821398	-1.313700
H	-0.046296	-3.945698	-2.403200
H	-2.284696	-5.080299	-2.426300
H	-3.921996	-1.839299	-0.150600
H	-4.205796	-3.995099	-1.286400

C	-3.608497	0.141501	1.681400
C	-4.856097	0.720501	1.910500
C	-5.463197	1.490700	0.925200
C	-4.818597	1.673801	-0.296700
C	-3.577697	1.091301	-0.526900
H	-3.076897	1.224601	-1.481600
H	-3.165197	-0.469899	2.461100
H	-5.350897	0.563900	2.863800
H	-6.433197	1.942900	1.105300
H	-5.284997	2.267700	-1.076400
C	1.659903	2.424402	-1.069000
C	2.414003	3.408602	-1.699800
C	1.938202	4.714802	-1.799300
C	0.696302	5.042902	-1.263300
C	-0.065398	4.063202	-0.633700
H	-1.037998	4.316501	-0.218500
H	2.040003	1.408802	-0.977800
H	0.318902	6.058002	-1.335200
H	2.350604	-2.048198	3.197900
H	3.474003	-0.032298	3.438300
H	5.097903	0.610903	-0.468800
H	4.549603	1.318703	1.745900
H	3.384503	3.151302	-2.112700
H	2.536002	5.476002	-2.290900

TS-C-2

M06-2X/def2-TZVPP-SMD(toluene) Energy = -1741.54825711

Number of Imaginary Frequencies = 1

Lowest Frequency = 371.7011i

M06-2X/6-31G* Geometry

C	-1.196897	-0.732694	1.981695
C	-1.731596	-0.533393	0.228495
C	-1.306893	0.593806	2.436595
H	-0.177197	-1.084797	1.811695
H	-1.874498	-1.469893	2.406095
C	-0.415991	1.579404	1.939195
H	-2.221992	0.919708	2.930595
N	-0.855994	0.417205	-0.274405
C	-1.584800	-1.930493	-0.348705
C	-3.193495	-0.091389	0.185795
C	-0.935790	1.700105	0.266495
C	-0.106487	2.800303	-0.334905
H	-1.974489	2.021708	0.348095
H	0.107206	0.071502	-0.510405
H	0.619409	1.246401	1.832395
H	-0.535288	2.585604	2.338195
C	5.572001	-1.714312	-0.345605
C	4.384599	-2.318909	-0.452105
C	5.826004	-0.613112	0.579095
C	4.923006	0.335690	0.845895
O	3.334500	-2.058106	0.384195
O	3.731506	0.434393	0.180895
P	2.509704	-0.646704	0.380895
O	1.676304	-0.512102	-0.867005
O	1.852004	-0.498902	1.711195
C	-4.096095	-0.210987	1.241195
C	-5.432494	0.153116	1.077695
C	-5.881793	0.644218	-0.142005
C	-4.987493	0.762815	-1.204605
C	-3.658494	0.391712	-1.044305
H	-3.774496	-0.595988	2.203795
H	-6.119094	0.051818	1.912295
H	-6.920892	0.931520	-0.266505

H	-2.960693	0.476810	-1.872705
H	-5.326092	1.142416	-2.163405
C	-2.389802	-2.957591	0.158395
C	-2.309806	-4.243192	-0.358105
C	-1.429906	-4.520194	-1.402805
C	-0.642204	-3.500496	-1.922805
C	-0.716000	-2.208096	-1.405805
H	-0.076098	-1.439797	-1.819605
H	-3.097402	-2.748990	0.956195
H	-2.938608	-5.027290	0.051495
H	-1.365009	-5.524394	-1.809805
H	0.042796	-3.701498	-2.740105
C	-0.633984	4.094104	-0.289805
C	0.091819	5.171902	-0.784505
C	1.356018	4.962299	-1.329805
C	1.882915	3.674198	-1.377305
C	1.162012	2.591599	-0.880705
H	1.588109	1.594298	-0.939105
H	-1.622184	4.257207	0.135195
H	2.867514	3.500195	-1.799305
H	4.190797	-3.125708	-1.152805
H	6.380700	-2.073414	-0.975305
H	5.101208	1.144589	1.548295
H	6.791504	-0.548115	1.071895
H	-0.330879	6.171103	-0.747305
H	1.927420	5.800398	-1.716705

TS-C-3

M06-2X/def2-TZVPP-SMD(toluene) Energy = -1741.54823838

Number of Imaginary Frequencies = 1

Lowest Frequency = 353.7638i

M06-2X/6-31G* Geometry

C	-1.289596	-0.726703	2.030504
C	-1.731997	-0.510104	0.300304
C	-1.459298	0.584397	2.533704
H	-0.251696	-1.045702	1.914404
H	-1.959395	-1.495204	2.410604
C	-0.560299	1.594698	2.131804
H	-2.408198	0.868596	2.987204
N	-0.850398	0.468097	-0.148996
C	-1.538995	-1.891203	-0.309196
C	-3.195797	-0.079205	0.184904
C	-0.951999	1.735697	0.405104
C	-0.044300	2.789798	-0.168396
H	-1.985899	2.083196	0.424804
H	0.115803	0.181198	-0.441796
H	0.480102	1.269299	2.072104
H	-0.723700	2.593098	2.533904
C	5.343605	-1.943296	-0.447096
C	4.082805	-2.364297	-0.584896
C	5.741804	-0.941395	0.537604
C	4.983103	0.111604	0.858104
O	3.079905	-1.990998	0.268404
O	3.825402	0.432202	0.205404
P	2.457603	-0.478899	0.280804
O	1.700003	-0.179600	-0.980696
O	1.764703	-0.291400	1.593004
C	-4.156597	-0.251506	1.180204
C	-5.484997	0.109992	0.956504
C	-5.868498	0.651292	-0.264496
C	-4.915898	0.822893	-1.267596
C	-3.594498	0.454894	-1.047196
H	-3.886996	-0.676706	2.142204

H	-6.217197	-0.032808	1.745004
H	-6.901398	0.936591	-0.435896
H	-2.850598	0.582295	-1.828996
H	-5.203098	1.241393	-2.227096
C	-2.365394	-2.935604	0.122404
C	-2.236593	-4.210704	-0.410396
C	-1.283092	-4.460703	-1.395496
C	-0.472193	-3.423902	-1.839796
C	-0.594795	-2.141102	-1.306896
H	0.064904	-1.360902	-1.667296
H	-3.128494	-2.749705	0.873504
H	-2.884492	-5.007705	-0.059496
H	-1.179491	-5.456603	-1.814796
H	0.270107	-3.602501	-2.611296
C	-0.626101	3.791298	-0.948596
C	0.166198	4.766499	-1.545796
C	1.546598	4.745400	-1.362996
C	2.127899	3.754401	-0.576096
C	1.337300	2.782900	0.027704
H	1.802401	2.031400	0.655604
H	-1.703301	3.797796	-1.097796
H	3.202799	3.724702	-0.431396
H	3.776106	-3.095098	-1.327396
H	6.098805	-2.378995	-1.094496
H	5.276102	0.842504	1.606304
H	6.701404	-1.042694	1.035804
H	-0.294103	5.538998	-2.153696
H	2.167897	5.502501	-1.831396

TS-C-4

M06-2X/def2-TZVPP-SMD(toluene) Energy = -1741.54823516

Number of Imaginary Frequencies = 1

Lowest Frequency = 353.7992i

M06-2X/6-31G* Geometry

C	-1.289602	-0.726798	2.030499
C	-1.731901	-0.510195	0.300299
C	-1.459295	0.584403	2.533699
H	-0.251704	-1.045703	1.914399
H	-1.959406	-1.495294	2.410599
C	-0.560290	1.594699	2.131799
H	-2.408294	0.868508	2.987199
N	-0.850396	0.468100	-0.149001
C	-3.195699	-0.079288	0.184899
C	-1.538908	-1.891196	-0.309201
C	-0.952090	1.735701	0.405099
C	-0.044384	2.789796	-0.168401
H	-1.985888	2.083106	0.424799
H	0.115903	0.181295	-0.441801
H	0.480108	1.269293	2.072099
H	-0.723785	2.593100	2.533999
C	5.741797	-0.941433	0.537499
C	4.983102	0.111571	0.858199
C	5.343592	-1.943231	-0.447301
C	4.082790	-2.364125	-0.585001
O	3.825404	0.432276	0.205599
O	3.079892	-1.991020	0.268299
P	2.457599	-0.478817	0.280799
O	1.700101	-0.179413	-0.980701
O	1.764600	-0.291413	1.592999
C	-2.365313	-2.935692	0.122399
C	-2.236420	-4.210793	-0.410301
C	-1.282921	-4.460798	-1.395401
C	-0.472016	-3.423902	-1.839701

C	-0.594709	-2.141101	-1.306801
H	-3.128412	-2.749688	0.873399
H	-2.884324	-5.007689	-0.059401
H	-1.179226	-5.456698	-1.814701
H	0.064995	-1.360904	-1.667201
H	0.270383	-3.602506	-2.611201
C	-4.156500	-0.251483	1.180199
C	-5.484898	0.109924	0.956399
C	-5.868495	0.651126	-0.264601
C	-4.915894	0.822621	-1.267701
C	-3.594496	0.454714	-1.047201
H	-2.850595	0.582010	-1.829101
H	-3.887002	-0.676684	2.142199
H	-6.217099	-0.032872	1.744899
H	-6.901394	0.936331	-0.436001
H	-5.203092	1.241122	-2.227201
C	1.337216	2.782989	0.027699
C	2.127721	3.754585	-0.576001
C	1.546326	4.745588	-1.363001
C	0.166026	4.766595	-1.545701
C	-0.626279	3.791299	-0.948501
H	-1.703579	3.797805	-1.097801
H	1.802312	2.031587	0.655599
H	-0.294370	5.538997	-2.153701
H	5.276206	0.842469	1.606399
H	6.701396	-1.042738	1.035699
H	3.775986	-3.094923	-1.327601
H	6.098790	-2.378935	-1.094701
H	3.202621	3.724980	-0.431301
H	2.167530	5.502685	-1.831401

TS-C-5

M06-2X/def2-TZVPP-SMD(toluene) Energy = -1741.54822640

Number of Imaginary Frequencies = 1

Lowest Frequency = 359.7525i

M06-2X/6-31G* Geometry

C	-1.366312	-0.797005	1.984704
C	-1.772112	-0.502705	0.267004
C	-1.484712	0.499195	2.544204
H	-0.341412	-1.156005	1.872104
H	-2.072712	-1.552205	2.324004
C	-0.535812	1.480695	2.199204
H	-2.426712	0.806695	2.996804
N	-0.845312	0.457295	-0.137296
C	-3.212512	0.000095	0.143504
C	-1.626412	-1.876305	-0.374096
C	-0.903312	1.703795	0.463404
C	0.050188	2.746795	-0.054796
H	-1.922912	2.090195	0.492504
H	0.109988	0.155895	-0.444596
H	0.489188	1.110495	2.131504
H	-0.659812	2.470595	2.634704
C	5.421088	-2.011705	0.428504
C	4.193688	-2.492705	0.650104
C	5.681688	-0.848905	-0.415896
C	4.875388	0.216195	-0.453296
O	3.079688	-2.028905	0.006204
O	3.809088	0.367495	0.391904
P	2.446388	-0.539305	0.250104
O	1.702488	-0.179105	-1.003996
O	1.732788	-0.433505	1.560604
C	-2.571812	-2.860205	-0.058196
C	-2.478612	-4.135405	-0.598896

C	-1.439112	-4.447305	-1.472896
C	-0.504812	-3.471705	-1.797896
C	-0.591312	-2.189105	-1.257196
H	-3.397112	-2.626505	0.608604
H	-3.221112	-4.883805	-0.340196
H	-1.362612	-5.443505	-1.897296
H	0.165488	-1.461005	-1.528396
H	0.310888	-3.698205	-2.476996
C	-4.193612	-0.143505	1.123304
C	-5.498912	0.290895	0.892404
C	-5.838512	0.877295	-0.320696
C	-4.865712	1.020595	-1.308696
C	-3.567912	0.580395	-1.080996
H	-2.808512	0.686195	-1.850996
H	-3.959112	-0.605505	2.077504
H	-6.247612	0.168695	1.668904
H	-6.853212	1.219295	-0.497596
H	-5.118912	1.473295	-2.262296
C	1.420188	2.721895	0.208804
C	2.248888	3.695595	-0.338196
C	1.718488	4.702595	-1.140396
C	0.349788	4.738395	-1.394696
C	-0.481112	3.764695	-0.849996
H	-1.549712	3.785395	-1.051496
H	1.848588	1.955895	0.845604
H	-0.071712	5.522995	-2.015196
H	3.998988	-3.346705	1.291904
H	6.256688	-2.523405	0.896704
H	5.048588	1.072495	-1.098796
H	6.570088	-0.836505	-1.040296
H	3.313588	3.658895	-0.131096
H	2.369288	5.461495	-1.563696

TS-C-6

M06-2X/def2-TZVPP-SMD(toluene) Energy = -1741.54822568

Number of Imaginary Frequencies = 1

Lowest Frequency = 359.8176i

M06-2X/6-31G* Geometry

C	-1.366392	-0.796909	1.984701
C	-1.772094	-0.502610	0.267001
C	-1.484797	0.499291	2.544201
H	-0.341491	-1.155905	1.872201
H	-2.072790	-1.552112	2.324101
C	-0.535901	1.480694	2.199201
H	-2.426799	0.806787	2.996801
N	-0.845197	0.457293	-0.137299
C	-1.626388	-1.876210	-0.374099
C	-3.212495	0.000184	0.143401
C	-0.903302	1.703793	0.463301
C	0.050294	2.746796	-0.054799
H	-1.922903	2.090289	0.492401
H	0.110104	0.155897	-0.444599
H	0.489100	1.110598	2.131501
H	-0.659905	2.470694	2.634601
C	5.681508	-0.848882	-0.416299
C	4.875104	0.216115	-0.453499
C	5.421112	-2.011683	0.428201
C	4.193814	-2.492688	0.650201
O	3.809103	0.367311	0.392101
O	3.079612	-2.029092	0.006601
P	2.446307	-0.539394	0.250301
O	1.702405	-0.179297	-1.003799
O	1.732706	-0.433497	1.560801

C	-4.193695	-0.143520	1.123301
C	-5.498997	0.290875	0.892301
C	-5.838599	0.877374	-0.320699
C	-4.865699	1.020578	-1.308799
C	-3.567898	0.580483	-1.080999
H	-3.959093	-0.605519	2.077501
H	-6.247596	0.168673	1.668801
H	-6.853200	1.219270	-0.497699
H	-2.808498	0.686286	-1.850999
H	-5.118901	1.473377	-2.262299
C	-2.571685	-2.860214	-0.057999
C	-2.478480	-4.135413	-0.598699
C	-1.439079	-4.447209	-1.472999
C	-0.504982	-3.471506	-1.798199
C	-0.591487	-2.188906	-1.257399
H	0.165110	-1.460803	-1.528799
H	-3.396885	-2.626617	0.609001
H	-3.220877	-4.883816	-0.339899
H	-1.362675	-5.443409	-1.897399
H	0.310519	-3.697903	-2.477499
C	1.420294	2.721902	0.208901
C	2.248990	3.695505	-0.338099
C	1.718787	4.702503	-1.140399
C	0.350087	4.738398	-1.394799
C	-0.480910	3.764694	-0.850099
H	-1.549410	3.785390	-1.051699
H	1.848597	1.955803	0.845701
H	-0.071416	5.522896	-2.015299
H	5.048100	1.072515	-1.098999
H	6.569708	-0.836479	-1.040899
H	3.999417	-3.346788	1.292001
H	6.256914	-2.523280	0.896101
H	3.313791	3.658709	-0.130899
H	2.369584	5.461305	-1.563699

TS-C-7

M06-2X/def2-TZVPP-SMD(toluene) Energy = -1741.54822365

Number of Imaginary Frequencies = 1

Lowest Frequency = 359.8620i

M06-2X/6-31G* Geometry

C	-1.366294	-0.796997	1.984706
C	-1.772095	-0.502698	0.267006
C	-1.484698	0.499203	2.544306
H	-0.341393	-1.155994	1.872106
H	-2.072592	-1.552298	2.324006
C	-0.535700	1.480605	2.199206
H	-2.426598	0.806701	2.996806
N	-0.845297	0.457305	-0.137294
C	-3.212496	0.000099	0.143506
C	-1.626392	-1.876297	-0.374094
C	-0.903400	1.703804	0.463406
C	0.050097	2.746807	-0.054794
H	-1.923001	2.090202	0.492606
H	0.110003	0.155907	-0.444594
H	0.489201	1.110508	2.131406
H	-0.659802	2.470605	2.634706
C	5.681806	-0.848979	-0.415794
C	4.875503	0.216119	-0.453294
C	5.421009	-2.011680	0.428706
C	4.193610	-2.492683	0.650206
O	3.809203	0.367516	0.391806
O	3.079709	-2.028886	0.006106
P	2.446405	-0.539287	0.250006

O	1.702504	-0.178989	-1.004094
O	1.732805	-0.433489	1.560506
C	-2.571689	-2.860300	-0.058194
C	-2.478586	-4.135399	-0.598894
C	-1.439085	-4.447297	-1.472994
C	-0.504788	-3.471695	-1.797994
C	-0.591291	-2.189095	-1.257194
H	-3.397090	-2.626502	0.608706
H	-3.221084	-4.883801	-0.340194
H	-1.362583	-5.443497	-1.897394
H	0.165507	-1.460993	-1.528394
H	0.310913	-3.698193	-2.477094
C	-4.193596	-0.143604	1.123406
C	-5.498897	0.290793	0.892506
C	-5.838498	0.877192	-0.320594
C	-4.865699	1.020495	-1.308694
C	-3.567898	0.580298	-1.080894
H	-2.808498	0.686200	-1.850994
H	-3.958995	-0.605603	2.077606
H	-6.247497	0.168591	1.669006
H	-6.853199	1.219190	-0.497594
H	-5.119000	1.473194	-2.262194
C	1.420097	2.722010	0.208806
C	2.248795	3.695812	-0.338194
C	1.718292	4.702711	-1.140494
C	0.349592	4.738407	-1.394694
C	-0.481205	3.764705	-0.849994
H	-1.549806	3.785303	-1.051594
H	1.848599	1.956011	0.845606
H	-0.071910	5.522906	-2.015194
H	5.048801	1.072419	-1.098794
H	6.570306	-0.836577	-1.040094
H	3.998812	-3.346684	1.292006
H	6.256610	-2.523378	0.896906
H	3.313495	3.659115	-0.130994
H	2.369090	5.461612	-1.563694

TS-B-6

M06-2X/def2-TZVPP-SMD(toluene) Energy = -1741.54817887

Number of Imaginary Frequencies = 1

Lowest Frequency = 373.5139i

M06-2X/6-31G* Geometry

C	-1.150798	-0.748388	1.815990
C	-1.820295	-0.319285	0.207990
C	-0.903190	0.525610	2.380290
H	-0.259001	-1.289194	1.500390
H	-1.906801	-1.375484	2.283090
C	0.142314	1.317504	1.860290
H	-1.670088	0.997515	2.993990
N	-0.802191	0.457210	-0.367310
C	-2.029603	-1.672083	-0.460510
C	-3.118491	0.462223	0.368090
C	-0.510784	1.675808	0.234590
C	0.500421	2.569002	-0.424110
H	-1.421881	2.229613	0.455290
H	0.037806	-0.078795	-0.637310
H	1.054511	0.787099	1.574790
H	0.295420	2.295903	2.311990
C	4.732009	0.426978	0.230290
C	4.512605	-0.319221	-0.865910
C	4.256308	0.261381	1.602090
C	3.682902	-0.827016	2.125890
O	3.744398	-1.421616	-1.035310

O	3.436195	-1.982115	1.441590
P	2.583496	-1.916710	0.029790
O	1.594802	-0.777104	0.176790
O	2.149788	-3.271607	-0.356610
C	-3.951991	0.350428	1.480390
C	-5.174788	1.018035	1.521490
C	-5.581183	1.804037	0.448690
C	-4.759282	1.914532	-0.670810
C	-3.541386	1.244925	-0.713210
H	-3.666395	-0.270674	2.323590
H	-5.809188	0.917838	2.396390
H	-6.532980	2.324342	0.482290
H	-2.903986	1.320022	-1.589910
H	-5.068479	2.518934	-1.517810
C	-3.310906	-2.120576	-0.797910
C	-3.476813	-3.363275	-1.405210
C	-2.376017	-4.172281	-1.672810
C	-1.099815	-3.733789	-1.327810
C	-0.930608	-2.494190	-0.724710
H	0.075094	-2.198395	-0.453310
H	-4.183402	-1.508271	-0.598710
H	-4.476115	-3.696969	-1.667110
H	-2.514823	-5.141881	-2.141010
H	-0.216618	-4.339594	-1.503910
C	1.791519	2.136995	-0.738510
C	2.676524	3.016090	-1.353610
C	2.290031	4.322092	-1.649110
C	1.007234	4.755499	-1.325410
C	0.115929	3.881004	-0.710910
H	-0.887569	4.216910	-0.460210
H	2.101813	1.121993	-0.499710
H	0.699040	5.771801	-1.549610
H	5.009206	-0.060724	-1.796910
H	5.393614	1.272274	0.062990
H	3.391102	-0.882014	3.170990
H	4.424813	1.093680	2.278690
H	3.677022	2.668984	-1.592910
H	2.988235	5.002588	-2.126710

TS-B-7

M06-2X/def2-TZVPP-SMD(toluene) Energy = -1741.54812017

Number of Imaginary Frequencies = 1

Lowest Frequency = 368.4798i

M06-2X/6-31G* Geometry

C	-0.627698	-0.943202	1.706198
C	-1.464698	-0.681104	0.123598
C	-0.889701	0.279398	2.362998
H	0.396002	-1.069000	1.349098
H	-1.070496	-1.848203	2.116298
C	-0.268203	1.460199	1.894998
H	-1.755001	0.362096	3.020298
N	-0.865501	0.477898	-0.380802
C	-1.138796	-1.952003	-0.652502
C	-2.961399	-0.499407	0.350398
C	-1.064604	1.663197	0.328198
C	-0.523207	2.933398	-0.263002
H	-2.114104	1.784695	0.591998
H	0.107899	0.355200	-0.698802
H	0.764497	1.346701	1.560998
H	-0.483205	2.380999	2.433798
C	3.485206	-2.729793	0.161198
C	3.903004	-1.962192	-0.859302
C	3.101605	-2.369794	1.524698

C	3.271103	-1.188893	2.130898
O	4.049101	-0.617191	-0.933002
O	3.831200	-0.083692	1.563098
P	3.294699	0.437507	0.087698
O	1.814200	0.121704	0.045398
O	3.809996	1.792708	-0.173902
C	-3.646098	-1.017009	1.449298
C	-5.031398	-0.895512	1.544498
C	-5.750399	-0.256613	0.540098
C	-5.075801	0.256788	-0.565702
C	-3.694600	0.131491	-0.662402
H	-3.111097	-1.533707	2.239698
H	-5.545497	-1.304613	2.408298
H	-6.828600	-0.160716	0.616398
H	-3.167301	0.523493	-1.527702
H	-5.625802	0.753187	-1.358902
C	-2.155394	-2.839905	-1.019202
C	-1.855091	-3.997405	-1.733402
C	-0.540590	-4.284902	-2.083702
C	0.475408	-3.409199	-1.708502
C	0.185805	-2.253400	-0.992702
H	1.001204	-1.595498	-0.696702
H	-3.187794	-2.634807	-0.759802
H	-2.657090	-4.672606	-2.014702
H	-0.308388	-5.187701	-2.640202
H	1.510008	-3.620297	-1.960302
C	0.825893	3.093801	-0.584202
C	1.269390	4.295802	-1.124802
C	0.375288	5.341300	-1.345302
C	-0.970412	5.185397	-1.020302
C	-1.417909	3.985696	-0.475702
H	-2.468209	3.863094	-0.220702
H	1.544795	2.301503	-0.409402
H	-1.671813	5.996996	-1.187002
H	4.204005	-2.428091	-1.793502
H	3.458308	-3.791693	-0.066202
H	2.989602	-1.031494	3.168698
H	2.669607	-3.161694	2.129298
H	2.324190	4.399505	-1.357802
H	0.726086	6.279701	-1.763902

TS-B-8

M06-2X/def2-TZVPP-SMD(toluene) Energy = -1741.54790053

Number of Imaginary Frequencies = 1

Lowest Frequency = 414.5679i

M06-2X/6-31G* Geometry

C	-1.145498	-0.798290	2.037195
C	-1.651897	-0.693989	0.277895
C	-1.529895	0.471111	2.513695
H	-0.077398	-0.942692	1.867895
H	-1.666099	-1.668289	2.430895
C	-0.845292	1.622009	2.060595
H	-2.502795	0.594913	2.988395
N	-0.983295	0.434510	-0.175305
C	-1.124900	-1.998090	-0.290505
C	-3.166397	-0.587586	0.164195
C	-1.343492	1.667110	0.343695
C	-0.659990	2.877609	-0.222105
H	-2.425392	1.796113	0.390995
H	0.051405	0.303507	-0.164105
H	0.231807	1.516707	1.921695
H	-1.166590	2.579010	2.467195
C	5.518901	-1.635204	0.328195

C	4.405300	-2.050602	-0.283805
C	5.523103	-0.584504	1.341995
C	4.730405	0.490497	1.283395
O	3.156501	-1.625399	0.074695
O	3.938406	0.780199	0.207895
P	2.620904	-0.099598	-0.209805
O	1.507004	0.114004	0.789895
O	2.336504	0.147003	-1.648605
C	-4.064598	-0.895984	1.184495
C	-5.439998	-0.826581	0.963495
C	-5.931997	-0.444180	-0.278605
C	-5.040696	-0.138182	-1.305805
C	-3.670796	-0.215785	-1.088805
H	-3.707198	-1.202985	2.162395
H	-6.123598	-1.071580	1.770195
H	-7.002397	-0.386178	-0.447905
H	-2.973496	0.014214	-1.889405
H	-5.412796	0.158719	-2.281205
C	-1.727903	-3.200289	0.094795
C	-1.250205	-4.413290	-0.383405
C	-0.163705	-4.439692	-1.256605
C	0.426797	-3.245793	-1.654305
C	-0.052100	-2.025392	-1.183305
H	0.428502	-1.118093	-1.536505
H	-2.582203	-3.187587	0.766995
H	-1.727307	-5.338089	-0.075005
H	0.213893	-5.387593	-1.626905
H	1.270497	-3.244295	-2.337005
C	-1.208187	4.131010	0.065495
C	-0.607885	5.289509	-0.412205
C	0.548515	5.201006	-1.184905
C	1.089612	3.953105	-1.480305
C	0.493210	2.787706	-1.004505
H	0.935208	1.831405	-1.273905
H	-2.113887	4.197512	0.665595
H	1.985312	3.870803	-2.087305
H	4.402398	-2.818302	-1.052305
H	6.455700	-2.113006	0.057395
H	4.723507	1.262097	2.047895
H	6.205103	-0.664606	2.183395
H	-1.043783	6.257510	-0.185905
H	1.021317	6.103305	-1.560105

TS-C-8

M06-2X/def2-TZVPP-SMD(toluene) Energy = -1741.54783008

Number of Imaginary Frequencies = 1

Lowest Frequency = 369.8984i

M06-2X/6-31G* Geometry

C	-0.902497	-0.978600	1.948199
C	-1.413797	-0.880500	0.200299
C	-1.412998	0.227100	2.470699
H	0.181003	-0.994799	1.810399
H	-1.331397	-1.908700	2.315299
C	-0.869199	1.460100	2.035899
H	-2.384298	0.235899	2.965499
N	-0.936698	0.351600	-0.240301
C	-2.937997	-0.973301	0.106399
C	-0.754297	-2.110600	-0.400101
C	-1.475899	1.479100	0.375999
C	-1.163500	2.847300	-0.160801
H	-2.554399	1.374199	0.493299
H	0.076702	0.422001	-0.487101
H	0.213001	1.464901	1.885299

H	-1.276200	2.362400	2.488899
C	5.847702	0.063005	-0.343701
C	5.012501	1.104004	-0.267201
C	5.607103	-1.207895	0.333999
C	4.389103	-1.742996	0.461799
O	3.922301	1.136303	0.556899
O	3.281803	-1.210997	-0.141901
P	2.598702	0.194803	0.357099
O	1.784202	0.669702	-0.819101
O	1.935702	0.062202	1.686599
C	-1.282696	-3.368900	-0.082201
C	-0.700895	-4.528100	-0.576101
C	0.421005	-4.448999	-1.399601
C	0.943804	-3.203799	-1.724701
C	0.360803	-2.035399	-1.236001
H	-2.162896	-3.442801	0.550499
H	-1.125394	-5.493400	-0.318601
H	0.881006	-5.354199	-1.783601
H	0.806103	-1.084999	-1.508101
H	1.822004	-3.122498	-2.356901
C	-3.785897	-1.376402	1.136399
C	-5.161497	-1.478603	0.925799
C	-5.705597	-1.175603	-0.316001
C	-4.864697	-0.775202	-1.353401
C	-3.494597	-0.681102	-1.145701
H	-2.836598	-0.372801	-1.953101
H	-3.389597	-1.627101	2.114999
H	-5.803797	-1.795603	1.741399
H	-6.776097	-1.251504	-0.477301
H	-5.276498	-0.537703	-2.329201
C	0.106900	3.227401	-0.600501
C	0.311899	4.526201	-1.057901
C	-0.729002	5.451600	-1.069001
C	-1.993001	5.075499	-0.623301
C	-2.206800	3.777699	-0.171401
H	-3.195500	3.481599	0.171999
H	0.924800	2.510901	-0.607601
H	-2.812302	5.787299	-0.630701
H	5.188001	2.040604	-0.788301
H	6.750102	0.183005	-0.935801
H	4.199204	-2.677896	0.980699
H	6.449203	-1.754795	0.747699
H	1.298499	4.814302	-1.406701
H	-0.556102	6.462700	-1.424601

TS-C-9

M06-2X/def2-TZVPP-SMD(toluene) Energy = -1741.54782995

Number of Imaginary Frequencies = 1

Lowest Frequency = 369.9219i

M06-2X/6-31G* Geometry

C	-0.902502	-0.978499	1.948288
C	-1.413802	-0.880501	0.200388
C	-1.413005	0.227199	2.470688
H	0.180998	-0.994797	1.810388
H	-1.331399	-1.908701	2.315288
C	-0.869308	1.460101	2.035888
H	-2.384305	0.235897	2.965488
N	-0.936705	0.351600	-0.240312
C	-2.938002	-0.973305	0.106388
C	-0.754299	-2.110599	-0.400112
C	-1.475908	1.479099	0.375888
C	-1.163512	2.847300	-0.160812
H	-2.554408	1.374196	0.493288

H	0.076695	0.422003	-0.487112
H	0.212992	1.464903	1.885288
H	-1.276210	2.362400	2.488888
C	5.847696	0.063018	-0.343912
C	5.012493	1.104016	-0.267212
C	5.607099	-1.207882	0.333888
C	4.389200	-1.743086	0.461688
O	3.922393	1.136213	0.556988
O	3.281799	-1.211088	-0.141812
P	2.598695	0.194810	0.357188
O	1.784294	0.669708	-0.819012
O	1.935696	0.062208	1.686688
C	-1.282795	-3.368900	-0.082212
C	-0.700992	-4.528099	-0.576112
C	0.420908	-4.449096	-1.399612
C	0.943904	-3.203795	-1.724612
C	0.360801	-2.035396	-1.236012
H	-2.162995	-3.442803	0.550388
H	-1.125490	-5.493400	-0.318712
H	0.881010	-5.354295	-1.783512
H	0.806099	-1.084995	-1.508012
H	1.822004	-3.122592	-2.356812
C	-3.786001	-1.376307	1.136388
C	-5.161500	-1.478511	0.925788
C	-5.705601	-1.175512	-0.316112
C	-4.864702	-0.775210	-1.353412
C	-3.494602	-0.681106	-1.145712
H	-2.836603	-0.372805	-1.953112
H	-3.389700	-1.627106	2.114988
H	-5.803799	-1.795512	1.741388
H	-6.776101	-1.251515	-0.477412
H	-5.276503	-0.537711	-2.329312
C	0.106887	3.227403	-0.600412
C	0.311984	4.526204	-1.057812
C	-0.728918	5.451601	-1.069012
C	-1.992917	5.075398	-0.623312
C	-2.206814	3.777697	-0.171512
H	-3.195513	3.481595	0.171888
H	0.924889	2.510905	-0.607512
H	-2.812319	5.787296	-0.630912
H	5.187891	2.040617	-0.788412
H	6.749995	0.183121	-0.936012
H	4.199303	-2.677986	0.980688
H	6.449200	-1.754780	0.747488
H	1.298583	4.814306	-1.406612
H	-0.556021	6.462701	-1.424612

TS-C-10

M06-2X/def2-TZVPP-SMD(toluene) Energy = -1741.54782799

Number of Imaginary Frequencies = 1

Lowest Frequency = 369.9249i

M06-2X/6-31G* Geometry

C	-0.902512	-0.978498	1.948295
C	-1.413812	-0.880497	0.200395
C	-1.413009	0.227203	2.470695
H	0.180988	-0.994800	1.810395
H	-1.331414	-1.908697	2.315295
C	-0.869307	1.460102	2.035895
H	-2.384309	0.235906	2.965495
N	-0.936709	0.351602	-0.240305
C	-0.754314	-2.110598	-0.400105
C	-2.938012	-0.973293	0.106395
C	-1.475907	1.479104	0.375895

C	-1.163504	2.847303	-0.160805
H	-2.554407	1.374206	0.493295
H	0.076691	0.422000	-0.487105
H	0.212993	1.464900	1.885295
H	-1.276205	2.362403	2.488895
C	5.847690	0.062988	-0.343905
C	5.012492	1.104090	-0.267205
C	5.607188	-1.207912	0.333795
C	4.389186	-1.743109	0.461695
O	3.922393	1.136192	0.556995
O	3.281787	-1.211107	-0.141805
P	2.598690	0.194795	0.357195
O	1.784292	0.669697	-0.819005
O	1.935690	0.062196	1.686695
C	-3.786013	-1.376292	1.136395
C	-5.161513	-1.478489	0.925795
C	-5.705612	-1.175487	-0.316105
C	-4.864712	-0.775189	-1.353505
C	-3.494611	-0.681092	-1.145705
H	-3.389713	-1.627092	2.114995
H	-5.803814	-1.795487	1.741395
H	-6.776113	-1.251485	-0.477405
H	-2.836611	-0.372794	-1.953105
H	-5.276511	-0.537688	-2.329305
C	-1.282817	-3.368897	-0.082205
C	-0.701020	-4.528098	-0.576105
C	0.420881	-4.449100	-1.399605
C	0.943883	-3.203802	-1.724605
C	0.360786	-2.035400	-1.236005
H	0.806188	-1.085001	-1.508005
H	-2.163017	-3.442795	0.550395
H	-1.125522	-5.493397	-0.318705
H	0.880979	-5.354301	-1.783505
H	1.821983	-3.122603	-2.356705
C	0.106997	3.227400	-0.600405
C	0.312000	4.526200	-1.057805
C	-0.728898	5.451602	-1.069005
C	-1.992899	5.075405	-0.623405
C	-2.206802	3.777705	-0.171505
H	-3.195502	3.481607	0.171795
H	0.924895	2.510898	-0.607405
H	-2.812298	5.787306	-0.630905
H	5.187794	2.040589	-0.788405
H	6.749990	0.183086	-0.936105
H	4.199384	-2.678009	0.980695
H	6.449286	-1.754813	0.747395
H	1.298600	4.814298	-1.406505
H	-0.555996	6.462702	-1.424605

TS-C-11

M06-2X/def2-TZVPP-SMD(toluene) Energy = -1741.54782730

Number of Imaginary Frequencies = 1

Lowest Frequency = 369.9845i

M06-2X/6-31G* Geometry

C	-0.902513	-0.978492	1.948293
C	-1.413812	-0.880489	0.200393
C	-1.413006	0.227211	2.470693
H	0.180987	-0.994898	1.810393
H	-1.331418	-1.908690	2.315293
C	-0.869199	1.460108	2.035893
H	-2.384306	0.235916	2.965493
N	-0.936705	0.351608	-0.240307
C	-2.938012	-0.973281	0.106393

C	-0.754419	-2.110593	-0.400107
C	-1.475899	1.479111	0.375893
C	-1.163491	2.847309	-0.160807
H	-2.554399	1.374217	0.493293
H	0.076695	0.422002	-0.487107
H	0.213001	1.464902	1.885293
H	-1.276194	2.362410	2.488893
C	5.607186	-1.207929	0.333793
C	4.389183	-1.743122	0.461693
C	5.847693	0.062970	-0.343907
C	5.012499	1.103975	-0.267207
O	3.281786	-1.211116	-0.141807
O	3.922399	1.136181	0.556993
P	2.598694	0.194788	0.357193
O	1.784297	0.669693	-0.819007
O	1.935693	0.062192	1.686693
C	-1.282826	-3.368890	-0.082207
C	-0.701132	-4.528093	-0.576107
C	0.420868	-4.449099	-1.399607
C	0.943875	-3.203802	-1.724507
C	0.360782	-2.035399	-1.235907
H	-2.163126	-3.442785	0.550393
H	-1.125638	-5.493391	-0.318707
H	0.880963	-5.354302	-1.783507
H	0.806187	-1.085002	-1.508007
H	1.821975	-3.122607	-2.356707
C	-3.786015	-1.376276	1.136393
C	-5.161515	-1.478468	0.925793
C	-5.705614	-1.175465	-0.316107
C	-4.864711	-0.775170	-1.353507
C	-3.494611	-0.681077	-1.145707
H	-2.836609	-0.372781	-1.953107
H	-3.389716	-1.627078	2.114993
H	-5.803817	-1.795465	1.741393
H	-6.776114	-1.251359	-0.477407
H	-5.276510	-0.537667	-2.329307
C	-2.206786	3.777715	-0.171607
C	-1.992879	5.075414	-0.623407
C	-0.728876	5.451607	-1.069007
C	0.312018	4.526201	-1.057807
C	0.107011	3.227402	-0.600407
H	0.924907	2.510898	-0.607407
H	-3.195487	3.481621	0.171793
H	1.298720	4.814296	-1.406507
H	4.199378	-2.678021	0.980593
H	6.449283	-1.754833	0.747393
H	5.187804	2.040574	-0.788407
H	6.749994	0.183065	-0.936207
H	-2.812275	5.787319	-0.630907
H	-0.555971	6.462706	-1.424607

TS-C-12

M06-2X/def2-TZVPP-SMD(toluene) Energy = -1741.54782244

Number of Imaginary Frequencies = 1

Lowest Frequency = 369.8680i

M06-2X/6-31G* Geometry

C	-0.902501	-0.978494	1.948302
C	-1.413801	-0.880492	0.200402
C	-1.412998	0.227208	2.470702
H	0.180999	-0.994897	1.810402
H	-1.331404	-1.908692	2.315302
C	-0.869194	1.460106	2.035902
H	-2.384298	0.235911	2.965502

N	-0.936697	0.351606	-0.240298
C	-0.754304	-2.110594	-0.400098
C	-2.938001	-0.973288	0.106402
C	-1.475894	1.479108	0.376002
C	-1.163490	2.847307	-0.160798
H	-2.554394	1.374211	0.493302
H	0.076703	0.422003	-0.487098
H	0.213006	1.464803	1.885302
H	-1.276191	2.362407	2.488902
C	5.607098	-1.207913	0.333902
C	4.389097	-1.743109	0.461702
C	5.847702	0.062987	-0.343798
C	5.012505	1.103989	-0.267198
O	3.281798	-1.211106	-0.141898
O	3.922405	1.136192	0.556902
P	2.598702	0.194796	0.357102
O	1.784204	0.669699	-0.819098
O	1.935602	0.062198	1.686702
C	-3.786002	-1.376285	1.136402
C	-5.161503	-1.478481	0.925802
C	-5.705602	-1.175480	-0.316098
C	-4.864701	-0.775182	-1.353398
C	-3.494600	-0.681086	-1.145698
H	-3.389703	-1.627086	2.115002
H	-5.803804	-1.795479	1.741402
H	-6.776102	-1.251477	-0.477398
H	-2.836599	-0.372788	-1.953098
H	-5.276500	-0.537681	-2.329298
C	-1.282808	-3.368893	-0.082198
C	-0.701012	-4.528094	-0.576098
C	0.420889	-4.449098	-1.399598
C	0.943792	-3.203799	-1.724598
C	0.360796	-2.035397	-1.235998
H	0.806098	-1.084999	-1.508098
H	-2.163008	-3.442790	0.550502
H	-1.125414	-5.493393	-0.318598
H	0.880986	-5.354299	-1.783498
H	1.821893	-3.122502	-2.356798
C	-2.206687	3.777710	-0.171498
C	-1.992884	5.075510	-0.623298
C	-0.728882	5.451606	-1.068998
C	0.312015	4.526103	-1.057898
C	0.106911	3.227403	-0.600498
H	0.924909	2.510901	-0.607598
H	-3.195388	3.481613	0.172002
H	1.298616	4.814200	-1.406698
H	4.199294	-2.677909	0.980702
H	6.449197	-1.754815	0.747602
H	5.187908	2.040589	-0.788398
H	6.750102	0.182984	-0.935898
H	-2.812281	5.787312	-0.630798
H	-0.555980	6.462705	-1.424598

TS-F

M06-2X/def2-TZVPP-SMD(toluene) Energy = -1741.54755982

Number of Imaginary Frequencies = 1

Lowest Frequency = 389.2245i

M06-2X/6-31G* Geometry

C	-1.342899	-0.774900	1.944100
C	-1.882600	-0.364901	0.258000
C	-1.017202	0.502701	2.445100
H	-0.480198	-1.408198	1.730900
H	-2.189198	-1.295901	2.385700

C	0.119297	1.175603	1.939400
H	-1.773503	1.080100	2.977700
N	-0.794301	0.315401	-0.294800
C	-2.147298	-1.728001	-0.366300
C	-3.136702	0.502697	0.328600
C	-0.451204	1.530502	0.281800
C	0.589295	2.399604	-0.368800
H	-1.338805	2.128300	0.485600
H	-0.012100	-0.265297	-0.674600
H	1.000898	0.561705	1.752700
H	0.336895	2.154604	2.362600
C	5.529202	-1.457787	0.775400
C	4.600204	-2.407389	0.635100
C	5.418799	-0.136287	0.164600
C	4.264998	0.529111	0.042600
O	3.526003	-2.268391	-0.204900
O	3.082799	0.105708	0.578600
P	2.281901	-1.275993	0.153500
O	1.519801	-1.059394	-1.123400
O	1.530402	-1.687394	1.375700
C	-4.046202	0.467796	1.385500
C	-5.221703	1.214793	1.336500
C	-5.506904	2.004493	0.227800
C	-4.609305	2.039395	-0.837000
C	-3.438203	1.291497	-0.788800
H	-3.857301	-0.150204	2.257000
H	-5.915203	1.174092	2.170500
H	-6.422006	2.586691	0.191900
H	-2.741603	1.310598	-1.622200
H	-4.821206	2.647194	-1.710900
C	-3.416197	-2.057003	-0.854200
C	-3.641495	-3.297404	-1.445400
C	-2.608093	-4.221702	-1.552300
C	-1.346694	-3.902200	-1.056400
C	-1.115596	-2.668799	-0.458900
H	-0.130396	-2.446697	-0.063500
H	-4.234598	-1.349605	-0.784700
H	-4.630794	-3.535706	-1.823500
H	-2.785191	-5.187902	-2.014500
H	-0.531892	-4.615198	-1.127900
C	0.645892	3.733704	0.049400
C	1.551291	4.620406	-0.519100
C	2.404992	4.182207	-1.529200
C	2.342694	2.859307	-1.956700
C	1.445996	1.960906	-1.379800
H	1.432597	0.927105	-1.711700
H	-0.032908	4.082303	0.825600
H	2.999695	2.511208	-2.748200
H	4.664705	-3.383089	1.106500
H	6.408302	-1.692185	1.368300
H	4.196196	1.510911	-0.418500
H	6.318299	0.349914	-0.201400
H	1.582989	5.651606	-0.182100
H	3.109690	4.871409	-1.984100

TS-F-2

M06-2X/def2-TZVPP-SMD(toluene) Energy = -1741.54755885

Number of Imaginary Frequencies = 1

Lowest Frequency = 389.0811*i*

M06-2X/6-31G* Geometry

C	-1.342807	-0.774896	1.944106
C	-1.882606	-0.364794	0.258006
C	-1.017103	0.502603	2.445006

H	-0.480010	-1.408199	1.730906
H	-2.189009	-1.295993	2.385606
C	0.119300	1.175598	1.939306
H	-1.773501	1.080005	2.977606
N	-0.794303	0.315502	-0.294794
C	-2.147211	-1.727993	-0.366294
C	-3.136703	0.502710	0.328706
C	-0.451299	1.530600	0.281906
C	0.589204	2.399697	-0.368794
H	-1.338797	2.128304	0.485706
H	-0.012106	-0.265301	-0.674594
H	1.000998	0.561595	1.752706
H	0.337003	2.154598	2.362506
C	5.529190	-1.457822	0.775406
C	4.600287	-2.407418	0.634806
C	5.418795	-0.136121	0.165006
C	4.264897	0.529283	0.043106
O	3.526087	-2.268314	-0.205094
O	3.082596	0.105687	0.578806
P	2.281891	-1.276010	0.153406
O	1.519892	-1.059207	-1.123494
O	1.530389	-1.687807	1.375506
C	-4.046303	0.467214	1.385506
C	-5.222000	1.214118	1.336506
C	-5.506997	2.004219	0.228006
C	-4.609297	2.039516	-0.836594
C	-3.438100	1.291811	-0.788494
H	-3.857505	-0.150987	2.256806
H	-5.915500	1.173121	2.170506
H	-6.422295	2.586322	0.192206
H	-2.741500	1.311209	-1.621794
H	-4.821195	2.647617	-1.710294
C	-3.416012	-2.056989	-0.854494
C	-3.641317	-3.297288	-1.445794
C	-2.607820	-4.221592	-1.552494
C	-1.346519	-3.902196	-1.056394
C	-1.115514	-2.668797	-0.458794
H	-0.130314	-2.446701	-0.063194
H	-4.234410	-1.349486	-0.785094
H	-4.630518	-3.535484	-1.823994
H	-2.784924	-5.187791	-2.014794
H	-0.531722	-4.615199	-1.127794
C	0.645809	3.733896	0.049306
C	1.551113	4.620493	-0.519194
C	2.404911	4.182290	-1.529294
C	2.342606	2.859390	-1.956794
C	1.445903	1.960993	-1.379794
H	1.432499	0.927193	-1.711694
H	-0.033089	4.082399	0.825506
H	2.999705	2.511288	-2.748194
H	4.664883	-3.383218	1.106006
H	6.408389	-1.692325	1.368306
H	4.196101	1.511183	-0.417794
H	6.318197	0.350275	-0.200694
H	1.582716	5.651693	-0.182294
H	3.109513	4.871487	-1.984194

TS-F-3

M06-2X/def2-TZVPP-SMD(toluene) Energy = -1741.54755850

Number of Imaginary Frequencies = 1

Lowest Frequency = 389.1361*i*

M06-2X/6-31G* Geometry

C	-1.342996	-0.774903	1.944097
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C	-1.882697	-0.364804	0.257997
C	-1.017099	0.502598	2.445097
H	-0.480395	-1.408301	1.730797
H	-2.189295	-1.295905	2.385597
C	0.119400	1.175400	1.939397
H	-1.773400	1.079996	2.977697
N	-0.794198	0.315398	-0.294803
C	-2.147494	-1.727904	-0.366303
C	-3.136599	0.502994	0.328597
C	-0.451001	1.530399	0.281897
C	0.589598	2.399401	-0.368803
H	-1.338502	2.128297	0.485697
H	-0.012197	-0.265500	-0.674503
H	1.001001	0.561402	1.752697
H	0.337098	2.154301	2.362597
C	5.529005	-1.457889	0.775697
C	4.600107	-2.407491	0.635097
C	5.418703	-0.136189	0.165097
C	4.264801	0.529109	0.042897
O	3.526007	-2.268393	-0.205103
O	3.082502	0.105606	0.578597
P	2.281805	-1.276095	0.153297
O	1.519705	-1.059497	-1.123603
O	1.530306	-1.687697	1.375497
C	-4.045998	0.468192	1.385597
C	-5.221500	1.215389	1.336597
C	-5.506602	2.004989	0.227797
C	-4.609102	2.039790	-0.836903
C	-3.438100	1.291793	-0.788803
H	-3.857197	-0.149808	2.257197
H	-5.914900	1.174788	2.170697
H	-6.421703	2.587287	0.191997
H	-2.741500	1.310694	-1.622303
H	-4.821003	2.647590	-1.710903
C	-3.416493	-2.056907	-0.853903
C	-3.641991	-3.297208	-1.445003
C	-2.608589	-4.221505	-1.552203
C	-1.347089	-3.902103	-1.056603
C	-1.115792	-2.668702	-0.459103
H	-0.130492	-2.446600	-0.064003
H	-4.234895	-1.349409	-0.784203
H	-4.631390	-3.535510	-1.822903
H	-2.785887	-5.187706	-2.014403
H	-0.532288	-4.615101	-1.128303
C	1.445898	1.960703	-1.380103
C	2.342697	2.858905	-1.957103
C	2.405394	4.181705	-1.529503
C	1.551993	4.620003	-0.519003
C	0.646595	3.733501	0.049597
H	-0.031906	4.082000	0.825997
H	1.432201	0.926903	-1.712103
H	1.583991	5.651103	-0.181903
H	4.664609	-3.383190	1.106297
H	6.408106	-1.692287	1.368697
H	4.196099	1.511009	-0.418103
H	6.318202	0.350113	-0.200703
H	2.999397	2.510806	-2.748803
H	3.110092	4.870906	-1.984503

TS-F-4

M06-2X/def2-TZVPP-SMD(toluene) Energy = -1741.54755681

Number of Imaginary Frequencies = 1

Lowest Frequency = 389.2543i

M06-2X/6-31G* Geometry

C	-1.343006	-0.774908	1.944099
C	-1.882706	-0.364809	0.257999
C	-1.017107	0.502592	2.445099
H	-0.480305	-1.408207	1.730899
H	-2.189205	-1.295909	2.385599
C	0.119392	1.175494	1.939399
H	-1.773408	1.080091	2.977699
N	-0.794207	0.315393	-0.294801
C	-3.136607	0.502989	0.328599
C	-2.147404	-1.727909	-0.366301
C	-0.451109	1.530493	0.281799
C	0.589490	2.399495	-0.368801
H	-1.338610	2.128292	0.485599
H	-0.012206	-0.265406	-0.674601
H	1.000993	0.561495	1.752699
H	0.337090	2.154494	2.362599
C	5.418694	-0.136299	0.164999
C	4.264893	0.529100	0.042799
C	5.528995	-1.457898	0.775599
C	4.600097	-2.407500	0.635099
O	3.082593	0.105698	0.578499
O	3.525997	-2.268401	-0.205101
P	2.281795	-1.276103	0.153399
O	1.519695	-1.059504	-1.123501
O	1.530296	-1.687704	1.375599
C	-3.416404	-2.056811	-0.854101
C	-3.641902	-3.297211	-1.445301
C	-2.608401	-4.221510	-1.552201
C	-1.347001	-3.902108	-1.056501
C	-1.115803	-2.668708	-0.459001
H	-4.234805	-1.349312	-0.784601
H	-4.631102	-3.535513	-1.823201
H	-2.785699	-5.187710	-2.014501
H	-0.130503	-2.446706	-0.063701
H	-0.532300	-4.615207	-1.128101
C	-3.438108	1.291789	-0.788701
C	-4.609109	2.039787	-0.836801
C	-5.506709	2.004886	0.227899
C	-5.221608	1.215087	1.336499
C	-4.046107	0.467988	1.385499
H	-3.857306	-0.150112	2.256999
H	-2.741508	1.310790	-1.622201
H	-4.821110	2.647687	-1.710801
H	-6.421810	2.587085	0.191999
H	-5.915108	1.174386	2.170599
C	1.445991	1.960696	-1.380001
C	2.342789	2.858997	-1.957001
C	2.405388	4.181797	-1.529301
C	1.551887	4.620096	-0.519101
C	0.646488	3.733595	0.049499
H	-0.032212	4.082094	0.825799
H	1.432292	0.926996	-1.712001
H	1.583786	5.651196	-0.182001
H	4.196191	1.511000	-0.418201
H	6.318193	0.350003	-0.200801
H	4.664498	-3.383200	1.106399
H	6.408096	-1.692297	1.368699
H	2.999690	2.510798	-2.748501
H	3.110187	4.870998	-1.984301

TS-F-5

M06-2X/def2-TZVPP-SMD(toluene) Energy = -1741.54755661

Number of Imaginary Frequencies = 1

Lowest Frequency = 389.0719i

M06-2X/6-31G* Geometry

C	-1.343110	-0.774788	1.944104
C	-1.882709	-0.364686	0.258004
C	-1.017205	0.502710	2.445104
H	-0.480513	-1.408192	1.730904
H	-2.189413	-1.295784	2.385604
C	0.119298	1.175505	1.939404
H	-1.773502	1.080214	2.977604
N	-0.794206	0.315409	-0.294796
C	-2.147515	-1.727785	-0.366296
C	-3.136605	0.503120	0.328604
C	-0.451000	1.530508	0.281904
C	0.589704	2.399403	-0.368796
H	-1.338498	2.128412	0.485604
H	-0.012208	-0.265394	-0.674496
H	1.000895	0.561401	1.752804
H	0.337103	2.154404	2.362604
C	5.418692	-0.136418	0.164804
C	4.264795	0.528987	0.042704
C	5.528986	-1.457919	0.775604
C	4.599982	-2.407515	0.635204
O	3.082593	0.105592	0.578504
O	3.525883	-2.268510	-0.204896
P	2.281687	-1.276104	0.153404
O	1.519588	-1.059601	-1.123496
O	1.530185	-1.687601	1.375604
C	-4.046205	0.468224	1.385504
C	-5.221702	1.215329	1.336404
C	-5.506598	2.005130	0.227704
C	-4.608998	2.039926	-0.836996
C	-3.438001	1.291921	-0.788796
H	-3.857408	-0.149877	2.257004
H	-5.915202	1.174732	2.170404
H	-6.421795	2.587434	0.191804
H	-2.741401	1.310918	-1.622196
H	-4.820895	2.647827	-1.710896
C	-3.416516	-2.056779	-0.853996
C	-3.642022	-3.297078	-1.445196
C	-2.608626	-4.221483	-1.552196
C	-1.347124	-3.902088	-1.056396
C	-1.115919	-2.668689	-0.458896
H	-0.130618	-2.446594	-0.063596
H	-4.234913	-1.349175	-0.784496
H	-4.631223	-3.535274	-1.823196
H	-2.785830	-5.187682	-2.014396
H	-0.532428	-4.615092	-1.127996
C	0.647010	3.733403	0.049704
C	1.552514	4.619699	-0.518896
C	2.405812	4.181495	-1.529396
C	2.342806	2.858695	-1.957196
C	1.445902	1.960599	-1.380196
H	1.431997	0.926799	-1.712296
H	-0.031489	4.082006	0.826104
H	2.999504	2.510492	-2.748896
H	4.196000	1.510787	-0.418496
H	6.318195	0.349878	-0.201096
H	4.664478	-3.383215	1.106604
H	6.408085	-1.692323	1.368604
H	1.584718	5.650899	-0.181596
H	3.110615	4.870492	-1.984296

TS-F-6

M06-2X/def2-TZVPP-SMD(toluene) Energy = -1741.54755592

Number of Imaginary Frequencies = 1
Lowest Frequency = 389.1076i
M06-2X/6-31G* Geometry

C	-1.343008	-0.774896	1.944097
C	-1.882706	-0.364694	0.257997
C	-1.017104	0.502603	2.445097
H	-0.480310	-1.408299	1.730797
H	-2.189209	-1.295894	2.385597
C	0.119398	1.175500	1.939397
H	-1.773402	1.080105	2.977697
N	-0.794204	0.315402	-0.294803
C	-3.136604	0.503009	0.328697
C	-2.147410	-1.727894	-0.366303
C	-0.451001	1.530501	0.281897
C	0.589602	2.399398	-0.368803
H	-1.338499	2.128404	0.485597
H	-0.012206	-0.265400	-0.674603
H	1.000996	0.561397	1.752697
H	0.337101	2.154399	2.362597
C	5.418694	-0.136316	0.165097
C	4.264796	0.529087	0.042897
C	5.528890	-1.457916	0.775697
C	4.600088	-2.407513	0.635097
O	3.082495	0.105691	0.578497
O	3.525988	-2.268410	-0.205103
P	2.281791	-1.276107	0.153297
O	1.519592	-1.059604	-1.123503
O	1.530290	-1.687704	1.375597
C	-3.416411	-2.056790	-0.854103
C	-3.641915	-3.297089	-1.445303
C	-2.608518	-4.221492	-1.552203
C	-1.347117	-3.902096	-1.056503
C	-1.115813	-2.668697	-0.459003
H	-4.234809	-1.349288	-0.784503
H	-4.631216	-3.535386	-1.823303
H	-2.785821	-5.187692	-2.014503
H	-0.130613	-2.446700	-0.063703
H	-0.532319	-4.615098	-1.128103
C	-4.046104	0.468012	1.385497
C	-5.221602	1.215115	1.336597
C	-5.506699	2.004916	0.227897
C	-4.609099	2.039914	-0.836803
C	-3.438002	1.291910	-0.788703
H	-2.741502	1.310908	-1.622103
H	-3.857306	-0.150089	2.256997
H	-5.915102	1.174517	2.170597
H	-6.421798	2.587219	0.191997
H	-4.820998	2.647814	-1.710703
C	1.445900	1.960696	-1.380103
C	2.342803	2.858893	-1.957103
C	2.405507	4.181693	-1.529403
C	1.552108	4.619995	-0.519103
C	0.646606	3.733498	0.049497
H	-0.031993	4.082100	0.825897
H	1.432297	0.926896	-1.712103
H	1.584111	5.651095	-0.181903
H	4.196099	1.510988	-0.418103
H	6.318196	0.350081	-0.200603
H	4.664485	-3.383314	1.106297
H	6.407990	-1.692319	1.368797
H	2.999602	2.510691	-2.748703
H	3.110209	4.870791	-1.984403

TS-C-13

M06-2X/def2-TZVPP-SMD(toluene) Energy = -1741.54752617

Number of Imaginary Frequencies = 1

Lowest Frequency = 427.5394i

M06-2X/6-31G* Geometry

C	-1.191192	-0.733404	2.098100
C	-1.636292	-0.691907	0.295100
C	-1.538901	0.571793	2.481700
H	-0.118391	-0.897996	2.020400
H	-1.760786	-1.567208	2.498800
C	-0.742809	1.645099	2.015700
H	-2.538003	0.777086	2.867000
N	-0.899100	0.376398	-0.197800
C	-3.146094	-0.490718	0.191500
C	-1.190482	-2.054104	-0.226100
C	-1.187109	1.644296	0.290900
C	-0.518318	2.851901	-0.300400
H	-2.261410	1.812888	0.343200
H	0.081802	0.169905	-0.516500
H	0.329992	1.447607	1.957900
H	-1.014216	2.644597	2.351100
C	5.828206	-0.398653	0.435700
C	4.980999	0.585441	0.753300
C	5.496614	-1.467456	-0.502900
C	4.280518	-2.015864	-0.576900
O	3.773697	0.766532	0.136200
O	3.279915	-1.714572	0.309000
P	2.509805	-0.265177	0.282300
O	1.703704	-0.118883	-0.978000
O	1.814604	-0.127082	1.599000
C	0.070622	-2.573995	0.082000
C	0.484830	-3.788992	-0.450500
C	-0.357064	-4.512398	-1.289700
C	-1.619468	-4.011007	-1.589800
C	-2.036677	-2.793110	-1.060700
H	0.741018	-2.048190	0.749800
H	1.472733	-4.160585	-0.197600
H	-0.034257	-5.462796	-1.703400
H	-3.024380	-2.421317	-1.309000
H	-2.288664	-4.566412	-2.239500
C	-4.052390	-1.031525	1.104600
C	-5.424691	-0.907535	0.902900
C	-5.913995	-0.247738	-0.220300
C	-5.018999	0.281968	-1.145800
C	-3.648098	0.156878	-0.944000
H	-2.950301	0.557283	-1.674400
H	-3.699986	-1.567922	1.979200
H	-6.111387	-1.333940	1.627300
H	-6.983796	-0.151746	-0.375500
H	-5.385303	0.790165	-2.032200
C	0.756682	2.834610	-0.869600
C	1.304174	4.016814	-1.362600
C	0.600265	5.215209	-1.287200
C	-0.671335	5.234300	-0.718700
C	-1.225227	4.057296	-0.230200
H	-2.219727	4.071388	0.211600
H	1.316089	1.907614	-0.956200
H	-1.232742	6.161496	-0.660000
H	5.224593	1.369342	1.464100
H	6.810806	-0.387046	0.897800
H	4.016723	-2.791066	-1.290500
H	6.266516	-1.844050	-1.169700

H	2.293674	3.991621	-1.807700
H	1.038058	6.131012	-1.672100

TS-D-7

M06-2X/def2-TZVPP-SMD(toluene) Energy = -1741.54714078

Number of Imaginary Frequencies = 1

Lowest Frequency = 340.6241i

M06-2X/6-31G* Geometry

C	-0.843601	-0.952401	1.881097
C	-1.444900	-0.857198	0.197697
C	-1.320095	0.252702	2.449397
H	0.237499	-1.016506	1.703197
H	-1.255205	-1.878799	2.279297
C	-0.825389	1.494999	1.990597
H	-2.248095	0.251106	3.021397
N	-1.014294	0.389000	-0.274403
C	-2.968501	-0.971990	0.168797
C	-0.778506	-2.055201	-0.459003
C	-1.538388	1.508003	0.366797
C	-1.245782	2.868801	-0.199503
H	-2.609289	1.397708	0.535997
H	0.015406	0.463995	-0.405903
H	0.233812	1.535094	1.726297
H	-1.208184	2.389501	2.478297
C	5.981304	-0.047334	0.382897
C	5.146305	0.224970	1.390097
C	5.579704	0.030968	-1.018603
C	4.368603	-0.331226	-1.454403
O	3.888308	0.724876	1.187797
O	3.430500	-0.938722	-0.668503
P	2.673103	-0.199918	0.596597
O	1.668408	0.789087	0.050997
O	2.229498	-1.256016	1.539697
C	-1.343612	-3.322698	-0.282503
C	-0.733918	-4.450201	-0.819503
C	0.453283	-4.327507	-1.536603
C	1.019989	-3.070310	-1.714703
C	0.407695	-1.938307	-1.186103
H	-2.269713	-3.430694	0.274497
H	-1.187322	-5.425499	-0.673203
H	0.936579	-5.208410	-1.947403
H	0.886799	-0.978509	-1.338703
H	1.956390	-2.956715	-2.250403
C	-3.762403	-1.371087	1.242197
C	-5.145603	-1.487980	1.098197
C	-5.750502	-1.203677	-0.119603
C	-4.963600	-0.807181	-1.200203
C	-3.586299	-0.698487	-1.058603
H	-2.969698	-0.393990	-1.899403
H	-3.316804	-1.610689	2.202197
H	-5.745505	-1.802777	1.946297
H	-6.826602	-1.291572	-0.229403
H	-5.423699	-0.585078	-2.157903
C	0.034920	3.267795	-0.594303
C	0.223626	4.547794	-1.106803
C	-0.844569	5.435599	-1.219103
C	-2.117271	5.041405	-0.816803
C	-2.314877	3.761706	-0.307703
H	-3.309979	3.450311	0.000997
H	0.876017	2.585691	-0.496703
H	-2.955868	5.725410	-0.900503
H	5.427305	0.149268	2.436297
H	7.001203	-0.328939	0.627497

H	4.072803	-0.249425	-2.497003
H	6.292506	0.393364	-1.753503
H	1.218328	4.853489	-1.415603
H	-0.684564	6.432898	-1.617003

TS-E-2

M06-2X/def2-TZVPP-SMD(toluene) Energy = -1741.54649791

Number of Imaginary Frequencies = 1

Lowest Frequency = 387.5805i

M06-2X/6-31G* Geometry

C	-0.157100	-0.895297	1.740899
C	-0.983600	-1.072596	0.143099
C	-1.042899	-0.045196	2.440399
H	0.772601	-0.442799	1.391699
H	-0.035802	-1.908897	2.116699
C	-1.188597	1.295804	2.025599
H	-1.801800	-0.476395	3.092599
N	-1.156098	0.242304	-0.286601
C	-2.297602	-1.828294	0.300399
C	0.026598	-1.858498	-0.672301
C	-2.001297	1.058206	0.449399
C	-2.251695	2.444706	-0.067701
H	-2.934398	0.554407	0.703099
H	-0.244098	0.707603	-0.496801
H	-0.278396	1.788903	1.679899
H	-1.869196	1.925305	2.595599
C	5.087800	-0.508006	1.102699
C	4.108800	-0.992304	0.332699
C	4.938002	0.718395	1.881199
C	4.258704	1.791496	1.457899
O	2.860901	-0.430202	0.319599
O	3.741504	1.938297	0.206899
P	2.586603	0.990598	-0.478001
O	1.227503	1.405901	0.053399
O	2.843403	0.894498	-1.930101
C	0.318696	-3.177398	-0.305101
C	1.289995	-3.897800	-0.985301
C	1.987296	-3.307801	-2.040801
C	1.689998	-2.004800	-2.419301
C	0.698499	-1.288699	-1.751401
H	-0.218805	-3.643497	0.516999
H	1.508393	-4.918800	-0.688101
H	2.759295	-3.865802	-2.562001
H	0.498601	-0.274598	-2.077301
H	2.238899	-1.509701	-3.212601
C	-2.651603	-2.583593	1.417099
C	-3.853204	-3.291591	1.443099
C	-4.715704	-3.249190	0.354699
C	-4.367803	-2.499591	-0.768201
C	-3.167402	-1.801393	-0.797701
H	-2.888901	-1.223593	-1.674501
H	-1.994103	-2.639794	2.278899
H	-4.110105	-3.875191	2.321499
H	-5.652005	-3.797489	0.377599
H	-5.031203	-2.461990	-1.626401
C	-1.219394	3.251404	-0.557501
C	-1.514392	4.526705	-1.028301
C	-2.822291	5.008407	-1.002601
C	-3.846592	4.209509	-0.503401
C	-3.560294	2.930108	-0.036401
H	-4.359995	2.300709	0.346899
H	-0.193394	2.887503	-0.562001
H	-4.867392	4.577510	-0.480301

H	4.199698	-1.887104	-0.277301
H	6.023100	-1.057607	1.153999
H	4.154705	2.685696	2.066599
H	5.408502	0.781494	2.858199
H	-0.713191	5.148704	-1.414401
H	-3.041389	6.006207	-1.369801

TS-B-9

M06-2X/def2-TZVPP-SMD(toluene) Energy = -1741.54626950

Number of Imaginary Frequencies = 1

Lowest Frequency = 397.4878i

M06-2X/6-31G* Geometry

C	-1.041309	-0.939795	2.044994
C	-1.410009	-0.894992	0.273394
C	-1.720000	0.205310	2.519194
H	0.043892	-0.851704	1.973494
H	-1.391417	-1.912693	2.383794
C	-1.255289	1.484106	2.147594
H	-2.730200	0.108619	2.915394
N	-0.974398	0.368904	-0.119706
C	-2.900210	-1.105480	0.029694
C	-0.576118	-2.049399	-0.257006
C	-1.637589	1.473210	0.398594
C	-1.220778	2.825606	-0.102606
H	-2.720190	1.350119	0.361994
H	0.062803	0.471695	-0.062306
H	-0.171688	1.598797	2.090294
H	-1.790282	2.346911	2.538994
C	4.862188	-1.345445	-1.016906
C	4.193296	-0.310239	-1.539706
C	4.489182	-1.979242	0.245194
C	4.028788	-1.286638	1.292194
O	3.020300	0.161971	-1.028206
O	3.986199	0.080163	1.309894
P	2.856106	0.897272	0.450894
O	1.478203	0.460084	0.908594
O	3.209918	2.330469	0.400394
C	0.625683	-1.840809	-0.934806
C	1.391974	-2.926516	-1.351106
C	0.962663	-4.226912	-1.108206
C	-0.245438	-4.440902	-0.447006
C	-1.008829	-3.359796	-0.024106
H	1.001192	-0.848112	-1.140606
H	2.333076	-2.735424	-1.858406
H	1.562156	-5.071317	-1.433806
H	-1.952531	-3.537288	0.484894
H	-0.596047	-5.450999	-0.260206
C	-3.796615	-1.612672	0.968794
C	-5.133916	-1.823561	0.632194
C	-5.590214	-1.525757	-0.646006
C	-4.699710	-1.021965	-1.592806
C	-3.366208	-0.819776	-1.260106
H	-2.668305	-0.432882	-1.997206
H	-3.465217	-1.861075	1.972294
H	-5.815920	-2.220656	1.377394
H	-6.631715	-1.686249	-0.905506
H	-5.043508	-0.788762	-2.595606
C	0.109826	3.248095	-0.064706
C	0.454336	4.496292	-0.570206
C	-0.525557	5.335800	-1.096806
C	-1.855960	4.923511	-1.118806
C	-2.203771	3.670714	-0.621806
H	-3.240673	3.343823	-0.647606

H	0.891621	2.624188	0.356094
H	-2.624055	5.574318	-1.524906
H	4.491800	0.177258	-2.463506
H	5.723284	-1.718852	-1.563406
H	3.729584	-1.751235	2.227594
H	4.599473	-3.054443	0.353594
H	1.497439	4.794383	-0.541606
H	-0.254849	6.312198	-1.486906

TS-B-10

M06-2X/def2-TZVPP-SMD(toluene) Energy = -1741.54626931

Number of Imaginary Frequencies = 1

Lowest Frequency = 397.5332i

M06-2X/6-31G* Geometry

C	-1.041220	-0.939794	2.044997
C	-1.410020	-0.894991	0.273397
C	-1.720011	0.205312	2.519197
H	0.043880	-0.851703	1.973497
H	-1.391428	-1.912691	2.383797
C	-1.255300	1.484108	2.147597
H	-2.730211	0.108620	2.915397
N	-0.974409	0.368906	-0.119703
C	-0.576129	-2.049398	-0.257003
C	-2.900122	-1.105478	0.029697
C	-1.637600	1.473211	0.398597
C	-1.220789	2.825608	-0.102603
H	-2.720201	1.350120	0.361997
H	0.062792	0.471697	-0.062303
H	-0.171699	1.598799	2.090297
H	-1.790293	2.346912	2.538997
C	4.862176	-1.345443	-1.016903
C	4.193285	-0.310237	-1.539603
C	4.489171	-1.979240	0.245197
C	4.028777	-1.286636	1.292197
O	3.020389	0.161972	-1.028203
O	3.986188	0.080164	1.309797
P	2.856095	0.897274	0.450897
O	1.478191	0.460085	0.908597
O	3.209907	2.330471	0.400397
C	-3.796626	-1.612671	0.968797
C	-5.133928	-1.823660	0.632197
C	-5.590225	-1.525856	-0.646003
C	-4.699721	-1.021963	-1.592803
C	-3.366219	-0.819874	-1.260103
H	-3.465228	-1.861074	1.972297
H	-5.815931	-2.220654	1.377397
H	-6.631726	-1.686247	-0.905503
H	-2.668316	-0.432880	-1.997203
H	-5.043519	-0.788760	-2.595503
C	-1.008840	-3.359794	-0.024103
C	-0.245349	-4.440900	-0.447003
C	0.962652	-4.226811	-1.108203
C	1.392063	-2.926514	-1.351103
C	0.625672	-1.840708	-0.934803
H	1.001181	-0.848011	-1.140703
H	-1.952542	-3.537286	0.484897
H	-0.596058	-5.450998	-0.260203
H	1.562245	-5.071316	-1.433803
H	2.333165	-2.735422	-1.858403
C	0.109815	3.248097	-0.064703
C	0.454325	4.496294	-0.570303
C	-0.525568	5.335802	-1.096803
C	-1.856071	4.923513	-1.118803

C	-2.203782	3.670716	-0.621803
H	-3.240684	3.343825	-0.647603
H	0.891609	2.624190	0.356097
H	-2.624066	5.574319	-1.524803
H	4.491789	0.177260	-2.463503
H	5.723273	-1.718850	-1.563403
H	3.729573	-1.751134	2.227597
H	4.599462	-3.054441	0.353697
H	1.497428	4.794385	-0.541603
H	-0.254960	6.312200	-1.486903

TS-B-11

M06-2X/def2-TZVPP-SMD(toluene) Energy = -1741.54620090

Number of Imaginary Frequencies = 1

Lowest Frequency = 400.0097i

M06-2X/6-31G* Geometry

C	-1.313102	-0.789796	1.936801
C	-1.862602	-0.480396	0.249301
C	-1.315401	0.507604	2.501701
H	-0.328602	-1.200997	1.708001
H	-2.018902	-1.516096	2.335101
C	-0.371501	1.455403	2.058701
H	-2.192001	0.856504	3.046201
N	-0.949301	0.466303	-0.221299
C	-1.742803	-1.854596	-0.387399
C	-3.296102	0.038104	0.233301
C	-0.955101	1.717403	0.375301
C	-0.044200	2.768103	-0.187199
H	-1.967401	2.098904	0.506701
H	0.012498	0.083903	-0.322699
H	0.625299	1.072503	1.833001
H	-0.398901	2.443203	2.514201
C	5.836398	-0.318400	0.164501
C	4.954698	0.005101	-0.786599
C	5.437398	-0.673900	1.523301
C	4.339498	-1.386099	1.800401
O	3.619898	0.160101	-0.526199
O	3.553797	-1.965399	0.847201
P	2.634098	-1.130798	-0.224699
O	1.459098	-0.507698	0.503401
O	2.416997	-1.971198	-1.423199
C	-4.184302	-0.047795	1.304101
C	-5.497901	0.403605	1.175101
C	-5.936801	0.948906	-0.025299
C	-5.056901	1.033205	-1.103399
C	-3.751201	0.576005	-0.977399
H	-3.871002	-0.480695	2.248901
H	-6.174902	0.325906	2.019901
H	-6.957801	1.303206	-0.123599
H	-3.065201	0.632704	-1.817799
H	-5.389601	1.452105	-2.047899
C	-2.746603	-2.801696	-0.151499
C	-2.635004	-4.088096	-0.664799
C	-1.515604	-4.448796	-1.413299
C	-0.517303	-3.510697	-1.651799
C	-0.632803	-2.216997	-1.151099
H	0.180298	-1.537097	-1.366599
H	-3.623203	-2.532595	0.431301
H	-3.423404	-4.810096	-0.476099
H	-1.424204	-5.457696	-1.803599
H	0.378797	-3.760997	-2.209999
C	1.305100	2.516202	-0.448799
C	2.101500	3.523402	-0.981699

C	1.566901	4.784102	-1.242299
C	0.225801	5.039503	-0.968899
C	-0.577800	4.033403	-0.440699
H	-1.627200	4.229004	-0.233499
H	1.737799	1.543502	-0.233499
H	-0.196899	6.019203	-1.168399
H	5.237198	0.240700	-1.808599
H	6.891298	-0.311400	-0.093499
H	4.043398	-1.636199	2.815501
H	6.061098	-0.363300	2.356401
H	3.146400	3.312901	-1.186299
H	2.194901	5.567602	-1.655099

TS-B-12

M06-2X/def2-TZVPP-SMD(toluene) Energy = -1741.54620013

Number of Imaginary Frequencies = 1

Lowest Frequency = 400.0156i

M06-2X/6-31G* Geometry

C	-1.313188	-0.789900	1.936699
C	-1.862689	-0.480403	0.249299
C	-1.315393	0.507499	2.501699
H	-0.328686	-1.201096	1.707899
H	-2.018885	-1.516203	2.334999
C	-0.371497	1.455303	2.058799
H	-2.192094	0.856396	3.046199
N	-0.949293	0.466201	-0.221301
C	-3.296091	0.038191	0.233299
C	-1.742883	-1.854502	-0.387401
C	-0.955098	1.717301	0.375299
C	-0.044202	2.768105	-0.187101
H	-1.967300	2.098897	0.506799
H	0.012509	0.083805	-0.322601
H	0.625305	1.072308	1.833099
H	-0.398901	2.443103	2.514299
C	5.836410	-0.318371	0.164299
C	4.954709	0.005126	-0.786701
C	5.437512	-0.673872	1.523199
C	4.339715	-1.386077	1.800399
O	3.619908	0.160120	-0.526201
O	3.553817	-1.965380	0.847299
P	2.634214	-1.130884	-0.224601
O	1.459111	-0.507689	0.503399
O	2.417017	-1.971285	-1.423101
C	-2.746779	-2.801606	-0.151701
C	-2.635274	-4.088006	-0.665001
C	-1.515872	-4.448801	-1.413401
C	-0.517376	-3.510697	-1.651801
C	-0.632782	-2.217098	-1.151001
H	-3.623480	-2.532410	0.430899
H	-3.423771	-4.809909	-0.476401
H	-1.424468	-5.457701	-1.803701
H	0.180315	-1.537294	-1.366301
H	0.378725	-3.761093	-2.209901
C	-4.184291	-0.047812	1.304099
C	-5.497993	0.403482	1.175099
C	-5.936695	0.949080	-0.025201
C	-5.056895	1.033584	-1.103301
C	-3.751193	0.576289	-0.977301
H	-3.065194	0.633192	-1.817601
H	-3.871089	-0.481011	2.248899
H	-6.174892	0.325779	2.019899
H	-6.957796	1.303376	-0.123501
H	-5.389497	1.452683	-2.047601

C	1.305199	2.516210	-0.448501
C	2.101594	3.523414	-0.981501
C	1.566989	4.784011	-1.242401
C	0.225788	5.039406	-0.969201
C	-0.577808	4.033303	-0.440801
H	-1.627208	4.228898	-0.233801
H	1.738003	1.543612	-0.233201
H	-0.196916	6.019004	-1.168801
H	5.237108	0.240727	-1.808701
H	6.891310	-0.311366	-0.093701
H	4.043616	-1.636078	2.815599
H	6.061311	-0.363170	2.356199
H	3.146495	3.312918	-1.186001
H	2.194986	5.567414	-1.655201

TS-G

M06-2X/def2-TZVPP-SMD(toluene) Energy = -1741.54607357

Number of Imaginary Frequencies = 1

Lowest Frequency = 314.5900i

M06-2X/6-31G* Geometry

C	-0.042089	-0.968203	1.344702
C	-1.263489	-0.906718	0.039602
C	-0.407103	0.148493	2.133102
H	0.866310	-0.848191	0.756502
H	-0.139076	-1.955104	1.792302
C	-0.231019	1.455195	1.620802
H	-1.068101	0.003185	2.987302
N	-1.109105	0.373184	-0.514498
C	-0.839275	-2.039913	-0.886798
C	-2.662187	-1.110935	0.611502
C	-1.402619	1.461180	0.310002
C	-1.343236	2.831881	-0.303198
H	-2.357817	1.315968	0.813302
H	-0.233907	0.496595	-1.041198
H	0.691579	1.618707	1.061902
H	-0.528829	2.277191	2.269602
C	4.942618	-1.498940	1.127802
C	4.159222	-1.799550	0.082602
C	4.945903	-0.332340	2.008202
C	4.032991	0.638948	2.082102
O	3.138113	-1.086063	-0.466098
O	2.891390	0.699634	1.326102
P	3.016092	0.564636	-0.327398
O	1.609889	0.832018	-0.798098
O	4.219784	1.245751	-0.832798
C	-2.921479	-1.753739	1.821202
C	-4.232476	-1.980255	2.238202
C	-5.300581	-1.567568	1.449702
C	-5.051089	-0.931165	0.235302
C	-3.743892	-0.710549	-0.182798
H	-2.106475	-2.100528	2.448602
H	-4.413170	-2.482257	3.183402
H	-6.320579	-1.741881	1.776702
H	-3.545998	-0.221646	-1.132398
H	-5.876193	-0.608576	-0.391698
C	-1.600561	-3.209222	-0.977598
C	-1.197648	-4.246817	-1.814398
C	-0.030149	-4.132802	-2.561598
C	0.736036	-2.973893	-2.465098
C	0.339423	-1.932998	-1.633798
H	0.972712	-1.053890	-1.555898
H	-2.514759	-3.317634	-0.404498
H	-1.802736	-5.145825	-1.878098

H	0.284361	-4.944599	-3.210198
H	1.657235	-2.873181	-3.030098
C	-0.242942	3.277695	-1.041998
C	-0.259258	4.557995	-1.586998
C	-1.353068	5.399381	-1.392798
C	-2.443263	4.959167	-0.647898
C	-2.436247	3.678367	-0.104098
H	-3.289543	3.330357	0.473502
H	0.622066	2.631706	-1.179598
H	-3.298571	5.608557	-0.490598
H	4.287934	-2.743648	-0.437998
H	5.693127	-2.252131	1.347302
H	4.125281	1.466850	2.778002
H	5.787102	-0.247230	2.689002
H	0.595438	4.900405	-2.161598
H	-1.353581	6.398081	-1.818398

TS-G-2

M06-2X/def2-TZVPP-SMD(toluene) Energy = -1741.54607026

Number of Imaginary Frequencies = 1

Lowest Frequency = 314.5752i

M06-2X/6-31G* Geometry

C	-0.041902	-0.968198	1.344495
C	-1.263302	-0.906700	0.039495
C	-0.406804	0.148401	2.132995
H	0.866398	-0.848097	0.756195
H	-0.138700	-1.955098	1.792095
C	-0.230806	1.455102	1.620795
H	-1.067703	0.003000	2.987295
N	-1.109104	0.373200	-0.514505
C	-0.839200	-2.039799	-0.887005
C	-2.661902	-1.111002	0.611595
C	-1.402606	1.461200	0.310095
C	-1.343408	2.831900	-0.303205
H	-2.357705	1.315898	0.813395
H	-0.234004	0.496802	-1.041405
H	0.691694	1.618803	1.061795
H	-0.528707	2.277101	2.269595
C	4.945697	-0.332190	2.008295
C	4.033096	0.639308	2.081895
C	4.942099	-1.499090	1.128295
C	4.158599	-1.799792	0.083095
O	2.891396	0.700006	1.325995
O	3.137798	-1.086093	-0.465905
P	3.016096	0.564607	-0.327605
O	1.609895	0.832105	-0.798205
O	4.219895	1.245508	-0.833005
C	-2.921101	-1.754002	1.821295
C	-4.231900	-1.980604	2.238495
C	-5.300201	-1.567806	1.450095
C	-5.050902	-0.931306	0.235795
C	-3.743802	-0.710604	-0.182405
H	-2.106000	-2.100801	2.448595
H	-4.412500	-2.482705	3.183595
H	-6.320201	-1.742208	1.777295
H	-3.546003	-0.221603	-1.132105
H	-5.876102	-0.608607	-0.391105
C	-1.600498	-3.209200	-0.977705
C	-1.197597	-4.246700	-1.814705
C	-0.030197	-4.132598	-2.562105
C	0.735901	-2.973597	-2.465605
C	0.339400	-1.932797	-1.634105
H	0.972698	-1.053696	-1.556205

H	-2.514498	-3.317702	-0.404505
H	-1.802595	-5.145701	-1.878305
H	0.284204	-4.944298	-3.210805
H	1.657001	-2.872895	-3.030805
C	-0.243008	3.277802	-1.041905
C	-0.259410	4.558102	-1.586905
C	-1.353412	5.399400	-1.392705
C	-2.443511	4.959098	-0.647805
C	-2.436509	3.678198	-0.104105
H	-3.289708	3.330197	0.473495
H	0.621893	2.631903	-1.179505
H	-3.298912	5.608397	-0.490605
H	4.125494	1.467408	2.777495
H	5.786897	-0.247089	2.688995
H	4.287001	-2.744091	-0.437105
H	5.692300	-2.252489	1.348095
H	0.595189	4.900603	-2.161505
H	-1.353913	6.398100	-1.818305

TS-H-

M06-2X/def2-TZVPP-SMD(toluene) Energy = -1741.54599221

Number of Imaginary Frequencies = 1

Lowest Frequency = 323.9716i

M06-2X/6-31G* Geometry

C	-1.581305	-0.566207	2.147707
C	-1.742705	-0.455308	0.399507
C	-1.748107	0.785892	2.553807
H	-0.558205	-0.932106	2.240007
H	-2.337004	-1.281008	2.466907
C	-0.724008	1.707794	2.270107
H	-2.740507	1.149591	2.819807
N	-0.749106	0.461194	0.016007
C	-3.139506	0.041391	0.034007
C	-1.467603	-1.867307	-0.107393
C	-0.833708	1.763094	0.480007
C	0.231591	2.699795	-0.021093
H	-1.829808	2.177792	0.326407
H	0.204694	0.093795	-0.089493
H	0.288493	1.312695	2.373807
H	-0.872909	2.739394	2.583107
C	3.946195	-0.830700	-1.889993
C	2.907394	-0.044602	-1.601793
C	4.369497	-2.026500	-1.163693
C	4.013497	-2.498500	0.040907
O	2.061095	-0.272203	-0.547793
O	3.152197	-1.990501	0.965607
P	2.713395	-0.400502	0.994207
O	1.486995	-0.338104	1.857907
O	3.873694	0.504899	1.123007
C	-2.435003	-2.581908	-0.818993
C	-2.148401	-3.856608	-1.302093
C	-0.899300	-4.427906	-1.081993
C	0.062599	-3.723105	-0.362193
C	-0.220903	-2.455906	0.132307
H	-3.411503	-2.150210	-1.008793
H	-2.907600	-4.399409	-1.856593
H	-0.678299	-5.419306	-1.465093
H	0.530797	-1.933905	0.716707
H	1.042299	-4.151704	-0.176893
C	-4.263606	-0.167011	0.833207
C	-5.527106	0.231388	0.400507
C	-5.684707	0.840588	-0.839793
C	-4.569807	1.044189	-1.649793

C	-3.310007	0.643291	-1.218693
H	-2.440307	0.790792	-1.853293
H	-4.172205	-0.653911	1.798907
H	-6.388706	0.060687	1.038207
H	-6.668907	1.151986	-1.174593
H	-4.680108	1.512089	-2.622993
C	1.554091	2.640997	0.415607
C	2.521890	3.445498	-0.177993
C	2.166189	4.336197	-1.187693
C	0.838789	4.421796	-1.604993
C	-0.125710	3.604094	-1.025293
H	-1.158410	3.654193	-1.363393
H	1.853092	1.972697	1.213507
H	0.554788	5.119895	-2.386293
H	2.648493	0.836398	-2.182093
H	4.534295	-0.559200	-2.760993
H	4.428898	-3.437700	0.393107
H	5.097597	-2.648399	-1.675693
H	3.550190	3.348199	0.154507
H	2.920388	4.966498	-1.648893

TS-B-13

M06-2X/def2-TZVPP-SMD(toluene) Energy = -1741.54587414

Number of Imaginary Frequencies = 1

Lowest Frequency = 399.4576i

M06-2X/6-31G* Geometry

C	-1.261804	-0.768499	1.950900
C	-1.840603	-0.489598	0.266800
C	-1.265301	0.537601	2.494500
H	-0.277705	-1.175901	1.713500
H	-1.956506	-1.492097	2.372700
C	-0.336699	1.486399	2.020600
H	-2.135000	0.888503	3.048800
N	-0.946701	0.459000	-0.233400
C	-1.709006	-1.869198	-0.355700
C	-3.281702	0.007106	0.265300
C	-0.951498	1.718400	0.343400
C	-0.053496	2.763498	-0.249300
H	-1.963097	2.098003	0.486900
H	0.016598	0.076098	-0.334500
H	0.659201	1.107296	1.783900
H	-0.364896	2.480299	2.462800
C	5.723195	-1.190115	0.930600
C	4.811993	-2.151713	0.749100
C	5.366398	0.216685	1.091000
C	4.368600	0.793488	0.413300
O	3.467093	-1.925010	0.833800
O	3.681198	0.163089	-0.586500
P	2.628495	-1.076708	-0.291700
O	1.447697	-0.506205	0.469500
O	2.420494	-1.812508	-1.558700
C	-4.150802	-0.068492	1.352300
C	-5.472601	0.362111	1.235800
C	-5.938500	0.876512	0.032100
C	-5.077600	0.950910	-1.062000
C	-3.763801	0.514207	-0.948400
H	-3.815803	-0.476193	2.301000
H	-6.134401	0.293012	2.093300
H	-6.965899	1.214714	-0.056500
H	-3.092601	0.562505	-1.801200
H	-5.431399	1.345811	-2.009100
C	-2.665609	-2.843696	-0.047100
C	-2.545012	-4.133296	-0.549500

C	-1.463213	-4.468799	-1.362200
C	-0.513210	-3.502901	-1.675100
C	-0.637407	-2.206001	-1.184000
H	0.135094	-1.501002	-1.462400
H	-3.513208	-2.592194	0.584800
H	-3.296413	-4.876994	-0.303000
H	-1.363815	-5.479499	-1.745800
H	0.350389	-3.734903	-2.289500
C	1.254904	2.476095	-0.647800
C	2.041306	3.475993	-1.208500
C	1.539909	4.768494	-1.356700
C	0.242710	5.060197	-0.944500
C	-0.552493	4.059099	-0.393500
H	-1.570092	4.283702	-0.082700
H	1.662901	1.479494	-0.513400
H	-0.154688	6.063898	-1.057400
H	5.071690	-3.196814	0.608800
H	6.769094	-1.479718	0.965700
H	4.084002	1.834588	0.552300
H	5.934200	0.832784	1.782200
H	3.049205	3.234091	-1.532200
H	2.158811	5.546293	-1.792900

TS-B-14

M06-2X/def2-TZVPP-SMD(toluene) Energy = -1741.54587202

Number of Imaginary Frequencies = 1

Lowest Frequency = 399.4515i

M06-2X/6-31G* Geometry

C	-1.261797	-0.768507	1.950898
C	-1.840598	-0.489608	0.266798
C	-1.265199	0.537593	2.494498
H	-0.277697	-1.175905	1.713398
H	-1.956496	-1.492108	2.372698
C	-0.336701	1.486395	2.020598
H	-2.135000	0.888492	3.048798
N	-0.946699	0.458994	-0.233402
C	-3.281698	0.007090	0.265298
C	-1.708996	-1.869208	-0.355702
C	-0.951501	1.718394	0.343398
C	-0.053503	2.763495	-0.249302
H	-1.963102	2.097992	0.486998
H	0.016602	0.076095	-0.334502
H	0.659200	1.107296	1.783898
H	-0.364802	2.480294	2.462798
C	5.723203	-1.190096	0.930598
C	4.812005	-2.151698	0.749098
C	5.366401	0.216703	1.090998
C	4.368600	0.793502	0.413298
O	3.467105	-1.925100	0.833798
O	3.681201	0.163101	-0.586502
P	2.628503	-1.076701	-0.291702
O	1.447702	-0.506203	0.469498
O	2.420504	-1.812501	-1.558702
C	-2.665594	-2.843609	-0.047202
C	-2.545092	-4.133309	-0.549502
C	-1.463192	-4.468807	-1.362202
C	-0.513193	-3.502906	-1.675102
C	-0.637495	-2.206006	-1.184002
H	-3.513294	-2.592110	0.584798
H	-3.296491	-4.877010	-0.303102
H	-1.363890	-5.479507	-1.745902
H	0.135104	-1.501005	-1.462402
H	0.350407	-3.734904	-2.289402

C	-4.150798	-0.068511	1.352398
C	-5.472599	0.362087	1.235898
C	-5.938500	0.876586	0.032098
C	-5.077600	0.950887	-1.061902
C	-3.763799	0.514189	-0.948402
H	-3.092699	0.562490	-1.801202
H	-3.815798	-0.476211	2.300998
H	-6.134399	0.292986	2.093398
H	-6.965900	1.214784	-0.056402
H	-5.431400	1.345887	-2.009002
C	1.254898	2.476097	-0.647802
C	2.041296	3.475998	-1.208502
C	1.539894	4.768497	-1.356702
C	0.242694	5.060195	-0.944602
C	-0.552505	4.059094	-0.393502
H	-1.570105	4.283693	-0.082802
H	1.662899	1.479498	-0.513402
H	-0.154708	6.063895	-1.057502
H	5.071707	-3.196797	0.608798
H	6.769104	-1.479695	0.965798
H	4.083999	1.834601	0.552298
H	5.934200	0.832804	1.782198
H	3.049197	3.234100	-1.532202
H	2.158793	5.546298	-1.793002

TS-B-15

M06-2X/def2-TZVPP-SMD(toluene) Energy = -1741.54587033

Number of Imaginary Frequencies = 1

Lowest Frequency = 399.4311i

M06-2X/6-31G* Geometry

C	-1.261799	-0.768511	1.950908
C	-1.840599	-0.489613	0.266808
C	-1.265302	0.537589	2.494608
H	-0.277697	-1.175908	1.713508
H	-1.956596	-1.492113	2.372708
C	-0.336805	1.486392	2.020608
H	-2.135103	0.888486	3.048808
N	-0.946702	0.458990	-0.233392
C	-1.708995	-1.869213	-0.355692
C	-3.281701	0.006983	0.265208
C	-0.951606	1.718390	0.343408
C	-0.053509	2.763492	-0.249292
H	-1.963207	2.097987	0.486908
H	0.016599	0.076093	-0.334392
H	0.659096	1.107295	1.784008
H	-0.364908	2.480291	2.462808
C	5.723203	-1.190090	0.930508
C	4.812006	-2.151693	0.749008
C	5.366499	0.216709	1.090908
C	4.368697	0.793506	0.413308
O	3.467105	-1.924997	0.833808
O	3.681099	0.163204	-0.586492
P	2.628502	-1.076700	-0.291692
O	1.447701	-0.506103	0.469508
O	2.420505	-1.812500	-1.558692
C	-4.150801	-0.068520	1.352308
C	-5.472602	0.362076	1.235808
C	-5.938503	0.876475	0.032008
C	-5.077604	0.950777	-1.062092
C	-3.763802	0.514081	-0.948392
H	-3.815799	-0.476219	2.301008
H	-6.134502	0.292874	2.093308
H	-6.965904	1.214572	-0.056592

H	-3.092603	0.562383	-1.801192
H	-5.431405	1.345676	-2.009192
C	-2.665492	-2.843715	-0.047092
C	-2.544888	-4.133315	-0.549392
C	-1.463087	-4.468812	-1.362192
C	-0.513090	-3.502809	-1.675092
C	-0.637394	-2.206009	-1.183992
H	0.135004	-1.501007	-1.462492
H	-3.513093	-2.592218	0.584908
H	-3.296186	-4.877117	-0.302892
H	-1.363684	-5.479512	-1.745792
H	0.350510	-3.734806	-2.289492
C	-0.552513	4.059091	-0.393492
C	0.242584	5.060193	-0.944492
C	1.539785	4.768597	-1.356592
C	2.041189	3.476099	-1.208492
C	1.254892	2.476096	-0.647792
H	1.662895	1.479498	-0.513292
H	-1.570214	4.283688	-0.082692
H	3.049189	3.234202	-1.532092
H	5.071709	-3.196792	0.608608
H	6.769104	-1.479687	0.965508
H	4.084094	1.834605	0.552308
H	5.934297	0.832810	1.782108
H	-0.154819	6.063892	-1.057392
H	2.158783	5.546299	-1.792892

TS-B-16

M06-2X/def2-TZVPP-SMD(toluene) Energy = -1741.54587002

Number of Imaginary Frequencies = 1

Lowest Frequency = 399.4269i

M06-2X/6-31G* Geometry

C	-1.261789	-0.768512	1.950900
C	-1.840590	-0.489614	0.266800
C	-1.265193	0.537588	2.494500
H	-0.277588	-1.176009	1.713400
H	-1.956487	-1.492114	2.372700
C	-0.336695	1.486290	2.020600
H	-2.134894	0.888486	3.048800
N	-0.946693	0.458989	-0.233400
C	-3.281691	0.007082	0.265300
C	-1.709086	-1.869213	-0.355700
C	-0.951496	1.718389	0.343400
C	-0.053399	2.763491	-0.249300
H	-1.963097	2.097986	0.487000
H	0.016608	0.076091	-0.334500
H	0.659206	1.107293	1.783900
H	-0.364798	2.480290	2.462800
C	5.366408	0.216706	1.091100
C	4.368607	0.793503	0.413300
C	5.723212	-1.190093	0.930700
C	4.812014	-2.151696	0.749100
O	3.681208	0.163101	-0.586500
O	3.467114	-1.925099	0.833800
P	2.628512	-1.076702	-0.291700
O	1.447710	-0.506205	0.469500
O	2.420614	-1.812502	-1.558800
C	-2.665684	-2.843616	-0.047200
C	-2.545180	-4.133216	-0.549700
C	-1.463279	-4.468813	-1.362300
C	-0.513182	-3.502910	-1.675100
C	-0.637485	-2.206010	-1.184000
H	-3.513284	-2.592118	0.584700

H	-3.296578	-4.876918	-0.303200
H	-1.363977	-5.479512	-1.746000
H	0.135113	-1.501108	-1.462300
H	0.350419	-3.734908	-2.289500
C	-4.150791	-0.068520	1.352400
C	-5.472592	0.362077	1.236000
C	-5.938494	0.876575	0.032200
C	-5.077594	0.950978	-1.061900
C	-3.763793	0.514281	-0.948300
H	-3.092693	0.562583	-1.801100
H	-3.815790	-0.476319	2.301000
H	-6.134392	0.292875	2.093500
H	-6.965895	1.214772	-0.056300
H	-5.431395	1.345977	-2.008900
C	1.254902	2.476095	-0.647800
C	2.041299	3.475997	-1.208500
C	1.539896	4.768495	-1.356700
C	0.242595	5.060192	-0.944700
C	-0.552502	4.059090	-0.393600
H	-1.570103	4.283687	-0.082900
H	1.662905	1.479496	-0.513300
H	-0.154808	6.063791	-1.057600
H	4.084004	1.834602	0.552300
H	5.934106	0.832807	1.782300
H	5.071717	-3.196795	0.608800
H	6.769113	-1.479690	0.965800
H	3.049300	3.234100	-1.532100
H	2.158794	5.546197	-1.793000

TS-G-3

M06-2X/def2-TZVPP-SMD(toluene) Energy = -1741.54572953

Number of Imaginary Frequencies = 1

Lowest Frequency = 313.6269i

M06-2X/6-31G* Geometry

C	-0.800296	-0.972497	1.442807
C	-1.756996	-0.283197	0.102407
C	-0.338196	0.195803	2.093407
H	-0.037796	-1.507097	0.877707
H	-1.482796	-1.620497	1.988607
C	0.618804	1.011903	1.447807
H	-0.903596	0.603503	2.931007
N	-0.836296	0.514003	-0.596093
C	-2.222296	-1.514897	-0.668093
C	-2.920196	0.537903	0.648207
C	-0.304796	1.615403	0.076307
C	0.627503	2.511003	-0.690293
H	-1.094996	2.202903	0.542507
H	-0.123196	-0.027597	-1.102593
H	1.413704	0.474803	0.928507
H	0.948104	1.901103	1.983207
C	4.247804	-0.984796	2.463307
C	3.349504	-1.945296	2.217907
C	4.343404	0.230404	1.660207
C	4.160404	0.244804	0.332507
O	2.352604	-1.798796	1.297407
O	3.979004	-0.878596	-0.414793
P	2.616804	-1.809096	-0.345993
O	1.453604	-0.984197	-0.847393
O	2.927404	-3.149796	-0.867493
C	-3.485396	0.335203	1.906907
C	-4.607496	1.059003	2.306507
C	-5.179996	1.994103	1.451107
C	-4.627296	2.197503	0.188407

C	-3.511396	1.471203	-0.211893
H	-3.068296	-0.401197	2.586707
H	-5.032696	0.886103	3.290107
H	-6.052397	2.558703	1.764007
H	-3.084296	1.620203	-1.199593
H	-5.068697	2.920003	-0.490793
C	-3.573296	-1.875497	-0.679893
C	-3.994396	-3.003897	-1.379393
C	-3.074696	-3.785897	-2.068993
C	-1.726796	-3.435597	-2.052093
C	-1.297196	-2.312697	-1.353693
H	-0.235296	-2.075297	-1.338793
H	-4.308496	-1.278297	-0.152393
H	-5.047596	-3.266797	-1.381593
H	-3.404196	-4.666597	-2.611593
H	-0.994196	-4.041297	-2.575493
C	1.680604	2.014403	-1.465593
C	2.504503	2.902604	-2.150893
C	2.299103	4.278104	-2.059993
C	1.258503	4.772403	-1.279193
C	0.426403	3.889803	-0.596993
H	-0.390897	4.275203	0.008207
H	1.859304	0.941903	-1.523293
H	1.090703	5.842003	-1.202393
H	3.298004	-2.869296	2.786807
H	4.935604	-1.126996	3.291607
H	4.235504	1.158004	-0.253993
H	4.608704	1.167204	2.142507
H	3.316303	2.512704	-2.757493
H	2.949803	4.962404	-2.595393

TS-B-17

M06-2X/def2-TZVPP-SMD(toluene) Energy = -1741.54548761

Number of Imaginary Frequencies = 1

Lowest Frequency = 378.3898i

M06-2X/6-31G* Geometry

C	-1.490294	-0.633208	2.009802
C	-1.929693	-0.317408	0.294102
C	-1.302293	0.679092	2.502202
H	-0.572694	-1.201808	1.858902
H	-2.315194	-1.216608	2.412402
C	-0.183993	1.422992	2.066902
H	-2.137093	1.201792	2.968402
N	-0.831393	0.407392	-0.191998
C	-3.225093	0.481593	0.221502
C	-2.068294	-1.712808	-0.303098
C	-0.604293	1.667892	0.350802
C	0.502207	2.498792	-0.232198
H	-1.526893	2.243592	0.402902
H	0.031107	-0.152408	-0.291898
H	0.744107	0.861992	1.941702
H	-0.071093	2.429692	2.464702
C	5.036607	0.275890	0.788402
C	4.303906	-0.470410	1.621702
C	5.274207	-0.094310	-0.604398
C	4.364706	-0.695810	-1.383098
O	3.803206	-1.691909	1.260302
O	3.068306	-0.913409	-1.040298
P	2.497006	-1.755109	0.271702
O	1.419806	-0.843409	0.827902
O	2.191806	-3.158309	-0.070798
C	-3.288794	-2.157407	-0.822198
C	-3.384394	-3.426107	-1.389598

C	-2.272395	-4.261608	-1.445498
C	-1.058494	-3.827208	-0.918798
C	-0.962694	-2.567408	-0.341998
H	-4.166694	-1.521407	-0.798698
H	-4.336594	-3.756807	-1.792698
H	-2.354595	-5.247208	-1.893498
H	-0.009594	-2.275108	0.081002
H	-0.167295	-4.446508	-0.940298
C	-4.207493	0.445293	1.210602
C	-5.414293	1.120693	1.038002
C	-5.655693	1.839093	-0.127998
C	-4.683893	1.873693	-1.125798
C	-3.481693	1.196093	-0.955098
H	-2.727193	1.211693	-1.736698
H	-4.051093	-0.121907	2.122702
H	-6.166093	1.079794	1.819802
H	-6.595293	2.365694	-0.260698
H	-4.862793	2.424793	-2.043598
C	1.802907	2.012691	-0.387098
C	2.778507	2.825891	-0.954598
C	2.470508	4.125091	-1.353698
C	1.178308	4.615991	-1.185398
C	0.196708	3.804192	-0.625098
H	-0.815192	4.183192	-0.500998
H	2.053707	1.006291	-0.066398
H	0.931908	5.627591	-1.492098
H	4.108007	-0.196009	2.654502
H	5.492707	1.180390	1.181302
H	4.582506	-0.980310	-2.408798
H	6.244007	0.117690	-1.044698
H	3.781507	2.429291	-1.082198
H	3.236808	4.756091	-1.793598

TS-H-2

M06-2X/def2-TZVPP-SMD(toluene) Energy = -1741.54548562

Number of Imaginary Frequencies = 1

Lowest Frequency = 378.6102i

M06-2X/6-31G* Geometry

C	-1.793198	-0.525496	2.091994
C	-1.889597	-0.292696	0.319594
C	-1.695094	0.804004	2.570494
H	-0.871000	-1.108499	2.128294
H	-2.686000	-1.086993	2.359394
C	-0.522491	1.540100	2.312794
H	-2.595192	1.336807	2.875094
N	-0.747395	0.452300	0.017594
C	-3.177195	0.429708	-0.062606
C	-1.863102	-1.717296	-0.209306
C	-0.653391	1.735900	0.530494
C	0.547912	2.540696	0.124194
H	-1.578189	2.297003	0.394394
H	0.129403	-0.088102	0.146894
H	0.408407	0.972997	2.356894
H	-0.467888	2.556199	2.697994
C	5.313401	-0.872520	-0.461406
C	4.895900	-0.985718	0.800294
C	4.511102	-0.399717	-1.586106
C	3.178603	-0.319813	-1.727606
O	3.632202	-0.626614	1.200594
O	2.178701	-0.679709	-0.885806
P	2.355399	-1.469410	0.583694
O	1.157401	-0.951706	1.339394
O	2.667594	-2.893611	0.367294

C	-2.974105	-2.538792	0.009294
C	-2.965009	-3.863692	-0.407306
C	-1.842111	-4.386596	-1.046106
C	-0.742508	-3.569400	-1.282206
C	-0.753904	-2.236900	-0.877806
H	-3.855603	-2.138689	0.503994
H	-3.834311	-4.488689	-0.229106
H	-1.827614	-5.425796	-1.359006
H	0.108198	-1.621802	-1.106406
H	0.144391	-3.960003	-1.769706
C	-4.287394	0.565312	0.769194
C	-5.445592	1.193416	0.310994
C	-5.504991	1.696516	-0.982806
C	-4.400791	1.561713	-1.823106
C	-3.250493	0.928609	-1.369606
H	-2.390794	0.815106	-2.024006
H	-4.270896	0.175212	1.782194
H	-6.299992	1.287619	0.973794
H	-6.405089	2.188519	-1.336906
H	-4.436690	1.946913	-2.837206
C	1.849611	2.097492	0.367294
C	2.932213	2.840588	-0.089906
C	2.722417	4.041189	-0.766006
C	1.425519	4.498793	-0.986306
C	0.339516	3.749397	-0.542806
H	-0.673983	4.097000	-0.728106
H	2.024308	1.172391	0.905594
H	1.257222	5.435994	-1.507406
H	5.524099	-1.349720	1.606594
H	6.344700	-1.141323	-0.667506
H	2.763704	0.096989	-2.640806
H	5.065404	-0.060119	-2.456206
H	3.936612	2.467885	0.085394
H	3.569019	4.622486	-1.118306

TS-H-3

M06-2X/def2-TZVPP-SMD(toluene) Energy = -1741.54548145

Number of Imaginary Frequencies = 1

Lowest Frequency = 378.5202i

M06-2X/6-31G* Geometry

C	-1.793203	-0.525404	2.092100
C	-1.889603	-0.292704	0.319700
C	-1.695105	0.803996	2.570500
H	-0.871002	-1.108403	2.128300
H	-2.686002	-1.086905	2.359400
C	-0.522506	1.540198	2.312700
H	-2.595306	1.336795	2.875000
N	-0.747404	0.452298	0.017600
C	-3.177204	0.429594	-0.062600
C	-1.863101	-1.717304	-0.209300
C	-0.653406	1.735998	0.530500
C	0.547892	2.540700	0.124100
H	-1.578307	2.296996	0.394300
H	0.129296	-0.088101	0.147000
H	0.408295	0.973099	2.356900
H	-0.468008	2.556298	2.698000
C	5.313398	-0.872593	-0.461200
C	4.895898	-0.985594	0.800400
C	4.511197	-0.399894	-1.586100
C	3.178697	-0.319996	-1.727700
O	3.632097	-0.626496	1.200600
O	2.178797	-0.679598	-0.885900
P	2.355398	-1.469398	0.583700

O	1.157298	-0.951599	1.339300
O	2.667701	-2.893497	0.367300
C	-2.974000	-2.538906	0.009400
C	-2.964898	-3.863706	-0.407300
C	-1.841997	-4.386604	-1.046100
C	-0.742398	-3.569402	-1.282200
C	-0.753800	-2.236802	-0.877900
H	-3.855601	-2.138807	0.504100
H	-3.834197	-4.488807	-0.229000
H	-1.827396	-5.425804	-1.359000
H	0.108199	-1.621701	-1.106500
H	0.144502	-3.959901	-1.769700
C	-4.287405	0.565092	0.769200
C	-5.445706	1.193191	0.311000
C	-5.505106	1.696390	-0.982800
C	-4.400806	1.561692	-1.823100
C	-3.250505	0.928694	-1.369600
H	-2.390705	0.815295	-2.023900
H	-4.271004	0.174992	1.782100
H	-6.300106	1.287189	0.973700
H	-6.405207	2.188289	-1.336900
H	-4.436707	1.946992	-2.837200
C	1.849593	2.097502	0.367300
C	2.932092	2.840603	-0.090000
C	2.722290	4.041303	-0.766100
C	1.425490	4.498801	-0.986300
C	0.339491	3.749399	-0.542800
H	-0.674010	4.097098	-0.728100
H	2.024295	1.172402	0.905600
H	1.257188	5.436101	-1.507300
H	5.524098	-1.349493	1.606800
H	6.344798	-1.141292	-0.667300
H	2.763896	0.096703	-2.640900
H	5.065596	-0.060494	-2.456200
H	3.936493	2.467905	0.085300
H	3.568889	4.622504	-1.118300

TS-B-18

M06-2X/def2-TZVPP-SMD(toluene) Energy = -1741.54538541

Number of Imaginary Frequencies = 1

Lowest Frequency = 363.8246i

M06-2X/6-31G* Geometry

C	-1.393603	-0.679304	2.117812
C	-1.593403	-0.606205	0.337712
C	-1.759510	0.629294	2.515212
H	-0.324402	-0.896798	2.152612
H	-2.029198	-1.499407	2.446212
C	-0.927916	1.715599	2.169112
H	-2.783311	0.831688	2.827912
N	-0.785809	0.467799	-0.046688
C	-3.057604	-0.395913	-0.034588
C	-1.084996	-1.965402	-0.115688
C	-1.147516	1.733597	0.396012
C	-0.323223	2.888802	-0.093488
H	-2.212817	1.921292	0.260312
H	0.225192	0.274905	0.112412
H	0.145785	1.523405	2.214112
H	-1.237222	2.705497	2.498812
C	3.424897	-0.718577	-2.131588
C	3.077991	0.369121	-1.429688
C	4.204303	-1.814073	-1.560588
C	4.038906	-2.234274	-0.300088
O	3.509190	0.611023	-0.159188

O	3.027203	-1.788080	0.495612
P	2.971295	-0.268480	1.143312
O	1.484393	0.000212	1.273612
O	3.911494	-0.074575	2.258112
C	-1.901790	-3.087807	0.063112
C	-1.456583	-4.350804	-0.305588
C	-0.187382	-4.510197	-0.859288
C	0.626212	-3.398093	-1.043088
C	0.181505	-2.130395	-0.677288
H	-2.896490	-2.973012	0.485212
H	-2.102878	-5.210808	-0.161088
H	0.162724	-5.497595	-1.143288
H	0.852901	-1.295692	-0.833088
H	1.622713	-3.497987	-1.463088
C	-4.132903	-0.590119	0.830912
C	-5.443904	-0.428826	0.382212
C	-5.694006	-0.067728	-0.936088
C	-4.624807	0.123978	-1.809988
C	-3.319706	-0.045115	-1.365188
H	-2.484407	0.096190	-2.045188
H	-3.966902	-0.882818	1.863012
H	-6.267403	-0.586731	1.071312
H	-6.714007	0.061367	-1.283188
H	-4.807709	0.401777	-2.843188
C	1.073278	2.866210	-0.045088
C	1.799572	3.945214	-0.536588
C	1.141066	5.057010	-1.060188
C	-0.250435	5.088202	-1.092488
C	-0.981429	4.005798	-0.609788
H	-2.068129	4.025392	-0.643988
H	1.591482	2.010812	0.378712
H	-0.768939	5.951899	-1.496288
H	2.491487	1.180117	-1.859488
H	3.132798	-0.760779	-3.177288
H	4.638210	-3.023471	0.145112
H	4.955706	-2.305469	-2.171288
H	2.884072	3.910620	-0.499488
H	1.711661	5.899613	-1.438188

TS-B-19

M06-2X/def2-TZVPP-SMD(toluene) Energy = -1741.54538316

Number of Imaginary Frequencies = 1

Lowest Frequency = 363.8079i

M06-2X/6-31G* Geometry

C	-1.393597	-0.679319	2.117798
C	-1.593398	-0.606222	0.337698
C	-1.759515	0.629276	2.515198
H	-0.324394	-0.896804	2.152598
H	-2.029185	-1.499528	2.446198
C	-0.927931	1.715588	2.169098
H	-2.783318	0.831662	2.827898
N	-0.785813	0.467790	-0.046702
C	-1.084979	-1.965414	-0.115702
C	-3.057601	-0.395942	-0.034602
C	-1.147531	1.733585	0.395998
C	-0.323247	2.888796	-0.093502
H	-2.212834	1.921370	0.260298
H	0.225190	0.274904	0.112398
H	0.145772	1.523403	2.214098
H	-1.237245	2.705483	2.498798
C	3.424904	-0.718551	-2.131602
C	3.077988	0.369144	-1.429602
C	4.204319	-1.814040	-1.560602

C	4.038925	-2.234242	-0.300102
O	3.509185	0.611050	-0.159202
O	3.027219	-1.788057	0.495598
P	2.971297	-0.268457	1.143298
O	1.484393	0.000122	1.273598
O	3.911494	-0.074544	2.258198
C	-4.132898	-0.590057	0.830898
C	-5.443901	-0.428776	0.382198
C	-5.694006	-0.067679	-0.936002
C	-4.624808	0.123936	-1.810002
C	-3.319706	-0.045146	-1.365202
H	-3.966894	-0.882855	1.862998
H	-6.267398	-0.586787	1.071298
H	-6.714007	0.061406	-1.283102
H	-2.484408	0.096166	-2.045202
H	-4.807712	0.401833	-2.843102
C	-1.901763	-3.087826	0.063098
C	-1.456545	-4.350820	-0.305602
C	-0.187443	-4.510202	-0.859302
C	0.626241	-3.398090	-1.043102
C	0.181523	-2.130497	-0.677202
H	0.852912	-1.295687	-0.833102
H	-2.896565	-2.972940	0.485198
H	-2.102933	-5.210829	-0.161102
H	0.162771	-5.497597	-1.143302
H	1.622743	-3.497976	-1.463102
C	1.073253	2.866216	-0.045002
C	1.799538	3.945226	-0.536602
C	1.141022	5.057017	-1.060202
C	-0.250378	5.088197	-1.092502
C	-0.981463	4.005787	-0.609802
H	-2.068063	4.025372	-0.644002
H	1.591465	2.010823	0.378798
H	-0.768990	5.951890	-1.496302
H	2.491477	1.180136	-1.859502
H	3.132804	-0.760755	-3.177302
H	4.638236	-3.023434	0.145098
H	4.955726	-2.305429	-2.171302
H	2.884138	3.910641	-0.499502
H	1.711610	5.899625	-1.438202

TS-B-20

M06-2X/def2-TZVPP-SMD(toluene) Energy = -1741.54537048

Number of Imaginary Frequencies = 1

Lowest Frequency = 331.5026i

M06-2X/6-31G* Geometry

C	-1.232897	-0.685501	2.126698
C	-1.585797	-0.635101	0.375698
C	-1.597099	0.622999	2.527598
H	-0.158197	-0.869300	2.094398
H	-1.817896	-1.515302	2.517598
C	-0.805000	1.719300	2.115598
H	-2.604199	0.808198	2.900698
N	-0.799798	0.430000	-0.092702
C	-1.128296	-1.997801	-0.131502
C	-3.072398	-0.393403	0.140298
C	-1.110500	1.707099	0.372398
C	-0.331401	2.851300	-0.209802
H	-2.180300	1.898298	0.300598
H	0.212302	0.233001	-0.077502
H	0.273900	1.546401	2.117198
H	-1.121501	2.706699	2.446998
C	4.103204	-2.042195	-1.392802

C	4.145504	-2.224495	-0.067002
C	3.199603	-1.090196	-2.033502
C	2.917802	0.104503	-1.499502
O	3.244604	-1.671896	0.792498
O	3.521601	0.568904	-0.365302
P	3.107702	-0.049396	1.114998
O	1.610902	0.143602	1.266798
O	4.079002	0.418505	2.115798
C	-4.064897	-0.728304	1.060798
C	-5.412397	-0.567505	0.742098
C	-5.784598	-0.071606	-0.502602
C	-4.800098	0.257995	-1.431902
C	-3.456498	0.092697	-1.115502
H	-3.802297	-1.132804	2.033198
H	-6.169697	-0.834206	1.472398
H	-6.833898	0.054993	-0.748802
H	-2.687098	0.339298	-1.841802
H	-5.077799	0.640395	-2.409102
C	-2.048895	-2.925902	-0.628002
C	-1.609694	-4.155001	-1.114202
C	-0.254493	-4.469900	-1.111102
C	0.663706	-3.552999	-0.604802
C	0.230405	-2.329399	-0.108002
H	0.964704	-1.648499	0.310698
H	-3.108495	-2.696703	-0.649802
H	-2.334993	-4.864302	-1.500702
H	0.083008	-5.427599	-1.495402
H	1.726506	-3.775898	-0.587702
C	1.064799	2.850302	-0.254302
C	1.739298	3.915502	-0.841102
C	1.029497	4.993301	-1.368102
C	-0.361503	5.004400	-1.308302
C	-1.040602	3.935199	-0.730602
H	-2.127502	3.938598	-0.693502
H	1.621000	2.024002	0.176598
H	-0.919904	5.842199	-1.713802
H	4.845305	-2.903894	0.411798
H	4.783905	-2.622395	-2.008702
H	2.244101	0.819203	-1.970702
H	2.758803	-1.336897	-2.995102
H	2.824098	3.897303	-0.874802
H	1.559796	5.825502	-1.820302

TS-B-21

M06-2X/def2-TZVPP-SMD(toluene) Energy = -1741.54518014

Number of Imaginary Frequencies = 1

Lowest Frequency = 333.0757i

M06-2X/6-31G* Geometry

C	-1.529300	-0.639306	2.077099
C	-1.810801	-0.361907	0.322599
C	-1.486406	0.688394	2.561099
H	-0.561397	-1.140001	2.028099
H	-2.349297	-1.274010	2.406099
C	-0.389609	1.516199	2.218899
H	-2.395608	1.148590	2.947499
N	-0.730105	0.441298	-0.066201
C	-1.780494	-1.763607	-0.275101
C	-3.148904	0.335787	0.106799
C	-0.647310	1.719898	0.490399
C	0.456186	2.604103	-0.015801
H	-1.606413	2.232794	0.429799
H	0.177598	-0.047798	-0.065001
H	0.584393	1.021304	2.211199

H	-0.394614	2.527199	2.622599
C	3.347800	-0.483783	-2.039801
C	2.449404	-1.329387	-1.520801
C	4.650999	-0.244177	-1.426701
C	4.842498	-0.193076	-0.102201
O	2.707907	-2.104086	-0.424901
O	3.833798	-0.188681	0.810499
P	2.754204	-1.419586	1.083299
O	1.439501	-0.686592	1.272099
O	3.259009	-2.413684	2.042699
C	-4.214904	0.258582	1.002299
C	-5.442506	0.843876	0.696599
C	-5.620109	1.512175	-0.509901
C	-4.563010	1.587380	-1.414501
C	-3.340307	0.999186	-1.111501
H	-4.107701	-0.270418	1.943999
H	-6.259906	0.773072	1.407199
H	-6.575612	1.969371	-0.745701
H	-2.516907	1.048790	-1.818601
H	-4.690512	2.101480	-2.361901
C	-2.929092	-2.333612	-0.831601
C	-2.875086	-3.604712	-1.400101
C	-1.681383	-4.318106	-1.421201
C	-0.536985	-3.758901	-0.856401
C	-0.588891	-2.496801	-0.277101
H	0.304907	-2.092797	0.186899
H	-3.868294	-1.791717	-0.836701
H	-3.774584	-4.032416	-1.831801
H	-1.644078	-5.306406	-1.868801
H	0.405217	-4.298097	-0.851601
C	1.785988	2.178609	-0.046201
C	2.766284	3.018614	-0.564301
C	2.430978	4.287012	-1.034201
C	1.107676	4.719006	-0.986901
C	0.121680	3.878302	-0.479201
H	-0.913922	4.209597	-0.452101
H	2.061392	1.201911	0.339499
H	0.840971	5.707305	-1.348101
H	1.477404	-1.512392	-1.977101
H	3.099697	0.013415	-2.973201
H	5.824798	-0.052572	0.340599
H	5.518198	-0.115073	-2.067601
H	3.793685	2.668419	-0.594801
H	3.200175	4.941016	-1.433401

TS-B-22

M06-2X/def2-TZVPP-SMD(toluene) Energy = -1741.54498136

Number of Imaginary Frequencies = 1

Lowest Frequency = 375.9738i

M06-2X/6-31G* Geometry

C	-1.487996	-0.750804	2.007698
C	-1.916197	-0.447305	0.294998
C	-1.458799	0.559596	2.541698
H	-0.507695	-1.208002	1.876098
H	-2.247894	-1.436006	2.376298
C	-0.415401	1.427498	2.159198
H	-2.357800	0.975594	2.995998
N	-0.894799	0.409797	-0.146202
C	-1.878894	-1.833905	-0.338102
C	-3.292498	0.200791	0.203998
C	-0.828502	1.670197	0.434598
C	0.178796	2.651500	-0.095902
H	-1.813503	2.131395	0.482598

H	0.031502	-0.046401	-0.236002
H	0.568900	0.969901	2.041398
H	-0.417504	2.429998	2.582798
C	5.147201	0.378212	-0.821502
C	3.915702	0.173309	-1.306602
C	5.815203	-0.547087	0.088398
C	5.172205	-1.225288	1.044498
O	3.194304	-0.961393	-1.094302
O	3.860004	-1.000992	1.353598
P	2.624806	-1.456395	0.373598
O	1.487703	-0.537797	0.779798
O	2.413209	-2.917695	0.303498
C	-4.293098	0.013589	1.156998
C	-5.563999	0.553586	0.967798
C	-5.852101	1.285085	-0.179402
C	-4.861801	1.468988	-1.142002
C	-3.595100	0.926891	-0.954502
H	-4.099397	-0.567211	2.053198
H	-6.328899	0.396884	1.721798
H	-6.841702	1.705883	-0.325102
H	-2.824800	1.058492	-1.709502
H	-5.076203	2.030987	-2.045502
C	-3.009492	-2.376208	-0.958102
C	-2.941889	-3.633808	-1.553702
C	-1.755987	-4.362505	-1.536102
C	-0.631689	-3.831402	-0.908802
C	-0.698592	-2.581502	-0.306602
H	0.190307	-2.213000	0.189498
H	-3.943094	-1.825610	-0.989702
H	-3.825588	-4.041010	-2.035302
H	-1.711885	-5.340805	-2.004902
H	0.312513	-4.365300	-0.868402
C	-0.301807	3.880998	-0.553802
C	0.575390	4.835901	-1.059002
C	1.941091	4.568604	-1.100702
C	2.422594	3.345705	-0.637502
C	1.550596	2.386603	-0.132202
H	1.928499	1.435104	0.235898
H	-1.369008	4.088396	-0.522302
H	3.486295	3.127008	-0.659602
H	3.437700	0.867307	-1.994502
H	5.680199	1.262313	-1.161002
H	5.663407	-1.937587	1.700798
H	6.885504	-0.700784	-0.011402
H	0.191688	5.786000	-1.416902
H	2.628589	5.313405	-1.489502

TS-B-23

M06-2X/def2-TZVPP-SMD(toluene) Energy = -1741.54483579

Number of Imaginary Frequencies = 1

Lowest Frequency = 391.6581i

M06-2X/6-31G* Geometry

C	-0.554705	-0.947294	1.560404
C	-1.571903	-0.657689	0.106304
C	-0.680499	0.275607	2.263504
H	0.406694	-1.107398	1.071504
H	-0.967609	-1.842692	2.020704
C	-0.089194	1.442304	1.738104
H	-1.447199	0.375510	3.031204
N	-1.012498	0.495308	-0.460396
C	-3.027302	-0.444982	0.507104
C	-1.368709	-1.930290	-0.701996
C	-1.097293	1.673809	0.266704

C	-0.591087	2.935806	-0.368196
H	-2.097692	1.818313	0.672504
H	-0.077099	0.348804	-0.872496
H	0.882206	1.313700	1.255304
H	-0.216590	2.363705	2.303104
C	5.624398	-0.416922	1.347704
C	5.395799	-0.187521	0.050204
C	4.565998	-0.400417	2.353304
C	3.336396	-0.872012	2.120004
O	4.183501	0.220284	-0.428596
O	2.988293	-1.524710	0.972604
P	2.862196	-0.753309	-0.483896
O	1.691301	0.203096	-0.386996
O	2.917791	-1.772610	-1.552896
C	-2.308114	-2.965186	-0.629796
C	-2.092620	-4.156987	-1.315496
C	-0.934220	-4.337792	-2.066496
C	0.006584	-3.314196	-2.135496
C	-0.213210	-2.116295	-1.465896
H	-3.213714	-2.846681	-0.044296
H	-2.833723	-4.947883	-1.254296
H	-0.763225	-5.275293	-2.586596
H	0.556693	-1.358899	-1.538396
H	0.936584	-3.428801	-2.682496
C	-3.575004	-0.852380	1.722804
C	-4.935804	-0.688374	1.979204
C	-5.765201	-0.113970	1.022804
C	-5.227899	0.289328	-0.198196
C	-3.873000	0.119222	-0.456196
H	-3.453098	0.424620	-1.410296
H	-2.953207	-1.319583	2.479904
H	-5.343105	-1.013872	2.931104
H	-6.823600	0.015835	1.224504
H	-5.866297	0.733331	-0.955496
C	0.666614	3.024301	-0.973896
C	1.062419	4.227099	-1.550496
C	0.225924	5.341403	-1.518396
C	-1.020076	5.255908	-0.904396
C	-1.425582	4.055510	-0.329496
H	-2.401282	3.984615	0.145404
H	1.332310	2.163198	-0.982896
H	-1.677172	6.119311	-0.873596
H	6.175999	-0.222225	-0.704496
H	6.645397	-0.619627	1.656804
H	2.546096	-0.846108	2.868104
H	4.779500	-0.004618	3.342104
H	2.037319	4.292894	-2.022796
H	0.547029	6.275901	-1.968096

TS-B-24

M06-2X/def2-TZVPP-SMD(toluene) Energy = -1741.54467300

Number of Imaginary Frequencies = 1

Lowest Frequency = 391.2786i

M06-2X/6-31G* Geometry

C	-1.613710	-0.519791	2.046004
C	-1.848808	-0.254489	0.281004
C	-1.451298	0.798707	2.533104
H	-0.702415	-1.118300	1.992904
H	-2.493215	-1.070283	2.373504
C	-0.296292	1.528697	2.183904
H	-2.312593	1.339715	2.923504
N	-0.722901	0.481001	-0.094496
C	-1.885420	-1.670389	-0.264796

C	-3.152601	0.489822	0.014804
C	-0.589990	1.758299	0.427704
C	0.558318	2.592989	-0.054596
H	-1.527285	2.312908	0.385404
H	0.155294	-0.073207	-0.010396
H	0.632803	0.958889	2.128704
H	-0.200383	2.536896	2.581904
C	4.922792	-0.295450	-1.005796
C	3.851987	-0.851740	-1.587396
C	4.951896	0.138550	0.388804
C	4.325290	-0.521944	1.369604
O	2.629186	-0.953429	-0.999196
O	3.711279	-1.723939	1.168104
P	2.275378	-1.822226	0.380704
O	1.273486	-0.912817	1.064704
O	1.989166	-3.233124	0.065804
C	-4.184800	0.641432	0.939004
C	-5.367294	1.290542	0.582704
C	-5.528589	1.798844	-0.700296
C	-4.502891	1.647934	-1.632396
C	-3.329096	0.993924	-1.280396
H	-4.089503	0.246331	1.945604
H	-6.160293	1.396249	1.316304
H	-6.447285	2.306752	-0.975396
H	-2.531098	0.867417	-2.006596
H	-4.618887	2.036736	-2.639196
C	-3.006827	-2.465579	0.001904
C	-3.051339	-3.785578	-0.424096
C	-1.970144	-4.333288	-1.113896
C	-0.859637	-3.546098	-1.390696
C	-0.822525	-2.214598	-0.984196
H	0.047380	-1.623506	-1.244996
H	-3.851824	-2.046771	0.542404
H	-3.927545	-4.389771	-0.210396
H	-1.994653	-5.371688	-1.428596
H	0.005459	-3.958806	-1.896896
C	1.851613	2.076378	-0.167696
C	2.872920	2.886069	-0.652896
C	2.619132	4.210871	-1.004096
C	1.334937	4.731582	-0.871096
C	0.306130	3.922591	-0.397996
H	-0.700967	4.322300	-0.305896
H	2.064604	1.049376	0.116504
H	1.130646	5.762984	-1.140696
H	3.863084	-1.187240	-2.620696
H	5.813393	-0.168458	-1.614096
H	4.330393	-0.192245	2.405004
H	5.525804	1.021345	0.658104
H	3.869217	2.468160	-0.757496
H	3.422038	4.837364	-1.380096

TS-I

M06-2X/def2-TZVPP-SMD(toluene) Energy = -1741.53852851

Number of Imaginary Frequencies = 1

Lowest Frequency = 533.1079i

M06-2X/6-31G* Geometry

C	2.816004	0.116477	-2.122894
C	1.895701	-0.285915	-0.581794
C	3.115417	1.485674	-1.960694
H	2.045602	-0.129616	-2.848794
H	3.636298	-0.597931	-2.128594
C	2.093326	2.439583	-2.005594
H	4.053119	1.765165	-1.484394

N	0.878209	0.653094	-0.593594
C	1.436588	-1.706411	-0.848394
C	2.823002	-0.150223	0.617606
C	1.158821	1.971592	-0.430494
C	-0.039070	2.876003	-0.274994
H	1.956823	2.176285	0.284706
H	-0.132593	0.374304	-0.885494
H	1.275724	2.295091	-2.708794
H	2.371635	3.478281	-1.845094
C	-5.279305	-0.854149	0.311806
C	-4.459595	0.201143	0.338306
C	-4.887717	-2.169453	0.811806
C	-3.657021	-2.672564	0.667106
O	-3.238195	0.166032	0.954306
O	-2.680116	-2.076473	-0.078594
P	-1.970203	-0.649680	0.301506
O	-1.593797	-0.025683	-1.024394
O	-0.936304	-0.769389	1.364406
C	4.214402	-0.107836	0.557906
C	4.967703	-0.043143	1.729906
C	4.334203	-0.026537	2.967406
C	2.942802	-0.088624	3.031106
C	2.185202	-0.156118	1.867106
H	4.733502	-0.136041	-0.395194
H	6.051003	-0.007753	1.669106
H	4.921604	0.026157	3.878806
H	1.098401	-0.248208	1.905206
H	2.440802	-0.093120	3.993506
C	1.999578	-2.778116	-0.151894
C	1.573066	-4.079312	-0.401994
C	0.582164	-4.323603	-1.346194
C	0.027573	-3.259998	-2.053894
C	0.464385	-1.962202	-1.821594
H	0.003693	-1.147798	-2.370894
H	2.758480	-2.601223	0.602106
H	2.011958	-4.900916	0.155206
H	0.240854	-5.337500	-1.530194
H	-0.755228	-3.434691	-2.784294
C	-0.243260	4.047205	-1.004494
C	-1.363452	4.838715	-0.761694
C	-2.289256	4.466623	0.207506
C	-2.088767	3.299422	0.939706
C	-0.967174	2.511811	0.708106
H	-0.819882	1.597810	1.279106
H	0.451443	4.354898	-1.777994
H	-2.808169	2.980928	1.687306
H	-4.725986	1.178146	-0.055794
H	-6.277503	-0.716240	-0.093294
H	-3.367030	-3.642967	1.059106
H	-5.624822	-2.781246	1.323606
H	-1.513044	5.743916	-1.341794
H	-3.165750	5.081631	0.387106

TS Structures of Full System

TS-1-major

M06-2X/6-31G* Energy = -8271.53713845

M06-2X/6-31G* Free Energy = -8270.650848

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.51448188

M06-2X/def2-TZVPP-SMD(toluene) Energy = -8277.52146070

Number of Imaginary Frequencies = 1

Lowest Frequency = 200.9430i

M06-2X/6-31G* Geometry

C	-0.082221	2.806156	0.129306
C	0.736342	2.474597	1.555294
C	0.943825	3.087229	-0.838346
H	-0.631388	1.885014	-0.065595
H	-0.769075	3.629743	0.327035
C	1.793561	2.061102	-1.276617
H	1.238695	4.122634	-1.009577
N	1.668455	1.434931	1.238308
C	1.478367	3.713161	2.060848
C	-0.344619	2.022143	2.541279
C	2.633685	1.763442	0.301649
C	3.693485	0.755187	-0.039095
H	3.090773	2.725943	0.526750
H	1.233532	0.516423	1.065197
H	1.352888	1.077297	-1.451685
H	2.578461	2.330788	-1.980889
C	-5.182552	-0.967876	-1.362801
C	-5.655733	0.069013	-2.178341
C	-3.908901	-0.850596	-0.768150
C	-3.086043	0.217087	-1.128002
C	-3.546822	1.266516	-1.929730
C	-4.845745	1.183263	-2.415756
C	-3.404904	-1.805488	0.263838
C	-4.082514	-1.985670	1.488272
C	-3.583788	-2.919457	2.407517
C	-2.399284	-3.598253	2.122437
C	-1.652993	-3.367884	0.967312
C	-2.187424	-2.457183	0.044562
O	-1.818442	0.280325	-0.609376
O	-1.500231	-2.171165	-1.115407
P	-0.639888	-0.771231	-1.149999
O	0.365300	-0.720394	-0.031990
O	-0.252508	-0.485170	-2.550684
C	-2.680359	2.443909	-2.206790
C	-0.356656	-4.061444	0.768692
C	-1.509718	2.303801	-3.003965
C	-0.716505	3.392762	-3.264239
C	-1.016412	4.672241	-2.720074
C	-2.175507	4.811873	-1.906899
C	-3.000615	3.677119	-1.684824
C	0.475877	-4.300073	1.900077
C	1.646158	-4.999872	1.787268
C	2.074235	-5.499217	0.530694
C	1.267178	-5.240992	-0.611535
C	0.052151	-4.526494	-0.462400
H	-5.224356	1.993185	-3.036336
H	-2.035080	-4.330239	2.839988
H	-1.241455	1.319728	-3.378110
H	0.168997	3.283426	-3.886894
H	-0.558280	-4.349017	-1.341683
H	2.272523	-5.168404	2.659531
H	0.179181	-3.895375	2.863125
H	-3.887092	3.785035	-1.063537

C	-0.923894	0.752734	2.430151
C	-1.929420	0.361832	3.309185
C	-2.384433	1.233623	4.295307
C	-1.824439	2.502514	4.398843
C	-0.810422	2.895230	3.528751
H	-0.616606	0.058303	1.652817
H	-2.355927	-0.633268	3.209280
H	-3.171456	0.926784	4.978313
H	-0.382240	3.886720	3.630174
H	-2.170472	3.193759	5.161101
C	2.452669	3.523502	3.049009
C	3.133120	4.605900	3.592857
C	2.844813	5.901310	3.165332
C	1.872366	6.100096	2.192630
C	1.192299	5.012966	1.642687
H	0.428354	5.205039	0.894342
H	2.670702	2.512885	3.382342
H	3.888266	4.438063	4.354367
H	3.374816	6.748002	3.589761
H	1.634984	7.103422	1.853244
C	5.016275	1.201484	-0.021699
C	6.035526	0.316068	-0.346658
C	5.766820	-0.999410	-0.697586
C	4.439011	-1.419485	-0.714064
Br	7.828121	0.918382	-0.314867
H	6.568437	-1.681169	-0.955354
C	3.392996	-0.562965	-0.390304
H	2.362640	-0.914942	-0.416777
H	5.256262	2.224885	0.248161
Br	4.050535	-3.200038	-1.197125
C	1.710175	-5.699109	-1.881624
C	2.895472	-6.378267	-2.007897
C	3.692428	-6.645308	-0.865730
C	3.288516	-6.216534	0.372973
H	1.097758	-5.485916	-2.753606
H	3.229226	-6.714409	-2.984745
H	3.900814	-6.405884	1.250989
H	4.627892	-7.184543	-0.978768
C	-2.452773	6.074209	-1.316362
C	-1.616335	7.142936	-1.517609
C	-0.464541	7.004787	-2.331634
C	-0.177035	5.800083	-2.922473
H	-3.340122	6.175671	-0.696702
H	-1.837042	8.101725	-1.058832
H	0.185422	7.859578	-2.491357
H	0.701600	5.689050	-3.553972
C	-7.043833	0.039249	-2.791178
C	-7.649411	-1.361233	-2.844038
H	-7.007304	0.480472	-3.793356
H	-7.702543	0.687380	-2.195515
C	-7.478237	-2.049391	-1.492346
H	-7.141945	-1.955322	-3.614985
H	-8.705607	-1.300799	-3.126031
C	-5.994271	-2.239707	-1.188087
H	-7.941553	-1.432993	-0.708841
H	-7.985197	-3.019649	-1.478962
H	-5.856859	-2.657513	-0.187716
H	-5.581337	-2.989784	-1.877856
C	-5.245332	-1.085286	1.871580
C	-6.101775	-1.652591	3.000810
H	-5.867786	-0.846645	1.007069
H	-4.814010	-0.125241	2.196207
C	-5.216777	-2.089623	4.164264

H	-6.830458	-0.901287	3.322443
H	-6.671905	-2.517751	2.634535
C	-4.297585	-3.221179	3.712438
H	-4.614709	-1.232681	4.497741
H	-5.817745	-2.412924	5.020464
H	-4.897700	-4.133005	3.583287
H	-3.556880	-3.450308	4.486586

TS-1-major-2

M06-2X/6-31G* Energy = -8271.53713853

M06-2X/6-31G* Free Energy = -8270.650849

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.51448180

M06-2X/def2-TZVPP-SMD(toluene) Energy = -8277.52146053

Number of Imaginary Frequencies = 1

Lowest Frequency = 201.0265i

M06-2X/6-31G* Geometry

C	-0.082388	2.806026	0.129019
C	0.735991	2.474705	1.555121
C	0.943748	3.087151	-0.838542
H	-0.631422	1.884812	-0.065895
H	-0.769380	3.629544	0.326563
C	1.793615	2.061093	-1.276665
H	1.238535	4.122578	-1.009786
N	1.668277	1.435108	1.238344
C	1.477801	3.713400	2.060663
C	-0.345026	2.022188	2.541017
C	2.633588	1.763643	0.301800
C	3.693510	0.755465	-0.038780
H	3.090547	2.726215	0.526859
H	1.233457	0.516554	1.065220
H	1.353076	1.077216	-1.451653
H	2.578593	2.330791	-1.980844
C	-4.082417	-1.985995	1.487904
C	-3.583645	-2.919651	2.407257
C	-3.404742	-1.805830	0.263503
C	-2.187168	-2.457395	0.044360
C	-1.652709	-3.367980	0.967210
C	-2.399054	-3.598346	2.122299
C	-3.908762	-0.851041	-0.768566
C	-5.182349	-0.968475	-1.363321
C	-5.655572	0.068341	-2.178929
C	-4.845690	1.182680	-2.416290
C	-3.546823	1.266095	-1.930143
C	-3.085995	0.216728	-1.128363
O	-1.499910	-2.171354	-1.115566
O	-1.818451	0.280113	-0.609620
P	-0.639743	-0.771308	-1.150164
O	0.365393	-0.720320	-0.032113
O	-0.252345	-0.485223	-2.550839
C	-0.356287	-4.061425	0.768737
C	-2.680505	2.443632	-2.207047
C	0.476174	-4.299900	1.900208
C	1.646521	-4.999612	1.787549
C	2.074741	-5.499016	0.531047
C	1.267762	-5.240934	-0.611269
C	0.052663	-4.526526	-0.462288
C	-1.509738	2.303784	-3.004083
C	-0.716665	3.392899	-3.264147
C	-1.016831	4.672275	-2.719876
C	-2.176064	4.811645	-1.906853
C	-3.001028	3.676744	-1.685014
H	-2.034819	-4.330238	2.839930
H	-5.224344	1.992555	-3.036905

H	0.179366	-3.895155	2.863202
H	2.272827	-5.168029	2.659876
H	-3.887603	3.784457	-1.063832
H	0.168934	3.283768	-3.886700
H	-1.241262	1.319783	-3.378273
H	-0.557709	-4.349164	-1.341634
C	-0.924124	0.752696	2.429920
C	-1.929709	0.361734	3.308862
C	-2.384956	1.233544	4.294857
C	-1.825137	2.502515	4.398361
C	-0.811063	2.895291	3.528363
H	-0.616661	0.058243	1.652675
H	-2.356076	-0.633428	3.208982
H	-3.172027	0.926657	4.977789
H	-0.383024	3.886846	3.629756
H	-2.171351	3.193778	5.160521
C	1.191616	5.013128	1.642339
C	1.871464	6.100400	2.192272
C	2.843805	5.901837	3.165125
C	3.132230	4.606506	3.592809
C	2.451997	3.523965	3.048971
H	2.670122	2.513409	3.382430
H	0.427751	5.205032	0.893869
H	1.633987	7.103662	1.852758
H	3.373634	6.748641	3.589550
H	3.887291	4.438842	4.354440
C	3.393176	-0.562730	-0.389961
C	4.439302	-1.419167	-0.713583
C	5.767072	-0.998974	-0.696971
C	6.035624	0.316540	-0.346062
Br	4.051037	-3.199762	-1.196656
H	6.568778	-1.680672	-0.954627
C	5.016258	1.201882	-0.021261
H	5.256125	2.225317	0.248575
H	2.362853	-0.914799	-0.416537
Br	7.828163	0.919009	-0.314072
C	-2.453592	6.073865	-1.316191
C	-1.617263	7.142729	-1.517162
C	-0.465325	7.004840	-2.331027
C	-0.177573	5.800256	-2.921991
H	-3.341045	6.175121	-0.696650
H	-1.838166	8.101426	-1.058285
H	0.701173	5.689429	-3.553372
H	0.184554	7.859737	-2.490531
C	1.710910	-5.699099	-1.881289
C	2.896275	-6.378166	-2.007412
C	3.693150	-6.645069	-0.865157
C	3.289093	-6.216247	0.373482
H	1.098551	-5.486015	-2.753339
H	3.230142	-6.714345	-2.984209
H	4.628667	-7.184236	-0.978077
H	3.901328	-6.405490	1.251565
C	-4.297465	-3.221304	3.712180
C	-5.216723	-2.089748	4.163872
H	-3.556768	-3.450324	4.486369
H	-4.897532	-4.133171	3.583098
C	-6.101749	-1.652923	3.000362
H	-4.614704	-1.232727	4.497236
H	-5.817669	-2.412978	5.020114
C	-5.245348	-1.085693	1.871061
H	-6.671815	-2.518171	2.634196
H	-6.830488	-0.901632	3.321898
H	-4.814140	-0.125550	2.195548

H	-5.867818	-0.847255	1.006505
C	-5.993958	-2.240377	-1.188624
C	-7.477924	-2.050197	-1.492967
H	-5.856560	-2.658148	-0.188235
H	-5.580921	-2.990432	-1.878355
C	-7.649080	-1.362116	-2.844701
H	-7.984809	-3.020495	-1.479565
H	-7.941330	-1.433800	-0.709516
C	-7.043617	0.038418	-2.791882
H	-7.141529	-1.956204	-3.615593
H	-8.705266	-1.301778	-3.126752
H	-7.702429	0.686539	-2.196322
H	-7.007038	0.479573	-3.794088

TS-1-major-3

M06-2X/6-31G* Energy = -8271.53920181

M06-2X/6-31G* Free Energy = -8270.651597

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.51576594

M06-2X/def2-TZVPP-SMD(toluene) Energy = -8277.52274658

Number of Imaginary Frequencies = 1

Lowest Frequency = 218.2641i

M06-2X/6-31G* Geometry

C	-0.158447	-2.876159	0.290395
C	-0.888148	-2.425443	1.723266
C	-1.229352	-3.067811	-0.655709
H	0.479538	-2.023554	0.057483
H	0.447730	-3.762237	0.483900
C	-1.976467	-1.971361	-1.098197
H	-1.619602	-4.071237	-0.833025
N	-1.717287	-1.299924	1.402688
C	-1.745260	-3.557648	2.291289
C	0.260572	-2.060907	2.668452
C	-2.741316	-1.550165	0.510192
C	-3.697629	-0.449033	0.157041
H	-3.285240	-2.456561	0.770757
H	-1.191609	-0.440880	1.184812
H	-1.448674	-1.033703	-1.282763
H	-2.797038	-2.174545	-1.783161
C	5.320223	0.320402	-1.365906
C	5.695220	-0.781723	-2.146303
C	4.045388	0.335304	-0.763468
C	3.126796	-0.665626	-1.083880
C	3.487216	-1.777543	-1.853557
C	4.788002	-1.826136	-2.341671
C	3.638691	1.365632	0.238293
C	4.344821	1.524125	1.449680
C	3.948906	2.533873	2.337718
C	2.833392	3.314355	2.035415
C	2.054936	3.115882	0.895450
C	2.486213	2.122005	0.004404
O	1.863075	-0.589845	-0.556156
O	1.763357	1.863014	-1.140080
P	0.782804	0.543043	-1.130529
O	-0.221818	0.619572	-0.012470
O	0.364669	0.251302	-2.521761
C	2.523404	-2.882363	-2.100894
C	0.837152	3.934785	0.677139
C	2.796688	-4.179065	-1.582460
C	1.907657	-5.210311	-1.750996
C	0.695771	-5.010010	-2.462898
C	0.437914	-3.724624	-3.019498
C	1.364186	-2.669766	-2.811711
C	0.055020	4.319833	1.804502

C	-1.029461	5.143225	1.670885
C	-1.419131	5.628069	0.396330
C	-0.667424	5.222988	-0.741038
C	0.461827	4.383473	-0.570717
H	5.090322	-2.685977	-2.936958
H	2.552311	4.106264	2.726087
H	3.717999	-4.333902	-1.027448
H	2.118571	-6.193765	-1.337890
H	1.033095	4.096601	-1.447284
H	-1.617611	5.423474	2.541001
H	0.319170	3.930404	2.783147
H	1.133212	-1.676755	-3.191604
C	0.961510	-0.859931	2.508604
C	2.024081	-0.551152	3.352563
C	2.416223	-1.440504	4.349925
C	1.735849	-2.644258	4.500163
C	0.663964	-2.952899	3.666345
H	0.706677	-0.158608	1.718455
H	2.544865	0.393344	3.216027
H	3.248389	-1.198166	5.004815
H	0.141636	-3.893682	3.804150
H	2.032500	-3.349048	5.270790
C	-2.642254	-3.235413	3.317858
C	-3.420473	-4.218478	3.915799
C	-3.309767	-5.546383	3.504526
C	-2.416360	-5.877023	2.493014
C	-1.638538	-4.888356	1.888936
H	-0.940786	-5.178782	1.109056
H	-2.721506	-2.200493	3.638246
H	-4.113057	-3.948328	4.706768
H	-3.916136	-6.315922	3.971454
H	-2.318508	-6.907418	2.166058
C	-5.058415	-0.758042	0.204990
C	-5.987690	0.215913	-0.136096
C	-5.592101	1.485639	-0.532103
C	-4.229069	1.768468	-0.577963
Br	-7.831268	-0.199259	-0.069925
H	-6.324449	2.236438	-0.803529
C	-3.270178	0.820737	-0.239042
H	-2.209697	1.063407	-0.294201
H	-5.396014	-1.743592	0.509097
Br	-3.672590	3.484033	-1.126585
C	-1.080039	5.662961	-2.027649
C	-2.184521	6.463248	-2.174277
C	-2.924679	6.876762	-1.037523
C	-2.547598	6.469641	0.216940
H	-0.511814	5.338003	-2.895030
H	-2.497499	6.783888	-3.163117
H	-3.118390	6.770968	1.091624
H	-3.796024	7.511329	-1.166826
C	-0.769482	-3.515613	-3.742818
C	-1.685620	-4.526239	-3.884236
C	-1.436558	-5.801585	-3.313982
C	-0.273274	-6.037623	-2.625304
H	-0.952837	-2.527570	-4.158473
H	-2.605608	-4.356509	-4.435322
H	-2.168586	-6.594430	-3.434170
H	-0.072592	-7.017401	-2.198356
C	7.076477	-0.895066	-2.765213
C	7.802469	0.444103	-2.868394
H	6.994450	-1.365100	-3.751460
H	7.679958	-1.577937	-2.150165
C	7.701428	1.189803	-1.540617

H	7.344209	1.054228	-3.657428
H	8.847324	0.281251	-3.152103
C	6.242151	1.521015	-1.238561
H	8.113230	0.561579	-0.737933
H	8.292348	2.111208	-1.562021
H	6.148745	1.984133	-0.253240
H	5.892933	2.280184	-1.953172
C	5.422925	0.532786	1.855280
C	6.343186	1.057371	2.954685
H	6.009708	0.205982	0.994771
H	4.908222	-0.370586	2.218882
C	5.518236	1.617130	4.109563
H	7.002572	0.253021	3.296860
H	6.986821	1.851550	2.551184
C	4.703252	2.813057	3.624773
H	4.843020	0.833196	4.480505
H	6.157811	1.913247	4.947436
H	5.384251	3.659500	3.457288
H	3.996419	3.137896	4.396345

TS-1-major-4

M06-2X/6-31G* Energy = -8271.53920178

M06-2X/6-31G* Free Energy = -8270.651593

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.51576519

M06-2X/def2-TZVPP-SMD(toluene) Energy = -8277.52274584

Number of Imaginary Frequencies = 1

Lowest Frequency = 218.1365i

M06-2X/6-31G* Geometry

C	-0.158379	-2.876137	0.290152
C	-0.887949	-2.425591	1.722978
C	-1.229299	-3.067774	-0.655976
H	0.479600	-2.023537	0.057195
H	0.447824	-3.762219	0.483559
C	-1.976436	-1.971331	-1.098369
H	-1.619551	-4.071199	-0.833299
N	-1.717172	-1.300063	1.402548
C	-1.745010	-3.557847	2.290988
C	0.260792	-2.061089	2.668170
C	-2.741220	-1.550297	0.510096
C	-3.697592	-0.449176	0.157055
H	-3.285097	-2.456737	0.770604
H	-1.191569	-0.440964	1.184697
H	-1.448679	-1.033639	-1.282855
H	-2.797039	-2.174476	-1.783304
C	4.344700	1.524401	1.449767
C	3.948697	2.534128	2.337790
C	3.638608	1.365853	0.238364
C	2.486097	2.122163	0.004438
C	2.054720	3.115997	0.895480
C	2.833123	3.314519	2.035472
C	4.045370	0.335528	-0.763375
C	5.320214	0.320680	-1.365793
C	5.695280	-0.781429	-2.146180
C	4.788111	-1.825882	-2.341567
C	3.487312	-1.777341	-1.853482
C	3.126828	-0.665443	-1.083807
O	1.763282	1.863133	-1.140067
O	1.863094	-0.589717	-0.556110
P	0.782774	0.543132	-1.130471
O	-0.221806	0.619642	-0.012377
O	0.364597	0.251345	-2.521684
C	0.836879	3.934804	0.677136
C	2.523535	-2.882187	-2.100858

C	0.054606	4.319666	1.804462
C	-1.029941	5.142968	1.670819
C	-1.419528	5.627905	0.396274
C	-0.667674	5.223007	-0.741062
C	0.461634	4.383574	-0.570714
C	2.796815	-4.178883	-1.582408
C	1.907807	-5.210143	-1.750983
C	0.695952	-5.009862	-2.462946
C	0.438102	-3.724482	-3.019561
C	1.364347	-2.669609	-2.811729
H	2.551949	4.106392	2.726148
H	5.090481	-2.685711	-2.936845
H	0.318708	3.930168	2.783093
H	-1.618204	5.423075	2.540904
H	1.133373	-1.676601	-3.191628
H	2.118715	-6.193593	-1.337865
H	3.718102	-4.333706	-1.027352
H	1.033014	4.096830	-1.447252
C	0.664268	-2.953166	3.665952
C	1.736175	-2.644565	4.499756
C	2.416493	-1.440768	4.349614
C	2.024270	-0.551332	3.352360
C	0.961669	-0.860067	2.508421
H	0.141987	-3.893989	3.803680
H	2.032891	-3.349424	5.270296
H	3.248674	-1.198466	5.004496
H	0.706769	-0.158673	1.718360
H	2.545011	0.393198	3.215887
C	-2.641949	-3.235706	3.317635
C	-3.420109	-4.218829	3.915556
C	-3.309399	-5.546704	3.504183
C	-2.416048	-5.877253	2.492594
C	-1.638284	-4.888526	1.888538
H	-0.940571	-5.178886	1.108596
H	-2.721202	-2.200809	3.638100
H	-4.112648	-3.948750	4.706588
H	-3.915723	-6.316288	3.971095
H	-2.318192	-6.907624	2.165562
C	-5.058369	-0.758192	0.205190
C	-5.987694	0.215753	-0.135789
C	-5.592167	1.485470	-0.531891
C	-4.229143	1.768302	-0.577949
Br	-7.831260	-0.199432	-0.069359
H	-6.324556	2.236253	-0.803251
C	-3.270205	0.820588	-0.239113
H	-2.209736	1.063277	-0.294387
H	-5.395923	-1.743739	0.509356
Br	-3.672717	3.483818	-1.126766
C	-0.769257	-3.515493	-3.742951
C	-1.685367	-4.526137	-3.884422
C	-1.436315	-5.801478	-3.314152
C	-0.273066	-6.037493	-2.625404
H	-0.952605	-2.527454	-4.158619
H	-2.605325	-4.356425	-4.435564
H	-0.072391	-7.017268	-2.198445
H	-2.168320	-6.594337	-3.434383
C	-1.080194	5.663089	-2.027666
C	-2.184719	6.463310	-2.174319
C	-2.925023	6.876645	-1.037595
C	-2.548044	6.469406	0.216859
H	-0.511853	5.338274	-2.895026
H	-2.497617	6.784039	-3.163156
H	-3.796401	7.511163	-1.166917

H	-3.118945	6.770599	1.091520
C	4.703016	2.813340	3.624848
C	5.517709	1.617284	4.109796
H	3.996218	3.138442	4.396340
H	5.384228	3.659598	3.457286
C	6.342860	1.057486	2.955081
H	4.842284	0.833429	4.480522
H	6.157120	1.913261	4.947841
C	5.422837	0.533096	1.855376
H	6.986720	1.851599	2.551811
H	7.002042	0.253015	3.297365
H	4.908151	-0.370425	2.218633
H	6.009840	0.206571	0.994909
C	6.242101	1.521321	-1.238451
C	7.701422	1.190044	-1.540207
H	6.148504	1.984591	-0.253221
H	5.893024	2.280376	-1.953252
C	7.802673	0.444391	-2.867993
H	8.292405	2.111413	-1.561461
H	8.113021	0.561765	-0.737461
C	7.076564	-0.894739	-2.765046
H	7.344627	1.054597	-3.657088
H	8.847572	0.281471	-3.151501
H	7.679962	-1.577759	-2.150084
H	6.994555	-1.364604	-3.751375

TS-1-major-5

M06-2X/6-31G* Energy = -8271.53965566

M06-2X/6-31G* Free Energy = -8270.650516

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.51628748

M06-2X/def2-TZVPP-SMD(toluene) Energy = -8277.52324665

Number of Imaginary Frequencies = 1

Lowest Frequency = 208.2065i

M06-2X/6-31G* Geometry

C	0.001256	-2.867468	0.402408
C	-0.770054	-2.343265	1.780358
C	-1.040420	-3.187809	-0.543115
H	0.601138	-2.006304	0.109772
H	0.648298	-3.704194	0.670308
C	-1.838635	-2.171603	-1.081040
H	-1.370972	-4.222486	-0.648519
N	-1.657082	-1.296534	1.360288
C	-1.570348	-3.470519	2.434441
C	0.337245	-1.828359	2.704301
C	-2.650429	-1.674750	0.477505
C	-3.659140	-0.652401	0.046194
H	-3.148201	-2.587059	0.802298
H	-1.172902	-0.434433	1.074011
H	-1.360608	-1.222233	-1.330620
H	-2.632581	-2.474609	-1.760801
C	5.383043	0.426050	-1.273545
C	5.862387	-0.738745	-1.888545
C	4.070807	0.441382	-0.757654
C	3.224426	-0.639909	-1.008276
C	3.688268	-1.812483	-1.616670
C	5.020166	-1.846128	-2.013900
C	3.544541	1.566932	0.070626
C	4.147331	1.924083	1.296289
C	3.637251	3.016088	2.012798
C	2.528306	3.705136	1.519034
C	1.862129	3.322235	0.357310
C	2.383903	2.226136	-0.342516
O	1.929943	-0.575761	-0.562123

O	1.735015	1.771065	-1.470056
P	0.815126	0.416556	-1.307506
O	-0.226917	0.581540	-0.233445
O	0.457459	-0.076863	-2.658131
C	2.796505	-2.988872	-1.791974
C	0.669213	4.067759	-0.111754
C	3.105886	-4.209272	-1.128482
C	2.276445	-5.297793	-1.225930
C	1.090379	-5.234901	-2.004195
C	0.799448	-4.029302	-2.704561
C	1.665936	-2.913423	-2.573293
C	0.522161	4.405732	-1.488594
C	-0.532433	5.166210	-1.913580
C	-1.514170	5.631463	-1.000083
C	-1.388697	5.282338	0.372742
C	-0.279361	4.502654	0.786106
H	5.402122	-2.751398	-2.482659
H	2.162674	4.572797	2.064353
H	4.004782	-4.257445	-0.519783
H	2.514149	-6.221016	-0.702987
H	-0.196929	4.228012	1.835295
H	-0.633410	5.422436	-2.964975
H	1.262109	4.052187	-2.197546
H	1.406183	-1.980007	-3.067812
C	0.946633	-0.591848	2.463075
C	1.964803	-0.138937	3.296053
C	2.407920	-0.919692	4.360691
C	1.822144	-2.160247	4.590094
C	0.791288	-2.611384	3.769455
H	0.658670	0.026521	1.616761
H	2.410699	0.832136	3.096748
H	3.206821	-0.564893	5.005857
H	0.339145	-3.577139	3.969775
H	2.160027	-2.782091	5.413325
C	-1.394702	-4.821180	2.136059
C	-2.126826	-5.798108	2.812395
C	-3.042535	-5.435673	3.792524
C	-3.222167	-4.087249	4.099595
C	-2.489669	-3.115420	3.429981
H	-2.622885	-2.064123	3.668584
H	-0.678690	-5.135952	1.382433
H	-1.975816	-6.844401	2.566159
H	-3.613135	-6.196401	4.315647
H	-3.933198	-3.792081	4.864844
C	-3.303615	0.654857	-0.294465
C	-4.310651	1.542522	-0.656355
C	-5.648304	1.158523	-0.708490
C	-5.969593	-0.151651	-0.382721
Br	-3.854503	3.322280	-1.078410
H	-6.417677	1.864564	-0.997088
C	-4.992747	-1.062496	-0.003279
H	-5.273589	-2.077598	0.258676
H	-2.262451	0.974552	-0.294997
Br	-7.776132	-0.706014	-0.450672
C	-2.392160	5.706182	1.283467
C	-3.470209	6.435478	0.851562
C	-3.595119	6.783228	-0.515804
C	-2.637017	6.392837	-1.418302
H	-2.294875	5.431104	2.330625
H	-4.236211	6.745527	1.555486
H	-2.729220	6.651172	-2.470336
H	-4.454729	7.357432	-0.847438
C	-0.384107	-3.955673	-3.491378

C	-1.246113	-5.020271	-3.560986
C	-0.964175	-6.215459	-2.850130
C	0.177005	-6.320421	-2.094547
H	-0.594022	-3.025102	-4.013476
H	-2.148289	-4.954334	-4.161478
H	-1.653282	-7.052092	-2.914187
H	0.402449	-7.239242	-1.558384
C	7.287054	-0.848811	-2.400258
C	7.952276	0.506544	-2.626451
H	7.296631	-1.440725	-3.322140
H	7.878806	-1.415167	-1.666860
C	7.725628	1.401908	-1.411408
H	7.519031	0.988649	-3.512298
H	9.020634	0.369887	-2.823119
C	6.234852	1.683569	-1.241512
H	8.113573	0.901297	-0.512874
H	8.270206	2.346274	-1.512802
H	6.053645	2.257643	-0.329585
H	5.897266	2.328838	-2.065370
C	5.241201	1.058688	1.900165
C	6.044322	1.771042	2.985728
H	5.909377	0.667337	1.130629
H	4.750599	0.174985	2.337710
C	5.103473	2.417163	3.998105
H	6.716380	1.057501	3.473691
H	6.674893	2.547667	2.530812
C	4.268367	3.492686	3.308459
H	4.442782	1.645437	4.417701
H	5.659194	2.852819	4.834850
H	4.914462	4.354517	3.089212
H	3.484243	3.862025	3.978687

TS-1-major-6

M06-2X/6-31G* Energy = -8271.53742689

M06-2X/6-31G* Free Energy = -8270.648760

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.51516231

M06-2X/def2-TZVPP-SMD(toluene) Energy = -8277.52180902

Number of Imaginary Frequencies = 1

Lowest Frequency = 75.4711i

M06-2X/6-31G* Geometry

C	-0.336105	2.804608	0.242090
C	0.648656	2.377691	1.652802
C	0.641267	3.216096	-0.689890
H	-0.801736	1.841088	0.042897
H	-1.053724	3.554849	0.570358
C	1.592528	2.270701	-1.194546
H	0.858047	4.279180	-0.796857
N	1.593993	1.446279	1.187233
C	1.322332	3.627726	2.213640
C	-0.380404	1.786715	2.610789
C	2.480695	1.919603	0.194199
C	3.607398	0.992921	-0.190237
H	2.908182	2.871384	0.512951
H	1.197684	0.525639	0.951043
H	1.179676	1.308485	-1.511632
H	2.298142	2.674835	-1.920902
C	-5.221204	-1.092664	-1.307714
C	-5.793368	-0.010686	-1.990836
C	-3.916670	-0.966496	-0.787029
C	-3.167428	0.169893	-1.094374
C	-3.724797	1.261457	-1.768857
C	-5.049041	1.157454	-2.177544
C	-3.295124	-1.997182	0.097275

C	-3.861086	-2.345803	1.342609
C	-3.249503	-3.346308	2.111856
C	-2.077941	-3.950261	1.651250
C	-1.452419	-3.566942	0.467746
C	-2.078800	-2.566693	-0.286590
O	-1.876891	0.252185	-0.641798
O	-1.473305	-2.108660	-1.436855
P	-0.668146	-0.679525	-1.324289
O	0.358134	-0.706941	-0.225317
O	-0.334389	-0.215573	-2.690653
C	-2.931854	2.499911	-1.995177
C	-0.187533	-4.205981	0.031555
C	-1.791719	2.482025	-2.846966
C	-1.065769	3.628094	-3.055628
C	-1.410347	4.848925	-2.411218
C	-2.539521	4.866663	-1.546006
C	-3.292314	3.674544	-1.373005
C	-0.015677	-4.615062	-1.322640
C	1.118321	-5.270230	-1.716934
C	2.159167	-5.550688	-0.793435
C	2.006962	-5.128057	0.555894
C	0.814714	-4.463220	0.938910
H	-5.502263	1.998724	-2.698430
H	-1.628168	-4.746145	2.241463
H	-1.488922	1.544679	-3.304998
H	-0.204243	3.611269	-3.720072
H	0.710333	-4.129554	1.968890
H	1.238845	-5.581973	-2.751112
H	-0.800260	-4.399680	-2.039203
H	-4.155200	3.689621	-0.710450
C	-0.861292	2.543941	3.683541
C	-1.815270	2.014661	4.548836
C	-2.298073	0.724687	4.354757
C	-1.827899	-0.030870	3.282964
C	-0.884554	0.496103	2.407322
H	-0.489315	3.548224	3.855675
H	-2.174843	2.615363	5.378449
H	-3.038545	0.311258	5.033660
H	-0.568524	-0.109063	1.560993
H	-2.194632	-1.039858	3.111963
C	0.913614	4.932204	1.935872
C	1.545916	6.016146	2.544740
C	2.592143	5.809559	3.436434
C	3.003383	4.508888	3.722368
C	2.370462	3.427839	3.120543
H	2.685225	2.412076	3.341426
H	0.092714	5.128052	1.251950
H	1.214244	7.023628	2.314343
H	3.085015	6.654838	3.905983
H	3.818790	4.334287	4.417228
C	3.399061	-0.360828	-0.460856
C	4.496251	-1.151212	-0.785012
C	5.782867	-0.627301	-0.873861
C	5.956965	0.725584	-0.619262
Br	4.236333	-2.994717	-1.091362
H	6.624556	-1.258528	-1.132037
C	4.887869	1.541485	-0.273119
H	5.058504	2.592472	-0.062308
H	2.401466	-0.795718	-0.425100
Br	7.691974	1.471849	-0.732123
C	3.064927	-5.364755	1.472767
C	4.218636	-5.986333	1.069001
C	4.369217	-6.409089	-0.274356

C	3.361067	-6.198606	-1.182013
H	2.946908	-5.032662	2.501081
H	5.024842	-6.152754	1.776620
H	3.472144	-6.514582	-2.216347
H	5.288420	-6.896883	-0.583827
C	-2.859391	6.067419	-0.856975
C	-2.091549	7.193430	-1.014568
C	-0.970253	7.177111	-1.880816
C	-0.643065	6.033973	-2.566022
H	-3.723988	6.075430	-0.198065
H	-2.344242	8.104560	-0.481237
H	-0.375098	8.076518	-2.005067
H	0.212356	6.017071	-3.237576
C	-7.217461	-0.053775	-2.513771
C	-7.762354	-1.472280	-2.662513
H	-7.269327	0.480168	-3.469047
H	-7.862287	0.501563	-1.817661
C	-7.469387	-2.273774	-1.396983
H	-7.282811	-1.965558	-3.517809
H	-8.836912	-1.439386	-2.869750
C	-5.961210	-2.415274	-1.206684
H	-7.906077	-1.757865	-0.530072
H	-7.929939	-3.265805	-1.445479
H	-5.737945	-2.918718	-0.262888
H	-5.562568	-3.074505	-1.991247
C	-5.030977	-1.556805	1.906986
C	-5.767995	-2.289582	3.025128
H	-5.729231	-1.263592	1.120428
H	-4.624614	-0.613019	2.303511
C	-4.773906	-2.792708	4.067494
H	-6.507496	-1.621292	3.478349
H	-6.318931	-3.143961	2.607836
C	-3.835039	-3.814669	3.431789
H	-4.193360	-1.940869	4.449020
H	-5.288888	-3.238903	4.924498
H	-4.392774	-4.745787	3.258108
H	-3.020836	-4.070923	4.118768

TS-1-major-7

M06-2X/6-31G* Energy = -8271.53742690

M06-2X/6-31G* Free Energy = -8270.648758

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.51516240

M06-2X/def2-TZVPP-SMD(toluene) Energy = -8277.52180912

Number of Imaginary Frequencies = 1

Lowest Frequency = 75.3539i

M06-2X/6-31G* Geometry

C	-0.336114	2.804720	0.242175
C	0.648555	2.377680	1.652842
C	0.641294	3.216227	-0.689763
H	-0.801788	1.841233	0.042916
H	-1.053687	3.554979	0.570497
C	1.592518	2.270836	-1.194477
H	0.858119	4.279308	-0.796661
N	1.593880	1.446253	1.187246
C	1.322277	3.627642	2.213794
C	-0.380581	1.786715	2.610759
C	2.480647	1.919617	0.194298
C	3.607337	0.992940	-0.190174
H	2.908140	2.871370	0.513123
H	1.197583	0.525622	0.950978
H	1.179653	1.308654	-1.511659
H	2.298163	2.675008	-1.920782
C	-3.861062	-2.345833	1.342594

C	-3.249507	-3.346374	2.111816
C	-3.295081	-1.997185	0.097277
C	-2.078770	-2.566714	-0.286597
C	-1.452407	-3.566987	0.467720
C	-2.077946	-3.950330	1.651207
C	-3.916603	-0.966476	-0.787015
C	-5.221133	-1.092632	-1.307716
C	-5.793279	-0.010650	-1.990847
C	-5.048932	1.157476	-2.177560
C	-3.724690	1.261463	-1.768861
C	-3.167341	0.169902	-1.094356
O	-1.473258	-2.108648	-1.436843
O	-1.876810	0.252195	-0.641756
P	-0.668046	-0.679556	-1.324159
O	0.358126	-0.707078	-0.225088
O	-0.334129	-0.215564	-2.690472
C	-0.187521	-4.206019	0.031524
C	-2.931734	2.499902	-1.995210
C	-0.015675	-4.615106	-1.322670
C	1.118329	-5.270257	-1.716974
C	2.159192	-5.550689	-0.793485
C	2.006998	-5.128048	0.555842
C	0.814741	-4.463232	0.938869
C	-1.791579	2.481977	-2.846971
C	-1.065635	3.628039	-3.055683
C	-1.410236	4.848904	-2.411349
C	-2.539430	4.866682	-1.546164
C	-3.292218	3.674567	-1.373112
H	-1.628187	-4.746233	2.241404
H	-5.502134	1.998746	-2.698463
H	-0.800271	-4.399741	-2.039224
H	1.238847	-5.582007	-2.751151
H	-4.155121	3.689676	-0.710581
H	-0.204085	3.611180	-3.720096
H	-1.488763	1.544608	-3.304945
H	0.710366	-4.129559	1.968847
C	-0.884593	0.496033	2.407408
C	-1.828020	-0.030889	3.282996
C	-2.298414	0.724783	4.354609
C	-1.815750	2.014827	4.548567
C	-0.861691	2.544056	3.683333
H	-0.568408	-0.109231	1.561209
H	-2.194644	-1.039932	3.112088
H	-3.038949	0.311390	5.033465
H	-0.489817	3.548393	3.855377
H	-2.175493	2.615622	5.378039
C	0.913682	4.932168	1.936066
C	1.546025	6.016028	2.545038
C	2.592174	5.809312	3.436793
C	3.003291	4.508592	3.722688
C	2.370325	3.427626	3.120763
H	2.684992	2.411827	3.341614
H	0.092845	5.128117	1.252098
H	1.214449	7.023549	2.314673
H	3.085080	6.654526	3.906422
H	3.818636	4.333890	4.417594
C	3.398999	-0.360797	-0.460852
C	4.496190	-1.151171	-0.785033
C	5.782806	-0.627258	-0.873862
C	5.956906	0.725616	-0.619208
Br	4.236275	-2.994668	-1.091430
H	6.624494	-1.258476	-1.132062
C	4.887811	1.541504	-0.273027

H	5.058449	2.592480	-0.062169
H	2.401406	-0.795694	-0.425095
Br	7.691915	1.471888	-0.732045
C	-2.859335	6.067480	-0.857221
C	-2.091510	7.193492	-1.014876
C	-0.970194	7.177134	-1.881100
C	-0.642970	6.033954	-2.566218
H	-3.723947	6.075521	-0.198332
H	-2.344230	8.104656	-0.481615
H	0.212467	6.017020	-3.237750
H	-0.375053	8.076543	-2.005399
C	3.064981	-5.364715	1.472702
C	4.218697	-5.986272	1.068925
C	4.369267	-6.409039	-0.274430
C	3.361099	-6.198587	-1.182074
H	2.946970	-5.032614	2.501014
H	5.024917	-6.152668	1.776534
H	5.288476	-6.896818	-0.583909
H	3.472167	-6.514572	-2.216406
C	-3.835074	-3.814774	3.431720
C	-4.773924	-2.792815	4.067454
H	-3.020890	-4.071083	4.118701
H	-4.392835	-4.745868	3.257989
C	-5.767988	-2.289621	3.025096
H	-4.193361	-1.941007	4.449024
H	-5.288928	-3.239032	4.924433
C	-5.030939	-1.556825	1.906987
H	-6.318947	-3.143969	2.607770
H	-6.507473	-1.621325	3.478335
H	-4.624554	-0.613064	2.303549
H	-5.729176	-1.263565	1.120432
C	-5.961146	-2.415240	-1.206702
C	-7.469317	-2.273745	-1.397059
H	-5.737921	-2.918677	-0.262894
H	-5.562473	-3.074477	-1.991243
C	-7.762244	-1.472231	-2.662586
H	-7.929860	-3.265778	-1.445587
H	-7.906044	-1.757853	-0.530156
C	-7.217367	-0.053727	-2.513792
H	-7.282664	-1.965488	-3.517874
H	-8.836795	-1.439344	-2.869863
H	-7.862203	0.501577	-1.817664
H	-7.269231	0.480252	-3.469049

TS-1-major-8

M06-2X/6-31G* Energy = -8271.53375667

M06-2X/6-31G* Free Energy = -8270.646339

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.51188284

M06-2X/def2-TZVPP-SMD(toluene) Energy = -8277.51850655

Number of Imaginary Frequencies = 1

Lowest Frequency = 86.9147i

M06-2X/6-31G* Geometry

C	-1.265033	-2.792987	0.101178
C	-1.903036	-2.106033	1.620905
C	-2.330519	-2.576026	-0.794705
H	-0.403378	-2.140447	-0.023311
H	-0.981705	-3.825755	0.299423
C	-2.726451	-1.233839	-1.126262
H	-3.017112	-3.390847	-1.030675
N	-2.293682	-0.796045	1.303825
C	-3.080779	-2.940246	2.114749
C	-0.699106	-2.174999	2.551261
C	-3.315461	-0.676822	0.329926

C	-3.857778	0.717571	0.138399
H	-4.143751	-1.337289	0.592809
H	-1.505041	-0.163944	1.116625
H	-1.902425	-0.556374	-1.372138
H	-3.537497	-1.175878	-1.852743
C	4.944888	-1.664094	-1.086391
C	4.963857	-2.853482	-1.827957
C	3.713744	-1.180228	-0.594770
C	2.529668	-1.800762	-0.989620
C	2.529332	-2.989298	-1.730836
C	3.762951	-3.511134	-2.103411
C	3.632225	-0.010180	0.329984
C	4.282291	-0.018925	1.584211
C	4.286024	1.151146	2.353914
C	3.674404	2.302134	1.852509
C	2.971495	2.322193	0.650559
C	2.898577	1.113758	-0.060509
O	1.343257	-1.266584	-0.555282
O	2.148345	1.046627	-1.214478
P	0.759443	0.167234	-1.172924
O	-0.158203	0.632348	-0.069950
O	0.260414	0.003367	-2.559361
C	1.261902	-3.681279	-2.080375
C	2.465915	3.606584	0.099087
C	1.033207	-5.009944	-1.622587
C	-0.148804	-5.655579	-1.884549
C	-1.176053	-5.010872	-2.623484
C	-0.935383	-3.696135	-3.116702
C	0.295852	-3.052252	-2.831718
C	1.184373	3.741202	-0.507407
C	0.808778	4.930586	-1.074270
C	1.656864	6.067778	-1.042707
C	2.922946	5.953483	-0.407955
C	3.299916	4.704254	0.144178
H	3.785971	-4.436570	-2.676284
H	3.719607	3.218187	2.437999
H	1.807995	-5.500233	-1.039114
H	-0.317817	-6.666088	-1.520371
H	4.291959	4.609390	0.579891
H	-0.161602	5.018067	-1.554150
H	0.505589	2.894644	-0.509650
H	0.450046	-2.032760	-3.177662
C	-0.595933	-3.201570	3.494959
C	0.502770	-3.267162	4.347853
C	1.506456	-2.306842	4.271556
C	1.412232	-1.287643	3.326553
C	0.327010	-1.226527	2.459760
H	-1.377328	-3.949760	3.576874
H	0.565688	-4.068955	5.076821
H	2.359896	-2.353961	4.942272
H	0.313869	-0.441753	1.707357
H	2.187277	-0.529814	3.247698
C	-3.869162	-2.378468	3.126887
C	-4.931918	-3.087956	3.672793
C	-5.218270	-4.376453	3.224666
C	-4.434424	-4.944582	2.227315
C	-3.371491	-4.230675	1.673999
H	-2.771789	-4.702920	0.901744
H	-3.639198	-1.375505	3.474433
H	-5.536718	-2.633691	4.451233
H	-6.047333	-4.932093	3.650949
H	-4.646204	-5.947741	1.871132
C	-5.238589	0.869526	0.013434

C	-5.774850	2.142358	-0.135167
C	-4.967693	3.271651	-0.140094
C	-3.594191	3.091051	-0.013802
Br	-7.646102	2.344566	-0.311457
H	-5.394045	4.262731	-0.236307
C	-3.019097	1.832202	0.103560
H	-1.937620	1.726188	0.156980
H	-5.897547	0.007399	0.041648
Br	-2.471302	4.606608	0.023552
C	3.777788	7.087116	-0.366698
C	3.390247	8.276727	-0.927042
C	2.127879	8.390224	-1.560570
C	1.284022	7.310882	-1.617334
H	4.746560	6.992750	0.117533
H	4.050596	9.137734	-0.889848
H	0.314928	7.390126	-2.103611
H	1.833347	9.336959	-2.002893
C	-1.961560	-3.031058	-3.844714
C	-3.173555	-3.638084	-4.057556
C	-3.415408	-4.944579	-3.560435
C	-2.439389	-5.614918	-2.865244
H	-1.763201	-2.023703	-4.203517
H	-3.952817	-3.122554	-4.610609
H	-4.376834	-5.416210	-3.739593
H	-2.619035	-6.619927	-2.490874
C	6.257790	-3.468307	-2.329022
C	7.411574	-2.471013	-2.394027
H	6.086073	-3.923197	-3.310787
H	6.538536	-4.290546	-1.655275
C	7.487897	-1.687607	-1.086654
H	7.249318	-1.770366	-3.223176
H	8.350072	-2.997884	-2.594889
C	6.219581	-0.859085	-0.897043
H	7.601269	-2.389507	-0.248213
H	8.362541	-1.029228	-1.074080
H	6.230705	-0.360827	0.074958
H	6.206451	-0.048962	-1.640428
C	4.872157	-1.306383	2.136468
C	5.842330	-1.075463	3.292726
H	5.355724	-1.887691	1.348260
H	4.036422	-1.931686	2.486440
C	5.215569	-0.147221	4.328972
H	6.117078	-2.036415	3.740022
H	6.768363	-0.620576	2.914065
C	4.970637	1.224822	3.706604
H	4.262478	-0.577633	4.667826
H	5.854270	-0.049815	5.212865
H	5.936832	1.734914	3.585870
H	4.376042	1.853475	4.378748

TS-1-major-9

M06-2X/6-31G* Energy = -8271.53285970

M06-2X/6-31G* Free Energy = -8270.645363

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.51040779

M06-2X/def2-TZVPP-SMD(toluene) Energy = -8277.51704189

Number of Imaginary Frequencies = 1

Lowest Frequency = 151.6080i

M06-2X/6-31G* Geometry

C	-0.930023	2.803538	0.048718
C	-0.122276	2.705215	1.523828
C	0.031554	3.370938	-0.848711
H	-1.179339	1.763610	-0.155662
H	-1.831395	3.396271	0.203887

C	1.181747	2.642041	-1.214827
H	0.004600	4.446142	-1.030142
N	1.050322	1.942265	1.264930
C	0.226201	4.095265	2.048558
C	-1.080513	1.951241	2.449144
C	1.977490	2.462321	0.378233
C	3.200039	1.605482	0.157354
H	2.255274	3.488144	0.625311
H	0.837024	0.964101	1.020656
H	1.040204	1.585659	-1.452336
H	1.885181	3.156565	-1.867065
C	-4.546184	-2.499154	-1.429510
C	-5.424591	-1.666324	-2.137693
C	-3.377153	-1.946871	-0.866786
C	-3.050327	-0.624469	-1.160958
C	-3.913042	0.224795	-1.859817
C	-5.111811	-0.313781	-2.309889
C	-2.474258	-2.703949	0.055492
C	-2.944711	-3.200080	1.290302
C	-2.064836	-3.926532	2.104040
C	-0.755276	-4.147043	1.675512
C	-0.239301	-3.624571	0.489255
C	-1.124808	-2.853596	-0.284255
O	-1.868584	-0.122178	-0.681459
O	-0.681204	-2.235631	-1.433113
P	-0.431609	-0.614292	-1.358144
O	0.554731	-0.273021	-0.270159
O	-0.255307	-0.095914	-2.734580
C	-3.542646	1.654235	-2.058433
C	1.153985	-3.951114	0.078134
C	-2.461741	2.000529	-2.918931
C	-2.083278	3.310756	-3.066505
C	-2.736703	4.350884	-2.350034
C	-3.820599	4.011123	-1.492590
C	-4.209642	2.648390	-1.379667
C	1.666894	-5.246075	0.390568
C	2.951037	-5.603953	0.077139
C	3.811973	-4.703854	-0.603357
C	3.295413	-3.432720	-0.967254
C	1.980566	-3.070082	-0.585772
H	-5.805636	0.327694	-2.849696
H	-0.091879	-4.716812	2.322374
H	-1.918087	1.209087	-3.425334
H	-1.260489	3.566964	-3.730791
H	1.657513	-2.060424	-0.796750
H	3.321948	-6.592881	0.334805
H	1.014270	-5.967818	0.872860
H	-5.026214	2.389440	-0.709279
C	-1.826661	2.632825	3.412882
C	-2.706486	1.940894	4.242811
C	-2.845728	0.562129	4.123547
C	-2.109209	-0.120567	3.158125
C	-1.242728	0.566812	2.316160
H	-1.719898	3.706570	3.527840
H	-3.276629	2.486133	4.988552
H	-3.525569	0.022329	4.776526
H	-0.719562	0.002645	1.548383
H	-2.199576	-1.197762	3.046474
C	1.187620	4.184852	3.062535
C	1.515421	5.413878	3.622566
C	0.878356	6.574534	3.186579
C	-0.086375	6.493067	2.188903
C	-0.411696	5.261183	1.621898

H	-1.180952	5.230622	0.854629
H	1.676592	3.276802	3.403879
H	2.267901	5.464790	4.403202
H	1.132440	7.534682	3.624195
H	-0.594357	7.388081	1.843536
C	4.215874	2.078140	-0.674757
C	5.376400	1.330736	-0.830498
C	5.568942	0.133781	-0.154010
C	4.550400	-0.315328	0.679196
Br	6.735422	1.959649	-1.984526
H	6.480388	-0.439576	-0.272886
C	3.364008	0.391911	0.830566
H	2.594340	-0.004349	1.480418
H	4.116265	3.023610	-1.198301
Br	4.798906	-1.923034	1.626758
C	4.126885	-2.525450	-1.676258
C	5.422818	-2.854971	-1.978953
C	5.946938	-4.113207	-1.590063
C	5.157295	-5.018693	-0.927316
H	3.713790	-1.560607	-1.962607
H	6.051609	-2.151611	-2.518440
H	5.551979	-5.989939	-0.639255
H	6.976361	-4.362137	-1.829637
C	-4.443516	5.037433	-0.733295
C	-4.005006	6.335530	-0.811765
C	-2.926389	6.673887	-1.665928
C	-2.313156	5.704559	-2.420508
H	-5.270128	4.772423	-0.079082
H	-4.486364	7.109771	-0.222489
H	-2.592697	7.705291	-1.726992
H	-1.491071	5.959113	-3.085927
C	-6.734743	-2.182615	-2.704406
C	-6.768554	-3.701146	-2.860097
H	-6.932123	-1.693576	-3.664733
H	-7.549966	-1.877597	-2.032707
C	-6.264456	-4.363987	-1.580826
H	-6.124825	-4.002169	-3.696595
H	-7.785143	-4.028691	-3.100903
C	-4.802518	-3.993635	-1.344406
H	-6.875340	-4.027038	-0.731261
H	-6.365526	-5.452641	-1.637133
H	-4.450271	-4.397166	-0.391689
H	-4.182457	-4.476224	-2.113428
C	-4.336913	-2.845289	1.787563
C	-4.813796	-3.739776	2.929508
H	-5.063022	-2.858281	0.972157
H	-4.310764	-1.800441	2.133879
C	-3.741609	-3.833269	4.010929
H	-5.751005	-3.347072	3.337312
H	-5.027206	-4.746875	2.545144
C	-2.495560	-4.504979	3.439777
H	-3.493504	-2.821289	4.361015
H	-4.103342	-4.391906	4.880321
H	-1.662043	-4.438907	4.147858
H	-2.702215	-5.576725	3.309474

TS-2-major

M06-2X/6-31G* Energy = -8271.54707643

M06-2X/6-31G* Free Energy = -8270.656049

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.51702981

M06-2X/def2-TZVPP-SMD(toluene) Energy = -8277.52315255

Number of Imaginary Frequencies = 1

Lowest Frequency = 271.6409i

M06-2X/6-31G* Geometry

C	-0.786664	3.211192	1.488010
C	-1.114539	3.466860	-0.210030
C	-2.018232	2.692880	1.980135
H	0.047018	2.503217	1.458881
H	-0.482925	4.182272	1.877745
C	-2.474103	1.418263	1.580951
H	-2.737711	3.373229	2.436183
N	-1.577498	2.221103	-0.683073
C	-2.176096	4.550207	-0.399482
C	0.224209	3.878910	-0.813214
C	-2.766362	1.754443	-0.144346
C	-3.329612	0.482809	-0.711669
H	-3.531540	2.530059	-0.131759
H	-0.845751	1.492754	-0.685126
H	-1.721267	0.630589	1.478887
H	-3.433043	1.089522	1.982194
C	1.739441	-3.929842	-0.652015
C	0.493186	-4.551628	-0.504278
C	2.088096	-2.881675	0.226392
C	1.124372	-2.381358	1.100552
C	-0.147704	-2.954466	1.230247
C	-0.406837	-4.077111	0.450320
C	3.450489	-2.267054	0.240459
C	4.590848	-3.055234	0.512497
C	5.861864	-2.473267	0.425889
C	5.970207	-1.113971	0.135839
C	4.861347	-0.288292	-0.025105
C	3.594799	-0.889130	0.034869
O	1.433022	-1.246357	1.818655
O	2.476449	-0.118190	-0.195071
P	1.339328	0.156350	0.969255
O	0.035305	0.204399	0.209906
O	1.705920	1.266846	1.886863
C	-1.206776	-2.349846	2.074491
C	5.059862	1.170099	-0.218364
C	-0.916552	-1.743451	3.333189
C	-1.905704	-1.153151	4.074049
C	-3.249551	-1.122694	3.615307
C	-3.556460	-1.752818	2.377724
C	-2.512984	-2.358605	1.632837
C	6.004409	1.633001	-1.178278
C	6.266375	2.970926	-1.324166
C	5.598341	3.933062	-0.520896
C	4.644608	3.476108	0.429100
C	4.398823	2.087666	0.565869
H	-1.370380	-4.572667	0.549136
H	6.959700	-0.662298	0.094993
H	0.104500	-1.743510	3.694505
H	-1.667317	-0.687961	5.027146
H	3.672751	1.762561	1.305566
H	6.988789	3.312473	-2.061586
H	6.512568	0.905493	-1.805848
H	-2.748601	-2.788926	0.662351
C	1.155190	2.928075	-1.247898
C	2.352825	3.333350	-1.826504
C	2.644327	4.686922	-1.970188
C	1.739977	5.635744	-1.507599
C	0.537119	5.236327	-0.933009
H	0.972981	1.863870	-1.145520
H	3.069735	2.579882	-2.140925
H	3.586684	4.998103	-2.409077
H	-0.165471	5.990259	-0.592695
H	1.969212	6.693705	-1.590969

C	-2.564184	5.458715	0.583676
C	-3.502750	6.452373	0.302973
C	-4.065553	6.547414	-0.963740
C	-3.678727	5.647013	-1.955548
C	-2.738723	4.663001	-1.677561
H	-2.428861	3.965174	-2.450104
H	-2.129045	5.419816	1.577158
H	-3.789324	7.151447	1.082262
H	-4.797852	7.318558	-1.180170
H	-4.107187	5.713901	-2.950583
C	-2.524666	-0.547290	-1.204747
C	-3.144468	-1.665964	-1.747911
C	-4.527843	-1.812380	-1.779084
C	-5.297869	-0.791758	-1.238415
Br	-2.072409	-3.084988	-2.385979
H	-4.987064	-2.707445	-2.181495
C	-4.719174	0.358217	-0.722223
H	-5.349654	1.137975	-0.306426
H	-1.441232	-0.509326	-1.126434
Br	-7.166583	-1.022248	-1.096329
C	3.932539	4.424863	1.210459
C	4.167731	5.766831	1.060121
C	5.130389	6.223823	0.124507
C	5.829140	5.328993	-0.645849
H	3.186910	4.053428	1.909267
H	3.614602	6.488975	1.653348
H	6.565739	5.675763	-1.367015
H	5.312835	7.289454	0.020508
C	-4.891602	-1.704507	1.895720
C	-5.866021	-1.027042	2.583629
C	-5.556892	-0.391220	3.812442
C	-4.282775	-0.451336	4.320872
H	-5.128005	-2.204241	0.960662
H	-6.874163	-0.980084	2.181961
H	-6.336113	0.134803	4.355724
H	-4.042192	0.025122	5.268117
C	0.073167	-5.716684	-1.379070
C	0.800901	-5.720717	-2.720154
H	-1.013201	-5.685059	-1.524413
H	0.285316	-6.659265	-0.855040
C	2.304472	-5.619830	-2.476233
H	0.470054	-4.859322	-3.317881
H	0.551581	-6.624793	-3.285013
C	2.650730	-4.287646	-1.814120
H	2.616971	-6.449235	-1.826460
H	2.863535	-5.719333	-3.412275
H	3.701016	-4.274607	-1.512416
H	2.551093	-3.481877	-2.555819
C	4.444217	-4.486283	1.006033
C	5.717525	-5.313518	0.846042
H	3.604578	-4.991248	0.524914
H	4.181947	-4.437898	2.073142
C	6.911233	-4.560226	1.424856
H	5.589060	-6.283471	1.337631
H	5.896901	-5.514174	-0.219758
C	7.134168	-3.273233	0.635570
H	6.708503	-4.319994	2.476616
H	7.816550	-5.175702	1.402186
H	7.552273	-3.530474	-0.348212
H	7.881233	-2.641902	1.129027

TS-2-major-2

M06-2X/6-31G* Energy = -8271.54707644

M06-2X/6-31G* Free Energy = -8270.656050

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.51665425

M06-2X/def2-TZVPP-SMD(toluene) Energy = -8277.52315256

Number of Imaginary Frequencies = 1

Lowest Frequency = 271.6359i

M06-2X/6-31G* Geometry

C	-0.786812	3.211115	1.488006
C	-1.114724	3.466741	-0.210159
C	-2.018392	2.692885	1.980063
H	0.046843	2.503115	1.458780
H	-0.483031	4.182225	1.877627
C	-2.474279	1.418249	1.580839
H	-2.737895	3.373272	2.436012
N	-1.577680	2.220983	-0.683095
C	-2.176258	4.550108	-0.399593
C	0.224056	3.878779	-0.813238
C	-2.766586	1.754349	-0.144319
C	-3.329842	0.482713	-0.711647
H	-3.531758	2.529974	-0.131789
H	-0.845973	1.492591	-0.685150
H	-1.721414	0.630597	1.478835
H	-3.433193	1.089474	1.982120
C	1.739664	-3.929890	-0.651945
C	0.493452	-4.551747	-0.504151
C	2.088285	-2.881664	0.226407
C	1.124554	-2.381368	1.100572
C	-0.147463	-2.954584	1.230359
C	-0.406561	-4.077266	0.450477
C	3.450637	-2.266951	0.240384
C	4.591064	-3.055046	0.512393
C	5.862036	-2.472998	0.425649
C	5.970269	-1.113710	0.135537
C	4.861347	-0.288108	-0.025355
C	3.594843	-0.889029	0.034713
O	1.433114	-1.246284	1.818582
O	2.476431	-0.118177	-0.195229
P	1.339320	0.156367	0.969101
O	0.035293	0.204328	0.209754
O	1.705877	1.266921	1.886656
C	-1.206529	-2.349973	2.074614
C	5.059781	1.170296	-0.218586
C	-0.916298	-1.743570	3.333305
C	-1.905435	-1.153218	4.074142
C	-3.249271	-1.122700	3.615370
C	-3.556187	-1.752842	2.377798
C	-2.512729	-2.358701	1.632946
C	6.004302	1.633287	-1.178484
C	6.266251	2.971226	-1.324269
C	5.598223	3.933292	-0.520910
C	4.644500	3.476251	0.429054
C	4.398733	2.087796	0.565719
H	-1.370082	-4.572859	0.549336
H	6.959729	-0.661975	0.094607
H	0.104751	-1.743662	3.694630
H	-1.667042	-0.688018	5.027233
H	3.672680	1.762635	1.305407
H	6.988650	3.312837	-2.061674
H	6.512462	0.905833	-1.806114
H	-2.748348	-2.789011	0.662456
C	1.154984	2.927964	-1.248085
C	2.352647	3.333281	-1.826607
C	2.644224	4.686862	-1.970051
C	1.739928	5.635655	-1.507295

C	0.537046	5.236199	-0.932787
H	0.972714	1.863750	-1.145889
H	3.069521	2.579832	-2.141153
H	3.586599	4.998069	-2.408880
H	-0.165507	5.990110	-0.592350
H	1.969225	6.693616	-1.590474
C	-2.738920	4.662852	-1.677661
C	-3.678904	5.646877	-1.955670
C	-4.065673	6.547340	-0.963898
C	-3.502833	6.452348	0.302803
C	-2.564288	5.458679	0.583531
H	-2.129127	5.419812	1.577004
H	-2.429101	3.964980	-2.450178
H	-4.107392	5.713726	-2.950696
H	-4.797955	7.318495	-1.180345
H	-3.789360	7.151471	1.082064
C	-2.524895	-0.547435	-1.204614
C	-3.144694	-1.666129	-1.747745
C	-4.528071	-1.812510	-1.778997
C	-5.298102	-0.791840	-1.238424
Br	-2.072621	-3.085258	-2.385561
H	-4.987290	-2.707598	-2.181358
C	-4.719407	0.358154	-0.722273
H	-5.349890	1.137936	-0.306526
H	-1.441462	-0.509509	-1.126217
Br	-7.166814	-1.022324	-1.096312
C	3.932439	4.424929	1.210512
C	4.167623	5.766912	1.060292
C	5.130264	6.223993	0.124703
C	5.829011	5.329235	-0.645743
H	3.186823	4.053421	1.909296
H	3.614503	6.488999	1.653595
H	6.565598	5.676072	-1.366888
H	5.312706	7.289634	0.020801
C	-4.891298	-1.704429	1.895728
C	-5.865692	-1.026856	2.583569
C	-5.556564	-0.391030	3.812381
C	-4.282474	-0.451241	4.320872
H	-5.127695	-2.204157	0.960666
H	-6.873804	-0.979807	2.181835
H	-6.335762	0.135085	4.355607
H	-4.041893	0.025229	5.268112
C	0.073447	-5.716815	-1.378930
C	0.801104	-5.720797	-2.720055
H	-1.012932	-5.685243	-1.524213
H	0.285665	-6.659393	-0.854921
C	2.304685	-5.619826	-2.476230
H	0.470157	-4.859428	-3.317765
H	0.551808	-6.624891	-3.284897
C	2.650933	-4.287656	-1.814077
H	2.617283	-6.449245	-1.826523
H	2.863685	-5.719253	-3.412318
H	2.551292	-3.481858	-2.555742
H	3.701224	-4.274626	-1.512384
C	4.444577	-4.486082	1.006016
C	5.717935	-5.313228	0.845974
H	3.604939	-4.991131	0.524980
H	4.182374	-4.437662	2.073140
C	6.911650	-4.559820	1.424627
H	5.589582	-6.283157	1.337641
H	5.897230	-5.513947	-0.219828
C	7.134415	-3.272863	0.635243
H	6.709017	-4.319546	2.476395

H	7.817003	-5.175241	1.401892
H	7.552432	-3.530135	-0.348568
H	7.881488	-2.641448	1.128580

TS-2-major-3

M06-2X/6-31G* Energy = -8271.54519792

M06-2X/6-31G* Free Energy = -8270.653471

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.51681923

M06-2X/def2-TZVPP-SMD(toluene) Energy = -8277.52282000

Number of Imaginary Frequencies = 1

Lowest Frequency = 266.9315i

M06-2X/6-31G* Geometry

C	-0.900787	3.271976	1.296513
C	-1.276467	3.421001	-0.410136
C	-2.096243	2.729406	1.842732
H	-0.046444	2.588157	1.287035
H	-0.625352	4.273655	1.624804
C	-2.498587	1.417568	1.509649
H	-2.834307	3.395675	2.289757
N	-1.694843	2.135303	-0.806737
C	-2.383200	4.450351	-0.630959
C	0.041024	3.849162	-1.047428
C	-2.848088	1.639838	-0.215322
C	-3.355205	0.309315	-0.702029
H	-3.653681	2.374152	-0.227439
H	-0.935581	1.433938	-0.790534
H	-1.710805	0.664894	1.421364
H	-3.421157	1.057512	1.966797
C	2.055460	-3.871813	-0.791104
C	0.849578	-4.582711	-0.810917
C	2.213131	-2.834249	0.150556
C	1.119520	-2.437744	0.921138
C	-0.113483	-3.110063	0.896588
C	-0.180352	-4.219789	0.055209
C	3.512258	-2.114641	0.328917
C	4.678129	-2.812353	0.713865
C	5.900269	-2.129233	0.761472
C	5.930489	-0.764010	0.479359
C	4.781623	-0.027594	0.205426
C	3.567362	-0.727862	0.145927
O	1.278098	-1.312300	1.699775
O	2.414673	-0.046517	-0.178777
P	1.175985	0.116480	0.898048
O	-0.059949	0.134018	0.034474
O	1.404504	1.199724	1.892133
C	-1.323217	-2.630565	1.617142
C	4.878380	1.439744	0.000829
C	-2.606366	-2.973921	1.092332
C	-3.763881	-2.497229	1.641938
C	-3.728713	-1.602591	2.740470
C	-2.465823	-1.294189	3.314615
C	-1.282396	-1.837214	2.748113
C	5.867921	1.963908	-0.879180
C	6.018923	3.316108	-1.048763
C	5.185110	4.232365	-0.354259
C	4.188869	3.713070	0.516288
C	4.063345	2.312284	0.685296
H	-1.091500	-4.810752	0.027161
H	6.881161	-0.236660	0.533782
H	-2.664910	-3.585176	0.198433
H	-4.727650	-2.756108	1.210868
H	3.304059	1.939239	1.367066
H	6.777210	3.704072	-1.724660

H	6.500075	1.270925	-1.428245
H	-0.333953	-1.575141	3.201161
C	1.025030	2.910329	-1.379872
C	2.213905	3.320505	-1.972111
C	2.444457	4.668935	-2.230498
C	1.484361	5.608873	-1.874115
C	0.289378	5.203876	-1.285971
H	0.890435	1.851407	-1.186316
H	2.972238	2.577394	-2.202755
H	3.380810	4.985596	-2.678301
H	-0.454383	5.949844	-1.025167
H	1.663946	6.665238	-2.049088
C	-2.780427	5.399021	0.309865
C	-3.762693	6.339953	-0.000641
C	-4.360351	6.341770	-1.255076
C	-3.965179	5.400590	-2.204682
C	-2.982005	4.468672	-1.897351
H	-2.666236	3.738787	-2.637141
H	-2.320176	5.431724	1.292161
H	-4.056408	7.071275	0.745709
H	-5.126770	7.071907	-1.494389
H	-4.421245	5.394448	-3.189629
C	-2.549630	-0.612526	-1.373946
C	-3.126957	-1.790003	-1.832915
C	-4.467884	-2.092078	-1.626637
C	-5.229934	-1.180615	-0.907958
Br	-2.029536	-3.076557	-2.680828
H	-4.892041	-3.027276	-1.972353
C	-4.698358	0.018097	-0.457780
H	-5.324715	0.711770	0.095503
H	-1.485872	-0.451180	-1.503305
Br	-7.004983	-1.630540	-0.440059
C	3.310333	4.611047	1.179560
C	3.426110	5.963992	0.993237
C	4.431719	6.484415	0.139529
C	5.290370	5.639394	-0.516533
H	2.541462	4.190071	1.823296
H	2.746278	6.646035	1.495436
H	6.059784	6.034485	-1.175958
H	4.518220	7.558861	0.006362
C	-2.417703	-0.380054	4.402302
C	-3.562453	0.218050	4.866898
C	-4.816885	-0.071593	4.272100
C	-4.898218	-0.968025	3.234797
H	-1.451344	-0.144995	4.840974
H	-3.511597	0.921713	5.692287
H	-5.712878	0.415892	4.644539
H	-5.850304	-1.192329	2.756947
C	0.607406	-5.732117	-1.770520
C	1.525818	-5.681093	-2.988141
H	-0.445066	-5.721922	-2.079565
H	0.763975	-6.683367	-1.242617
C	2.968943	-5.488335	-2.529818
H	1.235018	-4.838805	-3.630591
H	1.417383	-6.595026	-3.581124
C	3.127086	-4.138324	-1.833707
H	3.237411	-6.296724	-1.835286
H	3.661987	-5.549068	-3.375172
H	3.056711	-3.336865	-2.583400
H	4.127405	-4.045851	-1.403857
C	4.595996	-4.258308	1.176795
C	5.942481	-4.977654	1.149182
H	3.856694	-4.819107	0.601288

H	4.216228	-4.250091	2.208949
C	7.002021	-4.138846	1.857452
H	5.842494	-5.962116	1.617949
H	6.250218	-5.146932	0.107547
C	7.203457	-2.827449	1.103372
H	6.668701	-3.930073	2.882298
H	7.951511	-4.679355	1.929854
H	7.744577	-3.036760	0.169451
H	7.839406	-2.145249	1.678174

TS-2-major-4

M06-2X/6-31G* Energy = -8271.54519796

M06-2X/6-31G* Free Energy = -8270.653470

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.51681938

M06-2X/def2-TZVPP-SMD(toluene) Energy = -8277.52282003

Number of Imaginary Frequencies = 1

Lowest Frequency = 266.8594i

M06-2X/6-31G* Geometry

C	-0.900814	3.271879	1.296492
C	-1.276596	3.420988	-0.410107
C	-2.096249	2.729298	1.842744
H	-0.046477	2.588058	1.286945
H	-0.625356	4.273547	1.624797
C	-2.498609	1.417470	1.509636
H	-2.834284	3.395556	2.289833
N	-1.694969	2.135295	-0.806759
C	-2.383368	4.450320	-0.630814
C	0.040854	3.849202	-1.047451
C	-2.848161	1.639756	-0.215304
C	-3.355209	0.309217	-0.702039
H	-3.653794	2.374026	-0.227381
H	-0.935697	1.433957	-0.790670
H	-1.710821	0.664804	1.421320
H	-3.421164	1.057408	1.966811
C	4.678221	-2.812218	0.713871
C	5.900339	-2.129059	0.761488
C	3.512330	-2.114537	0.328932
C	3.567390	-0.727754	0.145958
C	4.781630	-0.027450	0.205455
C	5.930518	-0.763833	0.479384
C	2.213225	-2.834183	0.150555
C	2.055595	-3.871742	-0.791118
C	0.849740	-4.582686	-0.810943
C	-0.180209	-4.219805	0.055176
C	-0.113387	-3.110079	0.896561
C	1.119595	-2.437722	0.921132
O	2.414674	-0.046444	-0.178726
O	1.278137	-1.312298	1.699802
P	1.176017	0.116519	0.898142
O	-0.059938	0.134124	0.034602
O	1.404575	1.199711	1.892272
C	4.878343	1.439889	0.000840
C	-1.323148	-2.630625	1.617098
C	5.867856	1.964066	-0.879192
C	6.018803	3.316267	-1.048817
C	5.184956	4.232511	-0.354338
C	4.188746	3.713202	0.516237
C	4.063284	2.312417	0.685293
C	-2.606276	-2.974010	1.092255
C	-3.763816	-2.497351	1.641836
C	-3.728698	-1.602723	2.740376
C	-2.465830	-1.294296	3.314557
C	-1.282374	-1.837284	2.748079

H	6.881174	-0.236455	0.533812
H	-1.091336	-4.810800	0.027119
H	6.500030	1.271091	-1.428244
H	6.777069	3.704241	-1.724733
H	-0.333949	-1.575191	3.201151
H	-4.727568	-2.756249	1.210739
H	-2.664782	-3.585261	0.198350
H	3.304022	1.939361	1.367085
C	1.024929	2.910411	-1.379805
C	2.213762	3.320612	-1.972109
C	2.444206	4.669034	-2.230641
C	1.484042	5.608935	-1.874348
C	0.289097	5.203910	-1.286143
H	0.890418	1.851502	-1.186119
H	2.972148	2.577535	-2.202684
H	3.380529	4.985719	-2.678490
H	-0.454716	5.949851	-1.025411
H	1.663542	6.665295	-2.049437
C	-2.982304	4.468646	-1.897143
C	-3.965518	5.400559	-2.204366
C	-4.360599	6.341728	-1.254712
C	-3.762811	6.339907	-0.000339
C	-2.780504	5.398982	0.310058
H	-2.320150	5.431682	1.292306
H	-2.666605	3.738771	-2.636973
H	-4.421686	5.394419	-3.189265
H	-5.127051	7.071860	-1.493940
H	-4.056454	7.071222	0.746046
C	-2.549573	-0.612595	-1.373923
C	-3.126841	-1.790088	-1.832925
C	-4.467762	-2.092217	-1.626690
C	-5.229869	-1.180791	-0.908026
Br	-2.029345	-3.076587	-2.680822
H	-4.891871	-3.027430	-1.972425
C	-4.698358	0.017945	-0.457834
H	-5.324760	0.711591	0.095432
H	-1.485813	-0.451218	-1.503231
Br	-7.004907	-1.630798	-0.440163
C	-2.417761	-0.380172	4.402255
C	-3.562538	0.217898	4.866829
C	-4.816948	-0.071770	4.271994
C	-4.898232	-0.968193	3.234680
H	-1.451419	-0.145093	4.840955
H	-3.511721	0.921553	5.692227
H	-5.850299	-1.192517	2.756801
H	-5.712963	0.415688	4.644417
C	3.310168	4.611164	1.179475
C	3.425873	5.964106	0.993091
C	4.431454	6.484545	0.139359
C	5.290147	5.639539	-0.516669
H	2.541323	4.190175	1.823234
H	2.746007	6.646136	1.495262
H	4.517898	7.558989	0.006146
H	6.059538	6.034642	-1.176114
C	7.203537	-2.827243	1.103407
C	7.002099	-4.138567	1.857608
H	7.839508	-2.144992	1.678127
H	7.744629	-3.036649	0.169491
C	5.942634	-4.977472	1.149340
H	6.668700	-3.929698	2.882409
H	7.951599	-4.679040	1.930128
C	4.596115	-4.258180	1.176788
H	6.250453	-5.146835	0.107744

H	5.842647	-5.961896	1.618188
H	3.856917	-4.819018	0.601184
H	4.216207	-4.249985	2.208891
C	3.127227	-4.138212	-1.833724
C	2.969194	-5.488290	-2.529730
H	4.127547	-4.045596	-1.403911
H	3.056740	-3.336822	-2.583481
C	1.526099	-5.681146	-2.988108
H	3.662283	-5.549063	-3.375044
H	3.237663	-6.296606	-1.835114
C	0.607622	-5.732117	-1.770532
H	1.235299	-4.838920	-3.630639
H	1.417730	-6.595128	-3.581027
H	0.764152	-6.683349	-1.242586
H	-0.444833	-5.721927	-2.079636

TS-2-major-5

M06-2X/6-31G* Energy = -8271.54504815

M06-2X/6-31G* Free Energy = -8270.654061

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.51585078

M06-2X/def2-TZVPP-SMD(toluene) Energy = -8277.52199159

Number of Imaginary Frequencies = 1

Lowest Frequency = 262.2830i

M06-2X/6-31G* Geometry

C	-0.697950	3.183836	1.731302
C	-0.913944	3.529080	0.031062
C	-1.992453	2.755658	2.142101
H	0.073719	2.408412	1.715603
H	-0.334497	4.109585	2.175849
C	-2.534431	1.540455	1.668700
H	-2.673532	3.477912	2.592976
N	-1.462977	2.349295	-0.513495
C	-1.861602	4.712508	-0.163314
C	0.484087	3.834004	-0.497349
C	-2.712932	1.969650	-0.047957
C	-3.351586	0.778365	-0.703660
H	-3.407928	2.808857	-0.037726
H	-0.799714	1.558766	-0.510170
H	-1.844644	0.696482	1.569401
H	-3.535372	1.278499	2.013684
C	4.292188	-3.344792	0.583833
C	5.592599	-2.824076	0.571790
C	3.197925	-2.482809	0.345566
C	3.418640	-1.103103	0.252591
C	4.713039	-0.565869	0.274720
C	5.777401	-1.452470	0.395780
C	1.806653	-3.020935	0.247324
C	1.429414	-3.981292	-0.715789
C	0.143442	-4.533719	-0.654658
C	-0.763896	-4.070942	0.299111
C	-0.467759	-3.024247	1.166270
C	0.841611	-2.527532	1.124143
O	2.357792	-0.249781	0.049882
O	1.188926	-1.469541	1.934617
P	1.191995	-0.003116	1.195409
O	-0.076088	0.168647	0.393841
O	1.579751	1.011389	2.207809
C	4.971570	0.896094	0.212308
C	-1.521351	-2.396976	2.001362
C	4.404740	1.758595	1.193827
C	4.716617	3.091013	1.208799
C	5.583246	3.653976	0.236570
C	6.123564	2.806037	-0.769928

C	5.813315	1.420100	-0.742524
C	-1.251726	-1.889710	3.307641
C	-2.227372	-1.258221	4.032050
C	-3.536352	-1.084914	3.508493
C	-3.826526	-1.618975	2.222712
C	-2.798189	-2.272230	1.496841
H	6.787011	-1.046777	0.413641
H	-1.760203	-4.507449	0.325500
H	3.715770	1.352429	1.927119
H	4.281136	3.742752	1.962007
H	-3.015081	-2.625898	0.491733
H	-2.003570	-0.868344	5.021742
H	-0.255364	-1.996493	3.718608
H	6.241140	0.770260	-1.503377
C	0.930681	5.157477	-0.555857
C	2.189796	5.456772	-1.069986
C	3.020549	4.440240	-1.529582
C	2.594199	3.117418	-1.442205
C	1.339109	2.813373	-0.928698
H	0.288545	5.965234	-0.219095
H	2.516390	6.491219	-1.116270
H	4.002707	4.671754	-1.932146
H	1.053752	1.768879	-0.873402
H	3.246372	2.306910	-1.754335
C	-2.346964	4.924127	-1.460470
C	-3.178504	6.000881	-1.740805
C	-3.530872	6.896133	-0.731667
C	-3.043329	6.702428	0.554838
C	-2.214413	5.616021	0.837499
H	-1.835960	5.499976	1.847964
H	-2.063198	4.229634	-2.245944
H	-3.548744	6.144100	-2.751049
H	-4.178205	7.739453	-0.949783
H	-3.303862	7.395720	1.348298
C	-2.608792	-0.293473	-1.204974
C	-3.286982	-1.326171	-1.840552
C	-4.673307	-1.349709	-1.955606
C	-5.385301	-0.293605	-1.403352
Br	-2.300419	-2.799100	-2.495988
H	-5.181682	-2.180856	-2.429706
C	-4.743496	0.776034	-0.796675
H	-5.329418	1.587372	-0.376129
H	-1.532451	-0.353760	-1.065630
Br	-7.271635	-0.369615	-1.373552
C	-5.124062	-1.428370	1.677811
C	-6.074503	-0.705902	2.353653
C	-5.781456	-0.166843	3.631614
C	-4.546765	-0.365260	4.199207
H	-5.349555	-1.854810	0.704498
H	-7.051073	-0.548910	1.904437
H	-4.319588	0.036627	5.183625
H	-6.542529	0.394777	4.164942
C	6.944048	3.376885	-1.779409
C	7.215715	4.721744	-1.787641
C	6.686434	5.563587	-0.777807
C	5.891971	5.039172	0.209867
H	7.350857	2.726755	-2.550041
H	7.841351	5.146281	-2.566842
H	6.912283	6.625533	-0.792110
H	5.472303	5.679036	0.982234
C	6.817385	-3.703116	0.744835
C	6.511157	-5.032606	1.428508
H	7.583662	-3.150764	1.299753

H	7.245141	-3.906749	-0.247341
C	5.295547	-5.677495	0.769648
H	6.295486	-4.862132	2.491258
H	7.384794	-5.690687	1.377251
C	4.062138	-4.799005	0.965243
H	5.490808	-5.807358	-0.304292
H	5.106124	-6.673340	1.183650
H	3.209308	-5.222370	0.431441
H	3.777664	-4.815371	2.027590
C	2.357991	-4.308481	-1.873200
C	1.959253	-5.566989	-2.641455
H	3.396596	-4.379358	-1.540797
H	2.329503	-3.447353	-2.556583
C	0.462017	-5.559496	-2.939296
H	2.544705	-5.633209	-3.564215
H	2.199898	-6.457696	-2.044401
C	-0.311689	-5.606329	-1.624978
H	0.202827	-4.639629	-3.482679
H	0.181261	-6.404831	-3.575841
H	-0.173739	-6.594757	-1.164477
H	-1.388679	-5.499355	-1.801759

TS-2-major-6

M06-2X/6-31G* Energy = -8271.54504813

M06-2X/6-31G* Free Energy = -8270.654060

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.51585085

M06-2X/def2-TZVPP-SMD(toluene) Energy = -8277.52199157

Number of Imaginary Frequencies = 1

Lowest Frequency = 262.3223i

M06-2X/6-31G* Geometry

C	-0.697870	3.183887	1.731241
C	-0.913769	3.529047	0.031009
C	-1.992398	2.755708	2.142060
H	0.073788	2.408444	1.715681
H	-0.334443	4.109614	2.175861
C	-2.534404	1.540528	1.668693
H	-2.673459	3.477972	2.592947
N	-1.462864	2.349262	-0.513556
C	-1.861360	4.712514	-0.163488
C	0.484271	3.833873	-0.497468
C	-2.712815	1.969715	-0.048053
C	-3.351552	0.778439	-0.703687
H	-3.407759	2.808966	-0.037854
H	-0.799615	1.558717	-0.510148
H	-1.844668	0.696512	1.569401
H	-3.535373	1.278634	2.013641
C	1.429334	-3.981303	-0.715797
C	0.143360	-4.533726	-0.654642
C	1.806599	-3.020942	0.247302
C	0.841570	-2.527534	1.124133
C	-0.467809	-3.024225	1.166271
C	-0.763967	-4.070926	0.299126
C	3.197880	-2.482833	0.345540
C	4.292144	-3.344829	0.583761
C	5.592558	-2.824124	0.571722
C	5.777370	-1.452511	0.395765
C	4.713014	-0.565900	0.274750
C	3.418609	-1.103126	0.252606
O	1.188902	-1.469551	1.934610
O	2.357779	-0.249779	0.049906
P	1.191945	-0.003132	1.195396
O	-0.076125	0.168591	0.393798
O	1.579646	1.011392	2.207799

C	-1.521378	-2.396927	2.001372
C	4.971537	0.896068	0.212401
C	-1.251724	-1.889653	3.307642
C	-2.227344	-1.258132	4.032058
C	-3.536329	-1.084804	3.508519
C	-3.826536	-1.618879	2.222751
C	-2.798222	-2.272161	1.496869
C	4.404668	1.758519	1.193940
C	4.716517	3.090942	1.208978
C	5.583158	3.653962	0.236793
C	6.123519	2.806074	-0.769725
C	5.813301	1.420128	-0.742385
H	-1.760277	-4.507426	0.325534
H	6.786983	-1.046826	0.413633
H	-0.255359	-1.996455	3.718598
H	-2.003518	-0.868248	5.021741
H	6.241157	0.770330	-1.503256
H	4.281002	3.742640	1.962202
H	3.715689	1.352313	1.927200
H	-3.015136	-2.625837	0.491768
C	1.339182	2.813187	-0.928900
C	2.594278	3.117141	-1.442447
C	3.020749	4.439926	-1.529783
C	2.190108	5.456511	-1.070100
C	0.930987	5.157306	-0.555932
H	1.053742	1.768715	-0.873653
H	3.246359	2.306586	-1.754638
H	4.002910	4.671368	-1.932383
H	0.288938	5.965107	-0.219105
H	2.516795	6.490930	-1.116348
C	-2.346633	4.924098	-1.460682
C	-3.178122	6.000865	-1.741114
C	-3.530527	6.896168	-0.732033
C	-3.043072	6.702500	0.554510
C	-2.214207	5.616077	0.837267
H	-1.835825	5.500062	1.847762
H	-2.062840	4.229562	-2.246109
H	-3.548294	6.144055	-2.751387
H	-4.177821	7.739500	-0.950223
H	-3.303635	7.395831	1.347926
C	-4.743468	0.776168	-0.796626
C	-5.385352	-0.293456	-1.403244
C	-4.673435	-1.349607	-1.955507
C	-3.287102	-1.326129	-1.840527
Br	-7.271688	-0.369382	-1.373350
H	-5.181871	-2.180744	-2.429558
C	-2.608833	-0.293444	-1.205015
H	-1.532487	-0.353770	-1.065735
H	-5.329331	1.587544	-0.376070
Br	-2.300643	-2.799122	-2.495970
C	6.944007	3.376984	-1.779168
C	7.215636	4.721851	-1.787344
C	6.686313	5.563641	-0.777488
C	5.891845	5.039168	0.210151
H	7.350849	2.726895	-2.549817
H	7.841276	5.146435	-2.566517
H	5.472143	5.678990	0.982532
H	6.912133	6.625595	-0.791747
C	-5.124081	-1.428260	1.677875
C	-6.074495	-0.705764	2.353726
C	-5.781412	-0.166687	3.631671
C	-4.546712	-0.365117	4.199241
H	-5.349605	-1.854715	0.704576

H	-7.051072	-0.548763	1.904530
H	-6.542462	0.394957	4.165005
H	-4.319507	0.036780	5.183648
C	-0.311778	-5.606416	-1.624875
C	0.462058	-5.559891	-2.939128
H	-1.388738	-5.499348	-1.801787
H	-0.173998	-6.594786	-1.164200
C	1.959270	-5.567281	-2.641161
H	0.202907	-4.640165	-3.482766
H	0.181366	-6.405387	-3.575489
C	2.357877	-4.308549	-1.873217
H	2.199887	-6.457814	-2.043833
H	2.544804	-5.633741	-3.563852
H	3.396525	-4.379153	-1.540895
H	2.329150	-3.447577	-2.556788
C	4.062113	-4.799067	0.965082
C	5.295488	-5.677547	0.769245
H	3.209204	-5.222374	0.431360
H	3.777788	-4.815523	2.027467
C	6.511148	-5.032784	1.428137
H	5.106082	-6.673461	1.183087
H	5.490670	-5.807223	-0.304732
C	6.817353	-3.703170	0.744691
H	6.295549	-4.862509	2.490933
H	7.384777	-5.690862	1.376702
H	7.245165	-3.906621	-0.247498
H	7.583588	-3.150887	1.299737

TS-2-major-7

M06-2X/6-31G* Energy = -8271.54504815

M06-2X/6-31G* Free Energy = -8270.654060

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.51545757

M06-2X/def2-TZVPP-SMD(toluene) Energy = -8277.52199173

Number of Imaginary Frequencies = 1

Lowest Frequency = 262.3729i

M06-2X/6-31G* Geometry

C	-0.697825	3.183832	1.731367
C	-0.913762	3.529045	0.031157
C	-1.992347	2.755642	2.142209
H	0.073833	2.408392	1.715769
H	-0.334388	4.109550	2.175997
C	-2.534356	1.540466	1.668847
H	-2.673399	3.477902	2.593118
N	-1.462866	2.349274	-0.513425
C	-1.861361	4.712515	-0.163281
C	0.484266	3.833886	-0.497339
C	-2.712810	1.969719	-0.047916
C	-3.351562	0.778465	-0.703570
H	-3.407749	2.808972	-0.037660
H	-0.799617	1.558727	-0.510048
H	-1.844621	0.696456	1.569498
H	-3.535319	1.278561	2.013804
C	1.429318	-3.981253	-0.716023
C	0.143347	-4.533684	-0.654864
C	1.806605	-3.020941	0.247116
C	0.841596	-2.527582	1.123997
C	-0.467781	-3.024274	1.166138
C	-0.763959	-4.070932	0.298947
C	3.197888	-2.482836	0.345354
C	4.292157	-3.344845	0.583508
C	5.592570	-2.824137	0.571484
C	5.777376	-1.452513	0.395602
C	4.713017	-0.565897	0.274648

C	3.418613	-1.103124	0.252494
O	1.188949	-1.469645	1.934525
O	2.357775	-0.249769	0.049861
P	1.191969	-0.003184	1.195392
O	-0.076123	0.168577	0.393836
O	1.579691	1.011286	2.207841
C	-1.521329	-2.397019	2.001298
C	4.971537	0.896074	0.212362
C	-1.251639	-1.889814	3.307587
C	-2.227238	-1.258325	4.032059
C	-3.536235	-1.084966	3.508563
C	-3.826478	-1.618976	2.222777
C	-2.798185	-2.272224	1.496834
C	4.404685	1.758481	1.193952
C	4.716524	3.090905	1.209038
C	5.583136	3.653973	0.236854
C	6.123480	2.806130	-0.769711
C	5.813275	1.420180	-0.742421
H	-1.760267	-4.507437	0.325358
H	6.786989	-1.046828	0.413478
H	-0.255264	-1.996640	3.718512
H	-2.003385	-0.868490	5.021756
H	6.241116	0.770417	-1.503330
H	4.281024	3.742569	1.962300
H	3.715727	1.352238	1.927211
H	-3.015126	-2.625851	0.491722
C	1.339171	2.813209	-0.928805
C	2.594257	3.117173	-1.442371
C	3.020725	4.439959	-1.529692
C	2.190091	5.456535	-1.069978
C	0.930979	5.157321	-0.555792
H	1.053734	1.768736	-0.873570
H	3.246330	2.306621	-1.754588
H	4.002879	4.671409	-1.932305
H	0.288935	5.965116	-0.218941
H	2.516775	6.490955	-1.116216
C	-2.346684	4.924126	-1.460452
C	-3.178189	6.000895	-1.740829
C	-3.530559	6.896175	-0.731715
C	-3.043053	6.702481	0.554805
C	-2.214174	5.616055	0.837507
H	-1.835754	5.500017	1.847986
H	-2.062919	4.229609	-2.245906
H	-3.548402	6.144105	-2.751084
H	-4.177865	7.739508	-0.949862
H	-3.303588	7.395794	1.348246
C	-2.608855	-0.293394	-1.204966
C	-3.287141	-1.326052	-1.840506
C	-4.673477	-1.349525	-1.955449
C	-5.385380	-0.293400	-1.403120
Br	-2.300697	-2.799011	-2.496043
H	-5.181925	-2.180641	-2.429526
C	-4.743481	0.776197	-0.796471
H	-5.329333	1.587555	-0.375865
H	-1.532504	-0.353722	-1.065722
Br	-7.271716	-0.369323	-1.373187
C	6.943935	3.377088	-1.779153
C	7.215548	4.721959	-1.787285
C	6.686241	5.563704	-0.777383
C	5.891805	5.039183	0.210256
H	7.350765	2.727034	-2.549838
H	7.841163	5.146580	-2.566458
H	5.472114	5.678971	0.982672

H	6.912045	6.625662	-0.791609
C	-5.124039	-1.428327	1.677948
C	-6.074432	-0.705861	2.353860
C	-5.781311	-0.166846	3.631822
C	-4.546597	-0.365308	4.199348
H	-5.349593	-1.854736	0.704636
H	-7.051020	-0.548836	1.904698
H	-6.542345	0.394775	4.165204
H	-4.319362	0.036541	5.183769
C	-0.311806	-5.606349	-1.625118
C	0.462041	-5.559841	-2.939366
H	-1.388761	-5.499251	-1.802041
H	-0.174061	-6.594726	-1.164447
C	1.959252	-5.567211	-2.641390
H	0.202888	-4.640127	-3.483022
H	0.181358	-6.405350	-3.575714
C	2.357828	-4.308449	-1.873481
H	2.199875	-6.457721	-2.044032
H	2.544794	-5.633690	-3.564075
H	2.329013	-3.447488	-2.557064
H	3.396497	-4.378986	-1.541210
C	4.062133	-4.799108	0.964735
C	5.295510	-5.677571	0.768829
H	3.209225	-5.222383	0.430987
H	3.777811	-4.815638	2.027120
C	6.511171	-5.032850	1.427754
H	5.106108	-6.673515	1.182603
H	5.490682	-5.807171	-0.305159
C	6.817368	-3.703190	0.744390
H	6.295581	-4.862643	2.490563
H	7.384804	-5.690919	1.376270
H	7.245173	-3.906579	-0.247815
H	7.583605	-3.150941	1.299465

TS-2-major-8

M06-2X/6-31G* Energy = -8271.54334586

M06-2X/6-31G* Free Energy = -8270.651805

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.51513180

M06-2X/def2-TZVPP-SMD(toluene) Energy = -8277.52129283

Number of Imaginary Frequencies = 1

Lowest Frequency = 268.2549i

M06-2X/6-31G* Geometry

C	-0.628642	3.325087	1.506173
C	-0.871588	3.556404	-0.216635
C	-1.919164	2.945694	1.967436
H	0.122199	2.529178	1.530184
H	-0.238561	4.271987	1.877441
C	-2.479248	1.710563	1.574623
H	-2.582539	3.700121	2.390928
N	-1.450103	2.355110	-0.670346
C	-1.796311	4.744137	-0.475594
C	0.531697	3.792222	-0.764395
C	-2.695589	2.021679	-0.158971
C	-3.354824	0.787022	-0.712878
H	-3.386211	2.864755	-0.193772
H	-0.804704	1.547743	-0.623461
H	-1.797353	0.859452	1.503566
H	-3.467057	1.470162	1.970101
C	4.181493	-3.356541	0.787903
C	5.468670	-2.817779	0.913276
C	3.107803	-2.510430	0.431266
C	3.320625	-1.129004	0.358603
C	4.598792	-0.573625	0.503972

C	5.655438	-1.445325	0.743940
C	1.744405	-3.066289	0.166264
C	1.503706	-4.013193	-0.850383
C	0.225448	-4.575029	-0.953963
C	-0.789567	-4.147300	-0.099546
C	-0.628214	-3.108902	0.816951
C	0.675131	-2.597412	0.930548
O	2.271435	-0.291107	0.054205
O	0.936231	-1.556496	1.793589
P	1.008816	-0.072665	1.096059
O	-0.179877	0.125084	0.189435
O	1.301468	0.909209	2.172801
C	4.841532	0.890261	0.422752
C	-1.803018	-2.520963	1.516397
C	4.161324	1.778738	1.304255
C	4.438568	3.118995	1.286755
C	5.382811	3.663132	0.377893
C	6.043171	2.786303	-0.526755
C	5.763908	1.395183	-0.465486
C	-3.094387	-2.682345	0.927939
C	-4.208194	-2.086605	1.451404
C	-4.112807	-1.241712	2.585091
C	-2.848679	-1.115129	3.221422
C	-1.717377	-1.782107	2.681678
H	6.653673	-1.027584	0.859138
H	-1.761582	-4.621845	-0.199564
H	3.415687	1.384052	1.987159
H	3.916166	3.791460	1.962822
H	-0.766813	-1.657587	3.185462
H	-5.176455	-2.209604	0.972845
H	-3.189583	-3.246750	0.006792
H	6.278264	0.724983	-1.151451
C	1.365146	2.723867	-1.114301
C	2.640533	2.961317	-1.613555
C	3.108708	4.263801	-1.765299
C	2.294947	5.329464	-1.394316
C	1.015490	5.097356	-0.896291
H	1.049283	1.692596	-1.001454
H	3.276133	2.115028	-1.856722
H	4.111256	4.444063	-2.144082
H	0.388708	5.940914	-0.624093
H	2.654797	6.349206	-1.492251
C	-2.290180	4.881932	-1.779386
C	-3.104907	5.953867	-2.120562
C	-3.432163	6.917071	-1.167099
C	-2.936461	6.795984	0.125212
C	-2.123949	5.715036	0.469187
H	-1.739271	5.654767	1.482158
H	-2.027005	4.133545	-2.521266
H	-3.482344	6.039513	-3.134635
H	-4.066917	7.756344	-1.432604
H	-3.178420	7.542028	0.875549
C	-2.651951	-0.202218	-1.403613
C	-3.358760	-1.274441	-1.933950
C	-4.733457	-1.408473	-1.781164
C	-5.396350	-0.437713	-1.041759
Br	-2.405553	-2.652671	-2.811656
H	-5.262129	-2.264742	-2.182944
C	-4.731750	0.661552	-0.520485
H	-5.283154	1.405943	0.046501
H	-1.573168	-0.172921	-1.498588
Br	-7.229640	-0.674383	-0.646270
C	-2.736561	-0.255016	4.347995

C	-3.818733	0.462803	4.792434
C	-5.071459	0.354600	4.136293
C	-5.216000	-0.484264	3.058552
H	-1.768682	-0.158139	4.833175
H	-3.718527	1.123103	5.648573
H	-6.165854	-0.568523	2.533380
H	-5.916433	0.935635	4.493595
C	6.944728	3.334100	-1.478257
C	7.178079	4.685312	-1.528911
C	6.527256	5.556855	-0.620360
C	5.654242	5.054594	0.310888
H	7.444014	2.661095	-2.170984
H	7.866085	5.092302	-2.263643
H	6.723115	6.623809	-0.667117
H	5.142338	5.717108	1.004546
C	6.678793	-3.680111	1.221568
C	6.317526	-5.016013	1.864959
H	7.369998	-3.118675	1.859724
H	7.217992	-3.874482	0.283330
C	5.189965	-5.675357	1.076375
H	5.984685	-4.852330	2.898109
H	7.200564	-5.662001	1.908151
C	3.930696	-4.814371	1.139755
H	5.502220	-5.798039	0.029536
H	4.971261	-6.675372	1.465025
H	3.145817	-5.245370	0.515049
H	3.532950	-4.838559	2.164857
C	2.572975	-4.330924	-1.881002
C	2.289678	-5.607099	-2.670439
H	3.563150	-4.378329	-1.421521
H	2.614969	-3.480315	-2.576783
C	0.850825	-5.604742	-3.180039
H	3.000474	-5.692012	-3.498812
H	2.442225	-6.483388	-2.024838
C	-0.109937	-5.626374	-1.994582
H	0.679148	-4.696382	-3.773453
H	0.661346	-6.461463	-3.834892
H	-0.079916	-6.620516	-1.526748
H	-1.142961	-5.477144	-2.332028

TS-2-major-9

M06-2X/6-31G* Energy = -8271.54334587

M06-2X/6-31G* Free Energy = -8270.651805

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.51513085

M06-2X/def2-TZVPP-SMD(toluene) Energy = -8277.52129187

Number of Imaginary Frequencies = 1

Lowest Frequency = 268.1977i

M06-2X/6-31G* Geometry

C	-0.628719	3.325043	1.506187
C	-0.871620	3.556412	-0.216560
C	-1.919237	2.945567	1.967486
H	0.122142	2.529152	1.530277
H	-0.238676	4.271904	1.877605
C	-2.479305	1.710468	1.574620
H	-2.582610	3.699955	2.391053
N	-1.450131	2.355126	-0.670380
C	-1.796368	4.744130	-0.475529
C	0.531639	3.792264	-0.764409
C	-2.695584	2.021648	-0.159024
C	-3.354787	0.786974	-0.712932
H	-3.386245	2.864692	-0.193802
H	-0.804701	1.547792	-0.623517
H	-1.797406	0.859362	1.503505

H	-3.467131	1.470059	1.970045
C	1.503761	-4.013182	-0.850311
C	0.225516	-4.575047	-0.953893
C	1.744438	-3.066270	0.166335
C	0.675150	-2.597415	0.930613
C	-0.628186	-3.108925	0.817006
C	-0.789513	-4.147332	-0.099486
C	3.107824	-2.510382	0.431339
C	4.181537	-3.356471	0.787957
C	5.468706	-2.817686	0.913315
C	5.655444	-1.445227	0.743981
C	4.598777	-0.573547	0.504035
C	3.320618	-1.128951	0.358683
O	0.936226	-1.556499	1.793661
O	2.271413	-0.291072	0.054292
P	1.008780	-0.072662	1.096138
O	-0.179906	0.125074	0.189503
O	1.301404	0.909212	2.172888
C	-1.803009	-2.520996	1.516427
C	4.841488	0.890343	0.422798
C	-3.094362	-2.682386	0.927938
C	-4.208185	-2.086650	1.451374
C	-4.112830	-1.241755	2.585062
C	-2.848717	-1.115163	3.221423
C	-1.717399	-1.782136	2.681707
C	4.161239	1.778825	1.304263
C	4.438442	3.119089	1.286730
C	5.382684	3.663230	0.377868
C	6.043093	2.786393	-0.526737
C	5.763871	1.395266	-0.465433
H	-1.761519	-4.621895	-0.199509
H	6.653673	-1.027467	0.859161
H	-3.189532	-3.246795	0.006790
H	-5.176434	-2.209654	0.972792
H	6.278258	0.725065	-1.151372
H	3.916006	3.791558	1.962767
H	3.415602	1.384136	1.987167
H	-0.766848	-1.657611	3.185513
C	1.365122	2.723910	-1.114237
C	2.640485	2.961359	-1.613550
C	3.108613	4.263846	-1.765414
C	2.294818	5.329511	-1.394513
C	1.015378	5.097403	-0.896444
H	1.049304	1.692635	-1.001289
H	3.276103	2.115068	-1.856664
H	4.111151	4.444110	-2.144225
H	0.388574	5.940964	-0.624306
H	2.654628	6.349258	-1.492547
C	-2.290260	4.881931	-1.779313
C	-3.104995	5.953865	-2.120470
C	-3.432237	6.917065	-1.166997
C	-2.936516	6.795971	0.125307
C	-2.123995	5.715023	0.469262
H	-1.739300	5.654752	1.482226
H	-2.027093	4.133548	-2.521201
H	-3.482448	6.039516	-3.134536
H	-4.066996	7.756338	-1.432488
H	-3.178464	7.542011	0.875650
C	-2.651877	-0.202272	-1.403622
C	-3.358656	-1.274510	-1.933965
C	-4.733356	-1.408557	-1.781221
C	-5.396287	-0.437793	-1.041854
Br	-2.405405	-2.652742	-2.811621

H	-5.262004	-2.264841	-2.183001
C	-4.731717	0.661492	-0.520581
H	-5.283150	1.405888	0.046371
H	-1.573092	-0.172965	-1.498558
Br	-7.229585	-0.674481	-0.646418
C	6.944655	3.334190	-1.478234
C	7.177965	4.685408	-1.528925
C	6.527090	5.556958	-0.620417
C	5.654069	5.054699	0.310824
H	7.443979	2.661179	-2.170928
H	7.865977	5.092397	-2.263652
H	5.142125	5.717219	1.004448
H	6.722914	6.623917	-0.667204
C	-2.736631	-0.255045	4.347995
C	-3.818817	0.462770	4.792405
C	-5.071528	0.354556	4.136236
C	-5.216038	-0.484312	3.058494
H	-1.768764	-0.158161	4.833198
H	-3.718635	1.123073	5.648544
H	-5.916515	0.935587	4.493517
H	-6.165881	-0.568580	2.533301
C	-0.109837	-5.626405	-1.994507
C	0.850906	-5.604717	-3.179976
H	-1.142876	-5.477228	-2.331934
H	-0.079755	-6.620548	-1.526678
C	2.289763	-5.607052	-2.670389
H	0.679197	-4.696344	-3.773362
H	0.661441	-6.461425	-3.834851
C	2.573040	-4.330887	-1.880930
H	2.442336	-6.483350	-2.024807
H	3.000555	-5.691932	-3.498770
H	3.563212	-4.378289	-1.421443
H	2.615030	-3.480265	-2.576694
C	3.930805	-4.814318	1.139777
C	5.190082	-5.675269	1.076119
H	3.145810	-5.245287	0.515198
H	3.533263	-4.838569	2.164957
C	6.317692	-5.016026	1.864717
H	4.971445	-6.675358	1.464617
H	5.502238	-5.797756	0.029228
C	6.678868	-3.679986	1.221556
H	5.984940	-4.852558	2.897929
H	7.200759	-5.661989	1.907708
H	7.218146	-3.874150	0.283321
H	7.369987	-3.118597	1.859849

TS-3-major

M06-2X/6-31G* Energy = -8271.53575934

M06-2X/6-31G* Free Energy = -8270.648412

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.51298929

M06-2X/def2-TZVPP-SMD(toluene) Energy = -8277.51973184

Number of Imaginary Frequencies = 1

Lowest Frequency = 297.9054i

M06-2X/6-31G* Geometry

C	-1.063972	-3.278720	0.364052
C	-1.544361	-2.409780	1.739198
C	-2.208366	-3.270486	-0.506507
H	-0.218327	-2.693136	-0.003019
H	-0.740946	-4.262685	0.703676
C	-2.606255	-2.077454	-1.111622
H	-2.910990	-4.102314	-0.479200
N	-2.010793	-1.163111	1.249596
C	-2.658895	-3.139092	2.495974

C	-0.288915	-2.302986	2.603714
C	-3.113464	-1.188327	0.434205
C	-3.656052	0.134044	-0.035137
H	-3.906515	-1.829016	0.818820
H	-1.295819	-0.454579	0.964976
H	-1.816927	-1.403730	-1.454292
H	-3.493127	-2.094605	-1.741290
C	4.903956	-1.074439	-1.169408
C	5.022792	-2.229629	-1.954025
C	3.652087	-0.750779	-0.603135
C	2.525181	-1.491111	-0.963492
C	2.624745	-2.635842	-1.763350
C	3.889502	-3.003272	-2.208917
C	3.496774	0.383205	0.355767
C	4.212693	0.419976	1.572269
C	4.131819	1.568184	2.369122
C	3.351529	2.644212	1.942205
C	2.576066	2.608647	0.785016
C	2.627167	1.427371	0.030759
O	1.300855	-1.122964	-0.452888
O	1.834250	1.289638	-1.094141
P	0.554783	0.278596	-0.943736
O	-0.273747	0.673150	0.251203
O	-0.096935	0.096548	-2.269493
C	1.429172	-3.431569	-2.142347
C	1.829216	3.826648	0.370474
C	1.318523	-4.791122	-1.737093
C	0.211588	-5.534344	-2.059868
C	-0.845423	-4.966238	-2.819783
C	-0.716448	-3.621283	-3.266869
C	0.428540	-2.869823	-2.902036
C	0.462646	3.799593	-0.030749
C	-0.183189	4.961781	-0.361902
C	0.481551	6.215031	-0.330167
C	1.847625	6.250258	0.059480
C	2.491242	5.035890	0.404701
H	3.984107	-3.894552	-2.826666
H	3.311449	3.540057	2.558311
H	2.120917	-5.226269	-1.147253
H	0.127132	-6.568326	-1.733757
H	3.541941	5.067052	0.684770
H	-1.224536	4.931627	-0.668857
H	-0.073158	2.856012	-0.036730
H	0.493017	-1.827824	-3.204439
C	0.110154	-3.428207	3.333667
C	1.259018	-3.398765	4.114438
C	2.023967	-2.236681	4.183200
C	1.631945	-1.115076	3.460102
C	0.486156	-1.142650	2.666924
H	-0.489477	-4.333921	3.303009
H	1.550317	-4.281625	4.674837
H	2.919421	-2.207833	4.798010
H	0.233989	-0.252352	2.100920
H	2.219056	-0.201034	3.495943
C	-3.334802	-2.411964	3.484485
C	-4.338363	-3.003895	4.240375
C	-4.678893	-4.339961	4.030674
C	-4.005867	-5.072905	3.061390
C	-3.002718	-4.475103	2.297105
H	-2.486556	-5.075686	1.554281
H	-3.063300	-1.372801	3.648915
H	-4.853803	-2.422205	4.998161
H	-5.461932	-4.804104	4.621583

H	-4.257318	-6.115090	2.891597
C	-2.994232	0.941206	-0.959509
C	-3.541712	2.177039	-1.276645
C	-4.733987	2.624459	-0.718980
C	-5.383620	1.791495	0.183537
Br	-2.621890	3.269182	-2.506966
H	-5.145557	3.591050	-0.983377
C	-4.862705	0.551571	0.530764
H	-5.385668	-0.073799	1.247526
H	-2.063826	0.643778	-1.432697
Br	-7.014889	2.358859	0.952563
C	2.524073	7.498958	0.088157
C	1.871972	8.656415	-0.250217
C	0.508939	8.621580	-0.635924
C	-0.167531	7.429428	-0.674589
H	3.570092	7.519079	0.383816
H	2.397770	9.605994	-0.224688
H	-1.212782	7.394555	-0.971346
H	0.003563	9.544875	-0.902305
C	-1.762942	-3.042391	-4.035019
C	-2.895766	-3.759230	-4.323690
C	-3.034108	-5.094183	-3.863186
C	-2.032077	-5.683917	-3.135405
H	-1.649476	-2.012149	-4.363921
H	-3.693136	-3.309143	-4.907263
H	-3.935300	-5.651605	-4.099894
H	-2.128517	-6.711646	-2.793175
C	6.352625	-2.679871	-2.530251
C	7.384600	-1.557972	-2.610299
H	6.187536	-3.123340	-3.518355
H	6.753236	-3.484180	-1.896707
C	7.430806	-0.807452	-1.282574
H	7.109452	-0.857272	-3.409082
H	8.365955	-1.970574	-2.866109
C	6.087500	-0.133797	-1.013321
H	7.659538	-1.514581	-0.472539
H	8.225673	-0.054588	-1.284849
H	6.089675	0.340034	-0.029597
H	5.947918	0.686476	-1.732286
C	4.969771	-0.803704	2.059953
C	5.981335	-0.486315	3.158857
H	5.461144	-1.319473	1.232025
H	4.226958	-1.517025	2.447648
C	5.326354	0.352321	4.252619
H	6.385433	-1.418556	3.567247
H	6.827581	0.071842	2.734134
C	4.890898	1.697333	3.677070
H	4.451282	-0.186035	4.643021
H	6.007865	0.507888	5.095307
H	5.784855	2.313614	3.505741
H	4.276624	2.246301	4.399522

TS-3-major-2

M06-2X/6-31G* Energy = -8271.53988311

M06-2X/6-31G* Free Energy = -8270.651739

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.51361570

M06-2X/def2-TZVPP-SMD(toluene) Energy = -8277.51992240

Number of Imaginary Frequencies = 1

Lowest Frequency = 305.7659i

M06-2X/6-31G* Geometry

C	-0.830715	3.029460	0.110850
C	0.166328	2.631861	1.413801
C	0.054612	3.569555	-0.886775

H	-1.279447	2.070473	-0.160282
H	-1.587061	3.719918	0.485578
C	0.941182	2.722521	-1.549404
H	0.214806	4.646394	-0.926265
N	1.159143	1.772323	0.877039
C	0.807046	3.881379	2.022773
C	-0.751540	1.931485	2.417333
C	1.999649	2.274901	-0.077939
C	3.063444	1.327983	-0.582606
H	2.415689	3.247777	0.185428
H	0.877194	0.788515	0.657629
H	0.572307	1.728542	-1.812325
H	1.632889	3.157873	-2.268452
C	-4.789002	-2.264923	-0.917472
C	-5.644818	-1.395876	-1.607744
C	-3.532667	-1.797565	-0.480963
C	-3.096520	-0.531387	-0.885200
C	-3.938885	0.345012	-1.577816
C	-5.217596	-0.097405	-1.895249
C	-2.640849	-2.595548	0.412107
C	-3.029257	-2.980794	1.713073
C	-2.116949	-3.685524	2.513224
C	-0.825103	-3.930247	2.039760
C	-0.395335	-3.498931	0.788517
C	-1.338739	-2.851788	-0.016730
O	-1.842219	-0.096664	-0.527495
O	-0.954455	-2.351373	-1.247616
P	-0.474306	-0.786932	-1.189796
O	0.561805	-0.613780	-0.116234
O	-0.236223	-0.281110	-2.567510
C	-3.473669	1.710643	-1.938331
C	1.018783	-3.625455	0.359214
C	-2.425478	1.876799	-2.888125
C	-1.986834	3.130915	-3.222132
C	-2.531751	4.289661	-2.604773
C	-3.575229	4.128485	-1.650756
C	-4.039118	2.819600	-1.352028
C	1.348791	-4.157533	-0.918229
C	2.652738	-4.239865	-1.323723
C	3.707846	-3.783351	-0.489687
C	3.385119	-3.232945	0.780870
C	2.026028	-3.179950	1.182471
H	-5.885628	0.577525	-2.426763
H	-0.117378	-4.454791	2.678766
H	-1.960978	0.996345	-3.321376
H	-1.189606	3.252493	-3.952147
H	1.777670	-2.727493	2.139912
H	2.899308	-4.645703	-2.301304
H	0.548012	-4.489641	-1.570748
H	-4.831472	2.696390	-0.616935
C	-1.520937	2.712424	3.286015
C	-2.402788	2.119914	4.183332
C	-2.522246	0.733532	4.231016
C	-1.759449	-0.048112	3.369416
C	-0.885252	0.540266	2.458273
H	-1.424766	3.794285	3.270414
H	-2.989390	2.744567	4.849800
H	-3.204545	0.266850	4.936030
H	-0.334748	-0.112062	1.787398
H	-1.835788	-1.131909	3.389492
C	1.878165	3.683056	2.903353
C	2.496205	4.760402	3.525487
C	2.046728	6.058732	3.287646

C	0.976316	6.264806	2.426115
C	0.360218	5.182817	1.795852
H	-0.482080	5.375342	1.137442
H	2.221268	2.669235	3.091059
H	3.328364	4.586227	4.200401
H	2.527714	6.901713	3.773312
H	0.612855	7.269961	2.237001
C	2.876168	0.410989	-1.615409
C	3.924992	-0.437426	-1.951099
C	5.143325	-0.408731	-1.286469
C	5.294109	0.497854	-0.245833
Br	3.688445	-1.657351	-3.369316
H	5.943308	-1.084377	-1.559902
C	4.279303	1.376457	0.105199
H	4.426335	2.079316	0.919526
H	1.936909	0.315838	-2.150737
Br	6.927555	0.530571	0.706522
C	4.434142	-2.739740	1.602524
C	5.741297	-2.811325	1.193878
C	6.062603	-3.375889	-0.065930
C	5.068768	-3.842907	-0.889436
H	4.179946	-2.305343	2.566155
H	6.533681	-2.423459	1.825894
H	5.306468	-4.260867	-1.864689
H	7.101591	-3.428154	-0.379398
C	-4.089679	5.278840	-0.994975
C	-3.585864	6.526181	-1.264993
C	-2.548666	6.686888	-2.216941
C	-2.040138	5.594820	-2.873963
H	-4.887747	5.150615	-0.268023
H	-3.984842	7.397213	-0.754405
H	-2.163385	7.679641	-2.428419
H	-1.248009	5.710779	-3.610228
C	-7.040698	-1.813114	-2.032626
C	-7.226836	-3.327616	-2.089411
H	-7.275757	-1.360173	-3.002124
H	-7.762605	-1.394711	-1.316706
C	-6.673708	-3.965744	-0.817728
H	-6.690144	-3.734507	-2.956149
H	-8.286383	-3.568497	-2.223805
C	-5.169282	-3.723030	-0.725682
H	-7.174865	-3.527976	0.057282
H	-6.876359	-5.041488	-0.798976
H	-4.771303	-4.112899	0.214340
H	-4.666687	-4.298253	-1.516655
C	-4.350029	-2.509245	2.298684
C	-4.797432	-3.326054	3.508487
H	-5.137301	-2.490750	1.542580
H	-4.214247	-1.459542	2.603221
C	-3.660100	-3.436128	4.519524
H	-5.679998	-2.861430	3.960426
H	-5.093907	-4.333649	3.185510
C	-2.487380	-4.189528	3.896489
H	-3.341582	-2.426022	4.813258
H	-3.988863	-3.944564	5.431825
H	-2.753018	-5.253513	3.821336
H	-1.607288	-4.141007	4.547435

TS-3-major-3

M06-2X/6-31G* Energy = -8271.53745819

M06-2X/6-31G* Free Energy = -8270.649855

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.51079551

M06-2X/def2-TZVPP-SMD(toluene) Energy = -8277.51731748

Number of Imaginary Frequencies = 1

Lowest Frequency = 270.9932i

M06-2X/6-31G* Geometry

C	0.042592	-2.567112	1.903335
C	-0.676780	-1.359614	2.968128
C	-1.094216	-3.088379	1.231802
H	0.690915	-1.945152	1.286237
H	0.595968	-3.246981	2.548646
C	-1.810118	-2.274211	0.329096
H	-1.581695	-3.983596	1.617133
N	-1.365494	-0.486989	2.103914
C	-1.619845	-2.023532	3.967517
C	0.536694	-0.727293	3.646861
C	-2.441078	-1.014140	1.399107
C	-3.197554	-0.093938	0.477653
H	-3.120947	-1.567865	2.047051
H	-0.762146	0.142255	1.532640
H	-1.232359	-1.664093	-0.368173
H	-2.684380	-2.730022	-0.132286
C	4.604871	-1.393653	-2.140289
C	4.474319	-2.658472	-2.730544
C	3.541551	-0.876157	-1.370457
C	2.323240	-1.562650	-1.332781
C	2.167463	-2.810361	-1.953044
C	3.268538	-3.351411	-2.606297
C	3.662351	0.411075	-0.622479
C	4.624554	0.613787	0.390943
C	4.716959	1.871398	1.003394
C	3.816996	2.881659	0.649838
C	2.799687	2.676493	-0.275029
C	2.745893	1.425831	-0.899686
O	1.281487	-1.045950	-0.600207
O	1.702310	1.154698	-1.761417
P	0.459501	0.346291	-1.051315
O	0.130125	0.971160	0.277103
O	-0.578464	0.035735	-2.060915
C	0.852735	-3.501978	-1.936799
C	1.775021	3.709031	-0.561223
C	0.692514	-4.767999	-1.310446
C	-0.541937	-5.367122	-1.241430
C	-1.692401	-4.722533	-1.770849
C	-1.528656	-3.472112	-2.428664
C	-0.237297	-2.896739	-2.517568
C	1.494046	4.089065	-1.903823
C	0.549588	5.039576	-2.178054
C	-0.189612	5.653466	-1.133107
C	0.069944	5.264434	0.210134
C	1.073476	4.295271	0.465397
H	3.163551	-4.323053	-3.085768
H	3.891531	3.853243	1.134852
H	1.562040	-5.248621	-0.869158
H	-0.659032	-6.331796	-0.752842
H	1.250170	3.974000	1.489546
H	0.338490	5.324409	-3.205402
H	2.037110	3.604674	-2.708748
H	-0.137267	-1.920935	-2.981968
C	1.438120	0.048821	2.907167
C	2.538420	0.624514	3.533943
C	2.772854	0.415213	4.891117
C	1.893136	-0.373544	5.623600
C	0.780510	-0.941370	5.007139
H	1.288910	0.231283	1.844550
H	3.210759	1.239902	2.943953
H	3.636687	0.864844	5.372316

H	0.101861	-1.544982	5.599270
H	2.063312	-0.548226	6.681390
C	-2.554335	-1.203800	4.612088
C	-3.394723	-1.719179	5.592106
C	-3.308004	-3.061937	5.954194
C	-2.374168	-3.880510	5.328715
C	-1.535018	-3.364057	4.342502
H	-0.804117	-4.021526	3.882275
H	-2.614084	-0.155557	4.333550
H	-4.116611	-1.068677	6.075634
H	-3.962844	-3.465681	6.719633
H	-2.292754	-4.926843	5.605577
C	-4.329147	-0.603750	-0.167130
C	-5.016571	0.197292	-1.064528
C	-4.617342	1.500410	-1.339958
C	-3.503130	1.990606	-0.672095
Br	-6.540041	-0.504660	-1.944687
H	-5.157403	2.110418	-2.053824
C	-2.793658	1.216572	0.239654
H	-1.912405	1.635972	0.706263
H	-4.667585	-1.620184	0.010712
Br	-2.897764	3.745593	-1.005319
C	-0.713162	5.828462	1.251450
C	-1.711030	6.726842	0.972705
C	-1.967531	7.116354	-0.364684
C	-1.219300	6.596134	-1.391146
H	-0.515799	5.521302	2.275331
H	-2.312530	7.140749	1.776046
H	-1.415893	6.884495	-2.420843
H	-2.762097	7.825857	-0.574274
C	-2.675173	-2.753199	-2.863543
C	-3.933327	-3.255438	-2.646528
C	-4.098418	-4.512878	-2.008778
C	-3.006352	-5.232591	-1.590318
H	-2.527849	-1.771431	-3.306313
H	-4.807844	-2.678037	-2.931165
H	-5.099381	-4.902801	-1.848785
H	-3.133498	-6.192434	-1.094962
C	5.608945	-3.308024	-3.501204
C	6.651449	-2.308517	-3.995582
H	5.196707	-3.881155	-4.338957
H	6.103639	-4.038402	-2.844924
C	7.045140	-1.371061	-2.857669
H	6.234981	-1.715968	-4.820394
H	7.523361	-2.841408	-4.388726
C	5.837650	-0.548141	-2.415445
H	7.419998	-1.963669	-2.011088
H	7.855086	-0.700977	-3.163765
H	6.093685	0.071839	-1.553661
H	5.575671	0.159135	-3.215801
C	5.452757	-0.549618	0.909465
C	6.704593	-0.106510	1.662078
H	5.713090	-1.241152	0.105238
H	4.809971	-1.122965	1.594912
C	6.335246	0.925099	2.724250
H	7.191267	-0.976826	2.114308
H	7.423390	0.335698	0.958045
C	5.769406	2.175857	2.055177
H	5.583726	0.487999	3.396288
H	7.202276	1.189893	3.338308
H	6.592859	2.725304	1.577539
H	5.346715	2.856132	2.804344

TS-3-major-4

M06-2X/6-31G* Energy = -8271.53671069
 M06-2X/6-31G* Free Energy = -8270.648154
 M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.50956303
 M06-2X/def2-TZVPP-SMD(toluene) Energy = -8277.51609143
 Number of Imaginary Frequencies = 1
 Lowest Frequency = 321.1935i
 M06-2X/6-31G* Geometry

C	-1.706956	2.864414	0.142812
C	-0.617731	2.938646	1.416462
C	-1.062132	3.574551	-0.936021
H	-1.828189	1.793683	-0.043605
H	-2.640715	3.302847	0.496668
C	-0.000544	2.981399	-1.600155
H	-1.235698	4.644192	-1.043778
N	0.577600	2.352944	0.910485
C	-0.371616	4.382196	1.853326
C	-1.235166	2.094653	2.536015
C	1.232329	2.936258	-0.128899
C	2.439959	2.150119	-0.593147
H	1.395709	4.008330	-0.018032
H	0.605864	1.311957	0.829227
H	-0.047976	1.903457	-1.768208
H	0.515788	3.549941	-2.372088
C	-3.690516	-3.506017	-0.884001
C	-4.729586	-2.997753	-1.675629
C	-2.689491	-2.632615	-0.412621
C	-2.663328	-1.312593	-0.872250
C	-3.694054	-0.792155	-1.660891
C	-4.731006	-1.643796	-2.020914
C	-1.655251	-3.048108	0.581380
C	-2.002436	-3.474866	1.880233
C	-0.977495	-3.822584	2.772221
C	0.354655	-3.670164	2.384687
C	0.729112	-3.165185	1.140247
C	-0.310096	-2.887651	0.242749
O	-1.646547	-0.477626	-0.478930
O	-0.029177	-2.354575	-1.000616
P	-0.086378	-0.716593	-1.036235
O	0.757613	-0.164109	0.073885
O	0.038039	-0.246292	-2.440096
C	-3.667151	0.636032	-2.075465
C	2.156383	-2.884608	0.843461
C	-2.710571	1.075248	-3.034829
C	-2.674473	2.387691	-3.424125
C	-3.546084	3.349798	-2.845938
C	-4.494075	2.918425	-1.876320
C	-4.545275	1.542113	-1.528342
C	2.978231	-2.371194	1.889075
C	4.316552	-2.155666	1.705408
C	4.928199	-2.431458	0.454422
C	4.107606	-2.887862	-0.614560
C	2.724226	-3.112959	-0.390287
H	-5.543567	-1.249907	-2.628278
H	1.135308	-3.935069	3.094657
H	-1.993698	0.360614	-3.427144
H	-1.945422	2.718536	-4.160521
H	2.116711	-3.478923	-1.212128
H	4.926828	-1.754560	2.510270
H	2.517464	-2.128696	2.842023
H	-5.268584	1.212452	-0.785760
C	-1.915628	2.709771	3.589966
C	-2.511388	1.944237	4.589562

C	-2.429444	0.556072	4.552400
C	-1.756478	-0.061846	3.501678
C	-1.172961	0.696614	2.491846
H	-1.977692	3.791913	3.642881
H	-3.032955	2.440451	5.402147
H	-2.886402	-0.039852	5.337096
H	-0.676373	0.171068	1.681456
H	-1.672568	-1.144738	3.453884
C	-1.247063	5.433912	1.580237
C	-0.989879	6.715633	2.066209
C	0.144179	6.962031	2.831527
C	1.019604	5.915980	3.117498
C	0.759860	4.637976	2.637337
H	1.433705	3.817979	2.870403
H	-2.148503	5.269320	0.997045
H	-1.683050	7.520369	1.842476
H	0.344553	7.960801	3.205902
H	1.905031	6.094267	3.719516
C	2.527766	1.473857	-1.805270
C	3.623399	0.653715	-2.044317
C	4.654828	0.505721	-1.127655
C	4.555061	1.213929	0.063705
Br	3.661663	-0.328509	-3.652703
H	5.493896	-0.152561	-1.325995
C	3.467196	2.027423	0.346247
H	3.404779	2.532966	1.303969
H	1.734102	1.482265	-2.539017
Br	5.926360	1.048644	1.356725
C	4.703353	-3.120256	-1.882965
C	6.046535	-2.919067	-2.076310
C	6.866040	-2.487235	-1.003862
C	6.318357	-2.249169	0.232162
H	4.068039	-3.444035	-2.702754
H	6.486889	-3.089766	-3.053877
H	6.937613	-1.904645	1.055674
H	7.930283	-2.344278	-1.165376
C	-5.327684	3.885277	-1.253434
C	-5.216988	5.216459	-1.567954
C	-4.275594	5.645650	-2.536224
C	-3.466494	4.732038	-3.163719
H	-6.051474	3.550452	-0.514545
H	-5.856527	5.946326	-1.081178
H	-4.202879	6.700253	-2.783729
H	-2.744480	5.053282	-3.911013
C	-5.877073	-3.869932	-2.150773
C	-5.553241	-5.361669	-2.118716
H	-6.173237	-3.562246	-3.159731
H	-6.748012	-3.683169	-1.506279
C	-4.923085	-5.725526	-0.776934
H	-4.847159	-5.604769	-2.923199
H	-6.461985	-5.944936	-2.299678
C	-3.591252	-4.997407	-0.612560
H	-5.605956	-5.439102	0.035523
H	-4.765574	-6.806070	-0.697817
H	-3.165325	-5.188932	0.375510
H	-2.867172	-5.412790	-1.328205
C	-3.445185	-3.425944	2.355904
C	-3.700447	-4.288158	3.589845
H	-4.137594	-3.696069	1.556242
H	-3.675692	-2.376527	2.597145
C	-2.662448	-3.987696	4.667157
H	-4.714691	-4.108445	3.961184
H	-3.641100	-5.350839	3.316483

C	-1.271488	-4.361110	4.160429
H	-2.696556	-2.916049	4.909171
H	-2.882721	-4.531399	5.591686
H	-1.188013	-5.456895	4.136625
H	-0.500242	-4.011646	4.855767

TS-4-major

M06-2X/6-31G* Energy = -8271.53919153

M06-2X/6-31G* Free Energy = -8270.649752

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.51410240

M06-2X/def2-TZVPP-SMD(toluene) Energy = -8277.51999560

Number of Imaginary Frequencies = 1

Lowest Frequency = 341.3134i

M06-2X/6-31G* Geometry

C	-0.288949	3.456985	-1.618444
C	0.232595	3.659725	0.047858
C	0.923376	3.273772	-2.339467
H	-0.896084	2.551226	-1.545109
H	-0.866757	4.350472	-1.851218
C	1.699823	2.117681	-2.125287
H	1.395146	4.127624	-2.826402
N	1.074616	2.562593	0.307830
C	0.988833	4.978721	0.212420
C	-1.070261	3.651851	0.835683
C	2.231018	2.485208	-0.442560
C	3.268860	1.463979	-0.066848
H	2.708872	3.459345	-0.543667
H	0.613911	1.634756	0.421368
H	1.157378	1.185713	-1.963411
H	2.617228	2.021901	-2.703269
C	-1.961244	-4.295833	1.030574
C	-0.767388	-4.964403	1.332183
C	-1.942565	-3.300104	0.033997
C	-0.721766	-2.894853	-0.509470
C	0.497124	-3.512355	-0.191086
C	0.414458	-4.585406	0.699052
C	-3.196647	-2.650297	-0.456671
C	-4.239880	-3.418566	-1.020303
C	-5.455705	-2.798207	-1.332913
C	-5.593576	-1.425279	-1.128220
C	-4.545115	-0.625294	-0.684237
C	-3.335902	-1.260751	-0.372619
O	-0.756390	-1.850827	-1.406400
O	-2.283997	-0.504618	0.100961
P	-0.917802	-0.336631	-0.809547
O	0.172058	-0.024120	0.180324
O	-1.118770	0.555424	-1.987633
C	1.816908	-3.074293	-0.724517
C	-4.751664	0.841021	-0.554966
C	1.960394	-2.367867	-1.959838
C	3.193515	-1.986504	-2.418128
C	4.381115	-2.313432	-1.712965
C	4.256991	-3.047870	-0.503424
C	2.966113	-3.382034	-0.025447
C	-3.926593	1.760521	-1.263616
C	-4.194084	3.103417	-1.221726
C	-5.278052	3.616237	-0.462294
C	-6.086624	2.706096	0.271526
C	-5.804391	1.318146	0.192826
H	1.313484	-5.151383	0.926383
H	-6.537729	-0.945026	-1.377255
H	1.081231	-2.136228	-2.545193
H	3.277283	-1.447579	-3.359105

H	-6.433293	0.622501	0.744768
H	-3.572838	3.803130	-1.777136
H	-3.096332	1.376031	-1.849504
H	2.904692	-3.875939	0.938932
C	-1.754439	4.856883	1.036491
C	-2.964235	4.875489	1.719849
C	-3.519877	3.690494	2.196003
C	-2.850407	2.489528	1.988664
C	-1.630263	2.466534	1.317857
H	-1.334991	5.788668	0.669227
H	-3.486646	5.816154	1.863330
H	-4.482373	3.705605	2.699195
H	-1.143353	1.507080	1.182568
H	-3.278439	1.551123	2.326548
C	1.655573	5.165164	1.430476
C	2.342230	6.343779	1.690987
C	2.366740	7.365329	0.742284
C	1.699273	7.194211	-0.463984
C	1.015061	6.006803	-0.727969
H	0.492140	5.907838	-1.673721
H	1.630541	4.369252	2.169155
H	2.857694	6.466175	2.638286
H	2.901549	8.287599	0.945077
H	1.706075	7.983368	-1.209182
C	3.042614	0.469474	0.885781
C	4.125135	-0.288282	1.318508
C	5.406008	-0.122640	0.806349
C	5.588103	0.831891	-0.185497
Br	3.863395	-1.551010	2.697144
H	6.230946	-0.728597	1.158719
C	4.542781	1.634739	-0.614570
H	4.730507	2.410919	-1.350824
H	2.054454	0.285273	1.289904
Br	7.307224	1.078616	-0.928698
C	-7.143225	3.216423	1.072947
C	-7.383249	4.564937	1.142646
C	-6.583724	5.470997	0.401664
C	-5.560879	5.004544	-0.383746
H	-7.756740	2.515875	1.634123
H	-8.190901	4.944190	1.761235
H	-4.936257	5.694216	-0.946760
H	-6.786966	6.536090	0.459329
C	5.433461	-3.417898	0.201832
C	6.672980	-3.077359	-0.278669
C	6.795125	-2.332384	-1.477647
C	5.674101	-1.954860	-2.173636
H	5.331837	-3.975600	1.129237
H	7.567453	-3.373815	0.261358
H	7.779582	-2.049364	-1.836669
H	5.763291	-1.375901	-3.089973
C	-0.723644	-6.127247	2.307138
C	-1.911243	-6.154772	3.265982
H	0.219535	-6.099763	2.863899
H	-0.712188	-7.063792	1.731568
C	-3.208882	-5.962934	2.485977
H	-1.812815	-5.345972	4.001676
H	-1.920176	-7.097841	3.822252
C	-3.223284	-4.587357	1.823514
H	-3.291218	-6.744606	1.717407
H	-4.079575	-6.065337	3.141932
H	-3.303955	-3.816748	2.604138
H	-4.115559	-4.469880	1.205165
C	-4.017177	-4.878580	-1.381221

C	-5.316549	-5.660473	-1.557305
H	-3.372710	-5.374753	-0.653217
H	-3.457206	-4.898633	-2.327578
C	-6.257019	-4.911136	-2.496547
H	-5.093883	-6.661529	-1.940959
H	-5.804990	-5.791262	-0.581115
C	-6.643600	-3.572416	-1.873883
H	-5.747282	-4.741616	-3.453820
H	-7.156073	-5.498991	-2.708664
H	-7.345746	-3.756431	-1.048122
H	-7.181135	-2.950642	-2.598248

TS-4-major-2

M06-2X/6-31G* Energy = -8271.54087276

M06-2X/6-31G* Free Energy = -8270.649639

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.51458259

M06-2X/def2-TZVPP-SMD(toluene) Energy = -8277.52037843

Number of Imaginary Frequencies = 1

Lowest Frequency = 228.8721i

M06-2X/6-31G* Geometry

C	0.361603	3.349265	-0.699128
C	1.036171	3.274712	0.928242
C	1.502665	3.105936	-1.498308
H	-0.365526	2.537676	-0.685654
H	-0.101732	4.330538	-0.774061
C	2.113605	1.825471	-1.478947
H	2.066963	3.952497	-1.890187
N	1.657107	2.015033	1.015164
C	2.028839	4.414959	1.135401
C	-0.196405	3.407336	1.817229
C	2.730441	1.778930	0.155339
C	3.456849	0.465858	0.311114
H	3.447317	2.600067	0.188690
H	0.991889	1.226007	1.007307
H	1.421081	0.981609	-1.471493
H	2.979770	1.695135	-2.127013
C	-3.418827	-3.159477	1.346797
C	-2.513636	-4.113053	1.829234
C	-3.059071	-2.389582	0.223535
C	-1.773637	-2.508373	-0.317770
C	-0.871469	-3.498280	0.108490
C	-1.285742	-4.278136	1.190201
C	-3.996599	-1.392672	-0.380984
C	-5.227849	-1.752346	-0.965254
C	-6.071235	-0.745828	-1.460151
C	-5.658783	0.589879	-1.419064
C	-4.413710	0.957396	-0.925512
C	-3.602518	-0.055751	-0.411428
O	-1.415634	-1.623711	-1.312635
O	-2.362038	0.272194	0.085541
P	-1.054950	-0.084285	-0.857291
O	0.091399	-0.075166	0.124730
O	-0.977137	0.750152	-2.083581
C	0.445050	-3.768951	-0.530885
C	-3.891482	2.353791	-0.949944
C	0.954088	-5.104423	-0.504934
C	2.205716	-5.406923	-0.967883
C	3.031961	-4.404861	-1.542759
C	2.500557	-3.094294	-1.662480
C	1.224770	-2.798053	-1.120514
C	-4.080772	3.208801	0.168681
C	-3.503187	4.450781	0.212922
C	-2.693697	4.907713	-0.859008

C	-2.525099	4.069038	-1.996629
C	-3.140774	2.791101	-2.015137
H	-0.596846	-5.017516	1.591738
H	-6.313654	1.360278	-1.821014
H	0.329128	-5.899160	-0.109789
H	2.577569	-6.427112	-0.914136
H	-2.946593	2.124272	-2.848954
H	-3.630757	5.087879	1.083704
H	-4.670255	2.849348	1.007647
H	0.908089	-1.765959	-1.129921
C	-1.028910	2.307548	2.047078
C	-2.142344	2.431530	2.870175
C	-2.447263	3.651456	3.467594
C	-1.638284	4.756230	3.218843
C	-0.522528	4.638717	2.393995
H	-0.841639	1.345604	1.580892
H	-2.774875	1.563384	3.028424
H	-3.315402	3.744096	4.113367
H	0.101504	5.508444	2.218114
H	-1.868512	5.716328	3.670997
C	2.031529	5.587620	0.378652
C	2.922710	6.617910	0.675414
C	3.820723	6.489412	1.729336
C	3.817859	5.325370	2.494973
C	2.924688	4.300221	2.204893
H	2.914987	3.394099	2.803863
H	1.324768	5.724848	-0.435254
H	2.909826	7.523251	0.076667
H	4.516434	7.291116	1.955409
H	4.510707	5.214638	3.323114
C	2.896260	-0.642425	0.947555
C	3.659209	-1.799017	1.076965
C	4.948539	-1.897169	0.571104
C	5.473531	-0.788342	-0.078414
Br	2.904630	-3.305212	1.918453
H	5.508305	-2.821964	0.643345
C	4.755436	0.391741	-0.202034
H	5.204093	1.244519	-0.703334
H	1.873696	-0.640214	1.305625
Br	7.186099	-0.919930	-0.864238
C	-1.685681	4.505747	-3.057026
C	-1.038358	5.714266	-2.989001
C	-1.201957	6.548370	-1.852746
C	-2.010433	6.153337	-0.814657
H	-1.552824	3.849900	-3.913287
H	-0.399133	6.038378	-3.804869
H	-2.136366	6.784857	0.061715
H	-0.688816	7.505044	-1.809897
C	3.281674	-2.088850	-2.291603
C	4.544222	-2.363634	-2.749564
C	5.092859	-3.659884	-2.585564
C	4.348703	-4.658840	-2.007476
H	2.854771	-1.093097	-2.392720
H	5.144224	-1.584411	-3.210818
H	6.102867	-3.860087	-2.930561
H	4.757732	-5.660361	-1.898656
C	-2.835146	-4.994144	3.022199
C	-3.946991	-4.428704	3.902066
H	-1.923800	-5.156123	3.608535
H	-3.143738	-5.983731	2.656039
C	-5.125405	-4.003804	3.030252
H	-3.575219	-3.555493	4.453997
H	-4.252920	-5.173547	4.644044

C	-4.706744	-2.869184	2.098388
H	-5.465259	-4.863448	2.435973
H	-5.973274	-3.682906	3.644317
H	-4.543342	-1.958683	2.693885
H	-5.518365	-2.622518	1.409672
C	-5.582625	-3.216599	-1.160862
C	-7.073183	-3.446873	-1.397344
H	-5.229369	-3.821833	-0.322484
H	-5.021402	-3.575170	-2.035809
C	-7.579223	-2.512767	-2.493132
H	-7.246876	-4.494548	-1.663682
H	-7.630026	-3.253733	-0.469597
C	-7.438062	-1.061953	-2.039271
H	-6.988415	-2.675240	-3.403872
H	-8.623712	-2.726194	-2.742960
H	-8.199173	-0.856105	-1.272995
H	-7.647407	-0.376900	-2.868316

TS-4-major-3

M06-2X/6-31G* Energy = -8271.54087272

M06-2X/6-31G* Free Energy = -8270.649640

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.51416208

M06-2X/def2-TZVPP-SMD(toluene) Energy = -8277.52037725

Number of Imaginary Frequencies = 1

Lowest Frequency = 228.9812i

M06-2X/6-31G* Geometry

C	0.361388	3.349319	-0.699139
C	1.035869	3.274756	0.928275
C	1.502514	3.106092	-1.498264
H	-0.365690	2.537684	-0.685727
H	-0.102008	4.330564	-0.774060
C	2.113521	1.825665	-1.478936
H	2.066787	3.952705	-1.890068
N	1.656874	2.015109	1.015172
C	2.028455	4.415053	1.135536
C	-0.196774	3.407273	1.817183
C	2.730280	1.779118	0.155428
C	3.456766	0.466090	0.311178
H	3.447088	2.600310	0.188832
H	0.991697	1.226046	1.007201
H	1.421060	0.981751	-1.471513
H	2.979735	1.695400	-2.126950
C	-5.227741	-1.752766	-0.965134
C	-6.071271	-0.746329	-1.459952
C	-3.996465	-1.392973	-0.380990
C	-3.602507	-0.056016	-0.411500
C	-4.413844	0.957051	-0.925513
C	-5.658936	0.589416	-1.418927
C	-3.058809	-2.389782	0.223495
C	-3.418428	-3.159660	1.346814
C	-2.513122	-4.113134	1.829239
C	-1.285250	-4.278134	1.190141
C	-0.871115	-3.498287	0.108373
C	-1.773395	-2.508480	-0.317879
O	-2.362024	0.272060	0.085365
O	-1.415512	-1.623812	-1.312782
P	-1.054923	-0.084357	-0.857465
O	0.091414	-0.075160	0.124572
O	-0.977148	0.750073	-2.083760
C	-3.891737	2.353492	-0.950013
C	0.445407	-3.768850	-0.531040
C	-4.081219	3.208606	0.168499
C	-3.503715	4.450627	0.212678

C	-2.694139	4.907506	-0.859210
C	-2.525359	4.068726	-1.996727
C	-3.140934	2.790741	-2.015165
C	0.954547	-5.104283	-0.505116
C	2.206203	-5.406673	-0.968058
C	3.032380	-4.404530	-1.542891
C	2.500872	-3.094004	-1.662596
C	1.225050	-2.797880	-1.120652
H	-6.313919	1.359749	-1.820821
H	-0.596249	-5.017420	1.591676
H	-4.670777	2.849203	1.007434
H	-3.631428	5.087810	1.083377
H	0.908287	-1.765811	-1.130041
H	2.578137	-6.426835	-0.914330
H	0.329644	-5.899075	-0.109989
H	-2.946595	2.123828	-2.848878
C	-1.029219	2.307424	2.046951
C	-2.142726	2.431314	2.869961
C	-2.447777	3.651209	3.467378
C	-1.638851	4.756041	3.218715
C	-0.523020	4.638619	2.393954
H	-0.841843	1.345500	1.580769
H	-2.775211	1.563121	3.028144
H	-3.315975	3.743779	4.113081
H	0.100971	5.508389	2.218146
H	-1.869178	5.716114	3.670871
C	2.924241	4.300331	2.205083
C	3.817332	5.325523	2.495257
C	3.820176	6.489591	1.729661
C	2.922226	6.618072	0.675684
C	2.031125	5.587741	0.378828
H	1.324409	5.724952	-0.435120
H	2.914553	3.394189	2.804022
H	4.510133	5.214803	3.323440
H	4.515824	7.291329	1.955808
H	2.909328	7.523434	0.076968
C	4.755378	0.392078	-0.201921
C	5.473545	-0.787963	-0.078313
C	4.948600	-1.896847	0.571142
C	3.659247	-1.798797	1.076962
Br	7.186163	-0.919406	-0.864057
H	5.508424	-2.821609	0.643371
C	2.896227	-0.642250	0.947564
H	1.873651	-0.640116	1.305600
H	5.203998	1.244903	-0.703172
Br	2.904739	-3.305064	1.918385
C	3.281924	-2.088478	-2.291668
C	4.544509	-2.363145	-2.749596
C	5.093248	-3.659355	-2.585615
C	4.349157	-4.658388	-2.007575
H	2.854944	-1.092756	-2.392769
H	5.144462	-1.583862	-3.210812
H	4.758267	-5.659877	-1.898769
H	6.103283	-3.859466	-2.930585
C	-1.685876	4.505391	-3.057091
C	-1.038659	5.713970	-2.989131
C	-1.202432	6.548178	-1.852976
C	-2.010975	6.153188	-0.814923
H	-1.552884	3.849462	-3.913269
H	-0.399385	6.038051	-3.804973
H	-0.689372	7.504896	-1.810177
H	-2.137043	6.784790	0.061369
C	-7.438131	-1.062598	-2.038911

C	-7.579133	-2.513401	-2.492846
H	-7.647693	-0.377514	-2.867875
H	-8.199168	-0.856923	-1.272513
C	-7.072928	-3.447491	-1.397120
H	-6.988339	-2.675752	-3.403617
H	-8.623606	-2.726949	-2.742642
C	-5.582383	-3.217057	-1.160712
H	-7.629742	-3.254451	-0.469335
H	-7.246514	-4.495176	-1.663487
H	-5.229022	-3.822249	-0.322347
H	-5.021163	-3.575577	-2.035681
C	-4.706314	-2.869417	2.098483
C	-5.124771	-4.003946	3.030552
H	-4.542965	-1.958806	2.693825
H	-5.518029	-2.622951	1.409806
C	-3.946212	-4.428680	3.902249
H	-5.972570	-3.683016	3.644697
H	-5.464666	-4.863682	2.436430
C	-2.834481	-4.994177	3.022278
H	-3.574391	-3.555384	4.454013
H	-4.251999	-5.173444	4.644366
H	-3.143134	-5.983777	2.656204
H	-1.923063	-5.156139	3.608506

TS-5-major

M06-2X/6-31G* Energy = -8271.53777369

M06-2X/6-31G* Free Energy = -8270.648942

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.51098166

M06-2X/def2-TZVPP-SMD(toluene) Energy = -8277.51702803

Number of Imaginary Frequencies = 1

Lowest Frequency = 273.5597i

M06-2X/6-31G* Geometry

C	-3.425984	0.354500	2.253920
C	-3.768124	0.978696	0.692594
C	-3.678745	-1.048999	2.123851
H	-2.367709	0.587888	2.374889
H	-4.059069	0.898242	2.952912
C	-2.792372	-1.831248	1.370848
H	-4.665350	-1.442933	2.365791
N	-2.893308	0.257762	-0.169113
C	-5.229720	0.742721	0.321632
C	-3.419088	2.466019	0.736423
C	-3.094606	-1.104427	-0.269331
C	-2.203233	-1.877068	-1.199083
H	-4.141467	-1.345465	-0.444734
H	-1.903075	0.523402	-0.059661
H	-1.731237	-1.584584	1.459609
H	-3.018478	-2.889360	1.259174
C	4.393866	-1.732159	0.045819
C	4.157828	-3.054545	0.452386
C	3.671098	-0.690086	0.659694
C	2.639415	-0.994464	1.556160
C	2.288229	-2.321399	1.852800
C	3.119472	-3.318878	1.342104
C	3.880330	0.736593	0.270305
C	5.116434	1.398363	0.410949
C	5.243766	2.710163	-0.066643
C	4.134402	3.357239	-0.613496
C	2.875863	2.764570	-0.671740
C	2.781371	1.440612	-0.229288
O	1.960180	0.040144	2.147355
O	1.543840	0.829878	-0.192764
P	0.839384	0.909236	1.302086

O	-0.428191	0.098422	1.159475
O	0.812818	2.282517	1.849644
C	1.024153	-2.681448	2.545424
C	1.684924	3.522278	-1.128298
C	0.338159	-3.856881	2.111374
C	-0.847036	-4.247329	2.674913
C	-1.471471	-3.452956	3.671719
C	-0.820973	-2.256613	4.083212
C	0.441010	-1.915057	3.533178
C	0.707733	2.920893	-1.975226
C	-0.372127	3.635082	-2.419094
C	-0.551834	4.995964	-2.055313
C	0.409770	5.602205	-1.201174
C	1.516471	4.836045	-0.752509
H	2.915247	-4.354778	1.602722
H	4.249196	4.373904	-0.984241
H	0.757910	-4.431613	1.291000
H	-1.347844	-5.149045	2.329880
H	2.230911	5.298140	-0.075386
H	-1.107773	3.167861	-3.069123
H	0.835569	1.884776	-2.268509
H	0.926704	-1.010366	3.878769
C	-2.129358	2.849682	1.108290
C	-1.745218	4.183920	1.085796
C	-2.660408	5.162042	0.705990
C	-3.956802	4.791126	0.358594
C	-4.341904	3.451748	0.373408
H	-1.392385	2.122286	1.419733
H	-0.722510	4.425786	1.359207
H	-2.360713	6.205151	0.668138
H	-5.355543	3.187660	0.091820
H	-4.677715	5.547478	0.062585
C	-6.248192	0.652829	1.270183
C	-7.579129	0.528427	0.875501
C	-7.910510	0.495647	-0.474630
C	-6.901648	0.595142	-1.430493
C	-5.574579	0.723112	-1.035574
H	-4.787734	0.815580	-1.779280
H	-6.019040	0.692402	2.330477
H	-8.356322	0.459898	1.630077
H	-8.946943	0.397135	-0.781032
H	-7.147731	0.579230	-2.487613
C	-0.813105	-1.842871	-1.085733
C	-0.049689	-2.573058	-1.985852
C	-0.629351	-3.337573	-2.993595
C	-2.015782	-3.358841	-3.080354
Br	1.824690	-2.542240	-1.772655
H	-0.020383	-3.905231	-3.687028
C	-2.812250	-2.643876	-2.193762
H	-3.892862	-2.680539	-2.288443
H	-0.333179	-1.255556	-0.304902
Br	-2.839042	-4.391891	-4.433519
C	0.229186	6.958729	-0.819518
C	-0.842912	7.681410	-1.279728
C	-1.795486	7.077817	-2.137363
C	-1.653264	5.765192	-2.510203
H	0.962968	7.416516	-0.160820
H	-0.964946	8.720323	-0.988104
H	-2.386234	5.291978	-3.158823
H	-2.640645	7.658636	-2.494357
C	-1.482066	-1.399524	5.004462
C	-2.730683	-1.710077	5.481395
C	-3.371584	-2.909716	5.079555

C	-2.751291	-3.763015	4.201284
H	-0.984385	-0.482122	5.307911
H	-3.229785	-1.042119	6.176899
H	-4.352929	-3.153072	5.476070
H	-3.237711	-4.683771	3.886915
C	4.935906	-4.217002	-0.132006
C	5.433078	-3.921252	-1.544763
H	4.305970	-5.113244	-0.123512
H	5.800174	-4.437434	0.510312
C	6.193949	-2.598500	-1.544974
H	4.572336	-3.848957	-2.224512
H	6.064376	-4.740162	-1.904708
C	5.266786	-1.445774	-1.166130
H	7.020550	-2.660579	-0.823716
H	6.639708	-2.400396	-2.525160
H	4.578982	-1.246120	-2.003329
H	5.839930	-0.524688	-1.042195
C	6.254448	0.749987	1.180232
C	7.615650	1.367514	0.868741
H	6.276177	-0.330526	1.020032
H	6.040281	0.881966	2.250730
C	7.542706	2.886106	1.004530
H	8.373027	0.949879	1.540195
H	7.915315	1.107943	-0.156510
C	6.567561	3.451225	-0.025430
H	7.200247	3.138833	2.016332
H	8.529677	3.342034	0.874047
H	7.031485	3.393507	-1.020489
H	6.382259	4.514480	0.163058

TS-5-major-2

M06-2X/6-31G* Energy = -8271.55107429

M06-2X/6-31G* Free Energy = -8270.658418

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.51461779

M06-2X/def2-TZVPP-SMD(toluene) Energy = -8277.51987920

Number of Imaginary Frequencies = 1

Lowest Frequency = 337.5577i

M06-2X/6-31G* Geometry

C	-3.978012	-0.858539	1.736869
C	-4.093807	0.016535	0.229621
C	-3.775050	-2.198036	1.300128
H	-3.098255	-0.397323	2.185814
H	-4.896761	-0.640240	2.278067
C	-2.542264	-2.555549	0.734849
H	-4.635744	-2.850018	1.155447
N	-2.859938	-0.243268	-0.397527
C	-5.274655	-0.473012	-0.596396
C	-4.212831	1.480286	0.646552
C	-2.538639	-1.528149	-0.775586
C	-1.154606	-1.669619	-1.358892
H	-3.313283	-2.015172	-1.368640
H	-2.055865	0.189477	0.099160
H	-1.645148	-2.119611	1.184376
H	-2.449299	-3.586323	0.399357
C	4.074392	-0.761961	-0.297919
C	3.994428	-2.162804	-0.330679
C	3.248340	-0.058376	0.602994
C	2.316191	-0.752417	1.386741
C	2.169725	-2.145684	1.306180
C	3.062776	-2.818182	0.469444
C	3.266340	1.432450	0.695438
C	4.413694	2.164081	1.054447
C	4.372554	3.564646	0.995445

C	3.180439	4.203564	0.655881
C	1.996402	3.508453	0.412378
C	2.069487	2.111377	0.440972
O	1.548147	-0.025212	2.264713
O	0.924396	1.361756	0.270734
P	0.251303	0.816344	1.685968
O	-0.797528	-0.172873	1.238898
O	-0.074807	1.916822	2.616733
C	1.074742	-2.896173	1.974027
C	0.723526	4.232167	0.175491
C	0.488144	-2.499676	3.214045
C	-0.568979	-3.192057	3.745015
C	-1.122622	-4.321474	3.084526
C	-0.517852	-4.751656	1.873089
C	0.575220	-4.021907	1.351467
C	0.457898	5.423786	0.909061
C	-0.668953	6.165734	0.675777
C	-1.626088	5.751000	-0.286618
C	-1.396287	4.535830	-0.989256
C	-0.201175	3.810320	-0.755596
H	3.025914	-3.904101	0.426247
H	3.168161	5.290534	0.604449
H	0.880131	-1.633276	3.730663
H	-1.009564	-2.868371	4.684626
H	-0.002695	2.921714	-1.348049
H	-0.851686	7.078425	1.237645
H	1.162117	5.731792	1.675898
H	0.983409	-4.343243	0.399141
C	-5.343820	2.236124	0.329939
C	-5.402706	3.581380	0.687584
C	-4.340523	4.182674	1.355588
C	-3.213787	3.430387	1.678982
C	-3.158952	2.084393	1.340866
H	-6.175842	1.788941	-0.203621
H	-6.282560	4.162947	0.429048
H	-4.387076	5.235534	1.614436
H	-2.278058	1.525660	1.640202
H	-2.361613	3.869836	2.189696
C	-5.246374	-0.244870	-1.977103
C	-6.327303	-0.598336	-2.777522
C	-7.460640	-1.174811	-2.208749
C	-7.503972	-1.390412	-0.835180
C	-6.418748	-1.040241	-0.034623
H	-6.483135	-1.204172	1.036696
H	-4.367946	0.220007	-2.416089
H	-6.284746	-0.417866	-3.846986
H	-8.305433	-1.450298	-2.831773
H	-8.384817	-1.831318	-0.379365
C	-0.432704	-0.528656	-1.708166
C	0.848622	-0.653796	-2.225215
C	1.443067	-1.894402	-2.410462
C	0.703092	-3.017383	-2.064433
Br	1.784727	0.908371	-2.699723
H	2.450943	-1.984229	-2.798434
C	-0.585437	-2.929203	-1.555868
H	-1.115576	-3.838311	-1.290384
H	-0.846725	0.461816	-1.567898
Br	1.499208	-4.724510	-2.251778
C	-2.379325	4.081794	-1.909389
C	-3.519381	4.808408	-2.135870
C	-3.729070	6.036959	-1.461578
C	-2.804492	6.494126	-0.557987
H	-2.208612	3.141159	-2.428376

H	-4.267218	4.446579	-2.835070
H	-2.963836	7.430411	-0.027936
H	-4.630068	6.610289	-1.658898
C	-1.078151	-5.850255	1.166005
C	-2.200891	-6.482854	1.637646
C	-2.805053	-6.054897	2.846914
C	-2.273747	-5.005426	3.555113
H	-0.601616	-6.165376	0.239010
H	-2.628377	-7.317889	1.090969
H	-3.689111	-6.567498	3.213648
H	-2.733090	-4.677170	4.484347
C	4.886346	-3.013277	-1.218109
C	5.582071	-2.223605	-2.324743
H	4.284209	-3.825269	-1.643302
H	5.649685	-3.492276	-0.589356
C	6.138822	-0.918904	-1.762481
H	4.866945	-1.983846	-3.124532
H	6.370536	-2.832858	-2.778441
C	4.990495	-0.040824	-1.272215
H	6.823281	-1.139652	-0.931436
H	6.715780	-0.381026	-2.521802
H	5.370732	0.889261	-0.846811
H	4.383862	0.261323	-2.135254
C	5.633228	1.459584	1.623162
C	6.907687	2.293176	1.515499
H	5.772517	0.475882	1.168991
H	5.426415	1.263763	2.685364
C	6.665911	3.687567	2.088510
H	7.724814	1.790140	2.042949
H	7.208270	2.378496	0.461489
C	5.602394	4.411775	1.265921
H	6.327899	3.592105	3.128469
H	7.590359	4.274319	2.102195
H	6.041581	4.705731	0.301828
H	5.302023	5.342315	1.760171

TS-5-major-3

M06-2X/6-31G* Energy = -8271.53718042

M06-2X/6-31G* Free Energy = -8270.647532

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.51079281

M06-2X/def2-TZVPP-SMD(toluene) Energy = -8277.51649876

Number of Imaginary Frequencies = 1

Lowest Frequency = 276.8176i

M06-2X/6-31G* Geometry

C	-3.371144	0.309017	2.313328
C	-3.762005	0.925620	0.768734
C	-3.555934	-1.106756	2.178870
H	-2.324345	0.595631	2.426170
H	-4.021378	0.814079	3.025980
C	-2.644951	-1.842289	1.411694
H	-4.518070	-1.549859	2.433242
N	-2.864009	0.254224	-0.112811
C	-5.212930	0.624208	0.403908
C	-3.489529	2.427291	0.825158
C	-3.012306	-1.112471	-0.224765
C	-2.109705	-1.845596	-1.174007
H	-4.052028	-1.394358	-0.379988
H	-1.883214	0.554707	-0.004393
H	-1.595551	-1.543810	1.480577
H	-2.822541	-2.908885	1.294112
C	4.451411	-1.542412	0.025185
C	4.239586	-2.867340	0.435525
C	3.721132	-0.509584	0.647936

C	2.705127	-0.829241	1.557086
C	2.378100	-2.161424	1.861066
C	3.217119	-3.146267	1.338922
C	3.921415	0.920637	0.265065
C	5.168236	1.567261	0.373182
C	5.299672	2.868263	-0.129831
C	4.180984	3.526192	-0.639764
C	2.903986	2.964579	-0.640772
C	2.813649	1.634974	-0.204046
O	2.019897	0.195646	2.159395
O	1.586083	1.007981	-0.163950
P	0.872058	1.040095	1.326714
O	-0.365852	0.187914	1.157795
O	0.790414	2.400620	1.898459
C	1.137192	-2.542003	2.584805
C	1.719103	3.777886	-1.019843
C	0.475840	-3.745613	2.190955
C	-0.686321	-4.156854	2.786681
C	-1.314768	-3.358064	3.777242
C	-0.688463	-2.137261	4.152142
C	0.552853	-1.773211	3.570477
C	1.750491	5.183045	-0.775899
C	0.709704	5.997267	-1.132673
C	-0.462412	5.462437	-1.725980
C	-0.529896	4.057645	-1.929358
C	0.582420	3.245132	-1.594014
H	3.036448	-4.184615	1.606503
H	4.311457	4.533918	-1.026984
H	0.894659	-4.328455	1.376113
H	-1.167464	-5.079912	2.471207
H	0.518135	2.180769	-1.790089
H	0.760138	7.066185	-0.940192
H	2.611306	5.609629	-0.271545
H	1.020657	-0.850321	3.891140
C	-4.492481	3.367787	0.571452
C	-4.187146	4.726522	0.581684
C	-2.889724	5.159999	0.841500
C	-1.892803	4.227083	1.111652
C	-2.198986	2.871984	1.115000
H	-5.508118	3.054105	0.356490
H	-4.970928	5.448629	0.372940
H	-2.657173	6.220427	0.826881
H	-1.403259	2.178238	1.352798
H	-0.866802	4.521144	1.315319
C	-5.568750	0.649498	-0.950623
C	-6.889609	0.464227	-1.342048
C	-7.882121	0.262252	-0.384645
C	-7.540606	0.250258	0.963017
C	-6.214669	0.431328	1.354190
H	-5.977714	0.434953	2.413608
H	-4.794783	0.823472	-1.693534
H	-7.144906	0.484143	-2.396912
H	-8.914161	0.119416	-0.688368
H	-8.305591	0.102481	1.718696
C	-0.719855	-1.765207	-1.083789
C	0.051328	-2.465769	-2.000764
C	-0.519799	-3.242033	-3.004367
C	-1.905998	-3.307728	-3.069074
Br	1.926104	-2.378375	-1.815734
H	0.095884	-3.785153	-3.711409
C	-2.710100	-2.625898	-2.163638
H	-3.790374	-2.697887	-2.239853
H	-0.245846	-1.166528	-0.307728

Br	-2.717773	-4.356409	-4.416796
C	-1.733015	3.498135	-2.439552
C	-2.803033	4.297216	-2.748112
C	-2.718036	5.702148	-2.581717
C	-1.574181	6.269240	-2.082299
H	-1.791639	2.419253	-2.565192
H	-3.722949	3.857167	-3.121630
H	-1.506609	7.344844	-1.936319
H	-3.568878	6.325293	-2.840772
C	-1.353581	-1.279470	5.069938
C	-2.584728	-1.612116	5.576313
C	-3.202552	-2.834526	5.208591
C	-2.576858	-3.689373	4.335460
H	-0.873888	-0.344109	5.346317
H	-3.087680	-0.943734	6.268598
H	-4.170271	-3.094318	5.627526
H	-3.045392	-4.628006	4.048022
C	5.029280	-4.020124	-0.153039
C	5.517716	-3.720711	-1.567940
H	4.410594	-4.924133	-0.141115
H	5.898568	-4.229295	0.486299
C	6.255024	-2.384886	-1.574778
H	4.654622	-3.666054	-2.246176
H	6.162300	-4.529900	-1.926313
C	5.309140	-1.247562	-1.196052
H	7.085296	-2.429546	-0.856288
H	6.693572	-2.181841	-2.557209
H	5.866470	-0.315877	-1.083378
H	4.612010	-1.065375	-2.029541
C	6.318414	0.918839	1.124014
C	7.679315	1.504588	0.754898
H	6.317365	-0.165654	0.993958
H	6.139595	1.084538	2.196378
C	7.637144	3.027020	0.857158
H	8.450620	1.089186	1.411737
H	7.941715	1.215927	-0.272903
C	6.636654	3.586292	-0.151534
H	7.334559	3.308912	1.873955
H	8.626761	3.461883	0.682224
H	7.064355	3.496403	-1.160356
H	6.477499	4.656941	0.017898

TS-5-major-4

M06-2X/6-31G* Energy = -8271.55179167

M06-2X/6-31G* Free Energy = -8270.656954

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.51350153

M06-2X/def2-TZVPP-SMD(toluene) Energy = -8277.51909721

Number of Imaginary Frequencies = 1

Lowest Frequency = 350.4686i

M06-2X/6-31G* Geometry

C	-3.896309	-1.220651	1.721811
C	-4.043377	-0.439411	0.150525
C	-3.579153	-2.558509	1.366302
H	-3.065296	-0.664791	2.153975
H	-4.842155	-1.040884	2.228538
C	-2.306030	-2.843927	0.845138
H	-4.381773	-3.284600	1.240955
N	-2.783112	-0.647525	-0.436818
C	-5.173392	-1.063949	-0.654759
C	-4.271521	1.033514	0.480567
C	-2.361032	-1.928751	-0.724168
C	-0.966257	-2.014477	-1.294109
H	-3.090223	-2.507434	-1.292039

H	-2.023980	-0.120684	0.040416
H	-1.460148	-2.306953	1.284122
H	-2.115419	-3.882927	0.582696
C	4.180639	-0.267046	-0.212972
C	4.204100	-1.667727	-0.291981
C	3.268827	0.338347	0.675427
C	2.402851	-0.448767	1.442767
C	2.410865	-1.850181	1.373279
C	3.349865	-2.419921	0.511014
C	3.062829	1.817584	0.691841
C	4.047312	2.744675	1.074568
C	3.794833	4.115177	0.911719
C	2.553022	4.535246	0.433066
C	1.519617	3.642059	0.156889
C	1.800256	2.281476	0.306011
O	1.519458	0.206706	2.268561
O	0.782995	1.361056	0.155945
P	0.148965	0.839730	1.601602
O	-0.762780	-0.298390	1.213775
O	-0.327415	1.959925	2.440760
C	1.408615	-2.708907	2.057625
C	0.178096	4.110076	-0.269235
C	0.779735	-2.352725	3.289111
C	-0.192868	-3.147257	3.838546
C	-0.616434	-4.346186	3.204810
C	0.034939	-4.733696	2.003633
C	1.041367	-3.899298	1.465565
C	-0.470598	3.502753	-1.384403
C	-1.678398	3.964674	-1.831171
C	-2.320303	5.063189	-1.199787
C	-1.692105	5.662104	-0.073199
C	-0.439242	5.160744	0.369087
H	3.404159	-3.503410	0.431328
H	2.372208	5.599533	0.294109
H	1.070082	-1.435358	3.784622
H	-0.667387	-2.853463	4.771426
H	0.029622	5.611266	1.240831
H	-2.158353	3.504565	-2.691456
H	0.030213	2.684850	-1.893232
H	1.487056	-4.200019	0.525003
C	-3.299009	1.730636	1.205792
C	-3.436921	3.088826	1.455786
C	-4.565772	3.767931	1.003050
C	-5.549153	3.075774	0.302274
C	-5.408990	1.713569	0.039480
H	-2.412906	1.239102	1.590707
H	-2.642670	3.595832	1.995396
H	-4.668281	4.834144	1.182232
H	-6.180601	1.194851	-0.519858
H	-6.430546	3.598942	-0.056452
C	-5.126339	-0.951310	-2.049013
C	-6.168071	-1.431413	-2.835915
C	-7.280082	-2.022150	-2.240920
C	-7.342171	-2.124682	-0.854864
C	-6.296934	-1.646978	-0.067562
H	-6.376334	-1.725216	1.012272
H	-4.265116	-0.476420	-2.510508
H	-6.111350	-1.338382	-3.915841
H	-8.094069	-2.396559	-2.853302
H	-8.207129	-2.575945	-0.379177
C	-0.291938	-0.853355	-1.676840
C	0.990873	-0.947032	-2.196894
C	1.634763	-2.167992	-2.341906

C	0.945686	-3.308143	-1.955522
Br	1.877884	0.621337	-2.743550
H	2.641874	-2.230043	-2.736050
C	-0.346157	-3.255815	-1.450384
H	-0.839969	-4.175773	-1.153124
H	-0.744082	0.124576	-1.567818
Br	1.839802	-4.974010	-2.055246
C	-2.338871	6.749479	0.572910
C	-3.536175	7.233283	0.107300
C	-4.152412	6.645033	-1.024721
C	-3.559215	5.581348	-1.656630
H	-1.860700	7.198957	1.439595
H	-4.014763	8.071757	0.604341
H	-4.031759	5.116067	-2.518185
H	-5.098277	7.037398	-1.385980
C	-0.396136	-5.904231	1.321455
C	-1.442978	-6.646927	1.807559
C	-2.094488	-6.261268	3.006617
C	-1.685369	-5.143245	3.690867
H	0.114500	-6.182255	0.400642
H	-1.773238	-7.536728	1.280184
H	-2.917119	-6.860548	3.384779
H	-2.181357	-4.847110	4.612027
C	5.079395	-2.402132	-1.290066
C	5.493245	-1.502454	-2.451963
H	4.535652	-3.287639	-1.645705
H	5.984507	-2.777026	-0.792013
C	6.105359	-0.223544	-1.889289
H	4.613959	-1.233907	-3.055598
H	6.194848	-2.026075	-3.109121
C	5.055088	0.580478	-1.122070
H	6.933971	-0.490719	-1.219738
H	6.526762	0.397633	-2.686159
H	5.547293	1.375990	-0.558072
H	4.397224	1.095232	-1.831838
C	5.299934	2.278633	1.793595
C	6.444135	3.284974	1.702965
H	5.610417	1.289766	1.447496
H	5.031839	2.144806	2.851642
C	5.953217	4.661596	2.146965
H	7.283182	2.951931	2.322641
H	6.809471	3.343256	0.667842
C	4.856874	5.158855	1.206202
H	5.557550	4.585252	3.167937
H	6.776046	5.383619	2.173533
H	5.318392	5.461418	0.255297
H	4.381601	6.058200	1.613286

TS-6-major

M06-2X/6-31G* Energy = -8271.53351474

M06-2X/6-31G* Free Energy = -8270.645587

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.50718982

M06-2X/def2-TZVPP-SMD(toluene) Energy = -8277.51409360

Number of Imaginary Frequencies = 1

Lowest Frequency = 374.6414i

M06-2X/6-31G* Geometry

C	-0.766250	-1.658042	2.596426
C	-0.851346	-0.023396	3.319002
C	-2.080894	-1.809242	2.093722
H	0.004495	-1.501268	1.841393
H	-0.448229	-2.314094	3.404193
C	-2.485323	-1.040549	0.987045
H	-2.840810	-2.283278	2.713359

N	-1.195507	0.798202	2.234789
C	-1.902360	0.010986	4.423167
C	0.563490	0.177851	3.852976
C	-2.448698	0.625532	1.668623
C	-2.825914	1.506140	0.508208
H	-3.239308	0.577756	2.416670
H	-0.428752	0.991002	1.551428
H	-1.752051	-0.919601	0.191145
H	-3.502097	-1.190127	0.629634
C	2.488264	-3.564620	-2.198377
C	1.539681	-4.363794	-2.850317
C	2.046290	-2.501890	-1.380463
C	0.688580	-2.182833	-1.347072
C	-0.272999	-2.972299	-1.989054
C	0.181487	-4.072424	-2.708132
C	3.004619	-1.685141	-0.574773
C	3.825839	-2.266839	0.415087
C	4.827929	-1.489974	1.007130
C	4.986444	-0.160936	0.608957
C	4.113532	0.474724	-0.271632
C	3.088164	-0.311621	-0.820921
O	0.288557	-1.108435	-0.584913
O	2.163057	0.253922	-1.666955
P	0.639115	0.451745	-1.086252
O	0.696499	1.179663	0.235485
O	-0.237344	0.878327	-2.196932
C	-1.729167	-2.693134	-1.872336
C	4.334980	1.900841	-0.625059
C	-2.285491	-1.464240	-2.333778
C	-3.631814	-1.228859	-2.216068
C	-4.497648	-2.185074	-1.616590
C	-3.947996	-3.416750	-1.162340
C	-2.554804	-3.642836	-1.313661
C	5.658279	2.316679	-0.951209
C	5.937008	3.622798	-1.252340
C	4.910096	4.602513	-1.248138
C	3.586457	4.195098	-0.926521
C	3.325000	2.836196	-0.615263
H	-0.551043	-4.698278	-3.214089
H	5.786016	0.428039	1.056366
H	-1.628713	-0.709030	-2.757393
H	-4.058749	-0.292763	-2.568712
H	2.315263	2.547641	-0.338952
H	6.949684	3.924438	-1.508036
H	6.448504	1.571288	-0.978761
H	-2.133004	-4.580319	-0.956595
C	0.791608	0.252674	5.231372
C	2.083485	0.412913	5.725256
C	3.161178	0.500368	4.851604
C	2.940106	0.422012	3.478773
C	1.654314	0.248880	2.977142
H	-0.034131	0.194765	5.931088
H	2.239894	0.473283	6.797725
H	4.168159	0.630754	5.236176
H	1.517784	0.199167	1.898910
H	3.766548	0.495737	2.779868
C	-2.403115	1.263248	4.798452
C	-3.298096	1.381864	5.855974
C	-3.698080	0.251550	6.565200
C	-3.193164	-0.994623	6.209377
C	-2.299707	-1.113330	5.146623
H	-1.905585	-2.094851	4.902035
H	-2.080974	2.145240	4.252077

H	-3.679427	2.360888	6.128029
H	-4.396136	0.342538	7.391066
H	-3.491083	-1.881854	6.758936
C	-4.102085	1.360766	-0.048753
C	-4.433516	2.097542	-1.174670
C	-3.533925	2.969825	-1.778330
C	-2.285752	3.114102	-1.192354
Br	-6.135931	1.864940	-1.968370
H	-3.796927	3.507118	-2.681251
C	-1.930687	2.417736	-0.043159
H	-0.936363	2.553363	0.358798
H	-4.823081	0.661620	0.365638
Br	-1.000465	4.227619	-1.994299
C	2.549627	5.166644	-0.919238
C	2.816684	6.476663	-1.222045
C	4.136522	6.881947	-1.541960
C	5.156999	5.966184	-1.555585
H	1.538295	4.841898	-0.691127
H	2.016002	7.210181	-1.220220
H	6.170991	6.270521	-1.803075
H	4.335329	7.922639	-1.779585
C	-4.804123	-4.368209	-0.546729
C	-6.139583	-4.104625	-0.378186
C	-6.684047	-2.872753	-0.816592
C	-5.883225	-1.937730	-1.423023
H	-4.379137	-5.310755	-0.210274
H	-6.785150	-4.839180	0.093508
H	-7.741342	-2.672349	-0.672822
H	-6.291279	-0.986349	-1.753338
C	1.938383	-5.555119	-3.701743
C	3.388149	-5.495092	-4.174898
H	1.256445	-5.632886	-4.555550
H	1.796558	-6.471933	-3.111656
C	4.297494	-5.166677	-2.994573
H	3.496369	-4.715702	-4.940125
H	3.670092	-6.445730	-4.639095
C	3.971879	-3.778469	-2.448562
H	4.152967	-5.918093	-2.205344
H	5.351736	-5.208014	-3.286976
H	4.556943	-3.579763	-1.547864
H	4.292952	-3.020698	-3.177833
C	3.556882	-3.682422	0.897239
C	4.716282	-4.279200	1.691594
H	3.289609	-4.336769	0.063542
H	2.664131	-3.647220	1.539666
C	5.193263	-3.290146	2.751823
H	4.403187	-5.224712	2.146406
H	5.548926	-4.509741	1.012402
C	5.755962	-2.045930	2.070418
H	4.345836	-3.006304	3.390438
H	5.952411	-3.740277	3.399683
H	6.720875	-2.297040	1.607702
H	5.966001	-1.264595	2.810495

TS-6-major-2

M06-2X/6-31G* Energy = -8271.53317033

M06-2X/6-31G* Free Energy = -8270.644530

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.50591268

M06-2X/def2-TZVPP-SMD(toluene) Energy = -8277.51244357

Number of Imaginary Frequencies = 1

Lowest Frequency = 369.9127i

M06-2X/6-31G* Geometry

C	-1.677569	-2.129706	2.005819
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C	-1.474696	-0.786445	3.142317
C	-2.931878	-1.821519	1.418759
H	-0.814636	-1.982251	1.355745
H	-1.607592	-3.034223	2.607149
C	-3.035567	-0.722434	0.552097
H	-3.840990	-2.240520	1.847786
N	-1.503295	0.353411	2.321879
C	-2.601847	-0.780494	4.169674
C	-0.114023	-1.075692	3.768861
C	-2.683039	0.664083	1.672380
C	-2.651860	1.874925	0.777155
H	-3.552746	0.632124	2.328268
H	-0.640012	0.545404	1.761234
H	-2.218076	-0.574111	-0.152971
H	-4.021268	-0.525998	0.138487
C	1.945812	-3.387996	-2.651576
C	0.964491	-3.921915	-3.497843
C	1.573898	-2.432677	-1.678436
C	0.268398	-1.938934	-1.671544
C	-0.718338	-2.447159	-2.526717
C	-0.350096	-3.460265	-3.403354
C	2.567459	-1.898959	-0.696448
C	3.265815	-2.743624	0.194156
C	4.331477	-2.218969	0.933567
C	4.661580	-0.867647	0.796477
C	3.910452	0.016238	0.026158
C	2.828757	-0.526258	-0.684565
O	-0.076962	-0.989764	-0.736383
O	2.019346	0.299885	-1.429302
P	0.516531	0.577953	-0.823581
O	0.624290	0.934185	0.638508
O	-0.242875	1.390844	-1.796736
C	-2.107402	-1.919615	-2.500572
C	4.313211	1.444323	-0.072943
C	-2.346324	-0.546826	-2.795357
C	-3.615771	-0.034782	-2.741000
C	-4.719925	-0.853015	-2.378470
C	-4.492374	-2.232479	-2.108932
C	-3.167299	-2.739770	-2.187438
C	3.385659	2.511048	0.107428
C	3.806911	3.811735	0.034697
C	5.163930	4.139228	-0.221842
C	6.095320	3.080602	-0.402761
C	5.635564	1.741854	-0.320826
H	-1.105460	-3.866492	-4.073201
H	5.499062	-0.469605	1.366701
H	-1.507964	0.101713	-3.027254
H	-3.788911	1.017195	-2.953403
H	6.349042	0.936101	-0.480351
H	3.094288	4.619701	0.180738
H	2.348584	2.286874	0.333827
H	-2.990913	-3.789363	-1.959782
C	1.053444	-0.990415	3.000321
C	2.288239	-1.262961	3.580199
C	2.375226	-1.652815	4.914699
C	1.216105	-1.759057	5.674861
C	-0.022364	-1.470183	5.107664
H	1.024437	-0.686270	1.955656
H	3.182207	-1.161999	2.974303
H	3.342838	-1.870123	5.357369
H	-0.912948	-1.547622	5.720928
H	1.268161	-2.060855	6.716254
C	-3.326749	-1.917062	4.527994

C	-4.279011	-1.861075	5.543941
C	-4.516481	-0.667526	6.217292
C	-3.789723	0.470295	5.874033
C	-2.836382	0.412401	4.863560
H	-2.260477	1.295938	4.603037
H	-3.146988	-2.865729	4.031620
H	-4.833116	-2.756363	5.807340
H	-5.260265	-0.624127	7.006293
H	-3.960850	1.406106	6.396425
C	-3.712559	2.122029	-0.100882
C	-3.613199	3.172356	-0.999799
C	-2.480817	3.974680	-1.078125
C	-1.460635	3.730276	-0.172399
Br	-5.038676	3.482726	-2.208554
H	-2.394244	4.750312	-1.828896
C	-1.549521	2.725438	0.781067
H	-0.720819	2.573631	1.456817
H	-4.598869	1.495355	-0.115864
Br	0.146507	4.705202	-0.282858
C	7.455047	3.396850	-0.663611
C	7.869308	4.701734	-0.736961
C	6.941471	5.756559	-0.553838
C	5.621906	5.480001	-0.303177
H	8.161921	2.583034	-0.804980
H	8.911121	4.932703	-0.937133
H	4.904352	6.284647	-0.163901
H	7.281103	6.785951	-0.615141
C	-5.590531	-3.045081	-1.720436
C	-6.847620	-2.511183	-1.588014
C	-7.069293	-1.134581	-1.837650
C	-6.030812	-0.326251	-2.227767
H	-5.414793	-4.100167	-1.524611
H	-7.678646	-3.142300	-1.288166
H	-8.066832	-0.722226	-1.721413
H	-6.185375	0.734558	-2.410553
C	1.279880	-4.996051	-4.522599
C	2.759429	-5.058089	-4.891128
H	0.665871	-4.834327	-5.415303
H	0.976089	-5.970661	-4.114250
C	3.601392	-5.063000	-3.618978
H	3.027681	-4.182871	-5.496723
H	2.956884	-5.946179	-5.500240
C	3.406867	-3.757331	-2.852052
H	3.300079	-5.911049	-2.987771
H	4.663028	-5.197207	-3.850474
H	3.940355	-3.797723	-1.900408
H	3.875970	-2.936799	-3.414194
C	2.792706	-4.168980	0.422704
C	3.834225	-5.046885	1.112047
H	2.461990	-4.628472	-0.512308
H	1.896079	-4.114186	1.058834
C	4.397232	-4.329919	2.336302
H	3.383122	-6.005095	1.389876
H	4.653055	-5.267838	0.413000
C	5.139590	-3.071585	1.894258
H	3.570047	-4.053002	3.004379
H	5.069007	-4.982972	2.902936
H	6.080330	-3.364167	1.406749
H	5.424137	-2.466975	2.764138

TS-1-minor

M06-2X/6-31G* Energy = -8271.53796019

M06-2X/6-31G* Free Energy = -8270.651163

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.51298199

M06-2X/def2-TZVPP-SMD(toluene) Energy = -8277.52003464

Number of Imaginary Frequencies = 1

Lowest Frequency = 109.7759i

M06-2X/6-31G* Geometry

C	-3.116733	0.989661	-2.018756
C	-3.381310	2.150390	-0.797745
C	-3.538907	-0.233541	-1.405489
H	-2.042040	1.040980	-2.217148
H	-3.693270	1.308719	-2.886137
C	-2.777495	-0.779990	-0.352326
H	-4.564552	-0.577149	-1.539540
N	-2.623181	1.702355	0.322065
C	-2.862377	3.469553	-1.379530
C	-4.866340	2.237372	-0.443175
C	-3.007430	0.479480	0.870592
C	-2.248964	-0.006797	2.075955
H	-4.079281	0.454604	1.063867
H	-1.602901	1.800993	0.200568
H	-1.692954	-0.756570	-0.469748
H	-3.147826	-1.704554	0.088440
C	3.878005	-1.739733	0.877092
C	4.557030	-0.818613	1.683793
C	3.177532	-1.275478	-0.257756
C	3.048265	0.100297	-0.472959
C	3.742794	1.035573	0.309719
C	4.503266	0.539709	1.364707
C	2.549425	-2.229896	-1.220267
C	3.299074	-3.215067	-1.899838
C	2.630819	-4.161601	-2.688476
C	1.242902	-4.085221	-2.830258
C	0.499107	-3.060557	-2.258598
C	1.179372	-2.134469	-1.464554
O	2.291089	0.540695	-1.537638
O	0.474110	-1.111666	-0.873016
P	0.657233	0.416736	-1.494534
O	0.070261	1.271574	-0.401971
O	0.139760	0.526914	-2.881043
C	3.745235	2.494284	0.022806
C	-0.967177	-2.954285	-2.503322
C	2.534866	3.229783	-0.124085
C	2.566777	4.581975	-0.338979
C	3.796212	5.286534	-0.431855
C	5.009041	4.558297	-0.289373
C	4.948083	3.160020	-0.058438
C	-1.463834	-1.997370	-3.432112
C	-2.803612	-1.947393	-3.725223
C	-3.729565	-2.824947	-3.096544
C	-3.240981	-3.761845	-2.143855
C	-1.846256	-3.810190	-1.879109
H	5.034373	1.251091	1.993859
H	0.730440	-4.821408	-3.446275
H	1.587089	2.708224	-0.040323
H	1.637009	5.138992	-0.431520
H	-1.471694	-4.540862	-1.165567
H	-3.175147	-1.227798	-4.451964
H	-0.768324	-1.296922	-3.882945
H	5.879506	2.606133	0.038408
C	-5.888321	1.894094	-1.327880
C	-7.225001	2.079606	-0.977662
C	-7.557915	2.614365	0.261742
C	-6.544078	2.967791	1.150111
C	-5.211530	2.785336	0.798645
H	-5.658627	1.489686	-2.308784

H	-8.004602	1.805080	-1.681176
H	-8.598736	2.757006	0.533946
H	-4.418799	3.069208	1.485101
H	-6.790063	3.391319	2.118807
C	-1.521152	3.586579	-1.763036
C	-1.043071	4.779822	-2.293365
C	-1.894229	5.869661	-2.458913
C	-3.230328	5.755156	-2.092191
C	-3.715069	4.562849	-1.558918
H	-4.761561	4.498268	-1.283611
H	-0.837366	2.751737	-1.650834
H	0.000305	4.844587	-2.586406
H	-1.519876	6.798300	-2.878516
H	-3.906967	6.594219	-2.220832
C	-0.859607	-0.112718	2.060746
C	-0.204671	-0.577878	3.190997
C	-0.894641	-0.948585	4.340261
C	-2.280353	-0.838447	4.328690
Br	1.677206	-0.716738	3.097880
H	-0.373057	-1.314061	5.216775
C	-2.969278	-0.377175	3.212417
H	-4.051913	-0.304530	3.238131
H	-0.286188	0.169966	1.182431
Br	-3.254467	-1.334003	5.872734
C	-4.164978	-4.614348	-1.481774
C	-5.507836	-4.536786	-1.748902
C	-5.993827	-3.606663	-2.701221
C	-5.124517	-2.775351	-3.360950
H	-3.786023	-5.329844	-0.756451
H	-6.204703	-5.191624	-1.235335
H	-5.490036	-2.064398	-4.098709
H	-7.058090	-3.560246	-2.910415
C	6.243775	5.253620	-0.382994
C	6.271982	6.606689	-0.603141
C	5.063382	7.332539	-0.740902
C	3.856617	6.686345	-0.657136
H	7.167977	4.691063	-0.276775
H	7.221715	7.128116	-0.672938
H	5.098066	8.403818	-0.914002
H	2.925259	7.237359	-0.762020
C	5.337972	-1.244334	2.914123
C	4.903799	-2.603647	3.457839
H	5.239705	-0.472548	3.686181
H	6.405954	-1.287889	2.657693
C	4.826976	-3.612525	2.315416
H	3.914186	-2.513631	3.925417
H	5.599830	-2.936243	4.234772
C	3.758040	-3.190518	1.310477
H	5.803981	-3.670382	1.814965
H	4.600553	-4.615208	2.692650
H	2.765849	-3.294610	1.776256
H	3.754649	-3.865812	0.452182
C	4.818218	-3.190959	-1.859478
C	5.452989	-4.520268	-2.260847
H	5.182000	-2.876422	-0.879228
H	5.149632	-2.409865	-2.558899
C	4.855286	-5.011498	-3.575886
H	6.537923	-4.398993	-2.343502
H	5.271708	-5.268973	-1.476673
C	3.366036	-5.288851	-3.389940
H	4.995681	-4.240518	-4.344438
H	5.362675	-5.915546	-3.928036
H	3.248562	-6.206144	-2.795417

H 2.887158 -5.487450 -4.355092

TS-1-minor-2

M06-2X/6-31G* Energy = -8271.54110757

M06-2X/6-31G* Free Energy = -8270.653080

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.51351290

M06-2X/def2-TZVPP-SMD(toluene) Energy = -8277.52028094

Number of Imaginary Frequencies = 1

Lowest Frequency = 245.2005i

M06-2X/6-31G* Geometry

C	-3.021202	-0.172650	-2.001861
C	-3.782051	0.613019	-0.727125
C	-2.824255	-1.520189	-1.528328
H	-2.090154	0.379247	-2.162717
H	-3.677524	-0.078704	-2.867153
C	-1.894543	-1.780575	-0.517114
H	-3.575631	-2.279441	-1.745706
N	-2.904984	0.448915	0.393694
C	-3.919712	2.079457	-1.148607
C	-5.145564	-0.010388	-0.424344
C	-2.711524	-0.843500	0.836930
C	-1.797780	-1.058622	2.006164
H	-3.650417	-1.380467	0.960169
H	-2.038494	1.003971	0.326688
H	-0.952714	-1.233750	-0.537872
H	-1.808911	-2.807423	-0.165498
C	4.658856	-1.092647	-1.996973
C	4.515244	-2.215239	-2.824216
C	3.538900	-0.604727	-1.292097
C	2.279630	-1.159143	-1.548722
C	2.117414	-2.264622	-2.387683
C	3.254931	-2.796312	-2.983483
C	3.635541	0.492534	-0.283061
C	4.443550	0.387675	0.868034
C	4.490552	1.461433	1.770852
C	3.647665	2.557494	1.579251
C	2.759410	2.634247	0.510964
C	2.808614	1.608542	-0.437151
O	1.171152	-0.628307	-0.931570
O	1.989436	1.671868	-1.541962
P	0.584309	0.830343	-1.482722
O	-0.281899	1.282117	-0.339549
O	0.039892	0.734919	-2.859467
C	0.770263	-2.849482	-2.646063
C	1.721042	3.691504	0.450085
C	-0.128366	-2.198945	-3.537954
C	-1.344711	-2.762420	-3.830738
C	-1.748766	-3.991243	-3.240424
C	-0.864025	-4.632873	-2.329829
C	0.398531	-4.038656	-2.061891
C	0.882862	3.866528	1.587131
C	-0.112273	4.805972	1.587426
C	-0.330653	5.632282	0.453150
C	0.499162	5.457181	-0.690191
C	1.516813	4.468972	-0.664930
H	3.147963	-3.664500	-3.630789
H	3.642838	3.356276	2.318818
H	0.154396	-1.239449	-3.957451
H	-2.019732	-2.268582	-4.526912
H	2.135635	4.326955	-1.546527
H	-0.758850	4.924445	2.453125
H	1.026083	3.203102	2.436793
H	1.079333	-4.538283	-1.376134

C	-5.877878	-0.747993	-1.353716
C	-7.152262	-1.221423	-1.042591
C	-7.711888	-0.962016	0.202952
C	-6.991223	-0.219199	1.136797
C	-5.723510	0.256047	0.823572
H	-5.473644	-0.951373	-2.340341
H	-7.705021	-1.792929	-1.781492
H	-8.702813	-1.332464	0.445171
H	-5.164236	0.844536	1.545424
H	-7.419485	-0.004394	2.110853
C	-2.777580	2.873717	-1.304094
C	-2.896373	4.206433	-1.682231
C	-4.149919	4.762439	-1.923299
C	-5.286624	3.972918	-1.790900
C	-5.174967	2.637981	-1.407371
H	-6.075866	2.043016	-1.306482
H	-1.784459	2.466988	-1.131324
H	-1.999804	4.807779	-1.794830
H	-4.233860	5.804791	-2.216525
H	-6.270368	4.390722	-1.982208
C	-0.535111	-0.470323	2.049470
C	0.276061	-0.700599	3.149435
C	-0.128013	-1.504599	4.209633
C	-1.389392	-2.085055	4.138297
Br	1.982283	0.109343	3.127852
H	0.517582	-1.679821	5.061988
C	-2.229940	-1.877950	3.050242
H	-3.208694	-2.346389	3.026799
H	-0.176560	0.155682	1.234231
Br	-1.973881	-3.188917	5.558407
C	0.282675	6.281584	-1.827737
C	-0.708060	7.231038	-1.829704
C	-1.536430	7.400909	-0.692479
C	-1.351663	6.618051	0.418919
H	0.917274	6.141607	-2.698893
H	-0.862672	7.854858	-2.704804
H	-1.986890	6.739999	1.292558
H	-2.319223	8.153322	-0.705601
C	-1.274414	-5.843258	-1.709682
C	-2.504978	-6.387223	-1.976319
C	-3.385287	-5.749356	-2.884756
C	-3.013112	-4.582449	-3.503184
H	-0.593130	-6.330342	-1.016629
H	-2.808458	-7.311648	-1.495033
H	-4.354108	-6.192625	-3.093440
H	-3.680988	-4.092266	-4.208261
C	5.696569	-2.839436	-3.544301
C	6.882024	-1.889394	-3.695833
H	5.370906	-3.208000	-4.523315
H	6.022537	-3.723492	-2.977820
C	7.171961	-1.208695	-2.360914
H	6.648646	-1.122333	-4.445520
H	7.757026	-2.439088	-4.057800
C	5.982061	-0.347396	-1.945296
H	7.361530	-1.974103	-1.595041
H	8.071971	-0.588492	-2.424497
H	6.150204	0.090663	-0.959108
H	5.902009	0.505781	-2.634418
C	5.099072	-0.933515	1.230567
C	6.218998	-0.794409	2.258525
H	5.455881	-1.463442	0.345196
H	4.301733	-1.564418	1.653780
C	5.738182	0.024052	3.453445

H	6.552923	-1.788265	2.574271
H	7.083851	-0.295279	1.799314
C	5.382227	1.438061	2.999242
H	4.850012	-0.456807	3.885079
H	6.499648	0.063186	4.239223
H	6.309568	1.983248	2.773772
H	4.892109	1.989867	3.809843

TS-1-minor-3

M06-2X/6-31G* Energy = -8271.54110757

M06-2X/6-31G* Free Energy = -8270.653076

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.51351428

M06-2X/def2-TZVPP-SMD(toluene) Energy = -8277.52028270

Number of Imaginary Frequencies = 1

Lowest Frequency = 245.4371i

M06-2X/6-31G* Geometry

C	-3.020944	-0.172751	-2.002172
C	-3.781802	0.613063	-0.727555
C	-2.824088	-1.520300	-1.528500
H	-2.089807	0.378991	-2.163076
H	-3.677154	-0.078929	-2.867565
C	-1.894424	-1.780684	-0.517302
H	-3.575510	-2.279520	-1.745836
N	-2.904817	0.448948	0.393379
C	-3.919332	2.079522	-1.149061
C	-5.145403	-0.010169	-0.424772
C	-2.711592	-0.843390	0.836731
C	-1.798005	-1.058548	2.006062
H	-3.650539	-1.380293	0.959804
H	-2.038281	1.003957	0.326516
H	-0.952623	-1.233816	-0.537959
H	-1.808865	-2.807495	-0.165570
C	4.443525	0.387262	0.868376
C	4.490500	1.460997	1.771221
C	3.635646	0.492191	-0.282803
C	2.808824	1.608263	-0.436968
C	2.759620	2.633985	0.511132
C	3.647745	2.557146	1.579518
C	3.538999	-0.605053	-1.291856
C	4.658968	-1.093029	-1.996669
C	4.515327	-2.215575	-2.823971
C	3.254982	-2.796545	-2.983350
C	2.117464	-2.264802	-2.387598
C	2.279705	-1.159372	-1.548579
O	1.989723	1.671630	-1.541835
O	1.171229	-0.628476	-0.931470
P	0.584518	0.830237	-1.482613
O	-0.281661	1.282079	-0.339445
O	0.040109	0.734858	-2.859366
C	1.721378	3.691355	0.450099
C	0.770287	-2.849555	-2.646093
C	0.883141	3.866586	1.587070
C	-0.111908	4.806121	1.587193
C	-0.330143	5.632319	0.452807
C	0.499740	5.457020	-0.690454
C	1.517300	4.468724	-0.665013
C	-0.128199	-2.198969	-3.538092
C	-1.344573	-2.762336	-3.830960
C	-1.748808	-3.991083	-3.240613
C	-0.864213	-4.632759	-2.329910
C	0.398384	-4.038663	-2.061896
H	3.642907	3.355924	2.319089
H	3.147994	-3.664693	-3.630706

H	1.026238	3.203238	2.436814
H	-0.758534	4.924749	2.452834
H	1.079074	-4.538326	-1.376055
H	-2.019496	-2.268446	-4.527192
H	0.154693	-1.239517	-3.957601
H	2.136164	4.326551	-1.546555
C	-5.723396	0.256464	0.823081
C	-6.991167	-0.218627	1.136297
C	-7.711850	-0.961490	0.202501
C	-7.152182	-1.221093	-1.042980
C	-5.877735	-0.747817	-1.354094
H	-5.164107	0.844989	1.544893
H	-7.419464	-0.003665	2.110303
H	-8.702821	-1.331821	0.444711
H	-5.473473	-0.951357	-2.340674
H	-7.704952	-1.792636	-1.781843
C	-2.777131	2.873692	-1.304470
C	-2.895790	4.206425	-1.682594
C	-4.149274	4.762536	-1.923738
C	-5.286049	3.973101	-1.791424
C	-5.174523	2.638151	-1.407896
H	-6.075480	2.043262	-1.307070
H	-1.784058	2.466886	-1.131628
H	-1.999164	4.807702	-1.795117
H	-4.233113	5.804900	-2.216951
H	-6.269748	4.390983	-1.982791
C	-2.230565	-1.877451	3.050310
C	-1.390265	-2.084443	4.138575
C	-0.128763	-1.504263	4.209971
C	0.275713	-0.700695	3.149598
Br	-1.975293	-3.187729	5.558908
H	0.516622	-1.679367	5.062509
C	-0.535182	-0.470579	2.049393
H	-0.176290	0.155038	1.234003
H	-3.209444	-2.345627	3.026842
Br	1.982097	0.108906	3.128140
C	-1.274789	-5.843060	-1.709721
C	-2.505397	-6.386897	-1.976416
C	-3.385562	-5.748984	-2.884960
C	-3.013203	-4.582160	-3.503434
H	-0.593614	-6.330181	-1.016587
H	-2.809022	-7.311258	-1.495097
H	-3.680969	-4.091941	-4.208591
H	-4.354420	-6.192154	-3.093690
C	0.283401	6.281307	-1.828111
C	-0.707264	7.230832	-1.830264
C	-1.535707	7.400896	-0.693121
C	-1.351079	6.618158	0.418384
H	0.918053	6.141179	-2.699204
H	-0.861766	7.854560	-2.705449
H	-2.318446	8.153363	-0.706390
H	-1.986360	6.740256	1.291963
C	5.381965	1.437541	2.999769
C	5.738094	0.023524	3.453824
H	4.891581	1.989101	3.810379
H	6.309236	1.982959	2.774578
C	6.218950	-0.794804	2.258829
H	4.849990	-0.457463	3.885452
H	6.499579	0.062677	4.239581
C	5.098957	-0.933956	1.230957
H	7.083702	-0.295530	1.799585
H	6.553023	-1.788637	2.574491
H	5.455652	-1.463986	0.345603

H	4.301607	-1.564760	1.654296
C	5.982216	-0.347861	-1.944860
C	7.172090	-1.209134	-2.360609
H	6.150376	0.090013	-0.958592
H	5.902205	0.505448	-2.633824
C	6.882095	-1.889745	-3.695561
H	8.072094	-0.588923	-2.424192
H	7.361702	-1.974595	-1.594800
C	5.696657	-2.839803	-3.544018
H	6.648666	-1.122639	-4.445186
H	7.757085	-2.439405	-4.057607
H	6.022635	-3.723831	-2.977499
H	5.371007	-3.208405	-4.523020

TS-1-minor-4

M06-2X/6-31G* Energy = -8271.53961986

M06-2X/6-31G* Free Energy = -8270.651217

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.51348667

M06-2X/def2-TZVPP-SMD(toluene) Energy = -8277.52035011

Number of Imaginary Frequencies = 1

Lowest Frequency = 184.8135i

M06-2X/6-31G* Geometry

C	-3.147843	-0.739405	-1.700200
C	-3.761435	0.616223	-0.888541
C	-3.101706	-1.750146	-0.682100
H	-2.164375	-0.423722	-2.061685
H	-3.820684	-0.945098	-2.532311
C	-2.161567	-1.637638	0.354150
H	-3.944827	-2.430555	-0.556549
N	-2.865399	0.846869	0.199576
C	-3.745563	1.753303	-1.915029
C	-5.174333	0.343324	-0.369692
C	-2.799293	-0.159927	1.152541
C	-1.895649	0.036940	2.338718
H	-3.792945	-0.463536	1.478789
H	-1.941821	1.212004	-0.084791
H	-1.164895	-1.289530	0.081874
H	-2.170683	-2.416357	1.114964
C	4.396434	-0.381758	0.900168
C	4.822538	0.849925	1.412012
C	3.559617	-0.404231	-0.235991
C	3.027194	0.795397	-0.722919
C	3.450412	2.039469	-0.226405
C	4.374469	2.029445	0.814041
C	3.229310	-1.683124	-0.934728
C	4.228912	-2.521077	-1.476745
C	3.857387	-3.736824	-2.068522
C	2.504805	-4.072777	-2.167466
C	1.501165	-3.222153	-1.722873
C	1.889164	-2.030223	-1.107358
O	2.143787	0.755326	-1.778834
O	0.922534	-1.160501	-0.653931
P	0.619901	0.178083	-1.589805
O	-0.189817	1.043571	-0.658526
O	0.083337	-0.178649	-2.925588
C	2.985331	3.331683	-0.790836
C	0.061791	-3.537830	-1.951236
C	3.946448	4.323578	-1.136325
C	3.560194	5.535178	-1.646307
C	2.186560	5.835339	-1.842270
C	1.222266	4.853067	-1.486547
C	1.648639	3.608522	-0.960274
C	-0.567665	-3.063378	-3.137988

C	-1.880985	-3.353755	-3.393962
C	-2.657654	-4.099845	-2.467418
C	-2.036853	-4.570581	-1.275509
C	-0.661412	-4.288028	-1.055283
H	4.707753	2.984061	1.217075
H	2.223977	-5.009231	-2.645151
H	5.001540	4.095863	-1.010023
H	4.304158	6.279834	-1.918151
H	-0.187894	-4.650660	-0.145496
H	-2.355907	-2.985463	-4.300103
H	0.003330	-2.435978	-3.812435
H	0.899124	2.872909	-0.682818
C	-5.667168	1.170614	0.647793
C	-6.967480	1.024671	1.116456
C	-7.804103	0.052861	0.570092
C	-7.326541	-0.767743	-0.445140
C	-6.020805	-0.622936	-0.912928
H	-5.015287	1.932768	1.065685
H	-7.328914	1.674221	1.907500
H	-8.820019	-0.062235	0.934074
H	-5.679856	-1.276025	-1.710659
H	-7.968073	-1.527311	-0.880587
C	-2.536340	2.155277	-2.494058
C	-2.511333	3.194131	-3.419427
C	-3.689715	3.837273	-3.789823
C	-4.896474	3.427873	-3.233471
C	-4.927678	2.390619	-2.304143
H	-5.880997	2.088744	-1.885696
H	-1.603409	1.665560	-2.232899
H	-1.560975	3.496443	-3.848075
H	-3.666334	4.645787	-4.514079
H	-5.824097	3.914001	-3.519398
C	-0.530161	0.271610	2.187118
C	0.260219	0.413308	3.318184
C	-0.270109	0.330051	4.601157
C	-1.634501	0.095864	4.726031
Br	2.107649	0.695407	3.046737
H	0.357736	0.439539	5.477342
C	-2.454559	-0.059633	3.614256
H	-3.515116	-0.247818	3.747724
H	-0.083334	0.355811	1.200450
Br	-2.392379	-0.027062	6.454763
C	-2.829540	-5.253122	-0.314074
C	-4.173275	-5.445655	-0.516947
C	-4.789703	-4.982730	-1.707222
C	-4.045956	-4.334695	-2.661543
H	-2.352034	-5.611327	0.594834
H	-4.769007	-5.960729	0.230188
H	-4.509847	-3.980686	-3.579424
H	-5.851134	-5.150767	-1.862047
C	-0.156611	5.139084	-1.673646
C	-0.557514	6.338033	-2.203818
C	0.404257	7.316117	-2.561840
C	1.741807	7.070874	-2.382437
H	-0.884478	4.380992	-1.394774
H	-1.614443	6.541235	-2.350727
H	0.076047	8.263433	-2.978951
H	2.482410	7.818821	-2.654857
C	5.738885	0.947715	2.618517
C	5.719560	-0.308762	3.486292
H	5.460309	1.827060	3.210778
H	6.766150	1.125080	2.270051
C	5.882603	-1.544931	2.605977

H	4.761060	-0.371110	4.018907
H	6.508377	-0.253772	4.243544
C	4.698745	-1.666942	1.650051
H	6.816545	-1.462685	2.032027
H	5.959258	-2.452005	3.214458
H	3.794265	-1.906836	2.230384
H	4.842604	-2.505067	0.964174
C	5.677970	-2.063679	-1.524619
C	6.666271	-3.207217	-1.739884
H	5.944927	-1.498498	-0.629799
H	5.766428	-1.350851	-2.357274
C	6.228324	-4.066859	-2.921686
H	7.669386	-2.799266	-1.901199
H	6.713875	-3.830011	-0.835430
C	4.882872	-4.716007	-2.609782
H	6.136602	-3.433055	-3.813132
H	6.972201	-4.837775	-3.147775
H	5.037253	-5.508634	-1.863719
H	4.476421	-5.209512	-3.499482

TS-1-minor-5

M06-2X/6-31G* Energy = -8271.54767278

M06-2X/6-31G* Free Energy = -8270.655542

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.51087701

M06-2X/def2-TZVPP-SMD(toluene) Energy = -8277.51720732

Number of Imaginary Frequencies = 1

Lowest Frequency = 329.1333i

M06-2X/6-31G* Geometry

C	3.553762	1.897839	-0.836080
C	3.969941	0.846521	0.434154
C	2.887435	2.978818	-0.170210
H	2.890023	1.303506	-1.470090
H	4.482491	2.146788	-1.348166
C	1.608824	2.771326	0.339969
H	3.460988	3.841015	0.166523
N	2.727976	0.492954	1.021785
C	4.639241	-0.347185	-0.251308
C	4.889463	1.537172	1.437565
C	1.967376	1.451638	1.632297
C	0.617548	0.958486	2.103864
H	2.507075	2.066627	2.352525
H	2.136897	-0.185360	0.475909
H	0.917642	2.175410	-0.256925
H	1.152237	3.604214	0.869669
C	-3.648246	-1.924496	0.421080
C	-3.210791	-3.140163	0.962569
C	-2.902199	-1.341929	-0.631038
C	-1.728220	-1.954494	-1.068216
C	-1.254196	-3.144605	-0.504459
C	-2.034846	-3.723167	0.488717
C	-3.250872	-0.003030	-1.188675
C	-4.496942	0.267869	-1.788275
C	-4.847567	1.592360	-2.081657
C	-3.917863	2.609117	-1.858060
C	-2.626497	2.344645	-1.415974
C	-2.302573	1.022995	-1.085444
O	-0.972843	-1.299947	-2.026272
O	-1.055435	0.754368	-0.576481
P	0.051994	-0.192153	-1.382348
O	0.860365	-0.845115	-0.297687
O	0.724850	0.586933	-2.456522
C	0.065724	-3.725183	-0.846141
C	-1.616322	3.429285	-1.319959

C	0.916687	-4.123443	0.224334
C	2.134114	-4.696793	-0.019812
C	2.587008	-4.898343	-1.350107
C	1.758509	-4.469450	-2.424838
C	0.495494	-3.887840	-2.141915
C	-1.804165	4.514981	-0.420233
C	-0.866485	5.512585	-0.316492
C	0.316710	5.480243	-1.101673
C	0.494318	4.409508	-2.021805
C	-0.492568	3.397175	-2.114605
H	-1.691793	-4.650349	0.943938
H	-4.185526	3.636305	-2.099583
H	0.590687	-3.919465	1.240970
H	2.781795	-4.988564	0.803026
H	-0.322632	2.557366	-2.783360
H	-1.011213	6.333667	0.381471
H	-2.692286	4.526306	0.205198
H	-0.131848	-3.563955	-2.967493
C	5.756751	2.572849	1.086777
C	6.638188	3.110361	2.022219
C	6.667927	2.616967	3.322639
C	5.814496	1.576134	3.680308
C	4.937605	1.038239	2.744189
H	5.765242	2.964460	0.074161
H	7.303960	3.915808	1.728747
H	7.353267	3.037875	4.051297
H	4.282157	0.216478	3.018921
H	5.832923	1.177052	4.689577
C	5.970780	-0.676322	0.011130
C	6.569487	-1.753773	-0.639598
C	5.849315	-2.503659	-1.562109
C	4.523605	-2.172890	-1.834900
C	3.918950	-1.102816	-1.185911
H	2.879317	-0.875652	-1.407622
H	6.549576	-0.101122	0.725510
H	7.603807	-2.000448	-0.420044
H	6.310154	-3.345376	-2.070402
H	3.955448	-2.749177	-2.558926
C	-0.525269	1.754262	2.058331
C	-1.752041	1.202809	2.397845
C	-1.874917	-0.105781	2.838400
C	-0.718701	-0.871527	2.912869
Br	-3.311679	2.242688	2.155823
H	-2.838935	-0.520091	3.104570
C	0.518496	-0.364949	2.546246
H	1.392108	-1.005696	2.568085
H	-0.507870	2.768627	1.680052
Br	-0.846390	-2.653335	3.534916
C	1.699095	4.331407	-2.771053
C	2.684102	5.273930	-2.609424
C	2.504577	6.346991	-1.698736
C	1.348790	6.447948	-0.966375
H	1.827753	3.492411	-3.450682
H	3.604586	5.204840	-3.181730
H	1.208080	7.268130	-0.266534
H	3.287117	7.091407	-1.586255
C	2.227535	-4.630664	-3.756742
C	3.455084	-5.190380	-4.007764
C	4.274449	-5.625302	-2.936305
C	3.848064	-5.481065	-1.640046
H	1.595019	-4.294688	-4.574260
H	3.802846	-5.304505	-5.029917
H	5.241612	-6.072265	-3.146969

H	4.476016	-5.800996	-0.812070
C	-3.951045	-3.835452	2.086973
C	-4.766388	-2.862971	2.930541
H	-3.227133	-4.372336	2.710050
H	-4.624074	-4.594855	1.664644
C	-5.651183	-2.022578	2.014977
H	-4.080264	-2.220306	3.498791
H	-5.371076	-3.408047	3.662887
C	-4.825157	-1.183321	1.037865
H	-6.305129	-2.700006	1.449147
H	-6.305337	-1.362690	2.594376
H	-5.488211	-0.784589	0.267020
H	-4.434734	-0.289212	1.542783
C	-5.401451	-0.872205	-2.223601
C	-6.859599	-0.449087	-2.382536
H	-5.309880	-1.729570	-1.553125
H	-5.029122	-1.222973	-3.197148
C	-6.944731	0.785944	-3.276622
H	-7.442298	-1.275691	-2.802075
H	-7.290917	-0.217468	-1.398180
C	-6.218483	1.958321	-2.619968
H	-6.479380	0.557742	-4.244197
H	-7.986481	1.057678	-3.476317
H	-6.830588	2.329538	-1.785460
H	-6.123722	2.793358	-3.322916

TS-1-minor-6

M06-2X/6-31G* Energy = -8271.54709228

M06-2X/6-31G* Free Energy = -8270.654536

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.51105881

M06-2X/def2-TZVPP-SMD(toluene) Energy = -8277.51729245

Number of Imaginary Frequencies = 1

Lowest Frequency = 324.2510i

M06-2X/6-31G* Geometry

C	3.438688	1.996229	-0.965495
C	3.962139	1.009863	0.295506
C	2.703393	3.040461	-0.299641
H	2.808415	1.346630	-1.580211
H	4.328613	2.314753	-1.508227
C	1.458539	2.754646	0.246816
H	3.216629	3.952936	-0.000094
N	2.758416	0.557487	0.907058
C	4.724975	-0.143371	-0.361059
C	4.829256	1.781270	1.286705
C	1.943384	1.453163	1.537300
C	0.641938	0.862026	2.017082
H	2.448181	2.107991	2.246664
H	2.202673	-0.117126	0.335453
H	0.794849	2.102424	-0.317103
H	0.958642	3.556179	0.785738
C	-4.605865	0.278297	-1.592096
C	-5.011887	1.612386	-1.726511
C	-3.315012	-0.006773	-1.103946
C	-2.386459	1.033859	-0.969652
C	-2.766891	2.369804	-1.150256
C	-4.094635	2.632313	-1.470012
C	-2.897341	-1.379882	-0.699639
C	-3.565688	-2.085439	0.330929
C	-3.072099	-3.336095	0.722859
C	-1.925726	-3.849637	0.112161
C	-1.229062	-3.157371	-0.868262
C	-1.742518	-1.918303	-1.264479
O	-1.101637	0.751532	-0.576465

O	-1.052970	-1.171337	-2.201421
P	-0.026736	-0.062163	-1.559231
O	0.915081	-0.727778	-0.595127
O	0.487246	0.833836	-2.627191
C	-1.783754	3.478921	-1.047975
C	0.038062	-3.690858	-1.420058
C	-1.929109	4.492120	-0.059874
C	-1.026255	5.523573	0.028047
C	0.082027	5.595339	-0.857969
C	0.218911	4.593013	-1.858261
C	-0.735268	3.549231	-1.937504
C	0.219362	-3.825771	-2.824081
C	1.366555	-4.375312	-3.329353
C	2.411724	-4.800223	-2.466509
C	2.253832	-4.627845	-1.061860
C	1.044367	-4.077467	-0.566183
H	-4.404799	3.668508	-1.593255
H	-1.541121	-4.814254	0.437955
H	-2.756125	4.421655	0.641457
H	-1.139350	6.290362	0.790683
H	0.919119	-3.926003	0.504708
H	1.495562	-4.489594	-4.402567
H	-0.570729	-3.489239	-3.487616
H	-0.596355	2.765059	-2.677169
C	4.964023	1.272174	2.583428
C	5.801722	1.888490	3.506472
C	6.530761	3.019098	3.144669
C	6.416339	3.523329	1.853541
C	5.572270	2.907662	0.931277
H	4.406943	0.381492	2.860398
H	5.888364	1.480780	4.508681
H	7.186045	3.500703	3.863316
H	5.514635	3.309994	-0.075629
H	6.985552	4.398511	1.556662
C	4.036594	-1.073270	-1.150458
C	4.722821	-2.129524	-1.738345
C	6.097749	-2.265634	-1.563321
C	6.787642	-1.332430	-0.798675
C	6.106104	-0.274864	-0.199209
H	6.659944	0.437433	0.402575
H	2.960989	-1.000072	-1.303693
H	4.175548	-2.852928	-2.333478
H	6.620901	-3.099281	-2.022437
H	7.860193	-1.423596	-0.656669
C	-0.527510	1.614453	2.113750
C	-1.712967	0.980193	2.454060
C	-1.764811	-0.372931	2.759499
C	-0.581974	-1.096091	2.690796
Br	-3.321403	1.971961	2.408194
H	-2.696793	-0.849133	3.035259
C	0.613323	-0.502075	2.318535
H	1.510112	-1.104133	2.240062
H	-0.558658	2.664783	1.849376
Br	-0.593110	-2.937355	3.118937
C	3.320675	-5.001720	-0.202157
C	4.480948	-5.529663	-0.707959
C	4.629908	-5.719448	-2.104124
C	3.618130	-5.364063	-2.960651
H	3.200839	-4.853886	0.868036
H	5.291357	-5.804342	-0.039769
H	3.727581	-5.500957	-4.033709
H	5.548924	-6.147770	-2.493199
C	1.359397	4.608155	-2.705900

C	2.319068	5.579884	-2.566388
C	2.176710	6.588822	-1.579049
C	1.084916	6.596361	-0.747856
H	1.460418	3.816149	-3.444011
H	3.190616	5.583391	-3.214352
H	2.937589	7.357789	-1.484705
H	0.975034	7.365675	0.012665
C	-6.427481	1.982435	-2.129036
C	-7.164417	0.859134	-2.855951
H	-6.407452	2.889001	-2.743919
H	-6.989105	2.241982	-1.220129
C	-6.981570	-0.458477	-2.105864
H	-6.762181	0.749458	-3.871323
H	-8.224999	1.112730	-2.955217
C	-5.503946	-0.841841	-2.088527
H	-7.351404	-0.346811	-1.076586
H	-7.566911	-1.257496	-2.572553
H	-5.340266	-1.762844	-1.524861
H	-5.189143	-1.070565	-3.117161
C	-4.725440	-1.441686	1.077367
C	-5.450539	-2.379320	2.046441
H	-5.457619	-1.025204	0.382328
H	-4.339583	-0.563862	1.612562
C	-4.481162	-3.272947	2.813305
H	-6.066282	-1.785246	2.729857
H	-6.137619	-3.023661	1.481438
C	-3.720308	-4.148521	1.825405
H	-3.761148	-2.667747	3.380344
H	-5.017043	-3.893337	3.539275
H	-4.414177	-4.877431	1.383437
H	-2.946408	-4.728156	2.341005

TS-1-minor-7

M06-2X/6-31G* Energy = -8271.54423082

M06-2X/6-31G* Free Energy = -8270.653391

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.50899862

M06-2X/def2-TZVPP-SMD(toluene) Energy = -8277.51540642

Number of Imaginary Frequencies = 1

Lowest Frequency = 376.8105i

M06-2X/6-31G* Geometry

C	3.368447	2.098742	-1.187036
C	3.911418	1.183300	0.179373
C	2.637264	3.160190	-0.573687
H	2.745294	1.391979	-1.741491
H	4.270404	2.371001	-1.733038
C	1.391729	2.890393	-0.010627
H	3.151274	4.081175	-0.301320
N	2.717547	0.782127	0.815224
C	4.670730	0.002067	-0.426034
C	4.785722	2.042916	1.087166
C	1.888611	1.716289	1.372116
C	0.601131	1.148341	1.924904
H	2.387241	2.435396	2.021864
H	2.184732	-0.010931	0.361143
H	0.733538	2.202079	-0.542521
H	0.889187	3.721512	0.478708
C	-3.395453	-2.260806	0.595082
C	-2.860637	-3.387281	1.233501
C	-2.704884	-1.716458	-0.513074
C	-1.491797	-2.274876	-0.913491
C	-0.924154	-3.374237	-0.259512
C	-1.648527	-3.920883	0.792352
C	-3.154541	-0.462089	-1.183190

C	-4.412483	-0.340984	-1.805688
C	-4.848310	0.917920	-2.240558
C	-3.987106	2.011874	-2.137684
C	-2.686192	1.883294	-1.664544
C	-2.281560	0.633578	-1.186826
O	-0.794162	-1.647636	-1.931607
O	-1.019913	0.509280	-0.657228
P	0.149247	-0.418737	-1.393359
O	1.011490	-0.919060	-0.268146
O	0.755560	0.316781	-2.534796
C	0.435274	-3.872640	-0.575287
C	-1.742428	3.033039	-1.709105
C	1.336071	-4.091246	0.505693
C	2.601372	-4.560390	0.283261
C	3.053275	-4.831461	-1.035070
C	2.168543	-4.588468	-2.122852
C	0.858361	-4.111046	-1.861380
C	-0.702841	3.044830	-2.683270
C	0.147022	4.114943	-2.778567
C	0.032555	5.223524	-1.896834
C	-0.996967	5.212032	-0.913800
C	-1.880772	4.100740	-0.852764
H	-1.230365	-4.775173	1.321595
H	-4.317914	2.985769	-2.493087
H	1.007454	-3.828085	1.507734
H	3.287366	-4.712210	1.112754
H	-2.661040	4.086392	-0.095023
H	0.940441	4.116657	-3.522342
H	-0.573073	2.177739	-3.322481
H	0.190034	-3.924029	-2.697098
C	4.888762	1.687911	2.436761
C	5.736571	2.382544	3.293505
C	6.505943	3.438570	2.812079
C	6.422671	3.789175	1.468127
C	5.570819	3.094933	0.612454
H	4.301111	0.853484	2.809435
H	5.798364	2.093338	4.337874
H	7.168384	3.981518	3.478495
H	5.537492	3.376789	-0.435446
H	7.023743	4.604726	1.078636
C	4.012594	-0.877334	-1.295815
C	4.693664	-1.957218	-1.845482
C	6.037033	-2.169597	-1.543327
C	6.697863	-1.292387	-0.691235
C	6.020900	-0.208403	-0.135640
H	6.552896	0.463713	0.528609
H	2.964210	-0.738516	-1.543800
H	4.171173	-2.635248	-2.513985
H	6.558201	-3.019272	-1.974044
H	7.745591	-1.445620	-0.451265
C	-0.607337	1.838233	1.849294
C	-1.774690	1.211094	2.258473
C	-1.773528	-0.063419	2.804509
C	-0.553493	-0.717538	2.911906
Br	-3.426208	2.082675	1.963647
H	-2.692227	-0.536341	3.127271
C	0.627154	-0.138467	2.472216
H	1.552673	-0.699981	2.519568
H	-0.682028	2.818275	1.395556
Br	-0.512401	-2.445589	3.679733
C	-1.088463	6.296346	-0.000826
C	-0.198771	7.339175	-0.057549
C	0.824645	7.351536	-1.036843

C	0.933953	6.319852	-1.934929
H	-1.877341	6.281618	0.747211
H	-0.277168	8.161517	0.646807
H	1.715008	6.324995	-2.691607
H	1.520206	8.184309	-1.074934
C	2.630251	-4.822129	-3.446494
C	3.905258	-5.273794	-3.677591
C	4.782326	-5.522327	-2.592492
C	4.363659	-5.305265	-1.303835
H	1.953213	-4.628674	-4.274452
H	4.246829	-5.444881	-4.693861
H	5.787460	-5.885184	-2.786654
H	5.034476	-5.482920	-0.466719
C	-3.531370	-4.029094	2.431003
C	-4.412803	-3.047643	3.194376
H	-2.759773	-4.444472	3.088915
H	-4.145371	-4.876402	2.094730
C	-5.370469	-2.367600	2.220785
H	-3.773241	-2.303341	3.688034
H	-4.964946	-3.566766	3.984766
C	-4.621969	-1.559735	1.158813
H	-5.972982	-3.143688	1.729543
H	-6.070124	-1.710879	2.748277
H	-5.320020	-1.287013	0.364001
H	-4.299845	-0.595094	1.573808
C	-5.234499	-1.579174	-2.120226
C	-6.717184	-1.275670	-2.320096
H	-5.088610	-2.355669	-1.366189
H	-4.833322	-2.001118	-3.053223
C	-6.881326	-0.149290	-3.338025
H	-7.239626	-2.179434	-2.650420
H	-7.168760	-0.972936	-1.364611
C	-6.239055	1.131665	-2.809111
H	-6.397111	-0.445174	-4.277636
H	-7.938121	0.029104	-3.562379
H	-6.877880	1.544525	-2.015223
H	-6.199010	1.894118	-3.594890

TS-1-minor-8

M06-2X/6-31G* Energy = -8271.54340838

M06-2X/6-31G* Free Energy = -8270.652072

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.50888634

M06-2X/def2-TZVPP-SMD(toluene) Energy = -8277.51518087

Number of Imaginary Frequencies = 1

Lowest Frequency = 351.7553i

M06-2X/6-31G* Geometry

C	3.172784	2.284680	-1.360612
C	3.842263	1.499746	0.013519
C	2.319782	3.270561	-0.769943
H	2.635626	1.487413	-1.882055
H	4.019529	2.653589	-1.938268
C	1.129159	2.872968	-0.164254
H	2.715107	4.262194	-0.553237
N	2.714346	0.964898	0.678141
C	4.749147	0.406153	-0.551503
C	4.602693	2.485533	0.894951
C	1.786122	1.808398	1.228419
C	0.590249	1.095714	1.809905
H	2.206997	2.590356	1.859946
H	2.254364	0.155917	0.198265
H	0.547741	2.101367	-0.665211
H	0.536007	3.654245	0.306032
C	-3.175636	-2.567902	0.511211

C	-2.522166	-3.699662	1.014875
C	-2.609075	-1.888718	-0.594242
C	-1.397187	-2.327756	-1.124169
C	-0.727208	-3.447046	-0.620528
C	-1.323549	-4.122032	0.435111
C	-3.197675	-0.626681	-1.126423
C	-4.507839	-0.556644	-1.639245
C	-5.068267	0.695127	-1.925383
C	-4.282355	1.840822	-1.791220
C	-2.939173	1.778683	-1.435855
C	-2.406291	0.528893	-1.104401
O	-0.811435	-1.588713	-2.135426
O	-1.101021	0.450417	-0.684741
P	0.065404	-0.305064	-1.607021
O	1.087521	-0.763704	-0.603347
O	0.454981	0.557147	-2.751402
C	0.596290	-3.861803	-1.141542
C	-2.101878	3.009265	-1.460763
C	0.783561	-4.114337	-2.528323
C	1.993077	-4.546151	-3.001546
C	3.095041	-4.727767	-2.124007
C	2.925048	-4.436685	-0.740487
C	1.653615	-4.013888	-0.275622
C	-1.148517	3.184841	-2.504615
C	-0.420980	4.342686	-2.592079
C	-0.577994	5.383829	-1.637755
C	-1.520982	5.209600	-0.585514
C	-2.278886	4.008269	-0.530673
H	-0.815518	-4.991892	0.847290
H	-4.711308	2.811585	-2.031778
H	-0.051494	-3.961477	-3.204510
H	2.128530	-4.750737	-4.060445
H	-2.995947	3.872461	0.275938
H	0.305292	4.470237	-3.391518
H	-0.983141	2.372979	-3.205615
H	1.517325	-3.768613	0.776329
C	4.804322	2.147231	2.237848
C	5.559328	2.964869	3.071786
C	6.137871	4.129764	2.573432
C	5.957369	4.465982	1.235814
C	5.196326	3.648488	0.402789
H	4.365812	1.230595	2.622366
H	5.699311	2.687342	4.111734
H	6.728320	4.768438	3.222431
H	5.086562	3.922906	-0.642041
H	6.410223	5.366406	0.833102
C	6.136570	0.480580	-0.405024
C	6.952533	-0.529040	-0.911913
C	6.392157	-1.618582	-1.568117
C	5.010506	-1.688431	-1.728696
C	4.189846	-0.681790	-1.233621
H	3.113657	-0.771304	-1.370379
H	6.591628	1.316765	0.114361
H	8.028263	-0.459436	-0.782637
H	7.021852	-2.414889	-1.953862
H	4.563442	-2.534948	-2.239279
C	0.753038	-0.223558	2.239867
C	-0.344161	-0.934331	2.699699
C	-1.613249	-0.373875	2.732695
C	-1.751144	0.938512	2.301683
Br	-0.099392	-2.711849	3.295106
H	-2.467779	-0.942551	3.076032
C	-0.668618	1.691349	1.872059

H	-0.843249	2.698484	1.512957
H	1.721330	-0.705992	2.191761
Br	-3.484163	1.687459	2.202387
C	-1.659031	6.232325	0.390620
C	-0.896792	7.371107	0.327175
C	0.040845	7.544893	-0.720238
C	0.193615	6.575121	-1.678778
H	-2.381703	6.093614	1.190963
H	-1.010733	8.145786	1.079102
H	0.907750	6.704773	-2.488570
H	0.635669	8.452157	-0.762274
C	4.041409	-4.565176	0.128098
C	5.261589	-4.971278	-0.348346
C	5.425279	-5.279696	-1.721522
C	4.366084	-5.161726	-2.586245
H	3.909951	-4.327403	1.180562
H	6.108333	-5.058146	0.325589
H	6.393239	-5.610563	-2.086308
H	4.485457	-5.390963	-3.642359
C	-3.050989	-4.469973	2.207597
C	-3.914645	-3.602157	3.114822
H	-2.204001	-4.885515	2.765094
H	-3.645005	-5.325913	1.857489
C	-4.997262	-2.925897	2.279713
H	-3.276676	-2.852685	3.602268
H	-4.360136	-4.207702	3.911010
C	-4.405162	-2.005462	1.209395
H	-5.595930	-3.708502	1.794355
H	-5.682689	-2.350958	2.911170
H	-5.187475	-1.758609	0.488020
H	-4.133523	-1.035938	1.647814
C	-5.259858	-1.825504	-2.002335
C	-6.772420	-1.626354	-2.057009
H	-4.992674	-2.650394	-1.338358
H	-4.909784	-2.129920	-2.999453
C	-7.104143	-0.434807	-2.952789
H	-7.253906	-2.537814	-2.426146
H	-7.162094	-1.442439	-1.045610
C	-6.513542	0.844650	-2.363225
H	-6.682167	-0.611422	-3.950600
H	-8.186429	-0.323054	-3.076009
H	-7.111358	1.138363	-1.488481
H	-6.595060	1.670353	-3.078706

TS-2-minor

M06-2X/6-31G* Energy = -8271.54246470

M06-2X/6-31G* Free Energy = -8270.652040

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.51642887

M06-2X/def2-TZVPP-SMD(toluene) Energy = -8277.52257074

Number of Imaginary Frequencies = 1

Lowest Frequency = 348.0700i

M06-2X/6-31G* Geometry

C	2.214788	1.287773	2.963429
C	2.658718	2.234317	1.513032
C	3.022545	0.133047	2.827333
H	1.154960	1.104365	2.784957
H	2.416172	1.948553	3.803382
C	2.729234	-0.793296	1.804500
H	4.008647	0.105614	3.292170
N	2.425225	1.359472	0.436764
C	1.728162	3.443944	1.559102
C	4.130854	2.637398	1.604336
C	3.202432	0.210251	0.401028

C	3.140995	-0.722265	-0.776357
H	4.244116	0.438641	0.617960
H	1.447533	1.280121	0.080282
H	1.667962	-0.970550	1.605272
H	3.362853	-1.676396	1.727094
C	-4.708512	-1.903804	1.642050
C	-4.318133	-2.894833	2.553804
C	-3.761718	-1.412672	0.719338
C	-2.437302	-1.843042	0.800481
C	-2.015819	-2.791580	1.737090
C	-2.990582	-3.322121	2.578405
C	-4.109577	-0.374136	-0.295882
C	-5.097508	-0.602620	-1.275725
C	-5.493957	0.453617	-2.105569
C	-4.861054	1.690193	-1.982637
C	-3.800214	1.908817	-1.107517
C	-3.427353	0.848402	-0.270296
O	-1.512105	-1.235276	-0.028460
O	-2.420354	1.034889	0.654708
P	-0.996989	0.220929	0.531774
O	-0.143879	0.810894	-0.559236
O	-0.426109	0.097651	1.905964
C	-0.593797	-3.178826	1.899865
C	-3.107731	3.223568	-1.118279
C	-0.054439	-3.235519	3.217111
C	1.241681	-3.615434	3.439750
C	2.089717	-3.964455	2.356644
C	1.560712	-3.913005	1.036939
C	0.215155	-3.507111	0.834171
C	-3.862218	4.420673	-0.962878
C	-3.260035	5.649336	-1.048262
C	-1.866690	5.759668	-1.301401
C	-1.109711	4.566396	-1.454859
C	-1.755931	3.309154	-1.357191
H	-2.697834	-4.082520	3.300089
H	-5.163404	2.504885	-2.638199
H	-0.687347	-2.937662	4.047516
H	1.643097	-3.637364	4.449985
H	-1.165126	2.405881	-1.477344
H	-3.844335	6.557938	-0.924466
H	-4.928367	4.345262	-0.765765
H	-0.164823	-3.446633	-0.183513
C	4.809807	2.816495	2.809242
C	6.125023	3.277620	2.823146
C	6.779719	3.571324	1.631994
C	6.107819	3.404896	0.423034
C	4.795070	2.946762	0.410469
H	4.320904	2.610362	3.755551
H	6.634665	3.408335	3.772520
H	7.804128	3.929319	1.644582
H	4.266089	2.826786	-0.531080
H	6.603955	3.635969	-0.514367
C	0.342460	3.270703	1.643498
C	-0.508571	4.369714	1.668669
C	0.010261	5.660303	1.631608
C	1.387487	5.841585	1.567944
C	2.244375	4.744772	1.531900
H	3.313654	4.914385	1.478378
H	-0.083985	2.278456	1.723794
H	-1.581666	4.203648	1.700150
H	-0.655240	6.517846	1.637262
H	1.804091	6.843694	1.532140
C	1.944638	-1.119453	-1.373793

C	1.990766	-2.035329	-2.414196
C	3.184319	-2.567623	-2.888678
C	4.357575	-2.174044	-2.260668
Br	0.360835	-2.679876	-3.111073
H	3.194101	-3.294609	-3.692098
C	4.353078	-1.262226	-1.213144
H	5.289186	-0.987733	-0.736937
H	0.989714	-0.714878	-1.053816
Br	5.990583	-2.961145	-2.796237
C	0.289090	4.657925	-1.685413
C	0.903038	5.879838	-1.772746
C	0.147337	7.071095	-1.630944
C	-1.203215	7.011789	-1.398853
H	0.857448	3.734686	-1.772421
H	1.974586	5.942162	-1.938458
H	-1.786103	7.923083	-1.286694
H	0.645196	8.033562	-1.704740
C	2.409872	-4.239344	-0.054197
C	3.734344	-4.535259	0.145793
C	4.264727	-4.566273	1.460550
C	3.456059	-4.307034	2.539080
H	1.984067	-4.230630	-1.052851
H	4.385416	-4.732716	-0.701887
H	5.312068	-4.810786	1.609977
H	3.853483	-4.344849	3.550667
C	-5.301061	-3.528721	3.520489
C	-6.533197	-2.665045	3.777258
H	-4.787614	-3.758874	4.460642
H	-5.626125	-4.493409	3.105463
C	-7.104489	-2.178558	2.448514
H	-6.256390	-1.796343	4.388598
H	-7.277968	-3.234587	4.342828
C	-6.092697	-1.283992	1.736397
H	-7.341313	-3.045307	1.815477
H	-8.038592	-1.628109	2.601102
H	-6.467035	-0.996588	0.751932
H	-5.990499	-0.342474	2.295621
C	-5.653611	-1.999568	-1.497458
C	-6.983216	-2.003462	-2.248197
H	-5.745343	-2.543660	-0.554722
H	-4.910667	-2.557795	-2.085663
C	-6.874744	-1.151870	-3.509974
H	-7.265314	-3.032850	-2.492554
H	-7.774697	-1.597503	-1.602309
C	-6.603765	0.301372	-3.128990
H	-6.052073	-1.532253	-4.129333
H	-7.787961	-1.217189	-4.110530
H	-7.524471	0.735109	-2.713197
H	-6.361659	0.894449	-4.017733

TS-2-minor-2

M06-2X/6-31G* Energy = -8271.54246468

M06-2X/6-31G* Free Energy = -8270.652037

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.51642812

M06-2X/def2-TZVPP-SMD(toluene) Energy = -8277.52257025

Number of Imaginary Frequencies = 1

Lowest Frequency = 348.1540i

M06-2X/6-31G* Geometry

C	2.214804	1.287837	2.963458
C	2.658592	2.234423	1.513032
C	3.022566	0.133100	2.827343
H	1.154962	1.104404	2.785086
H	2.416214	1.948598	3.803424

C	2.729277	-0.793233	1.804515
H	4.008654	0.105641	3.292206
N	2.425079	1.359543	0.436794
C	1.727986	3.444008	1.559126
C	4.130722	2.637562	1.604196
C	3.202409	0.210394	0.400990
C	3.141012	-0.722178	-0.776345
H	4.244077	0.438840	0.617938
H	1.447419	1.280193	0.080214
H	1.668014	-0.970469	1.605235
H	3.362928	-1.676300	1.727026
C	-5.097451	-0.602748	-1.275791
C	-5.493922	0.453494	-2.105617
C	-4.109545	-0.374253	-0.295927
C	-3.427358	0.848306	-0.270305
C	-3.800245	1.908729	-1.107504
C	-4.861063	1.690089	-1.982646
C	-3.761673	-1.412792	0.719285
C	-4.708467	-1.903952	1.641981
C	-4.318074	-2.894976	2.553736
C	-2.990511	-3.322224	2.578357
C	-2.015750	-2.791652	1.737059
C	-2.437246	-1.843127	0.800443
O	-2.420369	1.034795	0.654712
O	-1.512057	-1.235336	-0.028488
P	-0.996980	0.220883	0.531745
O	-0.143916	0.810885	-0.559285
O	-0.426057	0.097618	1.905918
C	-3.107812	3.223507	-1.118218
C	-0.593718	-3.178851	1.899864
C	-3.862347	4.420578	-0.962787
C	-3.260212	5.649267	-1.048135
C	-1.866870	5.759661	-1.301263
C	-1.109843	4.566423	-1.454748
C	-1.756014	3.309153	-1.357122
C	-0.054392	-3.235534	3.217123
C	1.241737	-3.615397	3.439792
C	2.089814	-3.964380	2.356705
C	1.560838	-3.912945	1.036988
C	0.215271	-3.507105	0.834188
H	-5.163431	2.504787	-2.638192
H	-2.697751	-4.082616	3.300044
H	-4.928493	4.345118	-0.765679
H	-3.844548	6.557842	-0.924315
H	-0.164685	-3.446639	-0.183506
H	1.643130	-3.637317	4.450037
H	-0.687330	-2.937703	4.047514
H	-1.165173	2.405905	-1.477291
C	4.794671	2.947319	0.410279
C	6.107427	3.405426	0.422698
C	6.779610	3.571427	1.631564
C	6.125188	3.277317	2.822764
C	4.809959	2.816213	2.809005
H	4.265475	2.827652	-0.531189
H	6.603356	3.636806	-0.514737
H	7.804028	3.929399	1.644038
H	4.321277	2.609743	3.755354
H	6.635057	3.407685	3.772065
C	0.342294	3.270680	1.643521
C	-0.508805	4.369636	1.668764
C	0.009951	5.660260	1.631800
C	1.387166	5.841628	1.568173
C	2.244120	4.744869	1.532049

H	3.313390	4.914555	1.478574
H	-0.084082	2.278399	1.723762
H	-1.581890	4.203503	1.700221
H	-0.655602	6.517762	1.637508
H	1.803713	6.843764	1.532467
C	1.944682	-1.119388	-1.373822
C	1.990863	-2.035286	-2.414203
C	3.184442	-2.567563	-2.888639
C	4.357669	-2.173955	-2.260592
Br	0.360968	-2.679886	-3.111113
H	3.194264	-3.294559	-3.692049
C	4.353119	-1.262131	-1.213076
H	5.289204	-0.987622	-0.736834
H	0.989740	-0.714822	-1.053886
Br	5.990710	-2.961027	-2.796102
C	2.410039	-4.239241	-0.054129
C	3.734518	-4.535105	0.145892
C	4.264871	-4.566103	1.460662
C	3.456165	-4.306902	2.539172
H	1.984256	-4.230547	-1.052792
H	4.385618	-4.732535	-0.701773
H	3.853566	-4.344704	3.550769
H	5.312217	-4.810576	1.610113
C	0.288956	4.658015	-1.685282
C	0.902858	5.879953	-1.772572
C	0.147108	7.071177	-1.630749
C	-1.203444	7.011810	-1.398678
H	0.857351	3.734799	-1.772311
H	1.974406	5.942325	-1.938267
H	0.644930	8.033665	-1.704513
H	-1.786369	7.923079	-1.286497
C	-6.603705	0.301233	-3.129062
C	-6.874635	-1.152011	-3.510075
H	-6.361597	0.894329	-4.017792
H	-7.524432	0.734938	-2.713283
C	-6.983105	-2.003627	-2.248314
H	-6.051942	-1.532358	-4.129426
H	-7.787839	-1.217346	-4.110649
C	-5.653513	-1.999709	-1.497553
H	-7.774609	-1.597703	-1.602433
H	-7.265168	-3.033019	-2.492694
H	-4.910544	-2.557907	-2.085753
H	-5.745246	-2.543815	-0.554825
C	-6.092670	-1.284177	1.736310
C	-7.104446	-2.178766	2.448420
H	-6.467004	-0.996786	0.751840
H	-5.990502	-0.342654	2.295532
C	-6.533153	-2.665240	3.777169
H	-8.038565	-1.628343	2.600998
H	-7.341241	-3.045523	1.815382
C	-5.300998	-3.528890	3.520408
H	-6.256369	-1.796531	4.388509
H	-7.277917	-3.234794	4.342735
H	-5.626039	-4.493582	3.105375
H	-4.787554	-3.759036	4.460565

TS-2-minor-3

M06-2X/6-31G* Energy = -8271.54020740

M06-2X/6-31G* Free Energy = -8270.650313

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.51423232

M06-2X/def2-TZVPP-SMD(toluene) Energy = -8277.52089057

Number of Imaginary Frequencies = 1

Lowest Frequency = 361.9546i

M06-2X/6-31G* Geometry

C	1.950903	1.742904	2.897424
C	2.149446	2.726384	1.404658
C	3.025436	0.829242	2.799800
H	0.976937	1.287593	2.723049
H	1.969831	2.462323	3.712000
C	2.978958	-0.177690	1.811150
H	3.983869	1.070114	3.261241
N	2.166945	1.783186	0.365632
C	0.933328	3.651767	1.394526
C	3.464374	3.501766	1.500039
C	3.205266	0.862663	0.375786
C	3.387922	-0.091176	-0.771645
H	4.156059	1.347377	0.588865
H	1.246644	1.464990	-0.011430
H	1.995801	-0.617764	1.618482
H	3.810653	-0.880758	1.766198
C	-4.756650	-1.684352	-1.287328
C	-5.342555	-0.726141	-2.124295
C	-3.824433	-1.271159	-0.313515
C	-3.381794	0.057107	-0.301529
C	-3.937666	1.020350	-1.150768
C	-4.941434	0.606486	-2.021428
C	-3.277915	-2.216912	0.704933
C	-4.103208	-2.872794	1.641142
C	-3.518345	-3.754668	2.561513
C	-2.131682	-3.904027	2.585845
C	-1.285812	-3.201284	1.730920
C	-1.893814	-2.377900	0.778862
O	-2.426149	0.441529	0.616374
O	-1.113691	-1.617627	-0.072257
P	-0.874241	-0.083971	0.462961
O	-0.182454	0.648681	-0.653237
O	-0.263204	-0.083732	1.825973
C	-3.477422	2.436008	-1.182924
C	0.185707	-3.271234	1.904204
C	-2.171115	2.743635	-1.658942
C	-1.780307	4.045749	-1.820345
C	-2.648563	5.118294	-1.489940
C	-3.937470	4.818617	-0.968940
C	-4.332770	3.459596	-0.847121
C	0.712116	-3.178998	3.224887
C	2.058026	-3.253259	3.462138
C	2.972827	-3.427767	2.391419
C	2.457883	-3.525270	1.068670
C	1.057709	-3.432153	0.849855
H	-5.386473	1.347017	-2.682978
H	-1.689683	-4.575495	3.319659
H	-1.490308	1.929769	-1.882872
H	-0.782688	4.275770	-2.186697
H	0.685098	-3.476461	-0.171366
H	2.444334	-3.162865	4.474438
H	0.021116	-3.012126	4.045576
H	-5.330261	3.232533	-0.476607
C	4.097574	3.871931	0.306895
C	5.246517	4.655778	0.321769
C	5.779946	5.093214	1.531424
C	5.150916	4.742137	2.721358
C	4.001048	3.955657	2.705350
H	3.674811	3.541037	-0.637701
H	5.721379	4.928061	-0.615605
H	6.675903	5.705430	1.545907
H	3.523732	3.713770	3.648922
H	5.551099	5.082724	3.671108

C	-0.358177	3.142966	1.571038
C	-1.463712	3.985026	1.546250
C	-1.300083	5.354055	1.359434
C	-0.019729	5.870446	1.186254
C	1.090908	5.030155	1.205478
H	2.077682	5.459229	1.072508
H	-0.515975	2.087398	1.753232
H	-2.455101	3.555130	1.654617
H	-2.165788	6.010290	1.326795
H	0.120395	6.935939	1.030326
C	4.702254	-0.367341	-1.156140
C	4.939110	-1.277331	-2.177887
C	3.900241	-1.924631	-2.831832
C	2.604588	-1.651459	-2.408640
Br	6.720310	-1.709391	-2.639339
H	4.093780	-2.647824	-3.615177
C	2.326013	-0.747092	-1.394615
H	1.295156	-0.551432	-1.115009
H	5.540426	0.110972	-0.658962
Br	1.176734	-2.643643	-3.140799
C	3.368941	-3.687956	-0.009162
C	4.723839	-3.686729	0.205060
C	5.235529	-3.566877	1.521995
C	4.378960	-3.459770	2.589217
H	2.962102	-3.797832	-1.009791
H	5.411428	-3.763754	-0.633063
H	4.764411	-3.384954	3.603393
H	6.309470	-3.575819	1.682181
C	-4.786306	5.889578	-0.580342
C	-4.376179	7.192767	-0.705635
C	-3.096353	7.490702	-1.236944
C	-2.256713	6.476421	-1.620675
H	-5.769019	5.656198	-0.178035
H	-5.033023	8.002264	-0.402146
H	-2.784699	8.526085	-1.336371
H	-1.267779	6.694768	-2.016401
C	-6.414445	-1.088160	-3.135490
C	-6.421854	-2.570507	-3.500880
H	-6.291058	-0.470721	-4.032028
H	-7.394846	-0.823219	-2.714410
C	-6.360298	-3.415663	-2.231393
H	-5.550736	-2.801998	-4.127477
H	-7.314570	-2.806022	-4.089496
C	-5.045986	-3.161422	-1.497350
H	-7.205753	-3.154889	-1.579005
H	-6.452173	-4.481416	-2.465056
H	-4.219458	-3.574390	-2.093877
H	-5.022651	-3.708082	-0.551965
C	-5.581187	-2.535041	1.742780
C	-6.392954	-3.603378	2.471341
H	-6.011717	-2.335227	0.759593
H	-5.661053	-1.586658	2.294046
C	-5.728349	-3.954036	3.799547
H	-7.415933	-3.245517	2.627168
H	-6.459110	-4.506284	1.848157
C	-4.351458	-4.560247	3.540933
H	-5.624684	-3.041535	4.400924
H	-6.342543	-4.653377	4.376257
H	-4.482268	-5.574136	3.136661
H	-3.797597	-4.675429	4.479269

TS-3-minor

M06-2X/6-31G* Energy = -8271.54734437

M06-2X/6-31G* Free Energy = -8270.654753

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.51832189

M06-2X/def2-TZVPP-SMD(toluene) Energy = -8277.52444133

Number of Imaginary Frequencies = 1

Lowest Frequency = 196.6802i

M06-2X/6-31G* Geometry

C	3.428401	-0.852335	-1.153514
C	3.840108	-0.238337	0.435578
C	3.421097	0.345711	-1.914849
H	2.444781	-1.289802	-0.962803
H	4.194417	-1.585526	-1.398792
C	2.401973	1.310905	-1.724552
H	4.333174	0.637867	-2.435684
N	2.810338	0.676151	0.733938
C	3.816922	-1.454134	1.362433
C	5.212322	0.427088	0.400620
C	2.694106	1.808245	-0.073913
C	1.603216	2.769696	0.315232
H	3.646154	2.333629	-0.146626
H	1.907015	0.214719	0.891158
H	1.375479	0.934832	-1.669486
H	2.491818	2.219190	-2.320324
C	-4.875543	-2.343646	-0.635249
C	-5.865603	-1.387298	-0.892589
C	-3.583493	-1.913255	-0.262545
C	-3.266905	-0.548939	-0.295374
C	-4.247249	0.419990	-0.567294
C	-5.537488	-0.034456	-0.827212
C	-2.528397	-2.908381	0.101243
C	-2.664797	-3.806232	1.179675
C	-1.686870	-4.793347	1.371636
C	-0.578532	-4.842837	0.524522
C	-0.367422	-3.907129	-0.486013
C	-1.361733	-2.936433	-0.662572
O	-1.983139	-0.154116	0.016122
O	-1.178186	-1.940668	-1.594646
P	-0.709909	-0.486569	-0.979649
O	0.464451	-0.673250	-0.052427
O	-0.602627	0.462087	-2.119919
C	-3.966452	1.876369	-0.583431
C	0.883576	-3.891295	-1.282294
C	-4.848665	2.769009	0.088506
C	-4.607112	4.117844	0.110233
C	-3.472186	4.661906	-0.547250
C	-2.612743	3.777830	-1.255168
C	-2.880500	2.387523	-1.255308
C	0.890369	-3.537584	-2.665576
C	2.063452	-3.466378	-3.368041
C	3.313199	-3.708471	-2.736879
C	3.315346	-4.089389	-1.367105
C	2.081837	-4.202111	-0.679355
H	-6.307898	0.702443	-1.046467
H	0.155065	-5.634140	0.667999
H	-5.704818	2.360593	0.619242
H	-5.274783	4.788163	0.645989
H	2.107656	-4.468393	0.372074
H	2.051939	-3.191966	-4.419682
H	-0.048815	-3.311637	-3.155612
H	-2.209209	1.733155	-1.803282
C	6.217284	0.045159	-0.490283
C	7.484133	0.620437	-0.415028
C	7.764085	1.580757	0.552023
C	6.770913	1.956895	1.453110

C	5.507722	1.378689	1.382937
H	6.032413	-0.722306	-1.237223
H	8.253342	0.311798	-1.115913
H	8.750453	2.030148	0.606164
H	4.735026	1.660484	2.092837
H	6.979079	2.699199	2.217147
C	4.997517	-1.934685	1.938758
C	4.964855	-3.004675	2.829450
C	3.754475	-3.608649	3.157051
C	2.578511	-3.142082	2.575230
C	2.604881	-2.081891	1.673195
H	1.673412	-1.771387	1.202015
H	5.950202	-1.472274	1.706924
H	5.890832	-3.358721	3.271839
H	3.728294	-4.436987	3.858421
H	1.625383	-3.610870	2.805549
C	0.410297	2.341017	0.900195
C	-0.506386	3.290915	1.332284
C	-0.288533	4.654552	1.166441
C	0.887106	5.052213	0.546477
Br	-2.084663	2.714064	2.171804
H	-1.029958	5.379915	1.480608
C	1.839775	4.132329	0.127417
H	2.761939	4.480085	-0.328137
H	0.179369	1.288190	1.026534
Br	1.197970	6.894871	0.266864
C	4.554774	-4.237512	-0.689922
C	5.739668	-4.007112	-1.343762
C	5.739586	-3.645927	-2.715356
C	4.554025	-3.509406	-3.396258
H	4.542298	-4.498072	0.366286
H	6.682166	-4.101674	-0.812607
H	4.548550	-3.226247	-4.445926
H	6.683418	-3.480604	-3.226552
C	-1.483371	4.303949	-1.939773
C	-1.216404	5.647905	-1.914347
C	-2.060502	6.529299	-1.190996
C	-3.161433	6.048381	-0.527285
H	-0.834542	3.605661	-2.463895
H	-0.342004	6.045738	-2.421364
H	-1.825341	7.589174	-1.162527
H	-3.814378	6.723189	0.021344
C	-7.292476	-1.772264	-1.236325
C	-7.418412	-3.197843	-1.766230
H	-7.696793	-1.054513	-1.958494
H	-7.909213	-1.676342	-0.331214
C	-6.654110	-4.151362	-0.852751
H	-6.997867	-3.255787	-2.778571
H	-8.474073	-3.479639	-1.837844
C	-5.164136	-3.818078	-0.870598
H	-7.040817	-4.060372	0.172187
H	-6.801055	-5.192160	-1.159650
H	-4.629682	-4.448951	-0.157637
H	-4.751630	-4.078923	-1.856351
C	-3.799959	-3.645995	2.175730
C	-4.067184	-4.910127	2.988955
H	-4.712534	-3.308419	1.679241
H	-3.521586	-2.831682	2.860343
C	-2.763241	-5.435848	3.583099
H	-4.797768	-4.695231	3.775477
H	-4.508419	-5.680971	2.341456
C	-1.813391	-5.844268	2.459720
H	-2.302316	-4.645840	4.190349

H	-2.945870	-6.287933	4.246011
H	-2.182290	-6.774973	2.005774
H	-0.819307	-6.074914	2.859942

TS-3-minor-2

M06-2X/6-31G* Energy = -8271.54734426

M06-2X/6-31G* Free Energy = -8270.654752

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.51832176

M06-2X/def2-TZVPP-SMD(toluene) Energy = -8277.52444126

Number of Imaginary Frequencies = 1

Lowest Frequency = 196.6462i

M06-2X/6-31G* Geometry

C	3.428268	-0.852789	-1.153513
C	3.840108	-0.238817	0.435556
C	3.421126	0.345250	-1.914852
H	2.444589	-1.290103	-0.962760
H	4.194176	-1.586096	-1.398780
C	2.402134	1.310588	-1.724544
H	4.333239	0.637277	-2.435695
N	2.810464	0.675807	0.733932
C	3.816787	-1.454605	1.362418
C	5.212411	0.426420	0.400543
C	2.694356	1.807910	-0.073937
C	1.603600	2.769506	0.315229
H	3.646471	2.333170	-0.146666
H	1.907089	0.214492	0.891198
H	1.375590	0.934650	-1.669472
H	2.492092	2.218851	-2.320334
C	-2.665357	-3.805902	1.179671
C	-1.687571	-4.793156	1.371641
C	-2.528812	-2.908059	0.101251
C	-1.362135	-2.936262	-0.662538
C	-0.367969	-3.907107	-0.485978
C	-0.579227	-4.842795	0.524543
C	-3.583769	-1.912790	-0.262548
C	-4.875871	-2.343005	-0.635275
C	-5.865802	-1.386524	-0.892618
C	-5.537510	-0.033726	-0.827223
C	-4.247214	0.420546	-0.567285
C	-3.267002	-0.548515	-0.295360
O	-1.178425	-1.940512	-1.594595
O	-1.983191	-0.153864	0.016164
P	-0.709981	-0.486474	-0.979579
O	0.464331	-0.673297	-0.052323
O	-0.602555	0.462166	-2.119848
C	0.883036	-3.891445	-1.282253
C	-3.966215	1.876887	-0.583413
C	0.889882	-3.537737	-2.665535
C	2.062976	-3.466690	-3.367996
C	3.312689	-3.708944	-2.736827
C	3.314781	-4.089854	-1.367051
C	2.081253	-4.202420	-0.679308
C	-4.848300	2.769651	0.088526
C	-4.606556	4.118453	0.110250
C	-3.471556	4.662354	-0.547238
C	-2.612237	3.778156	-1.255153
C	-2.880193	2.387887	-1.255294
H	0.154256	-5.634205	0.668022
H	-6.307819	0.703277	-1.046480
H	-0.049270	-3.311666	-3.155575
H	2.051504	-3.192282	-4.419639
H	-2.208996	1.733424	-1.803269
H	-5.274133	4.788866	0.646006

H	-5.704510	2.361356	0.619264
H	2.107030	-4.468708	0.372119
C	5.507966	1.378011	1.382823
C	6.771242	1.956036	1.452954
C	7.764343	1.579724	0.551861
C	7.484234	0.619413	-0.415154
C	6.217301	0.044315	-0.490365
H	4.735324	1.659940	2.092729
H	6.979531	2.698335	2.216963
H	8.750778	2.028973	0.605969
H	6.032305	-0.723148	-1.237277
H	8.253385	0.310640	-1.116043
C	4.997318	-1.935245	1.938800
C	4.964529	-3.005212	2.829512
C	3.754082	-3.609072	3.157081
C	2.578182	-3.142417	2.575202
C	2.604679	-2.082252	1.673141
H	1.673259	-1.771681	1.201906
H	5.950052	-1.472919	1.706994
H	5.890457	-3.359330	3.271945
H	3.727802	-4.437392	3.858469
H	1.625004	-3.611118	2.805494
C	0.410628	2.340985	0.900202
C	-0.505928	3.291004	1.332293
C	-0.287897	4.654612	1.166447
C	0.887792	5.052117	0.546477
Br	-2.084280	2.714357	2.171812
H	-1.029227	5.380072	1.480612
C	1.840337	4.132108	0.127412
H	2.762543	4.479743	-0.328149
H	0.179562	1.288188	1.026542
Br	1.198899	6.894735	0.266858
C	-1.482790	4.304114	-1.939759
C	-1.215637	5.648033	-1.914341
C	-2.059614	6.529548	-1.190996
C	-3.160611	6.048786	-0.527281
H	-0.834058	3.605732	-2.463875
H	-0.341181	6.045741	-2.421358
H	-3.813463	6.723688	0.021344
H	-1.824309	7.589391	-1.162535
C	4.554187	-4.238120	-0.689857
C	5.739113	-4.007871	-1.343693
C	5.739084	-3.646703	-2.715291
C	4.553544	-3.510040	-3.396202
H	4.541674	-4.498664	0.366354
H	6.681595	-4.102539	-0.812530
H	6.682939	-3.481503	-3.226484
H	4.548110	-3.226890	-4.445872
C	-1.814256	-5.844070	2.459713
C	-2.764087	-5.435544	3.583069
H	-0.820212	-6.074844	2.859963
H	-2.183257	-6.774725	2.005747
C	-4.067940	-4.909635	2.988895
H	-2.303075	-4.645609	4.190350
H	-2.946851	-6.287617	4.245959
C	-3.800517	-3.645522	2.175706
H	-4.509259	-5.680404	2.341365
H	-4.798520	-4.694656	3.775398
H	-4.713032	-3.307800	1.679206
H	-3.522036	-2.831268	2.860345
C	-5.164654	-3.817397	-0.870645
C	-6.654671	-4.150489	-0.852834
H	-4.630298	-4.448347	-0.157678

H	-4.752160	-4.078287	-1.856392
C	-7.418831	-3.196854	-1.766312
H	-6.801745	-5.191262	-1.159754
H	-7.041388	-4.059465	0.172097
C	-7.292720	-1.771301	-1.236379
H	-6.998273	-3.254836	-2.778646
H	-8.474527	-3.478513	-1.837953
H	-7.909458	-1.675317	-0.331276
H	-7.696934	-1.053486	-1.958541

TS-3-minor-3

M06-2X/6-31G* Energy = -8271.54280749

M06-2X/6-31G* Free Energy = -8270.650785

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.51669787

M06-2X/def2-TZVPP-SMD(toluene) Energy = -8277.52316605

Number of Imaginary Frequencies = 1

Lowest Frequency = 192.7463i

M06-2X/6-31G* Geometry

C	-3.645028	-0.778329	-1.121267
C	-3.678558	-1.570771	0.439103
C	-3.130447	-1.817271	-1.940896
H	-2.955079	0.046769	-0.925341
H	-4.666338	-0.457053	-1.317429
C	-1.780405	-2.226461	-1.818123
H	-3.834259	-2.468226	-2.459691
N	-2.333894	-1.919771	0.677841
C	-4.180348	-0.512392	1.422045
C	-4.596208	-2.787641	0.391347
C	-1.738172	-2.843273	-0.180831
C	-0.307319	-3.189142	0.137400
H	-2.335870	-3.751762	-0.255322
H	-1.739079	-1.096257	0.829261
H	-1.026719	-1.432656	-1.774870
H	-1.480062	-3.060545	-2.452111
C	0.643606	4.540986	1.163870
C	-0.657286	4.998317	1.421098
C	0.862216	3.681378	0.068363
C	-0.232905	3.203046	-0.649252
C	-1.541363	3.641042	-0.409924
C	-1.714310	4.564769	0.618577
C	2.225959	3.248586	-0.364944
C	3.178183	4.201630	-0.787195
C	4.470677	3.775470	-1.116248
C	4.772726	2.416013	-1.060841
C	3.829214	1.443124	-0.740691
C	2.536762	1.883689	-0.413549
O	-0.003483	2.236404	-1.600707
O	1.571007	0.963544	-0.062689
P	0.242661	0.717758	-1.013378
O	-0.862250	0.357162	-0.052708
O	0.526509	-0.160491	-2.178491
C	-2.691012	3.090166	-1.167202
C	4.228521	0.013432	-0.733433
C	-2.600067	2.804983	-2.563199
C	-3.650234	2.240470	-3.236050
C	-4.849684	1.887431	-2.560860
C	-4.959804	2.189958	-1.176014
C	-3.874870	2.821350	-0.518212
C	3.440972	-0.972446	-1.392673
C	3.823037	-2.286760	-1.373993
C	4.991029	-2.707160	-0.686127
C	5.795661	-1.724031	-0.047050
C	5.391055	-0.365417	-0.099105

H	-2.712734	4.953251	0.811760
H	5.774584	2.088619	-1.331071
H	-1.678878	3.030497	-3.086776
H	-3.564587	2.026940	-4.298335
H	5.993135	0.378470	0.418694
H	3.214876	-3.037140	-1.875569
H	2.538246	-0.676246	-1.917772
H	-3.968953	3.022170	0.543952
C	-4.390758	-3.807351	1.326922
C	-5.249398	-4.900497	1.384078
C	-6.336477	-4.983050	0.517523
C	-6.559587	-3.962551	-0.401675
C	-5.696825	-2.870413	-0.463961
H	-3.549904	-3.733465	2.010970
H	-5.069465	-5.686091	2.111093
H	-7.007542	-5.834829	0.561639
H	-5.908305	-2.073157	-1.171701
H	-7.410006	-4.010706	-1.074446
C	-5.428499	-0.644708	2.039440
C	-5.855994	0.291762	2.977410
C	-5.043832	1.371251	3.312078
C	-3.806397	1.513942	2.689594
C	-3.378110	0.589528	1.740791
H	-2.424049	0.754381	1.242196
H	-6.072446	-1.484105	1.802808
H	-6.824866	0.167997	3.451168
H	-5.373135	2.096001	4.050337
H	-3.164283	2.358022	2.926893
C	0.157007	-4.450494	-0.237566
C	1.449432	-4.829356	0.106407
C	2.281917	-3.998631	0.841166
C	1.808536	-2.733597	1.173717
Br	2.109125	-6.512122	-0.453115
H	3.285370	-4.304230	1.114203
C	0.534562	-2.309986	0.822563
H	0.230022	-1.300093	1.074790
H	-0.480270	-5.138747	-0.784623
Br	2.942685	-1.554845	2.094331
C	6.959626	-2.140676	0.651360
C	7.299433	-3.467615	0.722454
C	6.489460	-4.447547	0.097083
C	5.365515	-4.073889	-0.596052
H	7.573448	-1.386701	1.137975
H	8.188969	-3.773938	1.264382
H	4.726087	-4.821237	-1.063094
H	6.763504	-5.495769	0.168421
C	-6.104953	1.752090	-0.459412
C	-7.093244	1.038169	-1.090556
C	-6.994843	0.754517	-2.476640
C	-5.902500	1.177662	-3.194820
H	-6.162310	1.959689	0.607038
H	-7.954769	0.688285	-0.529595
H	-7.789828	0.202303	-2.969162
H	-5.818663	0.956175	-4.255926
C	-0.951498	5.989119	2.532828
C	0.134376	6.029647	3.605310
H	-1.925487	5.756855	2.978751
H	-1.049843	6.991050	2.091407
C	1.506428	6.134861	2.944964
H	0.095967	5.112481	4.207473
H	-0.043065	6.869825	4.284611
C	1.781651	4.888442	2.107387
H	1.533102	7.026318	2.302524

H	2.294273	6.256632	3.695332
H	1.924037	4.029334	2.778889
H	2.723587	4.991015	1.563517
C	2.778589	5.653524	-0.998550
C	3.971235	6.605321	-1.054528
H	2.067801	5.986457	-0.239528
H	2.232721	5.707742	-1.951956
C	5.019440	6.080138	-2.030912
H	3.629975	7.604735	-1.343879
H	4.419417	6.695080	-0.054865
C	5.562318	4.745708	-1.527455
H	4.555891	5.943840	-3.016609
H	5.838605	6.796070	-2.154640
H	6.210849	4.933192	-0.659667
H	6.196793	4.275257	-2.286576

TS-4-minor

M06-2X/6-31G* Energy = -8271.54482040

M06-2X/6-31G* Free Energy = -8270.653321

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.51708612

M06-2X/def2-TZVPP-SMD(toluene) Energy = -8277.52312783

Number of Imaginary Frequencies = 1

Lowest Frequency = 181.4863i

M06-2X/6-31G* Geometry

C	-2.383569	-2.556261	1.138286
C	-3.073131	-2.326407	-0.434040
C	-3.035957	-1.547097	1.902582
H	-1.327890	-2.373972	0.920044
H	-2.588823	-3.586946	1.426287
C	-2.759456	-0.180729	1.670662
H	-3.926316	-1.816464	2.470150
N	-2.743526	-0.995145	-0.768655
C	-2.384656	-3.355733	-1.331684
C	-4.584959	-2.542917	-0.403896
C	-3.303471	0.016105	0.007226
C	-2.951140	1.420833	-0.400730
H	-4.384434	-0.097864	0.089309
H	-1.728481	-0.866652	-0.886695
H	-1.699723	0.090785	1.587918
H	-3.340890	0.529997	2.257947
C	4.540162	-1.579685	-1.253722
C	4.353416	-2.931673	-1.572323
C	3.797267	-1.022278	-0.193166
C	2.793005	-1.780255	0.410684
C	2.560721	-3.126385	0.087702
C	3.395692	-3.676992	-0.884854
C	4.045726	0.363423	0.312785
C	5.313473	0.727259	0.818263
C	5.547840	2.059711	1.179791
C	4.509325	2.984433	1.082080
C	3.219173	2.633032	0.694795
C	3.001446	1.296393	0.323833
O	2.009196	-1.153775	1.351400
O	1.752049	0.903383	-0.108078
P	0.844426	-0.144928	0.780606
O	-0.017468	-0.859155	-0.228351
O	0.216010	0.493583	1.970141
C	1.458128	-3.921408	0.687995
C	2.151114	3.663193	0.688749
C	0.863315	-4.963530	-0.083386
C	-0.190391	-5.698696	0.385968
C	-0.748970	-5.429344	1.660981
C	-0.147493	-4.418086	2.459722

C	0.965732	-3.694963	1.958938
C	2.399465	4.927138	0.082884
C	1.435727	5.901299	0.061487
C	0.165747	5.678392	0.656347
C	-0.072381	4.430753	1.295138
C	0.935818	3.436110	1.291747
H	3.294136	-4.730882	-1.132881
H	4.695361	4.015508	1.377021
H	1.225062	-5.148773	-1.088531
H	-0.640610	-6.466398	-0.237184
H	0.734408	2.490926	1.787526
H	1.628177	6.855706	-0.422450
H	3.361007	5.100449	-0.393427
H	1.399812	-2.924363	2.584957
C	-5.331888	-2.034920	-1.473260
C	-6.704684	-2.242082	-1.540609
C	-7.352472	-2.975595	-0.548392
C	-6.615175	-3.500710	0.506926
C	-5.239414	-3.285330	0.579855
H	-4.822332	-1.469799	-2.248659
H	-7.268877	-1.832276	-2.372408
H	-8.424059	-3.139105	-0.600838
H	-4.681508	-3.727508	1.401174
H	-7.106800	-4.082186	1.280460
C	-1.189628	-3.066217	-1.999346
C	-0.625048	-4.004830	-2.858147
C	-1.220127	-5.249005	-3.044301
C	-2.386858	-5.556590	-2.351125
C	-2.964559	-4.617111	-1.502215
H	-3.886662	-4.867264	-0.987881
H	-0.662504	-2.131796	-1.842653
H	0.298185	-3.756263	-3.373310
H	-0.775989	-5.974676	-3.718979
H	-2.861062	-6.525191	-2.477922
C	-3.920586	2.411238	-0.236886
C	-3.647163	3.706060	-0.658686
C	-2.439893	4.041016	-1.254374
C	-1.484544	3.039828	-1.393378
Br	-4.945778	5.052947	-0.396833
H	-2.231655	5.057296	-1.566893
C	-1.713473	1.738968	-0.963394
H	-0.927814	0.998261	-1.076709
H	-4.884989	2.179595	0.204725
Br	0.170792	3.459019	-2.177122
C	-1.327805	4.199002	1.920531
C	-2.303968	5.160868	1.905429
C	-2.075742	6.398380	1.250791
C	-0.870972	6.650042	0.643407
H	-1.489954	3.234513	2.396968
H	-3.269356	4.974271	2.367545
H	-0.690423	7.600895	0.147448
H	-2.865169	7.143792	1.229220
C	-0.733301	-4.098886	3.715300
C	-1.873832	-4.732781	4.140259
C	-2.476790	-5.734992	3.338151
C	-1.919958	-6.080618	2.131057
H	-0.272379	-3.322293	4.320186
H	-2.318099	-4.471924	5.096003
H	-3.375237	-6.234719	3.688195
H	-2.374476	-6.848246	1.509053
C	5.190178	-3.628526	-2.629979
C	5.834477	-2.662164	-3.620712
H	4.572352	-4.364897	-3.156263

H	5.983431	-4.199511	-2.126770
C	6.505718	-1.519675	-2.863415
H	5.067153	-2.247729	-4.287530
H	6.554226	-3.196609	-4.249359
C	5.460408	-0.713716	-2.096213
H	7.243678	-1.932651	-2.161125
H	7.048984	-0.860993	-3.548725
H	5.939866	0.057421	-1.489543
H	4.829376	-0.170408	-2.814589
C	6.379356	-0.327079	1.072893
C	7.784998	0.255495	1.198514
H	6.361851	-1.105565	0.307862
H	6.118370	-0.836012	2.012385
C	7.787516	1.413438	2.191888
H	8.481806	-0.530099	1.508881
H	8.124211	0.617309	0.217399
C	6.902641	2.540183	1.666162
H	7.402874	1.058894	3.156978
H	8.803133	1.784199	2.365103
H	7.419016	3.034170	0.830628
H	6.759757	3.308915	2.433527

TS-4-minor-2

M06-2X/6-31G* Energy = -8271.54482058

M06-2X/6-31G* Free Energy = -8270.653318

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.51708692

M06-2X/def2-TZVPP-SMD(toluene) Energy = -8277.52312865

Number of Imaginary Frequencies = 1

Lowest Frequency = 181.3103i

M06-2X/6-31G* Geometry

C	-2.383301	-2.556527	1.138265
C	-3.072878	-2.326678	-0.434137
C	-3.035846	-1.547471	1.902502
H	-1.327660	-2.374103	0.919965
H	-2.588479	-3.587262	1.426130
C	-2.759484	-0.181043	1.670563
H	-3.926222	-1.816931	2.469998
N	-2.743359	-0.995404	-0.768654
C	-2.384236	-3.355954	-1.331689
C	-4.584676	-2.543359	-0.404001
C	-3.303448	0.015777	0.007253
C	-2.951284	1.420547	-0.400731
H	-4.384406	-0.098307	0.089257
H	-1.728310	-0.866814	-0.886593
H	-1.699764	0.090551	1.587946
H	-3.340984	0.529610	2.257875
C	5.313382	0.727837	0.818212
C	5.547605	2.060312	1.179749
C	4.045659	0.363856	0.312778
C	3.001270	1.296705	0.323871
C	3.218854	2.633366	0.694839
C	4.508979	2.984913	1.082087
C	3.797343	-1.021870	-0.193178
C	4.540273	-1.579193	-1.253754
C	4.353670	-2.931200	-1.572357
C	3.396042	-3.676627	-0.884869
C	2.561031	-3.126115	0.087707
C	2.793183	-1.779963	0.410695
O	1.751903	0.903560	-0.108006
O	2.009339	-1.153575	1.351442
P	0.844429	-0.144869	0.780691
O	-0.017391	-0.859202	-0.228257
O	0.215956	0.493547	1.970244

C	2.150680	3.663410	0.688823
C	1.458532	-3.921258	0.688016
C	2.398894	4.927402	0.083000
C	1.435044	5.901452	0.061617
C	0.165081	5.678382	0.656450
C	-0.072911	4.430697	1.295203
C	0.935401	3.436170	1.291798
C	0.863845	-4.963463	-0.083351
C	-0.189776	-5.698748	0.386009
C	-0.748395	-5.429441	1.661015
C	-0.147038	-4.418103	2.459744
C	0.966105	-3.694856	1.958955
H	4.694904	4.016005	1.377035
H	3.294604	-4.730528	-1.132894
H	3.360421	5.100836	-0.393297
H	1.627391	6.855894	-0.422291
H	1.400095	-2.924203	2.584970
H	-0.639893	-6.466519	-0.237129
H	1.225618	-5.148680	-1.088491
H	0.734093	2.490952	1.787553
C	-5.331637	-2.035410	-1.473363
C	-6.704411	-2.242711	-1.540741
C	-7.352140	-2.976316	-0.548554
C	-6.614808	-3.501380	0.506765
C	-5.239071	-3.285861	0.579724
H	-4.822127	-1.470217	-2.248740
H	-7.268632	-1.832940	-2.372539
H	-8.423710	-3.139935	-0.601023
H	-4.681135	-3.727986	1.401049
H	-7.106387	-4.082921	1.280278
C	-1.189246	-3.066306	-1.999364
C	-0.624530	-4.004889	-2.858107
C	-1.219437	-5.249157	-3.044196
C	-2.386126	-5.556867	-2.351006
C	-2.963959	-4.617425	-1.502147
H	-3.886028	-4.867678	-0.987801
H	-0.662264	-2.131794	-1.842732
H	0.298671	-3.756222	-3.373281
H	-0.775196	-5.974802	-3.718834
H	-2.860194	-6.525541	-2.477754
C	-1.713647	1.738815	-0.963388
C	-1.484858	3.039697	-1.393383
C	-2.440320	4.040780	-1.254399
C	-3.647557	3.705694	-0.658718
Br	0.170437	3.459067	-2.177118
H	-2.232194	5.057079	-1.566929
C	-3.920839	2.410846	-0.236908
H	-4.885222	2.179099	0.204695
H	-0.927903	0.998197	-1.076688
Br	-4.946325	5.052439	-0.396895
C	-0.732884	-4.098962	3.715319
C	-1.873338	-4.732990	4.140285
C	-2.476178	-5.735278	3.338186
C	-1.919306	-6.080849	2.131095
H	-0.272055	-3.322308	4.320198
H	-2.317637	-4.472176	5.096026
H	-2.373731	-6.848539	1.509100
H	-3.374565	-6.235109	3.688235
C	-1.328319	4.198781	1.920569
C	-2.304594	5.160535	1.905477
C	-2.076502	6.398090	1.250878
C	-0.871752	6.649910	0.643521
H	-1.490362	3.234260	2.396978

H	-3.269967	4.973812	2.367574
H	-2.866015	7.143411	1.229314
H	-0.691305	7.600798	0.147591
C	6.902369	2.540944	1.666068
C	7.787429	1.414298	2.191698
H	6.759422	3.309623	2.433475
H	7.418628	3.035038	0.830527
C	7.784985	0.256377	1.198297
H	7.402906	1.059679	3.156808
H	8.803010	1.785187	2.364846
C	6.379407	-0.326371	1.072776
H	8.124072	0.618258	0.217163
H	8.481920	-0.529133	1.508590
H	6.118550	-0.835330	2.012289
H	6.361945	-1.104863	0.307750
C	5.460443	-0.713156	-2.096253
C	6.505992	-1.519051	-2.863191
H	5.939663	0.058173	-1.489642
H	4.829399	-0.170097	-2.814808
C	5.834984	-2.661604	-3.620599
H	7.049365	-0.860357	-3.548405
H	7.243821	-1.931953	-2.160720
C	5.190505	-3.627990	-2.630002
H	5.067799	-2.247226	-4.287610
H	6.554904	-3.196030	-4.249066
H	5.983654	-4.199084	-2.126754
H	4.572685	-4.364271	-3.156422

TS-4-minor-3

M06-2X/6-31G* Energy = -8271.54053444

M06-2X/6-31G* Free Energy = -8270.648804

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.51522667

M06-2X/def2-TZVPP-SMD(toluene) Energy = -8277.52144545

Number of Imaginary Frequencies = 1

Lowest Frequency = 179.0133i

M06-2X/6-31G* Geometry

C	3.640628	0.554997	-1.155940
C	3.780909	1.309235	0.397580
C	3.184079	1.633072	-1.967156
H	2.899732	-0.217523	-0.933293
H	4.620569	0.146294	-1.402366
C	1.886840	2.166195	-1.791701
H	3.918222	2.205913	-2.532897
N	2.474222	1.761128	0.678884
C	4.248809	0.204626	1.346180
C	4.784476	2.460190	0.361723
C	1.953670	2.761422	-0.136889
C	0.566905	3.229164	0.216089
H	2.634741	3.609361	-0.213631
H	1.812849	0.975957	0.785809
H	1.068864	1.435755	-1.724141
H	1.641191	3.028956	-2.410778
C	-1.194088	-4.597647	1.245493
C	0.008055	-5.204326	1.634954
C	-1.178321	-3.686109	0.170616
C	0.043371	-3.301885	-0.381748
C	1.265377	-3.868333	0.010705
C	1.198472	-4.849396	0.999910
C	-2.430083	-3.103913	-0.404794
C	-3.424544	-3.941382	-0.956538
C	-4.630225	-3.376427	-1.389463
C	-4.803172	-1.995574	-1.307153
C	-3.803176	-1.134294	-0.864179

C	-2.598988	-1.714134	-0.435161
O	0.017818	-2.316931	-1.340939
O	-1.583766	-0.905751	0.034536
P	-0.170285	-0.776273	-0.804223
O	0.872509	-0.457163	0.236185
O	-0.298409	0.076994	-2.017442
C	2.570103	-3.419159	-0.538959
C	-4.056251	0.328704	-0.841771
C	3.725081	-3.474593	0.295389
C	4.945935	-3.030381	-0.133211
C	5.098178	-2.467751	-1.425695
C	3.965318	-2.435977	-2.284760
C	2.720294	-2.936012	-1.824384
C	-3.131577	1.240705	-1.424589
C	-3.384168	2.585768	-1.408096
C	-4.552217	3.110667	-0.796345
C	-5.489573	2.203671	-0.229487
C	-5.216436	0.812148	-0.278919
H	2.112212	-5.355074	1.303798
H	-5.738286	-1.560325	-1.653738
H	3.623716	-3.836693	1.312865
H	5.802954	-3.060307	0.533530
H	-5.924236	0.124169	0.179048
H	-2.671588	3.278959	-1.851566
H	-2.229367	0.859987	-1.892776
H	1.870453	-2.893841	-2.495527
C	4.731070	3.395742	1.401556
C	5.648335	4.438092	1.464745
C	6.646297	4.553375	0.498804
C	6.719145	3.616829	-0.526146
C	5.793164	2.576579	-0.595406
H	3.956606	3.298135	2.157207
H	5.585314	5.159781	2.273014
H	7.363966	5.365935	0.548309
H	5.886198	1.842370	-1.391520
H	7.498068	3.690018	-1.278529
C	3.343507	-0.581441	2.066426
C	3.810139	-1.525803	2.976791
C	5.174931	-1.719765	3.165726
C	6.079590	-0.968063	2.421531
C	5.619742	-0.014524	1.518876
H	6.340194	0.578138	0.964475
H	2.273287	-0.496977	1.916885
H	3.090446	-2.117747	3.534343
H	5.530989	-2.453608	3.882453
H	7.148330	-1.111758	2.549499
C	0.217124	4.542340	-0.101783
C	-1.033747	5.021510	0.270197
C	-1.938251	4.236042	0.969567
C	-1.579674	2.920044	1.243662
Br	-1.531448	6.785727	-0.198350
H	-2.910761	4.617372	1.258127
C	-0.347424	2.401260	0.871485
H	-0.127681	1.361232	1.089470
H	0.912233	5.193564	-0.623087
Br	-2.818491	1.801516	2.102721
C	-6.653579	2.724143	0.395153
C	-6.869088	4.077016	0.464098
C	-5.928791	4.979964	-0.090672
C	-4.800595	4.506056	-0.711950
H	-7.368682	2.028444	0.827194
H	-7.760362	4.462664	0.949573
H	-4.063172	5.193543	-1.123100

H	-6.105910	6.049068	-0.022538
C	4.093210	-1.829161	-3.564304
C	5.278208	-1.259191	-3.956598
C	6.403976	-1.282770	-3.094069
C	6.316241	-1.881743	-1.861169
H	3.223668	-1.804866	-4.216036
H	5.360165	-0.789664	-4.932166
H	7.338308	-0.833771	-3.417939
H	7.173580	-1.905506	-1.192367
C	0.053623	-6.268259	2.716811
C	-1.155736	-6.231232	3.647807
H	0.983122	-6.166771	3.288308
H	0.097837	-7.255139	2.234514
C	-2.437941	-6.153163	2.823646
H	-1.095086	-5.350379	4.300197
H	-1.155337	-7.113813	4.295837
C	-2.470788	-4.850621	2.027915
H	-2.480390	-7.008964	2.135105
H	-3.321856	-6.214855	3.466717
H	-2.599192	-4.008926	2.723970
H	-3.345045	-4.822325	1.373859
C	-3.152612	-5.420003	-1.184457
C	-4.423444	-6.243015	-1.381559
H	-2.550860	-5.843925	-0.378139
H	-2.529718	-5.502854	-2.087175
C	-5.315923	-5.589265	-2.432239
H	-4.157795	-7.264825	-1.672010
H	-4.971143	-6.310774	-0.430825
C	-5.767648	-4.218092	-1.937451
H	-4.749209	-5.478591	-3.365852
H	-6.187548	-6.213451	-2.654936
H	-6.514361	-4.357838	-1.142669
H	-6.273326	-3.665947	-2.737210

TS-5-minor

M06-2X/6-31G* Energy = -8271.53352777

M06-2X/6-31G* Free Energy = -8270.645947

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.51274915

M06-2X/def2-TZVPP-SMD(toluene) Energy = -8277.51906569

Number of Imaginary Frequencies = 1

Lowest Frequency = 280.8187i

M06-2X/6-31G* Geometry

C	0.431320	-0.331280	2.324340
C	0.035194	-1.962261	2.326986
C	-0.812963	0.362627	2.552626
H	0.840022	-0.178531	1.322160
H	1.192751	-0.185975	3.091498
C	-1.796140	0.356772	1.563086
H	-1.079359	0.662404	3.566356
N	-0.967272	-2.102625	1.313855
C	1.327062	-2.701086	1.979266
C	-0.518259	-2.407064	3.680112
C	-2.163139	-1.460370	1.533119
C	-3.238329	-1.566958	0.496016
H	-2.550207	-1.639751	2.534321
H	-0.603697	-1.971057	0.362946
H	-1.442482	0.404384	0.532743
H	-2.740956	0.857756	1.765194
C	4.208612	3.062739	-0.076278
C	5.467603	2.647978	-0.528458
C	3.151529	2.127717	-0.047418
C	3.335276	0.859566	-0.599397
C	4.590522	0.423674	-1.046405

C	5.639814	1.334001	-0.968152
C	1.827189	2.468984	0.555809
C	1.716615	2.835571	1.914074
C	0.484330	3.298454	2.395358
C	-0.595455	3.400793	1.516894
C	-0.545147	2.952363	0.197119
C	0.676912	2.413848	-0.243169
O	2.266160	-0.001768	-0.607349
O	0.775404	1.872390	-1.496907
P	0.982943	0.231188	-1.631562
O	-0.128157	-0.471449	-0.881331
O	1.304250	-0.058593	-3.042795
C	4.823558	-0.949273	-1.561056
C	-1.757878	3.072690	-0.656007
C	5.888690	-1.724218	-1.022463
C	6.148224	-2.987793	-1.487405
C	5.358173	-3.557874	-2.521097
C	4.292909	-2.785647	-3.063463
C	4.048925	-1.479124	-2.568401
C	-2.206258	2.021478	-1.508794
C	-3.370616	2.146799	-2.219724
C	-4.154836	3.326811	-2.148318
C	-3.708299	4.389851	-1.316943
C	-2.507152	4.228647	-0.582426
H	6.622697	1.019875	-1.314838
H	-1.542961	3.779616	1.896039
H	6.487093	-1.304028	-0.218342
H	6.962248	-3.572953	-1.065884
H	-2.165340	5.054525	0.037542
H	-3.705015	1.331397	-2.855564
H	-1.623112	1.110888	-1.587588
H	3.236014	-0.900242	-3.000118
C	-1.186245	-3.637031	3.734157
C	-1.664760	-4.132835	4.940613
C	-1.472777	-3.413689	6.119599
C	-0.797925	-2.199592	6.078436
C	-0.323730	-1.699398	4.865505
H	-1.324342	-4.200439	2.815637
H	-2.183739	-5.085912	4.961349
H	-1.843915	-3.800896	7.063045
H	0.217697	-0.758090	4.866071
H	-0.634340	-1.634103	6.990308
C	2.076922	-3.329093	2.977989
C	3.279244	-3.957972	2.664208
C	3.744607	-3.966444	1.353472
C	3.004278	-3.338117	0.356055
C	1.806362	-2.704423	0.666473
H	1.277652	-2.180310	-0.122952
H	1.727125	-3.336463	4.004905
H	3.848582	-4.442206	3.451636
H	4.683870	-4.450442	1.103590
H	3.361421	-3.329246	-0.668323
C	-2.964752	-1.458133	-0.869684
C	-4.018435	-1.556635	-1.767325
C	-5.331847	-1.751286	-1.351321
C	-5.576121	-1.852081	0.012064
Br	-3.653537	-1.395093	-3.610772
H	-6.139509	-1.819564	-2.070077
C	-4.546950	-1.759567	0.941209
H	-4.768712	-1.842821	2.000336
H	-1.955568	-1.272212	-1.231773
Br	-7.345917	-2.118854	0.615478
C	-4.480667	5.580011	-1.246966

C	-5.642376	5.703004	-1.964213
C	-6.089185	4.641214	-2.789611
C	-5.361564	3.482504	-2.878927
H	-4.132057	6.392295	-0.614131
H	-6.225563	6.616765	-1.904421
H	-5.694876	2.665121	-3.513235
H	-7.010101	4.752145	-3.353644
C	3.480271	-3.346926	-4.085846
C	3.722489	-4.613552	-4.550211
C	4.787923	-5.380658	-4.014791
C	5.584339	-4.866601	-3.024020
H	2.662122	-2.747768	-4.477217
H	3.097230	-5.037458	-5.329897
H	4.969102	-6.382204	-4.393145
H	6.400678	-5.452942	-2.609260
C	6.665744	3.579115	-0.542500
C	6.278904	5.055043	-0.502787
H	7.295704	3.354441	0.330159
H	7.279072	3.365245	-1.424580
C	5.246727	5.284757	0.597270
H	5.847346	5.351357	-1.467501
H	7.169547	5.671624	-0.343803
C	3.963539	4.519248	0.282101
H	5.657437	4.940500	1.557181
H	5.021199	6.350369	0.708620
H	3.255990	4.610078	1.109941
H	3.467404	4.990622	-0.578555
C	2.890033	2.623465	2.856811
C	2.717799	3.307604	4.211539
H	3.826805	2.940100	2.392155
H	3.001151	1.538757	3.008581
C	1.319645	3.053114	4.767438
H	3.489058	2.952954	4.902575
H	2.862353	4.390803	4.098907
C	0.288958	3.697952	3.845489
H	1.143712	1.967546	4.820671
H	1.218839	3.445642	5.784298
H	0.370572	4.790132	3.936005
H	-0.730866	3.443860	4.158977

TS-5-minor-2

M06-2X/6-31G* Energy = -8271.54088633

M06-2X/6-31G* Free Energy = -8270.651184

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.51453297

M06-2X/def2-TZVPP-SMD(toluene) Energy = -8277.51992397

Number of Imaginary Frequencies = 1

Lowest Frequency = 261.4056i

M06-2X/6-31G* Geometry

C	0.729712	-0.294098	2.339471
C	0.087963	-1.888497	2.401851
C	-0.408403	0.537221	2.583613
H	1.112973	-0.245400	1.318277
H	1.527189	-0.252810	3.080853
C	-1.429116	0.606454	1.623976
H	-0.608451	0.892245	3.594481
N	-0.931276	-1.910676	1.412460
C	1.272747	-2.787635	2.058795
C	-0.487067	-2.200420	3.781099
C	-2.026743	-1.089990	1.615928
C	-3.122236	-1.094514	0.587350
H	-2.435320	-1.206792	2.618736
H	-0.567030	-1.857391	0.453532
H	-1.110862	0.626514	0.580257

H	-2.294697	1.221948	1.859848
C	4.123046	3.284053	-0.362476
C	5.430010	2.868939	-0.647451
C	3.103415	2.312584	-0.247818
C	3.382038	0.980871	-0.566978
C	4.685093	0.550031	-0.854507
C	5.688770	1.512640	-0.852591
C	1.724601	2.691282	0.192681
C	1.493840	3.310777	1.438493
C	0.217423	3.822463	1.712920
C	-0.804638	3.651406	0.780831
C	-0.656798	2.896289	-0.384542
C	0.642225	2.422315	-0.654756
O	2.363829	0.061377	-0.506774
O	0.890658	1.687891	-1.783708
P	1.135814	0.058294	-1.628682
O	0.001731	-0.541361	-0.834835
O	1.560188	-0.447467	-2.949100
C	5.010240	-0.869925	-1.142857
C	-1.851639	2.551444	-1.205155
C	6.041871	-1.516015	-0.406215
C	6.382985	-2.818243	-0.663514
C	5.716196	-3.555729	-1.677368
C	4.693807	-2.908383	-2.426186
C	4.358311	-1.561272	-2.138151
C	-1.767586	2.245642	-2.597884
C	-2.887691	1.919881	-3.314946
C	-4.174135	1.900826	-2.716254
C	-4.278440	2.212196	-1.334748
C	-3.099410	2.515460	-0.610282
H	6.706774	1.198127	-1.075474
H	-1.771542	4.099338	0.996275
H	6.546337	-0.963911	0.382438
H	7.164356	-3.307249	-0.086714
H	-3.210726	2.725077	0.450107
H	-2.800612	1.676306	-4.370475
H	-0.805140	2.269888	-3.090441
H	3.568292	-1.084311	-2.713064
C	-1.348515	-3.299423	3.888031
C	-1.857723	-3.684813	5.122317
C	-1.503905	-2.986535	6.275605
C	-0.637331	-1.903761	6.181348
C	-0.132361	-1.513346	4.941416
H	-1.614150	-3.848125	2.988945
H	-2.528511	-4.535908	5.183759
H	-1.898830	-3.288041	7.240419
H	0.558147	-0.676704	4.898882
H	-0.347269	-1.357008	7.072993
C	1.922102	-3.522544	3.054783
C	3.024097	-4.314137	2.739123
C	3.484933	-4.384187	1.428952
C	2.842279	-3.651996	0.434193
C	1.752657	-2.848391	0.746678
H	1.299885	-2.252129	-0.039434
H	1.570987	-3.488314	4.080506
H	3.516838	-4.878338	3.524948
H	4.343835	-4.998585	1.175845
H	3.192823	-3.697469	-0.590594
C	-2.875964	-1.221007	-0.782744
C	-3.958734	-1.258426	-1.652487
C	-5.271789	-1.141815	-1.210408
C	-5.483834	-0.970429	0.150397
Br	-3.640136	-1.480631	-3.497635

H	-6.099154	-1.153738	-1.909242
C	-4.430704	-0.953026	1.054691
H	-4.634163	-0.839406	2.115141
H	-1.864445	-1.258276	-1.176754
Br	-7.247895	-0.740560	0.785099
C	-5.560147	2.207916	-0.720739
C	-6.684160	1.916199	-1.449981
C	-6.576433	1.588470	-2.824700
C	-5.349977	1.574698	-3.440694
H	-5.635910	2.435263	0.340541
H	-7.657359	1.909426	-0.969708
H	-5.259212	1.315985	-4.492393
H	-7.472297	1.347956	-3.389349
C	3.993988	-3.641749	-3.422640
C	4.298666	-4.957172	-3.661714
C	5.320476	-5.601134	-2.919617
C	6.012257	-4.917150	-1.952501
H	3.203063	-3.136164	-3.970776
H	3.755439	-5.513833	-4.419070
H	5.551954	-6.642939	-3.119894
H	6.795678	-5.408326	-1.380105
C	6.588710	3.845798	-0.728360
C	6.144935	5.286619	-0.964708
H	7.153031	3.799184	0.214102
H	7.279959	3.521547	-1.513853
C	5.017020	5.638896	0.000308
H	5.783909	5.399263	-1.995114
H	6.995401	5.965455	-0.843899
C	3.795301	4.766314	-0.277732
H	5.359256	5.478560	1.032758
H	4.741195	6.695026	-0.085673
H	3.018029	4.960530	0.464664
H	3.356788	5.061398	-1.242042
C	2.586634	3.361999	2.492616
C	2.338247	4.416696	3.568167
H	3.567645	3.505420	2.035145
H	2.631289	2.369603	2.967816
C	0.915180	4.296722	4.106075
H	3.073557	4.305135	4.371478
H	2.479237	5.419293	3.140927
C	-0.081916	4.589442	2.987886
H	0.760995	3.276127	4.485014
H	0.749230	4.979083	4.945851
H	-0.057984	5.665711	2.766929
H	-1.105152	4.369556	3.314386

TS-5-minor-3

M06-2X/6-31G* Energy = -8271.53763666

M06-2X/6-31G* Free Energy = -8270.648866

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.51324130

M06-2X/def2-TZVPP-SMD(toluene) Energy = -8277.51881180

Number of Imaginary Frequencies = 1

Lowest Frequency = 260.1134i

M06-2X/6-31G* Geometry

C	0.828491	-0.869918	2.312921
C	0.219139	-2.461889	2.043267
C	-0.307559	-0.160504	2.810300
H	1.141081	-0.577488	1.308274
H	1.672152	-0.975755	2.994233
C	-1.392527	0.089344	1.954731
H	-0.448556	-0.056139	3.885985
N	-0.858408	-2.289251	1.135829
C	1.398688	-3.214152	1.433520

C	-0.259053	-3.099604	3.344547
C	-1.956092	-1.573708	1.582782
C	-3.100340	-1.357976	0.632489
H	-2.308763	-1.933905	2.548632
H	-0.550814	-1.993719	0.201027
H	-1.142522	0.367555	0.928784
H	-2.250571	0.604043	2.382200
C	3.880231	3.391605	0.312329
C	5.185092	3.112588	-0.113239
C	2.904481	2.371647	0.250029
C	3.214503	1.158733	-0.370622
C	4.515988	0.864807	-0.802515
C	5.482497	1.849468	-0.627887
C	1.536844	2.577042	0.820711
C	1.345965	2.891678	2.183355
C	0.066580	3.262242	2.619929
C	-0.995355	3.255933	1.715660
C	-0.874379	2.799385	0.402409
C	0.424760	2.454706	-0.020117
O	2.236279	0.201066	-0.471490
O	0.636153	1.996537	-1.293675
P	0.941579	0.382751	-1.501745
O	-0.119052	-0.422977	-0.793761
O	1.302599	0.184828	-2.919668
C	4.875114	-0.439149	-1.414919
C	-2.088209	2.614989	-0.437789
C	5.970667	-1.182286	-0.893493
C	6.337801	-2.380700	-1.447985
C	5.634495	-2.909782	-2.562321
C	4.549055	-2.161051	-3.097211
C	4.187990	-0.925587	-2.503316
C	-3.333186	2.332297	0.204770
C	-4.493178	2.180266	-0.503929
C	-4.495006	2.283549	-1.918754
C	-3.262331	2.541658	-2.577281
C	-2.077576	2.709592	-1.814820
H	6.498361	1.640976	-0.958793
H	-1.969163	3.587772	2.068247
H	6.503482	-0.793017	-0.029847
H	7.168026	-2.947851	-1.033959
H	-1.152845	2.916919	-2.340600
H	-5.422558	1.941259	0.009652
H	-3.364012	2.226238	1.284655
H	3.348710	-0.372109	-2.917298
C	-1.089081	-4.223130	3.244956
C	-1.509990	-4.897828	4.384733
C	-1.097409	-4.469615	5.645321
C	-0.260864	-3.364652	5.753097
C	0.155594	-2.684115	4.609338
H	-1.400197	-4.561012	2.260576
H	-2.157671	-5.763328	4.287318
H	-1.423414	-4.996978	6.536030
H	0.824963	-1.836627	4.720402
H	0.074522	-3.026359	6.728372
C	1.788933	-2.960367	0.114684
C	2.871429	-3.633065	-0.438606
C	3.597793	-4.544587	0.323208
C	3.226987	-4.787073	1.641357
C	2.131289	-4.128802	2.195318
H	1.850414	-4.338959	3.221764
H	1.270677	-2.219890	-0.486834
H	3.150478	-3.435777	-1.467301
H	4.450999	-5.053548	-0.115304

H	3.785369	-5.493960	2.247265
C	-2.922122	-1.270170	-0.750098
C	-4.030864	-1.054019	-1.557301
C	-5.308590	-0.903299	-1.030079
C	-5.451841	-0.950349	0.348969
Br	-3.789521	-0.884456	-3.414653
H	-6.156206	-0.710264	-1.677113
C	-4.370694	-1.187418	1.187453
H	-4.519502	-1.226786	2.262416
H	-1.937222	-1.311608	-1.201501
Br	-7.152646	-0.602599	1.098824
C	-3.248754	2.627143	-3.995580
C	-4.402194	2.459389	-4.717707
C	-5.629255	2.200437	-4.058281
C	-5.673742	2.115124	-2.690211
H	-2.302665	2.816446	-4.495367
H	-4.379653	2.520900	-5.801317
H	-6.611538	1.920589	-2.173648
H	-6.534526	2.068615	-4.643032
C	3.812924	-2.691140	-4.191616
C	4.142096	-3.910007	-4.726780
C	5.226202	-4.654446	-4.197437
C	5.954706	-4.165786	-3.142734
H	2.974741	-2.113756	-4.573382
H	3.570928	-4.313263	-5.557258
H	5.476575	-5.617792	-4.631395
H	6.786218	-4.734702	-2.733316
C	6.300980	4.137133	-0.021663
C	5.792575	5.571819	0.089362
H	6.914317	3.909715	0.862064
H	6.962629	4.028708	-0.887963
C	4.703069	5.647424	1.154704
H	5.375481	5.893179	-0.873733
H	6.622493	6.246429	0.323599
C	3.502123	4.800794	0.739489
H	5.103207	5.278754	2.110090
H	4.384123	6.681988	1.318421
H	2.756696	4.788368	1.537789
H	3.004428	5.280679	-0.115680
C	2.490140	2.760890	3.174489
C	2.254443	3.530692	4.471564
H	3.438341	3.057026	2.721100
H	2.603389	1.690695	3.408348
C	0.868773	3.215430	5.027419
H	3.035717	3.280971	5.196645
H	2.328756	4.609923	4.278405
C	-0.198564	3.698970	4.049079
H	0.779556	2.128699	5.169026
H	0.718643	3.679773	6.007333
H	-0.235939	4.796804	4.082147
H	-1.192020	3.352738	4.357968

TS-5-minor-4

M06-2X/6-31G* Energy = -8271.53407257

M06-2X/6-31G* Free Energy = -8270.644729

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.51318307

M06-2X/def2-TZVPP-SMD(toluene) Energy = -8277.51932579

Number of Imaginary Frequencies = 1

Lowest Frequency = 275.9367i

M06-2X/6-31G* Geometry

C	0.470888	-0.656989	2.115972
C	0.193883	-2.295876	1.872667
C	-0.810774	-0.106310	2.482637

H	0.829130	-0.319172	1.140215
H	1.248339	-0.573782	2.876222
C	-1.826659	-0.034311	1.528717
H	-1.061517	0.008845	3.537360
N	-0.835679	-2.354494	0.878960
C	1.517899	-2.869900	1.370884
C	-0.270178	-2.985568	3.154429
C	-2.064467	-1.844430	1.227784
C	-3.168675	-1.875398	0.216444
H	-2.399142	-2.204233	2.198880
H	-0.519610	-2.055927	-0.050538
H	-1.515325	0.198604	0.509759
H	-2.796488	0.356724	1.830596
C	3.775924	3.459489	0.219659
C	5.054638	3.245878	-0.309629
C	2.815965	2.428435	0.125643
C	3.106966	1.280748	-0.610803
C	4.385962	1.041629	-1.129136
C	5.342965	2.032672	-0.939088
C	1.484090	2.540460	0.793964
C	1.378759	2.686286	2.193431
C	0.122676	2.949890	2.756855
C	-0.985972	3.080422	1.918691
C	-0.931345	2.840799	0.545926
C	0.322502	2.492723	0.012069
O	2.130567	0.324510	-0.737918
O	0.437725	2.158304	-1.309725
P	0.807146	0.588460	-1.706444
O	-0.212416	-0.333064	-1.072282
O	1.134240	0.565928	-3.144480
C	4.740996	-0.228232	-1.813709
C	-2.172429	2.968162	-0.263878
C	4.023951	-0.669123	-2.962578
C	4.391672	-1.824463	-3.602769
C	5.471235	-2.619603	-3.130781
C	6.184159	-2.186539	-1.978136
C	5.798438	-0.976090	-1.346910
C	-2.542085	2.014128	-1.256897
C	-3.729622	2.131321	-1.929823
C	-4.617165	3.208855	-1.677361
C	-4.251698	4.176047	-0.701971
C	-3.023496	4.024089	-0.011558
H	6.341221	1.869151	-1.340378
H	-1.953464	3.306204	2.363698
H	3.183349	-0.082744	-3.324029
H	3.845750	-2.153357	-4.483404
H	-2.744486	4.779069	0.720219
H	-4.002819	1.389897	-2.675835
H	-1.878618	1.184637	-1.475347
H	6.338569	-0.652679	-0.459536
C	-0.854222	-4.253005	3.033993
C	-1.244881	-4.965051	4.161279
C	-1.047011	-4.428348	5.432759
C	-0.454923	-3.177842	5.563122
C	-0.069049	-2.460857	4.430400
H	-0.996960	-4.673437	2.042528
H	-1.699884	-5.943835	4.046944
H	-1.349422	-4.984344	6.314331
H	0.408909	-1.494901	4.562975
H	-0.287559	-2.752500	6.547579
C	1.947366	-2.600729	0.068696
C	3.167530	-3.087205	-0.384796
C	3.982196	-3.839942	0.456949

C	3.565373	-4.101641	1.758199
C	2.340484	-3.620258	2.215767
H	2.030974	-3.838832	3.232369
H	1.358379	-1.977135	-0.596156
H	3.481438	-2.864274	-1.398748
H	4.938609	-4.207781	0.095120
H	4.191013	-4.684678	2.427100
C	-2.953030	-1.563168	-1.128125
C	-4.031356	-1.608757	-2.000643
C	-5.314519	-1.941798	-1.578084
C	-5.501788	-2.241516	-0.235064
Br	-3.746211	-1.178682	-3.814813
H	-6.142667	-1.963319	-2.276136
C	-4.445886	-2.211318	0.667620
H	-4.622628	-2.452379	1.710964
H	-1.972645	-1.259391	-1.489342
Br	-7.229066	-2.697686	0.377930
C	-5.128933	5.264489	-0.449562
C	-6.312968	5.380908	-1.130490
C	-6.678409	4.414303	-2.100227
C	-5.849281	3.355157	-2.366317
H	-4.842556	6.004561	0.293482
H	-6.976382	6.216817	-0.931003
H	-6.119877	2.611770	-3.111806
H	-7.618041	4.519295	-2.633715
C	7.248254	-2.988631	-1.484875
C	7.585907	-4.164520	-2.105295
C	6.877647	-4.593878	-3.254982
C	5.847757	-3.838309	-3.754234
H	7.788973	-2.651898	-0.603690
H	8.400325	-4.770305	-1.719766
H	7.154874	-5.525548	-3.738399
H	5.299263	-4.163240	-4.634636
C	6.154052	4.286732	-0.206004
C	5.625095	5.693358	0.061008
H	6.831787	4.001968	0.611566
H	6.755768	4.268602	-1.121201
C	4.611775	5.651680	1.201135
H	5.135157	6.082656	-0.840725
H	6.455400	6.367636	0.294715
C	3.400529	4.813952	0.797529
H	5.085581	5.213269	2.091029
H	4.286331	6.660511	1.475207
H	2.715831	4.707662	1.642635
H	2.831325	5.354090	0.027295
C	2.594786	2.453755	3.074943
C	2.398395	2.908636	4.519618
H	3.482295	2.927400	2.648454
H	2.813937	1.374991	3.060077
C	1.048479	2.435290	5.051089
H	3.220469	2.534087	5.137766
H	2.434189	4.005497	4.569507
C	-0.067354	3.104398	4.253725
H	0.980560	1.341923	4.940596
H	0.940525	2.658493	6.117269
H	-0.090463	4.173004	4.509168
H	-1.047525	2.703836	4.539550

TS-5-minor-5

M06-2X/6-31G* Energy = -8271.54136278

M06-2X/6-31G* Free Energy = -8270.649986

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.51489847

M06-2X/def2-TZVPP-SMD(toluene) Energy = -8277.52043181

Number of Imaginary Frequencies = 1

Lowest Frequency = 279.5078i

M06-2X/6-31G* Geometry

C	0.707121	-0.759179	2.112667
C	0.161473	-2.365683	1.798077
C	-0.470376	-0.090447	2.569540
H	1.052933	-0.442596	1.126355
H	1.524386	-0.848557	2.827602
C	-1.518894	0.144773	1.668691
H	-0.664237	-0.012013	3.639124
N	-0.883237	-2.212466	0.848467
C	1.392648	-3.067131	1.233534
C	-0.349389	-3.037100	3.069539
C	-2.018142	-1.538549	1.263280
C	-3.148054	-1.362684	0.288557
H	-2.383863	-1.917465	2.216560
H	-0.553633	-1.908769	-0.076461
H	-1.233032	0.434717	0.656097
H	-2.413680	0.626033	2.057503
C	3.866373	3.511322	0.161292
C	5.171490	3.234512	-0.264663
C	2.889171	2.493062	0.091470
C	3.202027	1.284534	-0.535331
C	4.502520	0.992042	-0.964489
C	5.470252	1.973978	-0.786947
C	1.520553	2.691174	0.662571
C	1.326520	2.991871	2.026390
C	0.043063	3.349922	2.463553
C	-1.017116	3.341646	1.558541
C	-0.893778	2.892487	0.241952
C	0.409801	2.567165	-0.181618
O	2.228307	0.324665	-0.651341
O	0.635126	2.131544	-1.459641
P	0.956497	0.526452	-1.706865
O	-0.117109	-0.300457	-1.043707
O	1.354399	0.375853	-3.119205
C	4.861380	-0.317444	-1.570935
C	-2.109593	2.687626	-0.594712
C	4.256362	-0.742843	-2.788358
C	4.645677	-1.917432	-3.377985
C	5.624931	-2.755262	-2.777627
C	6.218755	-2.341726	-1.552654
C	5.823533	-1.104317	-0.981169
C	-2.077239	2.728779	-2.022184
C	-3.213456	2.521186	-2.757560
C	-4.467589	2.284167	-2.137131
C	-4.520773	2.249446	-0.718510
C	-3.324965	2.441023	0.016526
H	6.486160	1.763546	-1.115359
H	-1.991636	3.670100	1.911432
H	3.478744	-0.131486	-3.237645
H	4.187031	-2.234135	-4.311410
H	-3.396036	2.388302	1.099487
H	-3.164939	2.542814	-3.843011
H	-1.141145	2.924397	-2.527111
H	6.280953	-0.788833	-0.045782
C	-1.140170	-4.183280	2.921134
C	-1.583005	-4.888933	4.033574
C	-1.231911	-4.469089	5.315383
C	-0.434648	-3.341109	5.471899
C	0.003880	-2.629888	4.355439
H	-1.403292	-4.514309	1.920551
H	-2.199483	-5.771946	3.898198
H	-1.575077	-5.020558	6.184786

H	0.641766	-1.764211	4.504875
H	-0.147160	-3.008773	6.464364
C	1.847399	-2.749806	-0.049242
C	2.997982	-3.340985	-0.553790
C	3.720780	-4.249265	0.215787
C	3.275518	-4.565760	1.495270
C	2.118854	-3.978772	2.005151
H	1.788315	-4.239739	3.004862
H	1.329084	-2.014928	-0.656064
H	3.333625	-3.073689	-1.549102
H	4.629622	-4.692627	-0.182841
H	3.827349	-5.271918	2.108105
C	-2.946574	-1.135256	-1.075766
C	-4.057450	-1.023196	-1.902490
C	-5.357513	-1.097203	-1.415342
C	-5.527714	-1.278308	-0.049883
Br	-3.795909	-0.763995	-3.751543
H	-6.208359	-0.987346	-2.076344
C	-4.444131	-1.419523	0.806170
H	-4.613917	-1.581165	1.866332
H	-1.949883	-1.014095	-1.490091
Br	-7.276538	-1.319435	0.661931
C	-5.769763	2.022185	-0.079677
C	-6.911889	1.848011	-0.818270
C	-6.854340	1.866689	-2.234331
C	-5.659553	2.073148	-2.877625
H	-5.805581	1.985278	1.007102
H	-7.859564	1.669469	-0.320522
H	-5.606818	2.080234	-3.963175
H	-7.763544	1.716757	-2.808908
C	7.176073	-3.187229	-0.931344
C	7.520898	-4.389723	-1.494613
C	6.926189	-4.803680	-2.712251
C	6.003646	-4.003681	-3.337636
H	7.626580	-2.864591	0.004030
H	8.252206	-5.029464	-1.010011
H	7.205530	-5.757747	-3.148526
H	5.543102	-4.316254	-4.271361
C	6.287901	4.257670	-0.164055
C	5.780446	5.691806	-0.041660
H	6.900561	4.022478	0.718087
H	6.950043	4.155902	-1.030784
C	4.689303	5.759738	1.022588
H	5.365150	6.021621	-1.002662
H	6.610628	6.363636	0.199464
C	3.488497	4.917504	0.598256
H	5.087483	5.383013	1.975629
H	4.371003	6.793224	1.194090
H	2.741022	4.898987	1.394559
H	2.993279	5.404107	-0.254496
C	2.469216	2.859100	3.018681
C	2.226705	3.614988	4.322720
H	3.416884	3.164412	2.570267
H	2.587043	1.787379	3.242290
C	0.840415	3.289434	4.871255
H	3.006676	3.360458	5.047511
H	2.297917	4.696396	4.140958
C	-0.225087	3.779643	3.894287
H	0.753714	2.201117	5.001219
H	0.685965	3.743747	5.855195
H	-0.261052	4.877345	3.933298
H	-1.219237	3.432545	4.199432

TS-5-minor-6

M06-2X/6-31G* Energy = -8271.54136317
 M06-2X/6-31G* Free Energy = -8270.649977
 M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.51489969
 M06-2X/def2-TZVPP-SMD(toluene) Energy = -8277.52025649
 Number of Imaginary Frequencies = 1
 Lowest Frequency = 280.2172i
 M06-2X/6-31G* Geometry

C	0.706896	-0.759895	2.112845
C	0.161163	-2.366562	1.797524
C	-0.470650	-0.091492	2.569882
H	1.052735	-0.443073	1.126623
H	1.524127	-0.849684	2.827761
C	-1.518981	0.144270	1.668932
H	-0.664777	-0.013814	3.639471
N	-0.883290	-2.212751	0.847886
C	1.392489	-3.067667	1.232966
C	-0.349857	-3.038351	3.068706
C	-2.018331	-1.539018	1.262840
C	-3.148153	-1.362724	0.288113
H	-2.384110	-1.918205	2.215984
H	-0.553536	-1.908628	-0.076873
H	-1.232997	0.434569	0.656485
H	-2.413843	0.625370	2.057777
C	1.326699	2.991511	2.027103
C	0.043259	3.349415	2.464419
C	1.520656	2.691059	0.663220
C	0.409857	2.567155	-0.180919
C	-0.893694	2.892416	0.242778
C	-1.016975	3.341287	1.559469
C	2.889249	2.493093	0.092010
C	3.866418	3.511376	0.161930
C	5.171519	3.234675	-0.264147
C	5.470293	1.974230	-0.786643
C	4.502584	0.992287	-0.964274
C	3.202109	1.284671	-0.534989
O	0.635084	2.131745	-1.459033
O	2.228389	0.324808	-0.651087
P	0.956609	0.526745	-1.706609
O	-0.116929	-0.300452	-1.043693
O	1.354563	0.376522	-3.118975
C	-2.109534	2.687824	-0.593910
C	4.861459	-0.317091	-1.570950
C	-2.077211	2.729471	-2.021369
C	-3.213452	2.522170	-2.756789
C	-4.467573	2.284960	-2.136410
C	-4.520726	2.249758	-0.717799
C	-3.324897	2.441058	0.017276
C	4.256463	-0.742261	-2.788464
C	4.645787	-1.916741	-3.378304
C	5.625042	-2.754676	-2.778095
C	6.218845	-2.341370	-1.553034
C	5.823604	-1.104073	-0.981316
H	-1.991485	3.669644	1.912477
H	6.486188	1.763883	-1.115147
H	-1.141118	2.925231	-2.526244
H	-3.164962	2.544172	-3.842234
H	6.281011	-0.788762	-0.045864
H	4.187153	-2.233272	-4.311793
H	3.478847	-0.130821	-3.237641
H	-3.395937	2.387984	1.100221
C	-1.140969	-4.184242	2.919866
C	-1.583896	-4.890262	4.032042

C	-1.232561	-4.471081	5.313997
C	-0.434962	-3.343392	5.470936
C	0.003657	-2.631804	4.354753
H	-1.404266	-4.514779	1.919165
H	-2.200631	-5.773044	3.896334
H	-1.575800	-5.022837	6.183190
H	0.641780	-1.766354	4.504487
H	-0.147291	-3.011573	6.463520
C	2.118537	-3.979657	2.004330
C	3.275325	-4.566386	1.494438
C	3.720878	-4.249283	0.215206
C	2.998239	-3.340665	-0.554121
C	1.847519	-2.749757	-0.049570
H	1.329312	-2.014635	-0.656182
H	1.787771	-4.241112	3.003836
H	3.827021	-5.272829	2.107065
H	4.629818	-4.692449	-0.183420
H	3.334097	-3.072902	-1.549234
C	-2.946561	-1.134744	-1.076098
C	-4.057364	-1.022363	-1.902873
C	-5.357467	-1.096545	-1.415856
C	-5.527782	-1.278172	-0.050479
Br	-3.795670	-0.762537	-3.751816
H	-6.208259	-0.986425	-2.076884
C	-4.444271	-1.419750	0.805606
H	-4.614145	-1.581813	1.865690
H	-1.949820	-1.013456	-1.490260
Br	-7.276665	-1.319550	0.661179
C	7.176167	-3.186983	-0.931877
C	7.521017	-4.389360	-1.495381
C	6.926334	-4.803084	-2.713110
C	6.003785	-4.002978	-3.338347
H	7.626660	-2.864523	0.003565
H	8.252329	-5.029186	-1.010897
H	5.543257	-4.315372	-4.272140
H	7.205697	-5.757059	-3.149572
C	-5.769703	2.022284	-0.079017
C	-6.911843	1.848344	-0.817645
C	-6.854323	1.867498	-2.233700
C	-5.659552	2.074186	-2.876950
H	-5.805497	1.985014	1.007751
H	-7.859506	1.669625	-0.319938
H	-7.763538	1.717747	-2.808309
H	-5.606840	2.081636	-3.962498
C	-0.224822	3.778760	3.895275
C	0.840665	3.288134	4.872047
H	-1.218998	3.431671	4.200340
H	-0.260663	4.876453	3.934622
C	2.226951	3.613900	4.323629
H	0.753938	2.199766	5.001556
H	0.686230	3.742051	5.856173
C	2.469472	2.858545	3.019283
H	2.298162	4.695382	4.142310
H	3.006928	3.359078	5.048312
H	2.587481	1.786754	3.242454
H	3.417066	3.164182	2.570932
C	3.488523	4.917477	0.599135
C	4.689327	5.759670	1.023550
H	2.741078	4.898811	1.395463
H	2.993260	5.404205	-0.253519
C	5.780414	5.691952	-0.040770
H	4.371008	6.793119	1.195248
H	5.087569	5.382793	1.976504

C	6.287904	4.257851	-0.163440
H	5.365056	6.021921	-1.001692
H	6.610591	6.363763	0.200424
H	6.900628	4.022529	0.718622
H	6.949994	4.156250	-1.030229

TS-5-minor-7

M06-2X/6-31G* Energy = -8271.53800779

M06-2X/6-31G* Free Energy = -8270.647278

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.51344501

M06-2X/def2-TZVPP-SMD(toluene) Energy = -8277.51913406

Number of Imaginary Frequencies = 1

Lowest Frequency = 276.0029i

M06-2X/6-31G* Geometry

C	-0.828811	1.227603	1.992409
C	-0.330924	2.773852	1.395512
C	0.343910	0.729158	2.636354
H	-1.094136	0.707669	1.069340
H	-1.694529	1.410966	2.627871
C	1.460100	0.384985	1.857996
H	0.471204	0.870696	3.709486
N	0.774934	2.493272	0.551596
C	-1.554061	3.279969	0.638140
C	0.069004	3.705288	2.535235
C	1.911048	1.974736	1.148129
C	3.093948	1.647158	0.281487
H	2.210777	2.554478	2.020315
H	0.511226	1.988036	-0.303979
H	1.253816	-0.118399	0.911231
H	2.345109	0.038436	2.387402
C	-3.569999	-3.536565	0.829873
C	-4.870742	-3.434224	0.320599
C	-2.650311	-2.492591	0.583103
C	-3.006020	-1.456758	-0.283595
C	-4.302704	-1.339306	-0.798951
C	-5.219607	-2.325400	-0.453919
C	-1.295587	-2.485161	1.217925
C	-1.135898	-2.494224	2.619980
C	0.147824	-2.673545	3.153896
C	1.240158	-2.781738	2.293110
C	1.138829	-2.621383	0.910455
C	-0.163182	-2.464567	0.395576
O	-2.087077	-0.477578	-0.561411
O	-0.356864	-2.300912	-0.949677
P	-0.753693	-0.793264	-1.509466
O	0.233007	0.214559	-0.974447
O	-1.091485	-0.936204	-2.938343
C	-4.708862	-0.200388	-1.664269
C	2.367500	-2.533645	0.075954
C	-4.078235	0.016150	-2.923153
C	-4.509348	1.024358	-3.745625
C	-5.558140	1.900116	-3.352115
C	-6.176650	1.698909	-2.086706
C	-5.736741	0.624653	-1.270451
C	3.569267	-2.037019	0.669187
C	4.740424	-1.954363	-0.032694
C	4.797356	-2.350535	-1.393607
C	3.607535	-2.827837	-2.006834
C	2.410518	-2.914855	-1.250020
H	-6.232080	-2.249883	-0.845643
H	2.219529	-2.962199	2.730269
H	-3.247666	-0.619227	-3.218011
H	-4.031011	1.180442	-4.709387

H	1.519953	-3.292462	-1.738630
H	5.634546	-1.549043	0.437346
H	3.557158	-1.709309	1.703872
H	-6.213811	0.470335	-0.304901
C	0.822953	4.839175	2.208291
C	1.163766	5.769930	3.182644
C	0.745111	5.590958	4.499869
C	-0.016992	4.476280	4.830618
C	-0.353074	3.539640	3.853848
H	1.138427	4.981765	1.178662
H	1.753358	6.639715	2.910741
H	1.008761	6.318062	5.261164
H	-0.965771	2.688535	4.134603
H	-0.356566	4.329943	5.851081
C	-2.362295	4.290259	1.166982
C	-3.509172	4.699043	0.488514
C	-3.862856	4.105003	-0.718778
C	-3.057663	3.098604	-1.246846
C	-1.916675	2.684127	-0.573072
H	-1.332321	1.869789	-0.988503
H	-2.103762	4.766441	2.106781
H	-4.125861	5.485140	0.913333
H	-4.763903	4.408733	-1.245472
H	-3.321251	2.616577	-2.181156
C	2.965205	1.255181	-1.052870
C	4.110733	0.948140	-1.775051
C	5.378046	0.999894	-1.205243
C	5.474373	1.349758	0.133726
Br	3.940518	0.372296	-3.557054
H	6.255969	0.730817	-1.780680
C	4.354562	1.686471	0.882061
H	4.466321	1.963649	1.926051
H	1.994232	1.132010	-1.519430
Br	7.168549	1.285367	0.971808
C	3.648696	-3.211519	-3.374372
C	4.813406	-3.119866	-4.092054
C	5.997426	-2.641072	-3.478432
C	5.988714	-2.265546	-2.159408
H	2.734667	-3.568083	-3.841399
H	4.832589	-3.410619	-5.137803
H	6.893412	-1.900612	-1.677183
H	6.912036	-2.572114	-4.059440
C	-7.203382	2.588490	-1.672492
C	-7.591928	3.633042	-2.472420
C	-6.973140	3.836221	-3.730773
C	-5.983163	2.988241	-4.158965
H	-7.672022	2.428266	-0.704683
H	-8.376366	4.308611	-2.145040
H	-7.287636	4.666648	-4.355379
H	-5.503845	3.139711	-5.122814
C	-5.930487	-4.485426	0.595542
C	-5.347566	-5.830627	1.019329
H	-6.589929	-4.117710	1.394775
H	-6.562491	-4.601638	-0.291636
C	-4.297667	-5.614605	2.105047
H	-4.876145	-6.318771	0.156605
H	-6.147129	-6.492236	1.368181
C	-3.130637	-4.799947	1.552382
H	-4.754246	-5.080838	2.950851
H	-3.928520	-6.570535	2.490791
H	-2.417352	-4.574838	2.348465
H	-2.575241	-5.415044	0.829598
C	-2.321978	-2.237739	3.534083

C	-2.086010	-2.697777	4.970411
H	-3.232065	-2.688364	3.132702
H	-2.511508	-1.152895	3.531900
C	-0.744447	-2.175876	5.476962
H	-2.907651	-2.355499	5.607812
H	-2.084461	-3.795937	5.010384
C	0.386867	-2.779816	4.648837
H	-0.729874	-1.080273	5.384556
H	-0.601392	-2.410329	6.536653
H	0.492051	-3.840587	4.916157
H	1.344308	-2.307946	4.899586

TS-5-minor-8

M06-2X/6-31G* Energy = -8271.52998513

M06-2X/6-31G* Free Energy = -8270.640681

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.50900331

M06-2X/def2-TZVPP-SMD(toluene) Energy = -8277.51566469

Number of Imaginary Frequencies = 1

Lowest Frequency = 153.0786i

M06-2X/6-31G* Geometry

C	-1.787716	-2.074880	-0.380932
C	-0.916295	-3.356463	0.363384
C	-1.209005	-1.997262	-1.677368
H	-1.542650	-1.234136	0.257844
H	-2.838576	-2.343590	-0.329959
C	0.107075	-1.503379	-1.817118
H	-1.663338	-2.557008	-2.495751
N	0.443390	-2.970472	0.268659
C	-1.382474	-3.378244	1.817249
C	-1.204480	-4.664488	-0.364411
C	0.983656	-2.795219	-1.003027
C	2.442057	-2.431487	-1.019625
H	0.798005	-3.667361	-1.629387
H	0.698818	-2.226237	0.922919
H	0.356879	-0.655082	-1.171084
H	0.516767	-1.465915	-2.825464
C	-3.357463	4.250737	-0.202069
C	-4.674346	3.856109	0.064971
C	-2.358543	3.263190	-0.348749
C	-2.668954	1.934067	-0.066074
C	-3.980904	1.521060	0.188814
C	-4.968185	2.497889	0.214536
C	-0.983448	3.591492	-0.833032
C	-0.800855	4.205369	-2.091275
C	0.482217	4.625747	-2.457224
C	1.549188	4.385495	-1.595310
C	1.429224	3.673356	-0.400982
C	0.129370	3.261688	-0.049231
O	-1.652570	1.007538	-0.085325
O	-0.077727	2.591194	1.131581
P	-0.598522	1.030516	1.206443
O	0.459123	0.047936	0.774632
O	-1.308152	0.869124	2.498489
C	-4.322766	0.088151	0.411054
C	2.643444	3.430084	0.423426
C	-3.986350	-0.545111	1.641548
C	-4.347156	-1.848010	1.870118
C	-5.018278	-2.610612	0.876138
C	-5.335465	-1.990168	-0.366041
C	-4.991238	-0.624286	-0.558765
C	3.918057	3.405492	-0.222708
C	5.081748	3.303972	0.485450
C	5.063047	3.165278	1.897623

C	3.802416	3.144005	2.553416
C	2.611567	3.299318	1.796518
H	-5.995574	2.194729	0.406423
H	2.522270	4.778913	-1.875401
H	-3.417693	0.015874	2.378932
H	-4.091425	-2.329081	2.810972
H	1.666027	3.316260	2.325263
H	6.038061	3.278437	-0.031341
H	3.963801	3.445569	-1.305718
H	-5.244814	-0.145237	-1.502013
C	-0.250313	-5.686093	-0.312179
C	-0.510253	-6.927936	-0.883675
C	-1.735167	-7.172623	-1.499846
C	-2.696215	-6.166827	-1.538580
C	-2.434315	-4.919755	-0.976454
H	0.696848	-5.499146	0.186514
H	0.244072	-7.707240	-0.839048
H	-1.940309	-8.142622	-1.941513
H	-3.217126	-4.166099	-1.003924
H	-3.662142	-6.344846	-2.001442
C	-1.109990	-2.282246	2.641807
C	-1.517967	-2.277709	3.970159
C	-2.196477	-3.375289	4.496692
C	-2.475139	-4.467503	3.679181
C	-2.078464	-4.469375	2.342511
H	-2.312475	-5.325780	1.719166
H	-0.605488	-1.397433	2.264659
H	-1.314731	-1.397704	4.571626
H	-2.515496	-3.375730	5.534488
H	-3.005919	-5.326897	4.078134
C	3.292551	-3.163313	-1.847695
C	4.657880	-2.906686	-1.810152
C	5.193778	-1.955850	-0.952408
C	4.321555	-1.235716	-0.140085
Br	5.814496	-3.892857	-2.934646
H	6.261894	-1.778654	-0.915902
C	2.947818	-1.439204	-0.177804
H	2.288575	-0.818772	0.427883
H	2.905445	-3.936178	-2.503900
Br	5.010004	0.053071	1.048460
C	3.767344	2.963844	3.961686
C	4.925235	2.788492	4.675747
C	6.178857	2.790834	4.017063
C	6.245155	2.976583	2.658862
H	2.801409	2.952423	4.459478
H	4.885217	2.641413	5.750582
H	7.203429	2.976917	2.144889
H	7.087738	2.643505	4.592344
C	-5.950186	-2.769097	-1.383752
C	-6.235467	-4.096245	-1.177820
C	-5.927834	-4.710251	0.062176
C	-5.335828	-3.982648	1.063776
H	-6.190426	-2.292912	-2.331191
H	-6.705985	-4.679699	-1.963665
H	-6.161459	-5.759637	0.214348
H	-5.086971	-4.444159	2.015999
C	-5.810740	4.856898	0.168276
C	-5.335121	6.282735	0.434414
H	-6.376370	4.842516	-0.774450
H	-6.509133	4.532234	0.947516
C	-4.194336	6.630573	-0.517695
H	-4.976752	6.366777	1.468478
H	-6.170268	6.982125	0.323904

C	-2.994485	5.725462	-0.249918
H	-4.533465	6.499324	-1.555314
H	-3.896967	7.678577	-0.408039
H	-2.204530	5.912620	-0.980746
H	-2.558901	5.987092	0.725116
C	-1.952599	4.335735	-3.075068
C	-1.710190	5.394583	-4.148207
H	-2.896163	4.529246	-2.562082
H	-2.080736	3.357479	-3.562048
C	-0.343134	5.188146	-4.793325
H	-2.508749	5.349615	-4.896122
H	-1.750451	6.395031	-3.694646
C	0.750514	5.380579	-3.746506
H	-0.290126	4.171023	-5.203560
H	-0.190064	5.880954	-5.627280
H	0.832439	6.451815	-3.513841
H	1.725100	5.080499	-4.147323

TS-6-minor

M06-2X/6-31G* Energy = -8271.54211498

M06-2X/6-31G* Free Energy = -8270.651201

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.51469468

M06-2X/def2-TZVPP-SMD(toluene) Energy = -8277.52091380

Number of Imaginary Frequencies = 1

Lowest Frequency = 367.0504i

M06-2X/6-31G* Geometry

C	1.292073	1.785128	2.864806
C	1.541569	2.975722	1.532270
C	2.543104	1.129108	2.895356
H	0.480362	1.197911	2.437058
H	1.002645	2.382371	3.726332
C	2.894473	0.270614	1.830242
H	3.324195	1.493398	3.562405
N	1.872062	2.164412	0.436313
C	0.186065	3.662058	1.414729
C	2.661353	3.941813	1.896004
C	3.061600	1.451041	0.507935
C	3.474138	0.617251	-0.670376
H	3.885086	2.081143	0.840188
H	1.079998	1.596851	0.093487
H	2.091306	-0.345235	1.416628
H	3.863418	-0.224048	1.888107
C	-4.813609	-2.561298	-0.642259
C	-5.757756	-1.818847	-1.362627
C	-3.688956	-1.905205	-0.097940
C	-3.451720	-0.565302	-0.422278
C	-4.392310	0.192769	-1.132511
C	-5.547211	-0.453095	-1.560665
C	-2.737545	-2.602790	0.819100
C	-3.147270	-3.151611	2.052091
C	-2.206079	-3.831106	2.839218
C	-0.875645	-3.893240	2.424294
C	-0.423446	-3.275764	1.260306
C	-1.388219	-2.642895	0.467613
O	-2.306895	0.047263	0.039622
O	-1.008040	-2.001820	-0.689530
P	-0.833813	-0.371964	-0.593533
O	0.150103	-0.011588	0.493506
O	-0.630218	0.139532	-1.972545
C	-4.199064	1.644484	-1.382783
C	1.018750	-3.252733	0.915695
C	-3.048704	2.117761	-2.076364
C	-2.880672	3.458477	-2.299153

C	-3.825380	4.408710	-1.829861
C	-4.975355	3.942426	-1.134185
C	-5.142195	2.545481	-0.940717
C	1.464411	-3.415659	-0.429490
C	2.799615	-3.409182	-0.729308
C	3.779883	-3.212852	0.279355
C	3.347971	-3.054161	1.624868
C	1.958900	-3.085098	1.910051
H	-6.286405	0.123038	-2.113932
H	-0.159118	-4.432747	3.040491
H	-2.302802	1.405001	-2.416156
H	-1.999220	3.814870	-2.826058
H	1.635602	-2.931163	2.937451
H	3.122039	-3.535279	-1.760089
H	0.733631	-3.535406	-1.220941
H	-6.016680	2.190878	-0.398823
C	2.995430	4.270498	3.209538
C	3.962972	5.237428	3.474954
C	4.606620	5.891476	2.429661
C	4.272026	5.577472	1.114364
C	3.303506	4.615322	0.849867
H	2.495850	3.787042	4.043107
H	4.209413	5.478624	4.504089
H	5.361287	6.643061	2.637691
H	3.031209	4.378913	-0.174954
H	4.761676	6.085651	0.289735
C	0.063820	5.042979	1.601069
C	-1.176979	5.662062	1.461342
C	-2.307628	4.915782	1.145831
C	-2.192052	3.537303	0.978927
C	-0.958604	2.914145	1.115484
H	-0.901472	1.838289	0.986178
H	0.930885	5.647079	1.843528
H	-1.252197	6.736622	1.596761
H	-3.273161	5.399717	1.021414
H	-3.059925	2.933768	0.730667
C	2.554905	0.090742	-1.576016
C	3.014622	-0.753821	-2.579016
C	4.364953	-1.046517	-2.736609
C	5.260951	-0.491021	-1.832108
Br	1.755077	-1.606019	-3.687538
H	4.704465	-1.706146	-3.526810
C	4.834514	0.324616	-0.795152
H	5.557163	0.714150	-0.084402
H	1.492245	0.300222	-1.524765
Br	7.096362	-0.918319	-1.976773
C	4.322174	-2.829888	2.635489
C	5.655551	-2.746177	2.320009
C	6.084133	-2.902188	0.978069
C	5.166877	-3.147633	-0.012018
H	3.988333	-2.715878	3.664521
H	6.389657	-2.568000	3.100243
H	5.492307	-3.271158	-1.042014
H	7.139138	-2.827187	0.732670
C	-5.902802	4.891071	-0.626122
C	-5.696796	6.236633	-0.798879
C	-4.553393	6.700119	-1.495908
C	-3.643112	5.806021	-1.999745
H	-6.778616	4.529977	-0.092675
H	-6.411394	6.952330	-0.403888
H	-4.401801	7.767097	-1.627995
H	-2.760031	6.153776	-2.529678
C	-7.022938	-2.446683	-1.917654

C	-6.932434	-3.964545	-2.053226
H	-7.261777	-1.987375	-2.883170
H	-7.858696	-2.200785	-1.246938
C	-6.373940	-4.564640	-0.765922
H	-6.266834	-4.223007	-2.886958
H	-7.918764	-4.378494	-2.287089
C	-4.947647	-4.071281	-0.535041
H	-7.010397	-4.267975	0.079924
H	-6.383582	-5.658776	-0.806394
H	-4.567234	-4.434977	0.422270
H	-4.289702	-4.513085	-1.297421
C	-4.553177	-2.915228	2.577892
C	-4.965577	-3.909952	3.660268
H	-5.284199	-2.910653	1.767006
H	-4.577820	-1.898929	2.997960
C	-3.888053	-3.990923	4.737766
H	-5.927274	-3.609656	4.088979
H	-5.108562	-4.903949	3.213649
C	-2.594130	-4.527101	4.130909
H	-3.716980	-2.987818	5.149935
H	-4.205794	-4.631307	5.567168
H	-2.718510	-5.599926	3.925927
H	-1.769562	-4.447964	4.848191

TS-6-minor-2

M06-2X/6-31G* Energy = -8271.53400333

M06-2X/6-31G* Free Energy = -8270.644739

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.50635764

M06-2X/def2-TZVPP-SMD(toluene) Energy = -8277.51246017

Number of Imaginary Frequencies = 1

Lowest Frequency = 301.7076i

M06-2X/6-31G* Geometry

C	1.990246	1.519784	-2.876409
C	2.685238	0.076960	-2.355020
C	2.668309	2.569121	-2.150988
H	0.946514	1.409159	-2.576319
H	2.098120	1.543869	-3.960855
C	2.408520	2.728036	-0.797350
H	3.540106	3.050932	-2.592086
N	2.524783	0.104648	-0.941173
C	1.864991	-1.056227	-2.970986
C	4.163927	-0.009637	-2.715335
C	3.147420	1.080468	-0.223807
C	2.908780	0.958356	1.259483
H	4.193917	1.218992	-0.492693
H	1.564987	-0.063897	-0.608426
H	1.394545	2.492628	-0.466105
H	2.942847	3.500458	-0.245916
C	-4.985143	-1.619837	0.866436
C	-4.878387	-3.001174	1.079206
C	-3.899578	-0.923897	0.296610
C	-2.681719	-1.592271	0.129473
C	-2.557783	-2.976992	0.323422
C	-3.686409	-3.659846	0.762398
C	-3.995429	0.481783	-0.211132
C	-4.893768	0.835184	-1.240955
C	-4.882719	2.149141	-1.737348
C	-3.916952	3.048217	-1.287645
C	-2.958028	2.699544	-0.339499
C	-3.054065	1.421049	0.221383
O	-1.595322	-0.884104	-0.322109
O	-2.156206	1.042367	1.191006
P	-0.842396	0.189339	0.695373

O	0.001429	0.998856	-0.257474
O	-0.250029	-0.448674	1.895626
C	-1.270199	-3.653224	0.012983
C	-1.804058	3.586364	-0.048743
C	-1.211911	-4.711692	-0.934779
C	-0.006123	-5.237496	-1.329175
C	1.214242	-4.740675	-0.798918
C	1.152897	-3.729171	0.197569
C	-0.102234	-3.208571	0.588971
C	-1.301742	3.768541	1.271935
C	-0.194178	4.542230	1.501388
C	0.502246	5.162887	0.430222
C	0.009116	4.988011	-0.892769
C	-1.152431	4.201549	-1.096036
H	-3.619381	-4.735595	0.915844
H	-3.892437	4.050762	-1.710552
H	-2.137814	-5.075810	-1.373954
H	0.030684	-6.029424	-2.073727
H	-1.497990	4.036935	-2.114048
H	0.188452	4.653119	2.513253
H	-1.790946	3.265474	2.098336
H	-0.129508	-2.426869	1.342482
C	4.929022	-0.972917	-2.042979
C	6.271683	-1.149936	-2.352383
C	6.870915	-0.374751	-3.344926
C	6.114437	0.570842	-4.026946
C	4.766556	0.751272	-3.714521
H	4.449155	-1.593888	-1.288677
H	6.849994	-1.900088	-1.821863
H	7.919842	-0.512404	-3.587235
H	4.193553	1.485624	-4.272519
H	6.568088	1.173233	-4.807620
C	2.421649	-1.948215	-3.888225
C	1.654239	-2.994473	-4.398194
C	0.333595	-3.158907	-3.996303
C	-0.228498	-2.261052	-3.091141
C	0.527322	-1.209923	-2.590683
H	0.057177	-0.519094	-1.896628
H	3.454925	-1.844405	-4.201440
H	2.101129	-3.686599	-5.105309
H	-0.255962	-3.986100	-4.380306
H	-1.253625	-2.377017	-2.753092
C	1.961373	1.670571	1.980745
C	1.696793	1.292954	3.292080
C	2.363622	0.245671	3.909311
C	3.328765	-0.430647	3.171634
Br	0.287132	2.148978	4.203009
H	2.114182	-0.060073	4.917862
C	3.615121	-0.085978	1.861147
H	4.336149	-0.663440	1.290309
H	1.362476	2.449905	1.526389
Br	4.210213	-1.925583	3.918613
C	0.731890	5.558435	-1.975014
C	1.887847	6.264794	-1.754584
C	2.373593	6.446219	-0.435624
C	1.693088	5.910604	0.629891
H	0.352566	5.419495	-2.984659
H	2.430787	6.696724	-2.589992
H	2.058392	6.046142	1.645054
H	3.283400	7.015657	-0.271805
C	2.355106	-3.246545	0.782194
C	3.570734	-3.732661	0.374083
C	3.637408	-4.713811	-0.649915

C	2.489236	-5.207546	-1.217004
H	2.279852	-2.500201	1.569982
H	4.482446	-3.383302	0.854366
H	4.605400	-5.085190	-0.973816
H	2.540102	-5.967986	-1.992606
C	-6.040213	-3.820270	1.611725
C	-7.101022	-2.979239	2.318376
H	-5.658970	-4.598467	2.282111
H	-6.510478	-4.346939	0.768859
C	-7.447577	-1.757660	1.470533
H	-6.718759	-2.641631	3.290374
H	-7.989369	-3.588354	2.515307
C	-6.218842	-0.863255	1.326596
H	-7.787236	-2.086996	0.478106
H	-8.269327	-1.189883	1.919116
H	-6.427193	-0.016197	0.667638
H	-5.985225	-0.421495	2.305979
C	-5.760238	-0.216440	-1.916176
C	-6.945007	0.371285	-2.679136
H	-6.108041	-0.967280	-1.205736
H	-5.115354	-0.761491	-2.621652
C	-6.476832	1.491065	-3.603228
H	-7.445785	-0.421203	-3.244985
H	-7.680042	0.771661	-1.967076
C	-5.887520	2.625654	-2.770038
H	-5.713781	1.097741	-4.287598
H	-7.301083	1.866582	-4.218581
H	-6.706519	3.141711	-2.249028
H	-5.416494	3.375548	-3.415257

TS-6-minor-3

M06-2X/6-31G* Energy = -8271.53459639

M06-2X/6-31G* Free Energy = -8270.643860

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.50727387

M06-2X/def2-TZVPP-SMD(toluene) Energy = -8277.51383442

Number of Imaginary Frequencies = 1

Lowest Frequency = 270.5099i

M06-2X/6-31G* Geometry

C	-2.159478	0.371642	-2.998956
C	-2.517151	1.811611	-2.110839
C	-3.217337	-0.506861	-2.610284
H	-1.186269	0.093460	-2.592861
H	-2.120582	0.656596	-4.048972
C	-3.244000	-1.026999	-1.304372
H	-4.116285	-0.560138	-3.224470
N	-2.507950	1.386680	-0.765590
C	-1.358160	2.780912	-2.354263
C	-3.869616	2.380629	-2.520454
C	-3.438801	0.471520	-0.319029
C	-3.225084	0.079332	1.122966
H	-4.466701	0.756453	-0.546459
H	-1.563246	1.110237	-0.455678
H	-2.274155	-1.323653	-0.894174
H	-4.082540	-1.677713	-1.057817
C	4.029747	-2.462864	-1.847339
C	3.477695	-3.356972	-2.777358
C	3.258647	-2.076906	-0.731143
C	1.925881	-2.493703	-0.635481
C	1.322644	-3.294596	-1.615348
C	2.148178	-3.748468	-2.645104
C	3.788442	-1.107176	0.277208
C	4.971898	-1.328167	1.012793
C	5.530621	-0.273098	1.745498

C	4.892061	0.970977	1.760708
C	3.662283	1.175527	1.147758
C	3.107946	0.102151	0.440484
O	1.203281	-2.089553	0.458717
O	1.881757	0.265920	-0.163402
P	0.610241	-0.555596	0.513006
O	-0.482534	-0.395645	-0.514610
O	0.399712	-0.217697	1.939325
C	-0.133167	-3.589805	-1.648870
C	2.973360	2.493517	1.161489
C	-0.770022	-3.653687	-2.924737
C	-2.101998	-3.941044	-3.051505
C	-2.908006	-4.156851	-1.904761
C	-2.297427	-4.061096	-0.622339
C	-0.905871	-3.793021	-0.523422
C	1.671670	2.622626	1.727098
C	1.008056	3.818816	1.671466
C	1.585594	4.951342	1.035524
C	2.898902	4.837655	0.500102
C	3.575292	3.591029	0.591364
H	1.733583	-4.425747	-3.388543
H	5.343853	1.794105	2.311036
H	-0.180498	-3.447199	-3.812506
H	-2.563272	-3.987715	-4.035302
H	4.568922	3.498846	0.157094
H	0.021706	3.909296	2.122549
H	1.216438	1.757484	2.201688
H	-0.457286	-3.735250	0.462359
C	-4.538944	3.206693	-1.609760
C	-5.741885	3.813962	-1.952907
C	-6.290584	3.615881	-3.217924
C	-5.624825	2.809265	-4.134766
C	-4.421875	2.197053	-3.788411
H	-4.101746	3.372207	-0.629099
H	-6.248201	4.446975	-1.231099
H	-7.228778	4.090009	-3.487629
H	-3.914773	1.584230	-4.527249
H	-6.038213	2.653590	-5.126208
C	-1.572307	4.040791	-2.916593
C	-0.529468	4.964610	-2.978988
C	0.729620	4.643350	-2.482615
C	0.955831	3.371262	-1.960186
C	-0.075016	2.442196	-1.906249
H	0.134993	1.461977	-1.485566
H	-2.554438	4.321524	-3.282048
H	-0.715524	5.948033	-3.399703
H	1.529347	5.378643	-2.489362
H	1.930116	3.095227	-1.567613
C	-3.855475	-1.039731	1.673879
C	-3.594937	-1.374900	2.994468
C	-2.738305	-0.627518	3.796694
C	-2.147308	0.493563	3.235768
Br	-4.408093	-2.919178	3.732043
H	-2.534091	-0.917713	4.819880
C	-2.384496	0.856482	1.917240
H	-1.888248	1.733653	1.521053
H	-4.516242	-1.666570	1.085925
Br	-0.964675	1.546446	4.249238
C	3.477336	5.961062	-0.147845
C	2.782365	7.138812	-0.266143
C	1.473533	7.249984	0.263199
C	0.894151	6.182716	0.901892
H	4.482168	5.868788	-0.552902

H	3.234491	7.990974	-0.764681
H	-0.110464	6.261328	1.309580
H	0.931938	8.185652	0.162915
C	-3.116679	-4.189579	0.532381
C	-4.467092	-4.409817	0.414709
C	-5.067929	-4.522714	-0.863903
C	-4.303008	-4.399832	-1.996760
H	-2.664866	-4.081536	1.516025
H	-5.079206	-4.481887	1.308152
H	-6.135311	-4.706225	-0.941503
H	-4.755135	-4.478578	-2.982739
C	4.284959	-3.914017	-3.935266
C	5.471262	-3.033837	-4.319314
H	3.625524	-4.071391	-4.796061
H	4.660976	-4.907577	-3.652438
C	6.256337	-2.659629	-3.065786
H	5.111860	-2.117336	-4.805240
H	6.106472	-3.555841	-5.042511
C	5.385467	-1.832603	-2.122952
H	6.585152	-3.575864	-2.555584
H	7.158350	-2.094302	-3.322192
H	5.197469	-0.849655	-2.580008
H	5.926156	-1.622106	-1.199523
C	5.581463	-2.717852	1.078104
C	7.049203	-2.706006	1.497691
H	5.452647	-3.247146	0.130427
H	5.005247	-3.293910	1.816312
C	7.217186	-1.878793	2.769728
H	7.400163	-3.732206	1.648029
H	7.661951	-2.270059	0.695594
C	6.840504	-0.424258	2.497328
H	6.564790	-2.289725	3.550982
H	8.244320	-1.934384	3.145013
H	7.639437	0.043074	1.903847
H	6.787889	0.140256	3.434845

TS-6-minor-4

M06-2X/6-31G* Energy = -8271.53093788

M06-2X/6-31G* Free Energy = -8270.642592

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.50443590

M06-2X/def2-TZVPP-SMD(toluene) Energy = -8277.51151101

Number of Imaginary Frequencies = 1

Lowest Frequency = 302.5986i

M06-2X/6-31G* Geometry

C	2.027200	-2.331726	2.483734
C	2.824003	-0.846082	2.483093
C	2.672344	-3.105106	1.450725
H	1.000344	-2.057987	2.232428
H	2.107279	-2.724794	3.497075
C	2.427823	-2.777548	0.125049
H	3.513598	-3.748758	1.704965
N	2.671484	-0.365232	1.151901
C	2.075075	0.032986	3.487658
C	4.300884	-1.000146	2.834241
C	3.231335	-1.065057	0.123441
C	2.964137	-0.456438	-1.233995
H	4.273807	-1.334829	0.290715
H	1.710295	-0.068225	0.912491
H	1.421851	-2.408878	-0.088987
H	2.933537	-3.331825	-0.665227
C	-5.130355	1.175525	-0.588489
C	-5.236308	2.566830	-0.710524
C	-3.951729	0.621139	-0.047868

C	-2.851867	1.451446	0.195070
C	-2.940433	2.845955	0.082589
C	-4.159147	3.372157	-0.335377
C	-3.844023	-0.825371	0.317064
C	-4.708161	-1.409296	1.265938
C	-4.573316	-2.775184	1.555745
C	-3.525965	-3.496106	0.987984
C	-2.581701	-2.920221	0.136104
C	-2.796732	-1.581589	-0.219515
O	-1.672568	0.874753	0.615619
O	-1.953764	-0.962936	-1.109520
P	-0.790157	0.026404	-0.495243
O	0.152123	-0.794335	0.353578
O	-0.300935	0.870762	-1.609653
C	-1.801835	3.743985	0.410731
C	-1.387352	-3.702162	-0.277718
C	-1.983008	4.795708	1.351864
C	-0.954256	5.646699	1.664821
C	0.319004	5.503827	1.052713
C	0.499739	4.462728	0.101168
C	-0.579126	3.596616	-0.203216
C	-0.859428	-4.645209	0.655422
C	0.211523	-5.440766	0.351393
C	0.856259	-5.336573	-0.906941
C	0.366273	-4.378300	-1.838362
C	-0.760100	-3.576887	-1.502713
H	-4.250954	4.452944	-0.427950
H	-3.435328	-4.551470	1.234962
H	-2.951115	4.906632	1.833779
H	-1.100289	6.442487	2.391226
H	-1.110377	-2.847455	-2.227617
H	0.593508	-6.150727	1.081438
H	-1.311609	-4.712528	1.639759
H	-0.431545	2.813179	-0.941544
C	5.159061	0.058082	2.509645
C	6.504830	0.012297	2.853362
C	7.015303	-1.088384	3.539552
C	6.167987	-2.136310	3.880434
C	4.818818	-2.091658	3.530323
H	4.754254	0.923419	1.991624
H	7.154777	0.840734	2.590063
H	8.065717	-1.125190	3.809770
H	4.175471	-2.915372	3.824254
H	6.551808	-2.994585	4.422767
C	2.646344	0.353594	4.721091
C	1.957247	1.156395	5.627441
C	0.697503	1.652063	5.309717
C	0.119527	1.325399	4.085299
C	0.793718	0.509446	3.184144
H	0.300094	0.250924	2.250534
H	3.635492	-0.009560	4.979369
H	2.416982	1.400588	6.580055
H	0.168392	2.288891	6.011762
H	-0.860551	1.705101	3.814363
C	2.022407	-0.926107	-2.139066
C	1.753601	-0.187977	-3.285297
C	2.422390	0.990314	-3.573446
C	3.380183	1.427636	-2.664717
Br	0.333837	-0.742406	-4.388662
H	2.182447	1.570948	-4.455556
C	3.657793	0.728943	-1.500232
H	4.379730	1.120950	-0.791361
H	1.433331	-1.811868	-1.943648

Br	4.281186	3.058315	-2.990383
C	1.050973	-4.223510	-3.076218
C	2.165411	-4.971246	-3.361879
C	2.645328	-5.928979	-2.434179
C	2.001178	-6.107700	-1.236074
H	0.697756	-3.473387	-3.778498
H	2.683580	-4.831728	-4.305526
H	2.361772	-6.838866	-0.516314
H	3.523104	-6.520070	-2.676919
C	1.763300	4.313576	-0.532428
C	2.801102	5.154341	-0.225981
C	2.623959	6.187986	0.728433
C	1.413357	6.358839	1.350134
H	1.885087	3.520464	-1.266686
H	3.759491	5.028385	-0.720971
H	3.453236	6.849086	0.962408
H	1.273329	7.153359	2.079188
C	-6.502568	3.235199	-1.213988
C	-7.410866	2.292742	-2.000049
H	-6.235602	4.107106	-1.821241
H	-7.059800	3.623910	-0.349531
C	-7.578853	0.980783	-1.238222
H	-6.965409	2.081658	-2.980831
H	-8.378835	2.771428	-2.181389
C	-6.231708	0.272736	-1.117982
H	-7.979222	1.190184	-0.235868
H	-8.297695	0.324870	-1.740267
H	-6.325338	-0.632021	-0.512365
H	-5.921317	-0.073079	-2.114555
C	-5.693336	-0.562620	2.055105
C	-6.827996	-1.375881	2.673355
H	-6.096966	0.250017	1.449358
H	-5.126014	-0.071586	2.859639
C	-6.265293	-2.569245	3.439684
H	-7.424409	-0.733920	3.329911
H	-7.498389	-1.736190	1.880421
C	-5.539599	-3.501519	2.473459
H	-5.564500	-2.207683	4.203521
H	-7.058987	-3.114427	3.961057
H	-6.286868	-4.018736	1.854928
H	-5.002790	-4.284122	3.021223

TS-7-minor

M06-2X/6-31G* Energy = -8271.54164939

M06-2X/6-31G* Free Energy = -8270.650668

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.51369854

M06-2X/def2-TZVPP-SMD(toluene) Energy = -8277.51938139

Number of Imaginary Frequencies = 1

Lowest Frequency = 363.6528i

M06-2X/6-31G* Geometry

C	3.057395	-0.777097	0.720657
C	2.354089	-2.374171	0.393495
C	2.417409	-0.378289	1.920208
H	2.734098	-0.253212	-0.175342
H	4.136843	-0.924054	0.752235
C	1.030109	-0.116908	1.941035
H	2.917908	-0.552591	2.872573
N	0.966025	-2.159536	0.408258
C	2.947477	-2.718038	-0.967094
C	2.783631	-3.374136	1.465895
C	0.412960	-1.772733	1.614405
C	-1.083672	-1.672597	1.750001
H	0.818888	-2.348651	2.446238

H	0.553266	-1.667678	-0.419414
H	0.598962	0.402718	1.084156
H	0.603570	0.171313	2.900243
C	0.554578	4.647598	-0.192948
C	1.845598	5.171688	-0.345305
C	0.363044	3.254439	-0.297124
C	1.428041	2.449798	-0.699356
C	2.733276	2.945293	-0.812613
C	2.913185	4.309284	-0.608496
C	-0.941128	2.597006	0.022806
C	-1.491693	2.651164	1.321614
C	-2.742333	2.061004	1.550642
C	-3.421478	1.462950	0.488419
C	-2.877183	1.341198	-0.790417
C	-1.589267	1.863877	-0.974807
O	1.199943	1.105773	-0.875894
O	-0.925331	1.674753	-2.166864
P	0.268109	0.545078	-2.144879
O	-0.275700	-0.741725	-1.566114
O	1.003005	0.592873	-3.425165
C	3.876089	2.021104	-1.024435
C	-3.683806	0.710713	-1.866245
C	3.871439	1.071212	-2.087807
C	4.881431	0.151064	-2.194600
C	5.957958	0.126008	-1.266703
C	5.984025	1.090868	-0.221335
C	4.922125	2.028357	-0.127855
C	-5.075711	1.015886	-1.916081
C	-5.910797	0.390401	-2.801162
C	-5.409952	-0.578640	-3.710006
C	-4.017621	-0.864122	-3.691569
C	-3.175855	-0.204776	-2.760314
H	3.917152	4.719881	-0.698258
H	-4.396550	1.015463	0.676267
H	3.047937	1.066142	-2.797992
H	4.863069	-0.585021	-2.994523
H	-2.133236	-0.494656	-2.717605
H	-6.970143	0.633654	-2.823931
H	-5.471076	1.766701	-1.237872
H	4.920676	2.738663	0.696717
C	2.106846	-4.600284	1.485886
C	2.455701	-5.587834	2.398572
C	3.497051	-5.372972	3.300149
C	4.183261	-4.164937	3.277767
C	3.827859	-3.169932	2.366709
H	1.299235	-4.767002	0.778770
H	1.914780	-6.528785	2.403463
H	3.771720	-6.144465	4.012239
H	4.393270	-2.243270	2.359968
H	5.001033	-3.987764	3.969071
C	2.261522	-2.481732	-2.161727
C	2.864769	-2.769479	-3.383809
C	4.147920	-3.305298	-3.432216
C	4.837000	-3.537581	-2.244095
C	4.246127	-3.237173	-1.021758
H	4.801920	-3.416938	-0.106348
H	1.256413	-2.075701	-2.173044
H	2.316985	-2.560589	-4.296798
H	4.610211	-3.535914	-4.387131
H	5.839407	-3.954770	-2.263225
C	-1.569822	-1.435011	3.040401
C	-2.935665	-1.388262	3.262075
C	-3.841748	-1.614913	2.234538

C	-3.340517	-1.861025	0.961875
Br	-3.581944	-1.006676	4.994675
H	-4.909617	-1.600459	2.417939
C	-1.972154	-1.870864	0.692220
H	-1.619854	-2.018244	-0.322685
H	-0.889372	-1.297280	3.875595
Br	-4.577179	-2.196685	-0.419096
C	-3.503464	-1.834154	-4.593245
C	-4.332159	-2.482078	-5.472369
C	-5.718991	-2.191668	-5.493368
C	-6.244020	-1.261606	-4.633218
H	-2.437845	-2.046487	-4.571535
H	-3.928977	-3.220055	-6.159002
H	-7.306863	-1.033149	-4.645530
H	-6.364693	-2.709886	-6.195840
C	7.049516	1.058538	0.718251
C	8.040503	0.115048	0.623051
C	8.017037	-0.842701	-0.420977
C	7.000913	-0.834428	-1.342409
H	7.065444	1.798948	1.514345
H	8.851078	0.101417	1.345298
H	8.810832	-1.580247	-0.489503
H	6.974365	-1.562052	-2.149199
C	2.130844	6.655064	-0.198735
C	0.885397	7.524667	-0.352090
H	2.566280	6.831863	0.795249
H	2.897253	6.949146	-0.924210
C	-0.248268	6.956813	0.497612
H	0.571936	7.540297	-1.403821
H	1.113664	8.556989	-0.067791
C	-0.637368	5.570590	-0.010319
H	0.080778	6.890180	1.544382
H	-1.122235	7.615796	0.477399
H	-1.386917	5.116572	0.642992
H	-1.126904	5.672053	-0.989527
C	-0.683517	3.239661	2.468062
C	-1.487898	3.436119	3.753153
H	-0.216521	4.183416	2.174144
H	0.158378	2.559216	2.667963
C	-2.357397	2.215251	4.038508
H	-0.804599	3.641759	4.583768
H	-2.136707	4.316245	3.648969
C	-3.385647	2.068603	2.922456
H	-1.727506	1.313784	4.076473
H	-2.857522	2.295617	5.009059
H	-4.096333	2.905036	2.985911
H	-3.975689	1.155932	3.057965

TS-7-minor-2

M06-2X/6-31G* Energy = -8271.53497197

M06-2X/6-31G* Free Energy = -8270.644458

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.50909317

M06-2X/def2-TZVPP-SMD(toluene) Energy = -8277.51509211

Number of Imaginary Frequencies = 1

Lowest Frequency = 354.7926i

M06-2X/6-31G* Geometry

C	3.123075	-0.932799	0.599534
C	2.408224	-2.454193	0.109730
C	2.504373	-0.646797	1.848016
H	2.802641	-0.298856	-0.223407
H	4.202559	-1.086997	0.603872
C	1.126992	-0.361540	1.917500
H	3.016290	-0.922902	2.769866

N	1.020111	-2.233661	0.174172
C	2.947350	-2.661285	-1.301158
C	2.838612	-3.579469	1.049984
C	0.481094	-1.982678	1.415212
C	-1.017930	-1.895999	1.519831
H	0.880972	-2.642992	2.185446
H	0.587660	-1.641273	-0.577699
H	0.687351	0.238521	1.119173
H	0.719374	-0.169848	2.908225
C	0.825324	4.634318	0.271339
C	2.132755	5.115365	0.119249
C	0.566381	3.266595	0.043337
C	1.578164	2.452794	-0.466364
C	2.899628	2.904623	-0.581717
C	3.147726	4.235937	-0.263691
C	-0.769496	2.658430	0.323682
C	-1.308915	2.619655	1.626431
C	-2.603613	2.114755	1.801929
C	-3.334611	1.691559	0.691767
C	-2.802732	1.643585	-0.596079
C	-1.475482	2.079244	-0.732552
O	1.286312	1.141716	-0.748944
O	-0.817039	1.936377	-1.934480
P	0.273104	0.706374	-2.015021
O	-0.337546	-0.565679	-1.482873
O	0.981686	0.784460	-3.309139
C	4.001524	1.967366	-0.913267
C	-3.630040	1.195451	-1.745270
C	3.931148	1.101084	-2.043495
C	4.920900	0.179207	-2.266026
C	6.036608	0.065987	-1.392202
C	6.123909	0.944774	-0.276907
C	5.084905	1.887574	-0.065654
C	-3.432933	1.740954	-3.049799
C	-4.245630	1.384256	-4.090596
C	-5.316545	0.470183	-3.910039
C	-5.533421	-0.069039	-2.613550
C	-4.668139	0.309832	-1.556267
H	4.165685	4.609760	-0.356617
H	-4.366029	1.383389	0.845280
H	3.074315	1.158896	-2.711536
H	4.855081	-0.491409	-3.118940
H	-4.836345	-0.130997	-0.577799
H	-4.081733	1.808751	-5.077663
H	-2.628620	2.446848	-3.212867
H	5.133181	2.532969	0.809235
C	2.147771	-4.792672	0.934280
C	2.493147	-5.883369	1.721757
C	3.545028	-5.785765	2.631682
C	4.245050	-4.590711	2.742966
C	3.893198	-3.492559	1.957287
H	1.332491	-4.867494	0.220212
H	1.941761	-6.812987	1.622427
H	3.817171	-6.637868	3.246156
H	4.469238	-2.577402	2.052461
H	5.071047	-4.504020	3.441712
C	4.217366	-3.224907	-1.464085
C	4.747120	-3.416166	-2.735877
C	4.025741	-3.026611	-3.862231
C	2.773384	-2.440817	-3.703691
C	2.230591	-2.263872	-2.433373
H	1.243981	-1.819753	-2.363273
H	4.795595	-3.527895	-0.596145

H	5.726606	-3.872831	-2.842538
H	4.440382	-3.173253	-4.854898
H	2.202077	-2.106622	-4.563357
C	-1.585634	-1.607280	2.763789
C	-2.963241	-1.648491	2.913893
C	-3.799053	-2.013433	1.864689
C	-3.209956	-2.323027	0.644295
Br	-3.714553	-1.265775	4.605261
H	-4.871447	-2.084106	2.002801
C	-1.836115	-2.239325	0.444183
H	-1.421080	-2.454590	-0.531974
H	-0.966424	-1.379040	3.625218
Br	-4.296988	-2.953052	-0.761134
C	-6.612749	-0.972616	-2.418023
C	-7.428875	-1.325526	-3.461940
C	-7.208029	-0.791055	-4.755049
C	-6.176714	0.086721	-4.971187
H	-6.777074	-1.381269	-1.424484
H	-8.251692	-2.015362	-3.300639
H	-6.001853	0.503384	-5.959860
H	-7.860715	-1.079021	-5.573414
C	7.228974	0.827049	0.608513
C	8.200628	-0.116896	0.395363
C	8.115904	-0.990180	-0.717382
C	7.060025	-0.898770	-1.588369
H	7.290887	1.502946	1.457952
H	9.042282	-0.196439	1.076651
H	8.894213	-1.729822	-0.878427
H	6.986776	-1.561678	-2.446502
C	2.491970	6.565152	0.387761
C	1.284408	7.498345	0.354432
H	2.964468	6.632566	1.378244
H	3.249495	6.889197	-0.334292
C	0.154113	6.906570	1.191924
H	0.938698	7.620047	-0.680193
H	1.568677	8.490787	0.718967
C	-0.315487	5.588014	0.581653
H	0.513883	6.734056	2.216198
H	-0.689115	7.601341	1.260936
H	-1.060975	5.112679	1.224094
H	-0.836452	5.796262	-0.364026
C	-0.458329	3.025556	2.819583
C	-1.250748	3.168261	4.119252
H	0.091617	3.947751	2.612724
H	0.318694	2.257170	2.952449
C	-2.220320	2.001990	4.289914
H	-0.558007	3.237722	4.964471
H	-1.823817	4.105112	4.098687
C	-3.252509	2.046137	3.168751
H	-1.667610	1.052121	4.240336
H	-2.715918	2.031390	5.265881
H	-3.894620	2.926804	3.312787
H	-3.911491	1.173362	3.217232

TS-8-minor

M06-2X/6-31G* Energy = -8271.53840295

M06-2X/6-31G* Free Energy = -8270.648645

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.51234736

M06-2X/def2-TZVPP-SMD(toluene) Energy = -8277.51772670

Number of Imaginary Frequencies = 1

Lowest Frequency = 336.9783i

M06-2X/6-31G* Geometry

C	1.899164	-0.879062	2.226446
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C	1.227657	-2.450114	2.041669
C	0.877598	-0.151512	2.913942
H	2.052794	-0.566060	1.192465
H	2.840849	-1.014403	2.757027
C	-0.315785	0.166127	2.257898
H	0.908905	-0.087336	4.001680
N	0.006423	-2.236900	1.359214
C	2.250989	-3.200816	1.195571
C	0.989627	-3.112194	3.395931
C	-0.983405	-1.537321	2.001359
C	-2.276484	-1.411283	1.237617
H	-1.138244	-1.859951	3.030849
H	0.083571	-1.946289	0.365476
H	-0.269687	0.422215	1.197318
H	-1.060350	0.703522	2.839568
C	2.659140	4.241549	-0.217083
C	4.021491	4.253826	-0.543846
C	1.978536	3.005588	-0.156681
C	2.629850	1.841369	-0.568904
C	3.988263	1.839441	-0.912203
C	4.663969	3.053055	-0.853308
C	0.565175	2.914589	0.318458
C	0.193559	3.341497	1.613076
C	-1.162881	3.366163	1.961806
C	-2.117679	2.970101	1.022387
C	-1.773615	2.453568	-0.225467
C	-0.405556	2.377762	-0.535337
O	1.937571	0.655266	-0.538943
O	-0.005072	1.802108	-1.712537
P	0.720059	0.316996	-1.630879
O	-0.138980	-0.629045	-0.827097
O	1.237446	-0.005140	-2.975773
C	4.686571	0.597787	-1.331145
C	-2.847919	2.061537	-1.171846
C	5.831083	0.147688	-0.618009
C	6.484905	-0.998573	-0.990081
C	6.041353	-1.755090	-2.106024
C	4.917074	-1.288842	-2.841480
C	4.249818	-0.110805	-2.426580
C	-3.920061	2.975146	-1.387587
C	-4.991503	2.636536	-2.167995
C	-5.059961	1.359976	-2.785666
C	-3.968494	0.464259	-2.616529
C	-2.871023	0.838086	-1.799965
H	5.720609	3.070527	-1.114409
H	-3.173345	3.003063	1.291016
H	6.170232	0.718517	0.242696
H	7.348592	-1.347730	-0.429685
H	-2.072328	0.118941	-1.630120
H	-5.810277	3.336392	-2.315192
H	-3.876423	3.951333	-0.912032
H	3.371866	0.215733	-2.976990
C	0.128743	-4.216438	3.432651
C	-0.085825	-4.911241	4.616778
C	0.566465	-4.521814	5.785320
C	1.433119	-3.435339	5.755993
C	1.643446	-2.735279	4.568430
H	-0.371299	-4.525509	2.518886
H	-0.760730	-5.761195	4.625403
H	0.401483	-5.064363	6.710560
H	2.339239	-1.902111	4.570354
H	1.952576	-3.126571	6.657572
C	3.063537	-4.182173	1.767558

C	4.006809	-4.852461	0.991811
C	4.140820	-4.554627	-0.358986
C	3.335608	-3.572425	-0.932533
C	2.407623	-2.885081	-0.159102
H	1.813037	-2.102024	-0.624337
H	2.962464	-4.435415	2.817369
H	4.631171	-5.612741	1.450855
H	4.873727	-5.071785	-0.970324
H	3.434789	-3.334624	-1.985835
C	-3.178015	-0.373740	1.469282
C	-4.391801	-0.361863	0.794189
C	-4.758718	-1.373856	-0.082986
C	-3.851357	-2.404978	-0.287571
Br	-5.557985	1.097008	1.045900
H	-5.701940	-1.340855	-0.616202
C	-2.615773	-2.432896	0.345603
H	-1.930660	-3.249964	0.154462
H	-2.948393	0.446397	2.137989
Br	-4.304619	-3.807156	-1.467693
C	-4.026651	-0.816889	-3.226007
C	-5.129157	-1.200986	-3.945412
C	-6.217768	-0.309189	-4.111971
C	-6.179807	0.942570	-3.551420
H	-3.189062	-1.496005	-3.087112
H	-5.169868	-2.191431	-4.388542
H	-7.010973	1.631518	-3.679669
H	-7.083667	-0.621638	-4.687767
C	4.459162	-2.035679	-3.961493
C	5.081344	-3.204183	-4.320156
C	6.195789	-3.676697	-3.579884
C	6.665719	-2.967242	-2.503565
H	3.589600	-1.669655	-4.501391
H	4.722004	-3.775804	-5.170332
H	6.679815	-4.603247	-3.874416
H	7.521454	-3.325385	-1.936055
C	4.834123	5.535437	-0.564231
C	3.974939	6.790155	-0.695098
H	5.412660	5.598629	0.368662
H	5.568469	5.484951	-1.375506
C	2.820331	6.726942	0.300339
H	3.568192	6.856263	-1.712387
H	4.588347	7.682530	-0.533419
C	1.906681	5.548964	-0.029573
H	3.223087	6.610515	1.316712
H	2.240938	7.655909	0.289568
H	1.124947	5.452662	0.727316
H	1.377153	5.759505	-0.969995
C	1.260946	3.646449	2.650980
C	0.727915	4.404879	3.863745
H	2.102529	4.182262	2.206608
H	1.678424	2.682297	2.985505
C	-0.537179	3.734513	4.391365
H	1.500789	4.454017	4.637688
H	0.494126	5.439608	3.577530
C	-1.634205	3.814163	3.333092
H	-0.314985	2.681792	4.620654
H	-0.875757	4.200435	5.322292
H	-1.986825	4.852985	3.268058
H	-2.505987	3.218386	3.630401

Structures of Intermediates

A-1

M06-2X/6-31G* Energy = -8271.56668124

M06-2X/6-31G* Free Energy = -8270.684820

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.54512916

Lowest Frequency = 7.1455

M06-2X/6-31G* Geometry

C	-0.156024	3.009665	-0.365298
C	0.349829	2.585289	1.044500
C	0.874542	3.676945	-1.229280
H	-0.525409	2.116974	-0.876574
H	-1.025574	3.658258	-0.235641
C	1.382839	3.098379	-2.316673
H	1.211157	4.672380	-0.939597
N	1.440557	1.633328	0.763393
C	0.762843	3.780366	1.915213
C	-0.771297	1.854926	1.795378
C	2.624829	2.076856	0.628645
C	3.780785	1.277300	0.186336
H	2.854875	3.124786	0.848651
H	0.786700	0.230599	0.119597
H	1.054614	2.107398	-2.629124
H	2.125088	3.598255	-2.932825
C	-5.071653	-1.730025	-1.164678
C	-5.822383	-0.730625	-1.797714
C	-3.807869	-1.405156	-0.633137
C	-3.264479	-0.145642	-0.886222
C	-3.992938	0.862117	-1.519521
C	-5.283564	0.550911	-1.933392
C	-3.021139	-2.357874	0.202533
C	-3.506160	-2.815469	1.446123
C	-2.719109	-3.703075	2.191437
C	-1.490155	-4.127865	1.684588
C	-0.961309	-3.651220	0.486865
C	-1.745987	-2.730594	-0.215591
O	-1.969417	0.110914	-0.458562
O	-1.237836	-2.142885	-1.371644
P	-0.754466	-0.605302	-1.271162
O	0.395390	-0.654916	-0.201944
O	-0.474263	-0.013870	-2.587053
C	-3.419963	2.217642	-1.742654
C	0.352068	-4.133678	-0.003602
C	-2.500969	2.435313	-2.807213
C	-1.975997	3.681590	-3.023349
C	-2.300954	4.769277	-2.169529
C	-3.225463	4.558165	-1.107995
C	-3.786988	3.265402	-0.933046
C	0.537183	-4.453698	-1.379809
C	1.713600	-4.995982	-1.819955
C	2.782472	-5.252042	-0.922285
C	2.616226	-4.917601	0.449796
C	1.386135	-4.358956	0.877592
H	-5.871247	1.326151	-2.420476
H	-0.915650	-4.859464	2.248480
H	-2.198025	1.593064	-3.421051
H	-1.260860	3.843156	-3.824990
H	1.271904	-4.094123	1.926262
H	1.842726	-5.242188	-2.870578
H	-0.272952	-4.270963	-2.076793
H	-4.483780	3.097399	-0.114586
C	-2.014363	2.480238	1.936296
C	-3.047985	1.856863	2.623135

C	-2.853572	0.597547	3.189119
C	-1.620360	-0.030152	3.057842
C	-0.580258	0.602572	2.378248
H	-2.173312	3.473356	1.522388
H	-4.004572	2.360759	2.728804
H	-3.654949	0.120875	3.746351
H	0.377713	0.101750	2.289803
H	-1.458659	-1.015566	3.486570
C	0.369745	5.088769	1.628212
C	0.695369	6.134431	2.492816
C	1.418791	5.888973	3.653117
C	1.805710	4.583611	3.955625
C	1.472829	3.542572	3.099083
H	1.757623	2.523666	3.350818
H	-0.206362	5.312835	0.734573
H	0.376611	7.143599	2.249798
H	1.674109	6.704122	4.322927
H	2.359362	4.375704	4.866116
C	3.693004	-0.080388	-0.138589
C	4.840639	-0.744901	-0.549091
C	6.070135	-0.095537	-0.646085
C	6.133287	1.251653	-0.318984
Br	4.746820	-2.579692	-0.975302
H	6.955019	-0.631165	-0.968614
C	5.005155	1.944614	0.096558
H	5.077141	2.998044	0.347057
H	2.750203	-0.614191	-0.080354
Br	7.788317	2.156304	-0.439046
C	3.693616	-5.141696	1.347540
C	4.878891	-5.668398	0.903338
C	5.045171	-6.000053	-0.463952
C	4.019810	-5.798095	-1.354101
H	3.563289	-4.879307	2.394303
H	5.698571	-5.828287	1.596702
H	4.142264	-6.045744	-2.405497
H	5.989934	-6.411706	-0.805195
C	-3.501175	5.625493	-0.212352
C	-2.875287	6.838875	-0.352985
C	-1.949992	7.046766	-1.405747
C	-1.675224	6.037168	-2.294371
H	-4.207670	5.457696	0.597237
H	-3.085942	7.644442	0.343720
H	-1.458636	8.009744	-1.505534
H	-0.959361	6.185475	-3.098791
C	-7.222810	-0.990375	-2.320751
C	-7.519913	-2.471864	-2.542011
H	-7.375105	-0.424475	-3.246257
H	-7.943781	-0.588705	-1.594634
C	-7.077983	-3.278286	-1.323419
H	-6.975926	-2.831010	-3.425097
H	-8.587085	-2.611762	-2.741949
C	-5.565657	-3.166197	-1.146172
H	-7.586842	-2.894254	-0.427995
H	-7.360521	-4.330841	-1.426783
H	-5.241382	-3.683411	-0.239947
H	-5.071049	-3.691812	-1.975758
C	-4.803470	-2.259198	2.007192
C	-5.315929	-3.008315	3.236831
H	-5.583642	-2.233092	1.242917
H	-4.617901	-1.207268	2.262222
C	-4.178335	-3.295640	4.211709
H	-6.108231	-2.423301	3.715168
H	-5.766141	-3.961363	2.927368

C	-3.168411	-4.223253	3.542881
H	-3.686395	-2.353234	4.490190
H	-4.555112	-3.748941	5.134116
H	-3.626008	-5.214470	3.415991
H	-2.290763	-4.369598	4.182022

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M06-2X/6-31G* Energy = -8271.56668101

M06-2X/6-31G* Free Energy = -8270.684811

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.54512951

Lowest Frequency = 7.1907

M06-2X/6-31G* Geometry

C	-0.156585	3.008964	-0.365983
C	0.349130	2.585102	1.044047
C	0.873742	3.676900	-1.229681
H	-0.525120	2.115998	-0.877316
H	-1.026685	3.656865	-0.236717
C	1.383294	3.098361	-2.316501
H	1.209108	4.672848	-0.940312
N	1.440314	1.633521	0.763234
C	0.761444	3.780551	1.914596
C	-0.771773	1.854451	1.794995
C	2.624437	2.077478	0.628759
C	3.780643	1.278212	0.186571
H	2.854085	3.125465	0.848852
H	0.786668	0.230792	0.119474
H	1.056199	2.106953	-2.628765
H	2.125375	3.598682	-2.932492
C	-3.505159	-2.816076	1.446362
C	-2.717856	-3.703409	2.191717
C	-3.020329	-2.358515	0.202672
C	-1.745136	-2.731026	-0.215507
C	-0.960194	-3.651377	0.487010
C	-1.488821	-4.127958	1.684842
C	-3.807375	-1.406063	-0.633036
C	-5.071259	-1.731145	-1.164253
C	-5.822356	-0.731897	-1.797069
C	-5.283836	0.549754	-1.932911
C	-3.993119	0.861161	-1.519504
C	-3.264276	-0.146477	-0.886403
O	-1.237203	-2.143402	-1.371684
O	-1.969211	0.110464	-0.459057
P	-0.754073	-0.605736	-1.271425
O	0.395660	-0.654871	-0.202082
O	-0.473858	-0.014533	-2.587403
C	0.353239	-4.133610	-0.003556
C	-3.420434	2.216799	-1.742773
C	0.538157	-4.454034	-1.379703
C	1.714647	-4.996097	-1.819913
C	2.783820	-5.251459	-0.922400
C	2.617769	-4.916616	0.449600
C	1.387563	-4.358277	0.877491
C	-2.501273	2.434589	-2.807163
C	-1.976688	3.681005	-3.023436
C	-2.302152	4.768744	-2.169872
C	-3.226764	4.557503	-1.108446
C	-3.787952	3.264597	-0.933423
H	-0.914095	-4.859332	2.248797
H	-5.871841	1.324879	-2.419786
H	-0.272187	-4.271769	-2.076563
H	1.843618	-5.242674	-2.870467
H	-4.484871	3.096525	-0.115085
H	-1.261458	3.842654	-3.824978

H	-2.197912	1.592337	-3.420792
H	1.273451	-4.093175	1.926103
C	-0.580295	0.602269	2.378082
C	-1.620135	-0.030656	3.057888
C	-2.853550	0.596640	3.189107
C	-3.048448	1.855744	2.622819
C	-2.015079	2.479333	1.935808
H	0.377816	0.101721	2.289618
H	-1.458047	-1.015902	3.486856
H	-3.654741	0.119831	3.746486
H	-2.174423	3.472292	1.521685
H	-4.005220	2.359305	2.728401
C	0.367312	5.088618	1.627432
C	0.692178	6.134663	2.491854
C	1.415842	5.889920	3.652150
C	1.803759	4.584902	3.954840
C	1.471645	3.543466	3.098475
H	1.757214	2.524823	3.350381
H	-0.209015	5.312087	0.733788
H	0.372637	7.143551	2.248707
H	1.670586	6.705369	4.321812
H	2.357603	4.377557	4.865342
C	3.692882	-0.079284	-0.139166
C	4.840604	-0.743642	-0.549677
C	6.070176	-0.094305	-0.645836
C	6.133299	1.252688	-0.317908
Br	4.746729	-2.578191	-0.976889
H	6.955158	-0.629783	-0.968343
C	5.005070	1.945507	0.097611
H	5.077028	2.998784	0.348761
H	2.750042	-0.613061	-0.081547
Br	7.788487	2.157227	-0.436750
C	-3.502978	5.624892	-0.213024
C	-2.877498	6.838468	-0.353778
C	-1.952121	7.046496	-1.406441
C	-1.676856	6.036840	-2.294841
H	-4.209545	5.456982	0.596476
H	-3.088538	7.644091	0.342745
H	-0.960943	6.185271	-3.099195
H	-1.461100	8.009633	-1.506327
C	3.695479	-5.139923	1.347154
C	4.880867	-5.666281	0.902849
C	5.046928	-5.998410	-0.464353
C	4.021266	-5.797191	-1.354315
H	3.565279	-4.877232	2.393857
H	5.700788	-5.825574	1.596064
H	5.991781	-6.409790	-0.805676
H	4.143537	-6.045214	-2.405646
C	-3.166958	-4.223630	3.543216
C	-4.177115	-3.296248	4.212018
H	-2.289255	-4.369709	4.182338
H	-3.624301	-5.214972	3.416400
C	-5.314802	-3.009284	3.237146
H	-3.685407	-2.353703	4.490408
H	-4.553732	-3.749585	5.134471
C	-4.802562	-2.260080	2.007462
H	-5.764755	-3.962469	2.927737
H	-6.107266	-2.424463	3.715448
H	-4.617236	-1.208105	2.262471
H	-5.582780	-2.234167	1.243231
C	-5.565090	-3.167380	-1.145556
C	-7.077530	-3.279548	-1.321726
H	-5.240065	-3.684673	-0.239657

H	-5.071096	-3.692839	-1.975603
C	-7.520206	-2.473422	-2.540241
H	-7.360156	-4.332118	-1.424677
H	-7.585795	-2.895294	-0.426064
C	-7.222921	-0.991868	-2.319645
H	-6.976799	-2.832862	-3.423560
H	-8.587507	-2.613320	-2.739478
H	-7.943690	-0.589805	-1.593546
H	-7.375426	-0.426390	-3.245376

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M06-2X/6-31G* Energy = -8271.57366529

M06-2X/6-31G* Free Energy = -8270.688619

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.54809743

Lowest Frequency = 12.1055

M06-2X/6-31G* Geometry

C	-0.474689	3.238575	-0.374485
C	0.146405	2.805634	0.988994
C	0.518336	3.744964	-1.382739
H	-1.003637	2.369852	-0.787007
H	-1.238701	3.997060	-0.175456
C	0.805963	3.093682	-2.508722
H	1.026954	4.683390	-1.160648
N	1.200398	1.856782	0.598287
C	0.649218	3.978031	1.837682
C	-0.921912	2.053931	1.793337
C	2.435178	2.152972	0.584701
C	3.435914	1.259637	-0.034521
H	2.805456	3.087120	1.020641
H	0.696036	0.464314	0.059703
H	0.321916	2.148696	-2.756242
H	1.530741	3.484685	-3.217611
C	-4.803291	-2.464486	-0.858916
C	-5.716212	-1.647676	-1.540983
C	-3.587850	-1.912495	-0.410051
C	-3.258886	-0.607922	-0.783152
C	-4.151192	0.219815	-1.463761
C	-5.387507	-0.314905	-1.804763
C	-2.625359	-2.648908	0.461439
C	-2.964733	-3.050912	1.770053
C	-1.985200	-3.662004	2.566727
C	-0.691193	-3.826931	2.068362
C	-0.313308	-3.384864	0.802973
C	-1.313695	-2.804906	0.018707
O	-2.014093	-0.104475	-0.439360
O	-0.980468	-2.275618	-1.225863
P	-0.716088	-0.681069	-1.239948
O	0.433061	-0.502436	-0.199738
O	-0.537741	-0.140547	-2.596723
C	-3.758495	1.620266	-1.780846
C	1.095208	-3.461247	0.346577
C	-2.945830	1.889294	-2.916279
C	-2.518566	3.165039	-3.175138
C	-2.845962	4.233985	-2.300753
C	-3.671198	3.971328	-1.172184
C	-4.126229	2.647026	-0.945174
C	1.415344	-3.943562	-0.953785
C	2.716944	-4.025196	-1.366161
C	3.781580	-3.626188	-0.514807
C	3.469722	-3.122330	0.777465
C	2.111544	-3.057251	1.181194
H	-6.103072	0.316917	-2.326612
H	0.061528	-4.297904	2.697249

H	-2.634802	1.063670	-3.547792
H	-1.879643	3.367033	-4.030547
H	1.875176	-2.654220	2.163711
H	2.955249	-4.395772	-2.359599
H	0.610607	-4.247305	-1.614793
H	-4.726855	2.437872	-0.062940
C	-2.156174	2.673291	2.016991
C	-3.157657	2.021551	2.725028
C	-2.941808	0.737430	3.224497
C	-1.714668	0.118676	3.016137
C	-0.704700	0.780003	2.317562
H	-2.332769	3.679098	1.642863
H	-4.108789	2.519353	2.892248
H	-3.723075	0.232333	3.785593
H	0.244058	0.276873	2.163900
H	-1.533825	-0.886036	3.389822
C	1.290801	3.693538	3.050991
C	1.743526	4.711731	3.878953
C	1.548137	6.044506	3.516405
C	0.895419	6.339789	2.326523
C	0.449637	5.314444	1.490638
H	-0.069839	5.576117	0.574109
H	1.421975	2.655179	3.348230
H	2.238770	4.467230	4.813654
H	1.895857	6.843683	4.163443
H	0.726624	7.373133	2.039472
C	3.107703	0.507713	-1.166869
C	4.077503	-0.305533	-1.735060
C	5.365563	-0.378088	-1.217061
C	5.666123	0.375802	-0.089911
Br	3.654159	-1.317343	-3.267502
H	6.113152	-1.010684	-1.677714
C	4.725031	1.206169	0.501829
H	4.989347	1.796649	1.373279
H	2.121642	0.572715	-1.612899
Br	7.406378	0.262090	0.638489
C	4.529652	-2.708279	1.628104
C	5.836127	-2.814032	1.225561
C	6.145912	-3.322658	-0.060392
C	5.141769	-3.711377	-0.911861
H	4.285027	-2.315978	2.612108
H	6.638327	-2.491284	1.881091
H	5.370613	-4.090536	-1.905071
H	7.184801	-3.393558	-0.370269
C	-3.939569	5.023116	-0.255697
C	-3.385655	6.265994	-0.432483
C	-2.554808	6.524383	-1.552228
C	-2.302001	5.534631	-2.468299
H	-4.574494	4.816601	0.603178
H	-3.583128	7.057984	0.283396
H	-2.122203	7.511731	-1.682051
H	-1.657168	5.721202	-3.323083
C	-7.075154	-2.161288	-1.979558
C	-7.149177	-3.684507	-2.060101
H	-7.339322	-1.711628	-2.942938
H	-7.827805	-1.807522	-1.260668
C	-6.553668	-4.302123	-0.797274
H	-6.583093	-4.037440	-2.931738
H	-8.187999	-3.999698	-2.201369
C	-5.071406	-3.950624	-0.697876
H	-7.087164	-3.917415	0.083337
H	-6.676663	-5.389911	-0.797831
H	-4.642607	-4.327914	0.233981

H	-4.528592	-4.469976	-1.500765
C	-4.319214	-2.685081	2.352379
C	-4.649641	-3.422965	3.648077
H	-5.118606	-2.837016	1.623797
H	-4.302538	-1.601694	2.539681
C	-3.461699	-3.385132	4.604278
H	-5.538629	-2.976893	4.105819
H	-4.895838	-4.469994	3.424674
C	-2.285551	-4.129576	3.978115
H	-3.181171	-2.339612	4.795106
H	-3.718262	-3.831299	5.570465
H	-2.517096	-5.203836	3.957981
H	-1.385210	-4.021758	4.592930

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M06-2X/6-31G* Energy = -8271.56513838

M06-2X/6-31G* Free Energy = -8270.683267

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.54452838

Lowest Frequency = 8.0610

M06-2X/6-31G* Geometry

C	-0.127738	-3.096290	0.130821
C	-0.547458	-2.430851	1.478358
C	-1.247494	-3.762242	-0.615013
H	0.304785	-2.314942	-0.500412
H	0.683948	-3.804270	0.321363
C	-1.778249	-3.241478	-1.720136
H	-1.631518	-4.705298	-0.228325
N	-1.524381	-1.400644	1.078580
C	-1.090171	-3.432971	2.506722
C	0.662191	-1.746667	2.127516
C	-2.749572	-1.728102	0.975947
C	-3.810111	-0.866995	0.423397
H	-3.091794	-2.712851	1.310269
H	-0.747987	-0.153962	0.308080
H	-1.402146	-2.306705	-2.135623
H	-2.577344	-3.741921	-2.259603
C	5.277990	0.932645	-1.161015
C	5.900080	-0.213828	-1.673557
C	3.985604	0.823571	-0.611354
C	3.286680	-0.377978	-0.743206
C	3.878786	-1.525384	-1.272365
C	5.202598	-1.422978	-1.689203
C	3.330174	1.948644	0.116658
C	3.884439	2.475063	1.303441
C	3.218143	3.523168	1.951781
C	2.039632	4.034217	1.406343
C	1.443055	3.502714	0.265170
C	2.104816	2.429090	-0.339743
O	1.972857	-0.427362	-0.301515
O	1.517012	1.796563	-1.432595
P	0.843189	0.351342	-1.175426
O	-0.269803	0.648778	-0.108664
O	0.463439	-0.325380	-2.424023
C	3.137543	-2.807410	-1.421239
C	0.186851	4.082066	-0.268076
C	3.433350	-3.903233	-0.566121
C	2.777996	-5.100498	-0.708582
C	1.799502	-5.275734	-1.723811
C	1.525311	-4.191396	-2.602877
C	2.202137	-2.958827	-2.418267
C	0.021006	4.288741	-1.668136
C	-1.092708	4.916540	-2.155478
C	-2.114785	5.374889	-1.284090

C	-1.969691	5.154585	0.113205
C	-0.804086	4.504662	0.589725
H	5.685898	-2.309221	-2.095547
H	1.561934	4.882114	1.892308
H	4.180876	-3.771298	0.211803
H	3.000688	-5.933180	-0.045176
H	-0.706310	4.329196	1.658622
H	-1.206982	5.075369	-3.224513
H	0.796429	3.949832	-2.345963
H	1.956696	-2.120309	-3.064349
C	0.601849	-0.433877	2.594981
C	1.707366	0.153302	3.208149
C	2.876071	-0.577474	3.388893
C	2.942943	-1.892443	2.931422
C	1.843990	-2.471317	2.309645
H	-0.305480	0.146917	2.467475
H	1.647791	1.183925	3.547616
H	3.726404	-0.134627	3.899213
H	1.906635	-3.504050	1.977732
H	3.850084	-2.473240	3.070895
C	-1.746881	-2.946607	3.644516
C	-2.196039	-3.809207	4.635482
C	-1.983436	-5.182396	4.516693
C	-1.315476	-5.675327	3.402908
C	-0.872057	-4.807159	2.404505
H	-0.345704	-5.217813	1.548098
H	-1.897918	-1.875162	3.751876
H	-2.705291	-3.409355	5.506967
H	-2.331007	-5.858905	5.291101
H	-1.135500	-6.741293	3.302423
C	-5.089064	-1.423841	0.340694
C	-6.131034	-0.669184	-0.179241
C	-5.929412	0.633203	-0.614632
C	-4.647999	1.172721	-0.521015
Br	-7.859797	-1.424766	-0.295491
H	-6.748339	1.217709	-1.016730
C	-3.582906	0.443086	-0.010682
H	-2.596265	0.891243	0.040123
H	-5.269017	-2.440287	0.675594
Br	-4.364514	2.948221	-1.090889
C	-3.004603	5.580197	0.987663
C	-4.129967	6.191004	0.497770
C	-4.275097	6.409811	-0.894466
C	-3.289157	6.012838	-1.763295
H	-2.891201	5.404104	2.054283
H	-4.918604	6.504895	1.174315
H	-3.396453	6.172938	-2.833169
H	-5.172730	6.890050	-1.271423
C	0.571131	-4.366230	-3.639951
C	-0.092004	-5.556750	-3.785939
C	0.159524	-6.627645	-2.893315
C	1.082094	-6.490732	-1.887578
H	0.369408	-3.528974	-4.303012
H	-0.822483	-5.680872	-4.579455
H	-0.379402	-7.562673	-3.012869
H	1.286539	-7.314585	-1.207890
C	7.324010	-0.186505	-2.197066
C	7.802434	1.213480	-2.575659
H	7.410177	-0.867161	-3.051011
H	7.986744	-0.588469	-1.417550
C	7.458041	2.199836	-1.462445
H	7.310705	1.534822	-3.502856
H	8.879589	1.198783	-2.770533

C	5.942719	2.291470	-1.299855
H	7.913736	1.861235	-0.521180
H	7.866856	3.192139	-1.678379
H	5.679235	2.948318	-0.467601
H	5.518982	2.769592	-2.194891
C	5.118399	1.835161	1.916393
C	5.728273	2.639687	3.064301
H	5.882130	1.647380	1.158493
H	4.821235	0.840531	2.273439
C	4.644939	3.161168	4.003098
H	6.450460	2.016137	3.601409
H	6.285897	3.495137	2.659289
C	3.744541	4.126902	3.239003
H	4.047424	2.319669	4.380321
H	5.084688	3.660832	4.872183
H	4.315816	5.036517	3.006041
H	2.899283	4.445302	3.858975

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M06-2X/6-31G* Energy = -8271.57500021

M06-2X/6-31G* Free Energy = -8270.689141

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.54850653

Lowest Frequency = 8.0118

M06-2X/6-31G* Geometry

C	-3.638870	-1.066252	0.941980
C	-3.867752	-0.340984	-0.413790
C	-3.450656	-0.147424	2.117414
H	-2.746354	-1.693973	0.832973
H	-4.477830	-1.756778	1.096797
C	-2.434230	-0.262257	2.966006
H	-4.176528	0.653066	2.259188
N	-2.737008	0.596007	-0.556094
C	-3.767121	-1.399299	-1.525745
C	-5.237608	0.339711	-0.527910
C	-2.878416	1.854120	-0.441994
C	-1.772327	2.814056	-0.617411
H	-3.858510	2.300642	-0.244263
H	-1.301699	-0.143727	-0.347764
H	-1.677372	-1.032389	2.843257
H	-2.304782	0.416920	3.802545
C	2.772576	-3.594752	-1.431195
C	1.820498	-4.548940	-1.812504
C	2.511158	-2.785737	-0.305664
C	1.268937	-2.869789	0.318585
C	0.297048	-3.810729	-0.041977
C	0.625182	-4.655923	-1.100032
C	3.517177	-1.820122	0.231133
C	4.769387	-2.264687	0.705979
C	5.721776	-1.316942	1.102331
C	5.392980	0.037407	1.067950
C	4.130109	0.501023	0.706672
C	3.196794	-0.461973	0.300065
O	0.982299	-1.931553	1.307383
O	1.931483	-0.060838	-0.113365
P	0.622475	-0.449184	0.761778
O	-0.431774	-0.685029	-0.376547
O	0.281298	0.468659	1.858228
C	-1.013246	-3.931708	0.643337
C	3.834087	1.953300	0.758071
C	-2.164934	-4.304427	-0.109645
C	-3.371170	-4.516277	0.503080
C	-3.522405	-4.337984	1.902381
C	-2.388277	-3.937321	2.660586

C	-1.143276	-3.755320	2.006033
C	4.750789	2.873856	0.177214
C	4.501744	4.221215	0.195353
C	3.327616	4.734252	0.807192
C	2.427781	3.820043	1.420148
C	2.703144	2.431867	1.376854
H	-0.086822	-5.424393	-1.392475
H	6.133812	0.766201	1.390859
H	-2.089755	-4.392819	-1.189767
H	-4.238526	-4.795451	-0.089116
H	2.002464	1.755533	1.855721
H	5.197464	4.915466	-0.269320
H	5.641459	2.489568	-0.312985
H	-0.280916	-3.477484	2.604301
C	-5.554072	0.989566	-1.729728
C	-6.784056	1.606578	-1.909920
C	-7.737288	1.573782	-0.891390
C	-7.444514	0.917558	0.296704
C	-6.202116	0.305847	0.478603
H	-4.821315	0.996613	-2.533794
H	-7.005230	2.104625	-2.848850
H	-8.702439	2.050629	-1.030471
H	-6.004207	-0.207140	1.413534
H	-8.181601	0.874945	1.092622
C	-2.675276	-1.493759	-2.388310
C	-2.615025	-2.507399	-3.345427
C	-3.643662	-3.436000	-3.456560
C	-4.743907	-3.341058	-2.604757
C	-4.803540	-2.331103	-1.652168
H	-5.671212	-2.257293	-1.000387
H	-1.859334	-0.785041	-2.322114
H	-1.753897	-2.563713	-4.004463
H	-3.596704	-4.221496	-4.204681
H	-5.561241	-4.051743	-2.687114
C	-2.016834	4.154807	-0.310149
C	-1.019366	5.095885	-0.527902
C	0.215753	4.739640	-1.051272
C	0.437201	3.398894	-1.355505
Br	-1.347227	6.908009	-0.105266
H	0.995433	5.478809	-1.198019
C	-0.536429	2.433552	-1.151026
H	-0.333834	1.404874	-1.425166
H	-2.976659	4.463860	0.091185
Br	2.097380	2.890430	-2.077571
C	1.260295	4.315210	2.062031
C	0.998234	5.659981	2.089145
C	1.882827	6.572502	1.458940
C	3.019231	6.121186	0.835633
H	0.578095	3.597211	2.511227
H	0.097198	6.034476	2.565315
H	3.703195	6.819330	0.358988
H	1.651029	7.633378	1.470234
C	-2.535853	-3.725287	4.057991
C	-3.751626	-3.894994	4.667208
C	-4.881975	-4.290779	3.909750
C	-4.768471	-4.508714	2.560599
H	-1.666240	-3.415228	4.631839
H	-3.855014	-3.723509	5.734046
H	-5.839362	-4.421582	4.404725
H	-5.631431	-4.812774	1.973098
C	2.060617	-5.504162	-2.966775
C	3.134818	-5.018636	-3.936886
H	1.115886	-5.680236	-3.492993

H	2.367170	-6.476221	-2.555354
C	4.365197	-4.562720	-3.157347
H	2.750208	-4.175360	-4.525120
H	3.387626	-5.816028	-4.643058
C	4.014068	-3.366669	-2.275545
H	4.726788	-5.390457	-2.531169
H	5.181288	-4.293039	-3.835297
H	4.867571	-3.086852	-1.653991
H	3.819658	-2.493916	-2.915731
C	5.046769	-3.748194	0.885429
C	6.535523	-4.072468	0.983699
H	4.581979	-4.337975	0.092618
H	4.549918	-4.064586	1.814221
C	7.202912	-3.168645	2.016156
H	6.664755	-5.128034	1.243638
H	7.012341	-3.921057	0.005011
C	7.112455	-1.714767	1.560405
H	6.692883	-3.287594	2.980831
H	8.250404	-3.448169	2.167977
H	7.810571	-1.561174	0.725291
H	7.437421	-1.038312	2.358339

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M06-2X/6-31G* Energy = -8271.56513836

M06-2X/6-31G* Free Energy = -8270.683248

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.54453087

Lowest Frequency = 8.0672

M06-2X/6-31G* Geometry

C	-0.127634	-3.096128	0.130505
C	-0.547441	-2.431005	1.478248
C	-1.247371	-3.761737	-0.615637
H	0.305029	-2.314579	-0.500377
H	0.683945	-3.804221	0.320983
C	-1.778276	-3.240347	-1.720404
H	-1.631253	-4.705089	-0.229527
N	-1.524243	-1.400632	1.078643
C	-1.090318	-3.433366	2.506283
C	0.662193	-1.747047	2.127660
C	-2.749419	-1.728085	0.975729
C	-3.809916	-0.866890	0.423246
H	-3.091670	-2.712925	1.309734
H	-0.748225	-0.153715	0.308870
H	-1.402189	-2.305346	-2.135397
H	-2.577381	-3.740546	-2.260078
C	5.277610	0.932392	-1.161174
C	5.899370	-0.214081	-1.674160
C	3.985344	0.823402	-0.611245
C	3.286257	-0.378073	-0.742999
C	3.878031	-1.525460	-1.272494
C	5.201718	-1.423119	-1.689813
C	3.330090	1.948595	0.116746
C	3.884559	2.475242	1.303307
C	3.218735	3.523882	1.951275
C	2.040269	4.035009	1.405827
C	1.443390	3.503163	0.264972
C	2.104776	2.429164	-0.339685
O	1.972537	-0.427250	-0.300837
O	1.516664	1.796504	-1.432248
P	0.842879	0.351291	-1.174903
O	-0.270155	0.648858	-0.108260
O	0.463243	-0.325559	-2.423465
C	3.136834	-2.807541	-1.421168
C	0.187221	4.082572	-0.268297

C	3.432779	-3.903109	-0.565751
C	2.777680	-5.100537	-0.707988
C	1.799305	-5.276193	-1.723266
C	1.525013	-4.192127	-2.602631
C	2.201564	-2.959369	-2.418250
C	0.021390	4.289280	-1.668347
C	-1.092277	4.917183	-2.155661
C	-2.114331	5.375553	-1.284251
C	-1.969246	5.155214	0.113045
C	-0.803656	4.505243	0.589532
H	5.684752	-2.309354	-2.096486
H	1.562844	4.883227	1.891501
H	4.180229	-3.770835	0.212186
H	3.000461	-5.933017	-0.044358
H	-0.705818	4.329783	1.658426
H	-1.206558	5.076051	-3.224691
H	0.796798	3.950336	-2.346181
H	1.956045	-2.121030	-3.064539
C	0.601816	-0.434475	2.595669
C	1.707338	0.152492	3.209061
C	2.876081	-0.578288	3.389459
C	2.942965	-1.893103	2.931512
C	1.844019	-2.471757	2.309553
H	-0.305558	0.146333	2.468487
H	1.647694	1.182947	3.549007
H	3.726430	-0.135585	3.899887
H	1.906648	-3.504377	1.977295
H	3.850113	-2.473937	3.070781
C	-0.872198	-4.807533	2.403714
C	-1.315669	-5.675962	3.401860
C	-1.983691	-5.183323	4.515742
C	-2.196292	-3.810167	4.634886
C	-1.747074	-2.947303	3.644173
H	-1.898117	-1.875886	3.751813
H	-0.345784	-5.217945	1.547229
H	-1.135692	-6.741904	3.301110
H	-2.331303	-5.860036	5.289953
H	-2.705584	-3.410542	5.506452
C	-3.582745	0.443316	-0.010506
C	-4.647886	1.173064	-0.520567
C	-5.929291	0.633530	-0.614300
C	-6.130873	-0.668977	-0.179268
Br	-4.364507	2.948710	-1.090026
H	-6.748235	1.218123	-1.016242
C	-5.088855	-1.423738	0.340439
H	-5.268768	-2.440285	0.675060
H	-2.596102	0.891473	0.040343
Br	-7.859573	-1.424621	-0.295760
C	-3.004143	5.580819	0.987517
C	-4.129532	6.191599	0.497638
C	-4.274656	6.410445	-0.894588
C	-3.288689	6.013544	-1.763427
H	-2.890737	5.404699	2.054133
H	-4.918172	6.505451	1.174198
H	-3.396000	6.173695	-2.833293
H	-5.172290	6.890678	-1.271554
C	0.570957	-4.367406	-3.639745
C	-0.092013	-5.558051	-3.785451
C	0.159598	-6.628667	-2.892512
C	1.082095	-6.491344	-1.886763
H	0.369162	-3.530376	-4.303071
H	-0.822417	-5.682481	-4.578987
H	-0.379183	-7.563807	-3.011841

H	1.286627	-7.314983	-1.206842
C	7.323124	-0.186932	-2.198176
C	7.801961	1.213085	-2.576130
H	7.408703	-0.867090	-3.052579
H	7.985976	-0.589658	-1.419157
C	7.457955	2.199049	-1.462461
H	7.310274	1.535022	-3.503143
H	8.879097	1.198134	-2.771090
C	5.942672	2.291080	-1.299750
H	7.913582	1.859900	-0.521361
H	7.867069	3.191317	-1.677996
H	5.679453	2.947779	-0.467301
H	5.519015	2.769569	-2.194629
C	5.118189	1.834940	1.916527
C	5.728626	2.639689	3.063971
H	5.881732	1.646184	1.158678
H	4.820323	0.840741	2.274196
C	4.645671	3.162328	4.002578
H	6.450453	2.015965	3.601363
H	6.286762	3.494595	2.658504
C	3.745756	4.128140	3.237986
H	4.047712	2.321391	4.380347
H	5.085813	3.662266	4.871304
H	4.317692	5.037148	3.004261
H	2.900857	4.447629	3.857877

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M06-2X/6-31G* Energy = -8271.57228564

M06-2X/6-31G* Free Energy = -8270.687900

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.54678539

Lowest Frequency = 9.2008

M06-2X/6-31G* Geometry

C	-3.796160	-1.384244	-0.985432
C	-3.558261	-1.844399	0.490113
C	-3.363739	-2.367381	-2.036517
H	-3.240874	-0.446445	-1.108493
H	-4.857469	-1.131254	-1.095288
C	-2.218812	-2.267589	-2.711244
H	-4.023542	-3.209102	-2.240559
N	-2.101324	-1.978350	0.618928
C	-4.043833	-0.719647	1.423717
C	-4.309962	-3.126380	0.868196
C	-1.522795	-3.083027	0.362857
C	-0.058165	-3.230374	0.445242
H	-2.089881	-3.980155	0.095195
H	-1.236616	-0.641734	0.369103
H	-1.509889	-1.458911	-2.541797
H	-1.945770	-3.003669	-3.462728
C	0.053904	4.390618	1.103279
C	-1.309158	4.644368	1.306217
C	0.433901	3.530163	0.053118
C	-0.554460	2.857162	-0.659977
C	-1.924139	3.095056	-0.489276
C	-2.259177	4.029611	0.488813
C	1.860654	3.311437	-0.336822
C	2.653530	4.391145	-0.785304
C	4.005545	4.170224	-1.077288
C	4.524370	2.880218	-0.976662
C	3.745020	1.778341	-0.635022
C	2.401092	2.022641	-0.326894
O	-0.136093	1.853837	-1.529647
O	1.605016	0.955160	0.068513
P	0.321806	0.482586	-0.799088

O	-0.734544	0.253154	0.333937
O	0.552192	-0.599394	-1.768823
C	-2.968891	2.402390	-1.285700
C	4.352789	0.424826	-0.611052
C	-2.721320	2.008761	-2.636226
C	-3.680917	1.368915	-3.373118
C	-4.967715	1.112039	-2.834712
C	-5.246550	1.548761	-1.510910
C	-4.218231	2.161587	-0.749114
C	3.744189	-0.660580	-1.302374
C	4.335427	-1.894889	-1.310588
C	5.543202	-2.135654	-0.603766
C	6.157804	-1.055672	0.087042
C	5.542492	0.221857	0.050938
H	-3.307703	4.277769	0.635656
H	5.569012	2.710281	-1.228219
H	-1.755704	2.213835	-3.080248
H	-3.465736	1.053730	-4.390658
H	6.007981	1.042732	0.592497
H	3.865890	-2.722483	-1.839370
H	2.812245	-0.508948	-1.836669
H	-4.428354	2.405674	0.290724
C	-3.988841	-3.762231	2.074863
C	-4.678606	-4.891811	2.494640
C	-5.720052	-5.403570	1.720852
C	-6.064195	-4.768595	0.534359
C	-5.363940	-3.637973	0.111183
H	-3.191371	-3.356146	2.692261
H	-4.409601	-5.369374	3.431744
H	-6.261995	-6.285465	2.047514
H	-5.663931	-3.150359	-0.810808
H	-6.881026	-5.148868	-0.071350
C	-5.418786	-0.481984	1.524557
C	-5.912334	0.535068	2.333680
C	-5.037941	1.348103	3.052767
C	-3.670140	1.115294	2.964954
C	-3.176638	0.082826	2.167144
H	-2.108350	-0.080395	2.134673
H	-6.115138	-1.103860	0.967326
H	-6.985339	0.691678	2.402209
H	-5.422065	2.144500	3.683005
H	-2.971935	1.733022	3.521940
C	0.553943	-4.274724	-0.249308
C	1.930978	-4.427857	-0.153097
C	2.705047	-3.585924	0.630938
C	2.078764	-2.529227	1.284141
Br	2.806833	-5.773395	-1.153635
H	3.777079	-3.722696	0.710071
C	0.707014	-2.350680	1.219355
H	0.238899	-1.538702	1.763819
H	-0.031918	-4.945861	-0.868992
Br	3.144123	-1.302644	2.229992
C	7.358894	-1.296617	0.804883
C	7.913210	-2.550507	0.844474
C	7.291813	-3.628934	0.168126
C	6.136040	-3.424527	-0.542631
H	7.828311	-0.468233	1.329516
H	8.829277	-2.723584	1.400709
H	5.640994	-4.248532	-1.053336
H	7.735313	-4.618702	0.215293
C	-6.541262	1.315713	-0.974119
C	-7.492329	0.644392	-1.699668
C	-7.199491	0.179252	-3.006019

C	-5.968583	0.417631	-3.562474
H	-6.756964	1.672304	0.028303
H	-8.477152	0.469732	-1.276863
H	-7.958416	-0.356539	-3.567896
H	-5.737776	0.074307	-4.567529
C	-1.793317	5.608190	2.373849
C	-0.758243	5.864772	3.466450
H	-2.725540	5.228082	2.806764
H	-2.046599	6.563397	1.892732
C	0.596665	6.168824	2.832824
H	-0.664163	4.976283	4.104464
H	-1.088679	6.688572	4.107190
C	1.094781	4.953266	2.054653
H	0.496462	7.027570	2.154213
H	1.332621	6.445752	3.594379
H	1.355881	4.155383	2.764828
H	2.022362	5.188232	1.527060
C	2.028113	5.749452	-1.060716
C	3.050347	6.881718	-1.126742
H	1.251316	5.986743	-0.331427
H	1.508312	5.679588	-2.027511
C	4.195300	6.504636	-2.061911
H	2.557338	7.800834	-1.459433
H	3.450804	7.076756	-0.121934
C	4.934044	5.292527	-1.501863
H	3.787062	6.265736	-3.052435
H	4.891084	7.339732	-2.191896
H	5.520656	5.608273	-0.627474
H	5.655429	4.907784	-2.230833

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M06-2X/6-31G* Energy = -8271.57572857

M06-2X/6-31G* Free Energy = -8270.689724

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.54810216

Lowest Frequency = 13.0005

M06-2X/6-31G* Geometry

C	3.559145	-1.417601	1.032041
C	3.359700	-1.799155	-0.471302
C	3.078093	-2.446067	2.016778
H	3.014910	-0.478118	1.186049
H	4.620313	-1.188643	1.186174
C	1.915388	-2.358716	2.661512
H	3.715977	-3.310022	2.196016
N	1.905096	-1.931790	-0.639873
C	3.863059	-0.624334	-1.331868
C	4.129947	-3.054037	-0.899976
C	1.332602	-3.061192	-0.509013
C	-0.125366	-3.233501	-0.637514
H	1.908080	-3.974292	-0.326182
H	1.079969	-0.602195	-0.294854
H	1.228046	-1.526902	2.515147
H	1.606265	-3.127012	3.365050
C	0.043761	4.428168	-1.175188
C	1.424633	4.614578	-1.324685
C	-0.420565	3.630772	-0.109336
C	0.505270	2.948672	0.676328
C	1.890862	3.117945	0.558448
C	2.309332	3.995679	-0.440034
C	-1.873009	3.479882	0.214345
C	-2.647654	4.602971	0.579136
C	-4.019979	4.439436	0.811001
C	-4.578324	3.164258	0.740137
C	-3.821995	2.022763	0.488658

C	-2.458265	2.210417	0.227423
O	0.004701	1.994848	1.559893
O	-1.680249	1.105357	-0.093708
P	-0.458597	0.615640	0.850041
O	0.649755	0.328608	-0.215801
O	-0.774600	-0.433922	1.832288
C	2.868659	2.398683	1.414718
C	-4.462265	0.685843	0.514104
C	2.542139	2.025588	2.754411
C	3.433734	1.340278	3.534339
C	4.729098	1.017237	3.055775
C	5.091878	1.441252	1.748285
C	4.130261	2.100486	0.939378
C	-5.685132	0.477281	-0.182574
C	-6.289834	-0.752693	-0.190405
C	-5.717532	-1.847550	0.509394
C	-4.515958	-1.632758	1.238463
C	-3.906098	-0.355536	1.219401
H	3.373354	4.189072	-0.553420
H	-5.639607	3.042632	0.947613
H	1.570317	2.280939	3.155889
H	3.157298	1.041070	4.541856
H	-2.988708	-0.221353	1.783218
H	-7.212655	-0.908233	-0.743617
H	-6.119336	1.303034	-0.740119
H	4.399739	2.330295	-0.089729
C	3.866892	-3.602981	-2.162428
C	4.574248	-4.703891	-2.626141
C	5.576678	-5.272859	-1.840548
C	5.863980	-4.723412	-0.597798
C	5.145186	-3.621768	-0.130690
H	3.100923	-3.150282	-2.787481
H	4.350361	-5.113875	-3.606133
H	6.132974	-6.132115	-2.201617
H	5.401787	-3.200573	0.835845
H	6.650701	-5.148021	0.018189
C	5.239652	-0.379026	-1.386463
C	5.749340	0.680601	-2.128365
C	4.889745	1.530355	-2.823098
C	3.521153	1.289715	-2.782047
C	3.012366	0.212661	-2.055697
H	1.944879	0.042049	-2.061996
H	5.924004	-1.029521	-0.847168
H	6.823293	0.841749	-2.164546
H	5.286369	2.360997	-3.399315
H	2.833847	1.935106	-3.321357
C	-0.928246	-2.249041	-1.222884
C	-2.287777	-2.480060	-1.360972
C	-2.874270	-3.671663	-0.941230
C	-2.055221	-4.641745	-0.378886
Br	-3.366765	-1.167414	-2.166228
H	-3.943041	-3.830422	-1.042305
C	-0.689728	-4.441726	-0.223191
H	-0.071825	-5.218644	0.215330
H	-0.501104	-1.321828	-1.587627
Br	-2.817654	-6.283752	0.163928
C	-3.943043	-2.706771	1.971902
C	-4.538026	-3.941277	1.977735
C	-5.720821	-4.166384	1.227581
C	-6.296795	-3.145274	0.513399
H	-3.015625	-2.523887	2.509275
H	-4.091149	-4.762136	2.529073
H	-7.208509	-3.313223	-0.054707

H	-6.169394	-5.155393	1.223214
C	6.399123	1.147282	1.274639
C	7.280842	0.431132	2.043806
C	6.903228	-0.020181	3.333117
C	5.659492	0.276140	3.829447
H	6.681539	1.495393	0.285934
H	8.275935	0.210952	1.669078
H	7.607786	-0.591354	3.929792
H	5.364494	-0.055233	4.821630
C	1.998971	5.503060	-2.412724
C	1.027882	5.742278	-3.566134
H	2.934166	5.064081	-2.779137
H	2.268991	6.471350	-1.968327
C	-0.339863	6.136608	-3.015016
H	0.924047	4.824750	-4.160369
H	1.422951	6.515404	-4.232894
C	-0.927425	4.987118	-2.199756
H	-0.232295	7.025675	-2.377926
H	-1.027087	6.403041	-3.824325
H	-1.864736	5.290992	-1.727429
H	-1.195550	4.165593	-2.879762
C	-1.988739	5.949831	0.831637
C	-2.972075	7.117620	0.799565
H	-1.167906	6.129688	0.134733
H	-1.521354	5.903284	1.826209
C	-4.175334	6.818309	1.688485
H	-2.464009	8.032705	1.120525
H	-3.314445	7.284211	-0.231463
C	-4.927864	5.609787	1.139338
H	-3.826352	6.606940	2.707496
H	-4.846352	7.681163	1.748990
H	-5.456224	5.908242	0.222719
H	-5.699768	5.281539	1.843786

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M06-2X/6-31G* Energy = -8271.57452881

M06-2X/6-31G* Free Energy = -8270.688767

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.54774357

Lowest Frequency = 9.2687

M06-2X/6-31G* Geometry

C	-3.895488	0.048000	0.920746
C	-3.847272	0.570521	-0.549892
C	-3.753105	1.105599	1.978792
H	-3.083983	-0.684097	1.019079
H	-4.827417	-0.513501	1.051611
C	-2.646035	1.280420	2.697429
H	-4.604357	1.761061	2.155236
N	-2.512219	1.171249	-0.702813
C	-3.966398	-0.641621	-1.491549
C	-4.983675	1.537171	-0.909445
C	-2.338899	2.418142	-0.513520
C	-1.030788	3.083135	-0.648012
H	-3.180917	3.078263	-0.281086
H	-1.290788	0.138344	-0.450224
H	-1.757009	0.670259	2.553926
H	-2.587581	2.055709	3.456388
C	4.023895	-3.429433	0.604510
C	5.224147	-2.777266	0.916171
C	2.918436	-2.664876	0.171976
C	2.995825	-1.269527	0.200539
C	4.177853	-0.597855	0.539117
C	5.281534	-1.385902	0.855097
C	1.648740	-3.331002	-0.251339

C	1.589143	-4.234139	-1.332817
C	0.385356	-4.905089	-1.584078
C	-0.733314	-4.645414	-0.790048
C	-0.736859	-3.687905	0.222558
C	0.482289	-3.038280	0.450197
O	1.884635	-0.527790	-0.183476
O	0.536762	-1.993298	1.369203
P	0.527952	-0.519799	0.700470
O	-0.561113	-0.583507	-0.424874
O	0.415611	0.539983	1.715748
C	4.287407	0.880121	0.583581
C	-1.973028	-3.385823	0.987554
C	5.387242	1.523743	-0.049107
C	5.511186	2.888485	-0.027376
C	4.552386	3.694137	0.641676
C	3.471639	3.051694	1.305481
C	3.359600	1.641477	1.254836
C	-3.240632	-3.537140	0.352739
C	-4.406890	-3.350912	1.045020
C	-4.395299	-2.956818	2.407714
C	-3.138227	-2.766048	3.043463
C	-1.945100	-3.007348	2.315592
H	6.210105	-0.885546	1.122690
H	-1.645996	-5.203206	-0.985858
H	6.115970	0.917239	-0.580508
H	6.343593	3.373178	-0.531387
H	-0.998784	-2.889592	2.832031
H	-5.361666	-3.467301	0.537973
H	-3.282128	-3.773009	-0.706658
H	2.524973	1.177525	1.770294
C	-4.930021	2.196458	-2.145431
C	-5.955385	3.037808	-2.554128
C	-7.071652	3.227199	-1.739065
C	-7.148711	2.561524	-0.522818
C	-6.111539	1.722428	-0.110921
H	-4.072313	2.035261	-2.794121
H	-5.889503	3.539836	-3.514439
H	-7.876336	3.882551	-2.057056
H	-6.203806	1.203198	0.837191
H	-8.017199	2.690033	0.115834
C	-2.920325	-1.088663	-2.297830
C	-3.079928	-2.213712	-3.108975
C	-4.288928	-2.898392	-3.137850
C	-5.347010	-2.446612	-2.348602
C	-5.184457	-1.330315	-1.538213
H	-6.021461	-0.979570	-0.938708
H	-1.969987	-0.571271	-2.303838
H	-2.246721	-2.548027	-3.719951
H	-4.413085	-3.769521	-3.774052
H	-6.303112	-2.961551	-2.369610
C	0.068131	2.440534	-1.227610
C	1.255678	3.138377	-1.380246
C	1.380017	4.468200	-0.985358
C	0.271954	5.091444	-0.427688
Br	2.733172	2.277899	-2.162851
H	2.322167	4.994828	-1.095064
C	-0.930678	4.419396	-0.253618
H	-1.782655	4.932254	0.180942
H	0.000542	1.416351	-1.575455
Br	0.404827	6.903672	0.090717
C	-3.110875	-2.333887	4.396778
C	-4.275562	-2.096054	5.079013
C	-5.527760	-2.283409	4.443055

C	-5.585212	-2.705188	3.139282
H	-2.146831	-2.185580	4.876034
H	-4.243696	-1.759064	6.110346
H	-6.542746	-2.851329	2.645047
H	-6.442851	-2.091461	4.994887
C	2.518888	3.837197	2.008924
C	2.635268	5.201973	2.048708
C	3.696532	5.847795	1.363829
C	4.631983	5.112571	0.679393
H	1.691412	3.326301	2.495491
H	1.898481	5.799920	2.575547
H	3.763149	6.931530	1.384748
H	5.451666	5.604765	0.161613
C	6.474741	-3.536818	1.317642
C	6.185618	-4.944506	1.831510
H	7.024960	-2.956973	2.066587
H	7.133818	-3.608393	0.440776
C	5.230031	-5.652430	0.875750
H	5.723938	-4.889349	2.825823
H	7.121358	-5.502176	1.940353
C	3.887968	-4.925366	0.838981
H	5.668943	-5.669450	-0.131814
H	5.074589	-6.693790	1.175595
H	3.382203	-5.059727	1.806398
H	3.228629	-5.386724	0.101356
C	2.773915	-4.398673	-2.268281
C	2.713811	-5.686458	-3.086130
H	3.718064	-4.334356	-1.722405
H	2.772991	-3.538657	-2.953576
C	1.347138	-5.819061	-3.752529
H	3.515427	-5.687172	-3.831593
H	2.884037	-6.550808	-2.428919
C	0.261835	-5.941572	-2.685844
H	1.162083	-4.930492	-4.370105
H	1.315068	-6.687172	-4.418717
H	0.320849	-6.940863	-2.231938
H	-0.733776	-5.870720	-3.138180

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M06-2X/6-31G* Energy = -8271.57572841

M06-2X/6-31G* Free Energy = -8270.689747

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.54794640

Lowest Frequency = 12.9818

M06-2X/6-31G* Geometry

C	3.558431	-1.418751	1.032162
C	3.359024	-1.800244	-0.471163
C	3.076558	-2.446921	2.016823
H	3.014700	-0.478967	1.186076
H	4.619701	-1.190356	1.186518
C	1.914184	-2.358423	2.661973
H	3.713535	-3.311638	2.195614
N	1.904297	-1.932378	-0.639687
C	3.862832	-0.625682	-1.331809
C	4.128817	-3.055403	-0.899817
C	1.331446	-3.061668	-0.509557
C	-0.126588	-3.233396	-0.637851
H	1.906698	-3.975049	-0.327457
H	1.079913	-0.603324	-0.294987
H	1.227686	-1.525863	2.515949
H	1.604435	-3.126525	3.365447
C	-2.646017	4.603790	0.578774
C	-4.018331	4.440681	0.810833
C	-1.871771	3.480403	0.214012

C	-2.457344	2.211085	0.227209
C	-3.821126	2.023903	0.488636
C	-4.577051	3.165634	0.740151
C	-0.419276	3.630857	-0.109609
C	0.045373	4.428015	-1.175471
C	1.426323	4.613985	-1.324928
C	2.310765	3.994903	-0.440180
C	1.891937	3.117438	0.558410
C	0.506294	2.948536	0.676210
O	-1.679553	1.105912	-0.094015
O	0.005417	1.995000	1.559830
P	-0.458350	0.615765	0.850253
O	0.650228	0.327961	-0.215051
O	-0.775274	-0.433219	1.832825
C	-4.461911	0.687228	0.514294
C	2.869491	2.398028	1.414866
C	-5.684888	0.479073	-0.182320
C	-6.290035	-0.750673	-0.190058
C	-5.718114	-1.845689	0.509811
C	-4.516455	-1.631287	1.238846
C	-3.906101	-0.354291	1.219657
C	2.542812	2.025375	2.754644
C	3.434118	1.339858	3.534721
C	4.729333	1.016148	3.056217
C	5.092311	1.439731	1.748644
C	4.130986	2.099228	0.939607
H	-5.638331	3.044342	0.947817
H	3.374861	4.187907	-0.553506
H	-6.118764	1.304948	-0.739936
H	-7.212908	-0.905938	-0.743256
H	4.400551	2.328730	-0.089545
H	3.157587	1.041019	4.542320
H	1.571101	2.281227	3.156055
H	-2.988634	-0.220403	1.783410
C	5.143723	-3.623626	-0.130468
C	5.862177	-4.725466	-0.597644
C	5.574848	-5.274626	-1.840509
C	4.572749	-4.705162	-2.626168
C	3.865759	-3.604048	-2.162398
H	5.400379	-3.202689	0.836158
H	6.648660	-5.150426	0.018403
H	6.130881	-6.134014	-2.201662
H	3.100084	-3.150928	-2.787513
H	4.348854	-5.114926	-3.606250
C	5.239569	-0.381173	-1.386609
C	5.749763	0.677994	-2.128806
C	4.890565	1.528073	-2.823653
C	3.521852	1.288238	-2.782386
C	3.012528	0.211639	-2.055719
H	1.944943	0.041651	-2.061859
H	5.923602	-1.031994	-0.847300
H	6.823801	0.838532	-2.165168
H	5.287623	2.358329	-3.400131
H	2.834841	1.933896	-3.321753
C	-0.929067	-2.248622	-1.223208
C	-2.288708	-2.479106	-1.361200
C	-2.875654	-3.670419	-0.941268
C	-2.056969	-4.640819	-0.378932
Br	-3.367119	-1.166189	-2.166731
H	-3.944492	-3.828766	-1.042244
C	-0.691388	-4.441365	-0.223394
H	-0.073758	-5.218526	0.215080
H	-0.501537	-1.321625	-1.588070

Br	-2.819946	-6.282552	0.163928
C	6.399437	1.145101	1.275080
C	7.280860	0.428781	2.044426
C	6.903051	-0.022064	3.333842
C	5.659425	0.274865	3.830075
H	6.682012	1.492886	0.286305
H	8.275868	0.208113	1.669761
H	5.364290	-0.056139	4.822340
H	7.607368	-0.593381	3.930664
C	-3.943927	-2.705457	1.972346
C	-4.539343	-3.939760	1.978241
C	-5.722220	-4.164479	1.228118
C	-6.297843	-3.143196	0.513898
H	-3.016450	-2.522868	2.509714
H	-4.092755	-4.760737	2.529638
H	-6.171177	-5.153311	1.223820
H	-7.209630	-3.310854	-0.054173
C	-4.925789	5.611298	1.139344
C	-4.172744	6.819304	1.688904
H	-5.697923	5.283185	1.843598
H	-5.453895	5.910274	0.222747
C	-2.969553	7.118542	0.799873
H	-3.823683	6.607365	2.707766
H	-4.843414	7.682397	1.749863
C	-1.986578	5.950414	0.831122
H	-3.312109	7.285769	-0.230987
H	-2.461055	8.033281	1.121141
H	-1.166149	6.130197	0.133714
H	-1.518535	5.903513	1.825366
C	-0.925669	4.986959	-2.200202
C	-0.337684	6.135589	-3.016367
H	-1.862696	5.291715	-1.727872
H	-1.194462	4.165130	-2.879577
C	1.030073	5.740540	-3.566940
H	-1.024740	6.401460	-3.826006
H	-0.230006	7.025201	-2.380067
C	2.000852	5.502150	-2.413107
H	0.926208	4.822521	-4.160415
H	1.425388	6.513055	-4.234262
H	2.270367	6.470759	-1.969091
H	2.936328	5.063305	-2.778962

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M06-2X/6-31G* Energy = -8271.56227783

M06-2X/6-31G* Free Energy = -8270.682893

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.54104326

Number of Imaginary Frequencies = 1

Lowest Frequency = 211.3820i

M06-2X/6-31G* Geometry

C	2.875137	1.751521	-1.342573
C	3.516774	0.358536	-1.024462
C	2.809047	2.688620	-0.167945
H	1.871070	1.556768	-1.736242
H	3.438010	2.204272	-2.164674
C	1.719017	2.830995	0.586274
H	3.695288	3.274834	0.070295
N	2.669986	-0.176748	0.064088
C	3.408400	-0.579981	-2.231243
C	4.991773	0.425344	-0.615255
C	2.934707	0.042627	1.295276
C	2.057126	-0.272607	2.428249
H	3.899780	0.485672	1.545697
H	1.589414	-0.526898	-0.318289

H	0.801231	2.284442	0.368443
H	1.692238	3.530511	1.417088
C	-4.222315	-0.951579	0.764210
C	-4.166712	-2.292677	1.168868
C	-3.460676	-0.537855	-0.350200
C	-2.562202	-1.434651	-0.929952
C	-2.409951	-2.745489	-0.466160
C	-3.266446	-3.160172	0.548679
C	-3.528422	0.855223	-0.884063
C	-4.744560	1.427005	-1.317561
C	-4.779048	2.784681	-1.659595
C	-3.600248	3.531398	-1.619381
C	-2.368739	2.964136	-1.310928
C	-2.352727	1.610730	-0.957355
O	-1.786594	-0.997443	-1.984854
O	-1.151159	1.021184	-0.610125
P	-0.483850	-0.083961	-1.639343
O	0.415260	-0.898547	-0.707413
O	0.055751	0.513678	-2.875081
C	-1.328557	-3.634155	-0.953669
C	-1.133686	3.793241	-1.368782
C	-0.517861	-4.290599	0.015560
C	0.492315	-5.132202	-0.365611
C	0.757704	-5.370195	-1.740610
C	-0.036212	-4.702252	-2.714988
C	-1.073252	-3.833498	-2.290327
C	-0.151649	3.545973	-2.369448
C	0.944228	4.360577	-2.477213
C	1.145519	5.447130	-1.585927
C	0.174493	5.689972	-0.575801
C	-0.966515	4.847913	-0.501749
H	-3.190476	-4.185344	0.906672
H	-3.629567	4.585054	-1.889338
H	-0.700330	-4.079357	1.066843
H	1.110586	-5.625399	0.380322
H	-1.714451	5.041760	0.264327
H	1.686179	4.174005	-3.250690
H	-0.279421	2.699180	-3.036282
H	-1.669521	-3.321873	-3.039983
C	5.768986	1.571166	-0.775504
C	7.124629	1.564183	-0.443163
C	7.718408	0.413183	0.057904
C	6.952311	-0.742398	0.212781
C	5.607047	-0.736368	-0.128957
H	5.332006	2.480957	-1.172126
H	7.712004	2.466948	-0.578617
H	8.771890	0.409684	0.318998
H	5.020902	-1.647506	-0.033362
H	7.408130	-1.653084	0.588656
C	2.949798	-1.892281	-2.105748
C	2.921987	-2.739826	-3.210538
C	3.350407	-2.286751	-4.452376
C	3.822742	-0.983089	-4.582511
C	3.859296	-0.140368	-3.478206
H	4.255402	0.864604	-3.592347
H	2.585266	-2.266792	-1.154011
H	2.563978	-3.757177	-3.093386
H	3.316977	-2.948625	-5.312487
H	4.166744	-0.619024	-5.545686
C	0.742960	-0.720156	2.262426
C	-0.017399	-0.985793	3.389923
C	0.486802	-0.822085	4.676623
C	1.795641	-0.372954	4.817524

Br	-1.786958	-1.579169	3.110453
H	-0.122333	-1.034650	5.547345
C	2.585908	-0.092543	3.711216
H	3.602654	0.261666	3.847641
H	0.307481	-0.855070	1.276421
Br	2.508489	-0.138724	6.550456
C	0.381195	6.760541	0.333696
C	1.500660	7.548305	0.247767
C	2.468087	7.305811	-0.757978
C	2.291389	6.281288	-1.652783
H	-0.365181	6.942516	1.103008
H	1.649335	8.363054	0.949794
H	3.029265	6.090469	-2.428445
H	3.349445	7.937126	-0.817481
C	0.233281	-4.926678	-4.092076
C	1.238052	-5.775033	-4.481889
C	2.027091	-6.441434	-3.511093
C	1.792366	-6.241097	-2.174113
H	-0.369992	-4.405614	-4.830493
H	1.434850	-5.938522	-5.537018
H	2.820155	-7.110193	-3.831139
H	2.395884	-6.747551	-1.424962
C	-5.011243	-2.825692	2.312918
C	-5.489522	-1.736550	3.271431
H	-4.441183	-3.589738	2.855182
H	-5.887018	-3.339205	1.892231
C	-6.057721	-0.561971	2.480053
H	-4.645942	-1.383122	3.879949
H	-6.233324	-2.147223	3.961852
C	-4.966732	0.062802	1.614299
H	-6.880517	-0.914537	1.842173
H	-6.474159	0.195999	3.151406
H	-4.214650	0.529033	2.269777
H	-5.373904	0.874249	1.008255
C	-5.979433	0.561697	-1.509526
C	-7.277272	1.365323	-1.535171
H	-6.033676	-0.225929	-0.755210
H	-5.865048	0.038935	-2.470238
C	-7.156214	2.522912	-2.522277
H	-8.111751	0.708323	-1.801123
H	-7.487117	1.762394	-0.531743
C	-6.065662	3.484209	-2.057222
H	-6.901268	2.123909	-3.512559
H	-8.106570	3.056923	-2.624219
H	-6.437283	4.048323	-1.189877
H	-5.849120	4.226390	-2.833340

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M06-2X/6-31G* Energy = -8271.56623108

M06-2X/6-31G* Free Energy = -8270.683516

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.54398293

Lowest Frequency = 6.5210

M06-2X/6-31G* Geometry

C	1.482234	-3.342874	-0.451815
C	1.027889	-3.052145	1.010090
C	0.578490	-4.262949	-1.220398
H	1.548703	-2.383604	-0.976671
H	2.499031	-3.746011	-0.428919
C	-0.201748	-3.839204	-2.214515
H	0.567695	-5.314964	-0.934922
N	-0.313560	-2.462519	0.884023
C	1.052749	-4.289526	1.914744
C	1.925500	-1.963349	1.624178

C	-1.374034	-3.158907	0.832086
C	-2.690236	-2.516942	0.624479
H	-1.357542	-4.247762	0.949236
H	-0.289245	-1.036362	0.296257
H	-0.202639	-2.792393	-2.516300
H	-0.842532	-4.523106	-2.764262
C	3.482554	3.858567	-0.753734
C	4.760676	3.545876	-1.235922
C	2.607686	2.809914	-0.400219
C	2.977402	1.492724	-0.672605
C	4.247119	1.155278	-1.158245
C	5.125684	2.208542	-1.397526
C	1.285569	3.079306	0.246379
C	1.196588	3.703190	1.508519
C	-0.070551	3.991674	2.029620
C	-1.209611	3.673396	1.288429
C	-1.162281	3.012976	0.060541
C	0.117644	2.678808	-0.400749
O	2.073925	0.485805	-0.383229
O	0.254027	1.872364	-1.529192
P	0.682682	0.348661	-1.202075
O	-0.330581	-0.071075	-0.088406
O	0.768214	-0.482556	-2.416691
C	4.665393	-0.249670	-1.389243
C	-2.431775	2.744658	-0.670512
C	5.906475	-0.703567	-0.859445
C	6.305242	-2.006499	-1.006371
C	5.494686	-2.938400	-1.708797
C	4.278865	-2.477855	-2.285220
C	3.886007	-1.127327	-2.107113
C	-2.710376	1.521781	-1.346517
C	-3.934017	1.296670	-1.918986
C	-4.968350	2.263854	-1.857199
C	-4.695202	3.501284	-1.213248
C	-3.415870	3.712409	-0.641943
H	6.118364	1.976824	-1.779083
H	-2.186022	3.896161	1.712894
H	6.523227	-0.003521	-0.301200
H	7.245010	-2.346126	-0.577988
H	-3.217408	4.670552	-0.167364
H	-4.132598	0.347570	-2.411706
H	-1.971893	0.734940	-1.367413
H	2.946300	-0.803196	-2.545765
C	3.306761	-1.957894	1.415767
C	4.097661	-0.947593	1.954710
C	3.525149	0.076335	2.703887
C	2.153217	0.069293	2.931747
C	1.365018	-0.948906	2.405255
H	3.785646	-2.729013	0.817619
H	5.167359	-0.961118	1.773517
H	4.146777	0.868695	3.110816
H	0.293931	-0.931301	2.581641
H	1.686679	0.858722	3.514916
C	0.409457	-4.233451	3.157867
C	0.444941	-5.311808	4.032231
C	1.137347	-6.471057	3.685040
C	1.793209	-6.533155	2.461916
C	1.751833	-5.450607	1.582896
H	2.280406	-5.524862	0.637917
H	-0.118653	-3.327551	3.444724
H	-0.062541	-5.245060	4.989631
H	1.168236	-7.314923	4.366982
H	2.342895	-7.426602	2.182279

C	-3.701476	-3.235270	-0.015908
C	-4.931106	-2.625221	-0.230787
C	-5.190287	-1.333422	0.212363
C	-4.178023	-0.647303	0.878195
Br	-6.291630	-3.573962	-1.136204
H	-6.156096	-0.869424	0.049121
C	-2.926800	-1.214067	1.076088
H	-2.149295	-0.650055	1.579371
H	-3.525796	-4.248462	-0.362716
Br	-4.531841	1.083765	1.530607
C	-5.719435	4.483554	-1.150857
C	-6.956548	4.240151	-1.689156
C	-7.230430	3.002106	-2.321777
C	-6.257718	2.039060	-2.405429
H	-5.504958	5.431357	-0.663526
H	-7.733632	4.996139	-1.632689
H	-6.458080	1.088691	-2.894242
H	-8.214624	2.821899	-2.743067
C	3.458866	-3.393402	-2.998371
C	3.819219	-4.711638	-3.109372
C	5.026486	-5.173576	-2.526295
C	5.845877	-4.307441	-1.847434
H	2.525215	-3.029930	-3.421442
H	3.177136	-5.407481	-3.640706
H	5.302517	-6.219259	-2.623222
H	6.774445	-4.657163	-1.403227
C	5.775925	4.620869	-1.577051
C	5.144487	5.989485	-1.818692
H	6.357795	4.304817	-2.449713
H	6.490400	4.702212	-0.745533
C	4.161094	6.307428	-0.695885
H	4.607815	5.986480	-2.776150
H	5.925220	6.753701	-1.888475
C	3.011968	5.302208	-0.704634
H	4.684847	6.263017	0.269452
H	3.762812	7.321953	-0.798305
H	2.349946	5.472140	0.147727
H	2.391253	5.475231	-1.595700
C	2.448866	3.943038	2.333787
C	2.228469	4.904074	3.499535
H	3.271400	4.294393	1.706055
H	2.777569	2.966928	2.720235
C	0.976944	4.513329	4.280235
H	3.111840	4.905917	4.146200
H	2.109084	5.926985	3.116260
C	-0.248986	4.655020	3.382144
H	1.071851	3.472393	4.617876
H	0.860046	5.132734	5.175221
H	-0.452641	5.724029	3.227500
H	-1.138084	4.242113	3.871330

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M06-2X/6-31G* Energy = -8271.57154919

M06-2X/6-31G* Free Energy = -8270.687592

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.54510621

Lowest Frequency = 8.9295

M06-2X/6-31G* Geometry

C	-1.124587	3.262188	-0.590975
C	-0.512948	3.084704	0.832473
C	-0.200185	3.885051	-1.599149
H	-1.430276	2.267726	-0.940716
H	-2.042558	3.852340	-0.497438
C	0.280655	3.223186	-2.650660

H	0.088165	4.924717	-1.443152
N	0.722158	2.330133	0.580109
C	-0.294445	4.401937	1.582819
C	-1.464777	2.209791	1.658903
C	1.883835	2.843457	0.591176
C	3.034663	2.052645	0.099747
H	2.067539	3.861772	0.950088
H	0.605527	0.788195	0.188606
H	0.020959	2.179793	-2.830862
H	0.947731	3.701844	-3.362492
C	-3.970963	-3.375915	-0.659548
C	-5.012222	-2.860284	-1.444210
C	-2.932396	-2.519231	-0.245458
C	-2.890432	-1.217009	-0.745392
C	-3.914881	-0.685089	-1.528061
C	-4.981258	-1.519581	-1.839158
C	-1.867576	-2.929088	0.717365
C	-2.163664	-3.268628	2.054108
C	-1.108133	-3.566468	2.928579
C	0.210038	-3.494186	2.472260
C	0.532455	-3.114185	1.172510
C	-0.536160	-2.834235	0.317794
O	-1.816050	-0.407066	-0.418759
O	-0.271832	-2.342788	-0.959679
P	-0.363969	-0.734967	-1.082944
O	0.618532	-0.229748	0.022823
O	-0.194477	-0.245710	-2.460252
C	-3.836595	0.733681	-1.971421
C	1.944930	-2.965784	0.742963
C	-3.029071	1.086793	-3.087426
C	-2.894499	2.399249	-3.457085
C	-3.522213	3.433168	-2.714367
C	-4.340257	3.082836	-1.604679
C	-4.491107	1.713827	-1.264996
C	2.837618	-2.185953	1.530502
C	4.155031	-2.057237	1.179618
C	4.662048	-2.709583	0.024503
C	3.773448	-3.476793	-0.777279
C	2.412991	-3.580255	-0.394984
H	-5.796950	-1.122194	-2.439447
H	1.020900	-3.722832	3.161303
H	-2.490289	0.306704	-3.615464
H	-2.262606	2.670360	-4.298508
H	1.735244	-4.161076	-1.015225
H	4.828846	-1.431661	1.762508
H	2.446001	-1.669295	2.402364
H	-5.088289	1.447296	-0.396082
C	-1.045670	1.042364	2.295675
C	-1.953281	0.256187	3.005266
C	-3.283933	0.643989	3.109782
C	-3.704415	1.825509	2.499430
C	-2.802452	2.601152	1.782568
H	-0.013419	0.716991	2.225948
H	-1.608765	-0.665659	3.467243
H	-3.989429	0.039950	3.673537
H	-3.140963	3.525554	1.320388
H	-4.738918	2.146050	2.585887
C	0.333249	4.357741	2.835149
C	0.532902	5.513209	3.578421
C	0.090914	6.742432	3.089072
C	-0.552347	6.796655	1.859214
C	-0.743393	5.635029	1.109080
H	-1.262398	5.705395	0.158192

H	0.655694	3.396906	3.230919
H	1.022975	5.455022	4.545452
H	0.240476	7.647480	3.669370
H	-0.912230	7.745743	1.473941
C	4.249215	2.066474	0.789520
C	5.280821	1.255784	0.334707
C	5.146718	0.465673	-0.798793
C	3.922763	0.455754	-1.456316
Br	6.890359	1.134251	1.323948
H	5.958907	-0.161720	-1.143414
C	2.871214	1.254982	-1.036076
H	1.930807	1.246206	-1.576828
H	4.378663	2.668754	1.682861
Br	3.670771	-0.726680	-2.895893
C	4.273716	-4.111488	-1.945815
C	5.589409	-3.979962	-2.305266
C	6.475658	-3.215053	-1.506075
C	6.023893	-2.603568	-0.364501
H	3.587498	-4.693289	-2.555768
H	5.959968	-4.460778	-3.205235
H	6.695130	-2.009566	0.254058
H	7.517031	-3.122236	-1.799051
C	-4.909707	4.117465	-0.815112
C	-4.649991	5.435785	-1.093331
C	-3.826010	5.784104	-2.193684
C	-3.286111	4.805779	-2.989935
H	-5.537038	3.842605	0.030028
H	-5.076290	6.218496	-0.473316
H	-3.627407	6.830568	-2.404257
H	-2.643996	5.063735	-3.828011
C	-6.198946	-3.711485	-1.856889
C	-5.925233	-5.211597	-1.774715
H	-6.511081	-3.432133	-2.869142
H	-7.045176	-3.469047	-1.198449
C	-5.266912	-5.547701	-0.438966
H	-5.253787	-5.511106	-2.589737
H	-6.858931	-5.767988	-1.905499
C	-3.907372	-4.859745	-0.342889
H	-5.914027	-5.208204	0.382053
H	-5.142958	-6.629324	-0.324347
H	-3.452157	-5.032509	0.635720
H	-3.222986	-5.321250	-1.069288
C	-3.587514	-3.159844	2.572100
C	-3.802260	-3.852097	3.916205
H	-4.305516	-3.535147	1.839650
H	-3.810975	-2.087386	2.671363
C	-2.701708	-3.462981	4.898298
H	-4.790488	-3.590836	4.308520
H	-3.790559	-4.941742	3.776625
C	-1.355451	-3.955622	4.373947
H	-2.683047	-2.369540	5.007043
H	-2.893103	-3.881006	5.891834
H	-1.323417	-5.051127	4.456986
H	-0.535207	-3.578101	4.994412

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M06-2X/6-31G* Energy = -8271.57154809

M06-2X/6-31G* Free Energy = -8270.687533

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.54513471

Lowest Frequency = 9.1271

M06-2X/6-31G* Geometry

C	-1.121387	3.262248	-0.591950
C	-0.509718	3.084839	0.831454

C	-0.196596	3.883848	-1.600554
H	-1.428098	2.267937	-0.941268
H	-2.038773	3.853341	-0.498438
C	0.283083	3.221209	-2.652100
H	0.093035	4.923201	-1.444890
N	0.725054	2.329736	0.579025
C	-0.290426	4.402165	1.581419
C	-1.461827	2.210560	1.658235
C	1.887500	2.841279	0.592481
C	3.037760	2.049561	0.101133
H	2.072420	3.858638	0.953475
H	0.608077	0.788550	0.185122
H	0.022154	2.178082	-2.831992
H	0.950493	3.698954	-3.364231
C	-2.167537	-3.267110	2.054689
C	-1.112026	-3.565583	2.928996
C	-1.871436	-2.927876	0.717905
C	-0.540005	-2.833944	0.318123
C	0.528619	-3.114745	1.172578
C	0.206107	-3.494435	2.472410
C	-2.936003	-2.517124	-0.244828
C	-3.974949	-3.373034	-0.659447
C	-5.015447	-2.856596	-1.444670
C	-4.983342	-1.515917	-1.839537
C	-3.916627	-0.682092	-1.527632
C	-2.893054	-1.214790	-0.744454
O	-0.275619	-2.342295	-0.959254
O	-1.818154	-0.405776	-0.417182
P	-0.366484	-0.734356	-1.081904
O	0.616615	-0.230172	0.023851
O	-0.196935	-0.244649	-2.459035
C	1.941037	-2.967683	0.742521
C	-3.837015	0.736656	-1.970855
C	2.835168	-2.189666	1.530212
C	4.152557	-2.062291	1.178723
C	4.658141	-2.714177	0.022715
C	3.768064	-3.479362	-0.779352
C	2.407729	-3.581560	-0.396332
C	-3.029818	1.089005	-3.087321
C	-2.893891	2.401374	-3.456817
C	-3.520007	3.435888	-2.713588
C	-4.337773	3.086329	-1.603448
C	-4.489885	1.717454	-1.263804
H	1.016872	-3.723762	3.161346
H	-5.798384	-1.117965	-2.440338
H	2.444737	-1.673210	2.402728
H	4.827444	-1.438067	1.761817
H	-5.086769	1.451470	-0.394517
H	-2.262126	2.671887	-4.298530
H	-2.492241	0.308380	-3.615791
H	1.728965	-4.160920	-1.016811
C	-1.043280	1.043095	2.295267
C	-1.951321	0.257553	3.005035
C	-3.281772	0.646063	3.109491
C	-3.701652	1.827707	2.498946
C	-2.799278	2.602720	1.781917
H	-0.011284	0.717022	2.225256
H	-1.607302	-0.664396	3.467183
H	-3.987557	0.042501	3.673407
H	-3.137284	3.527232	1.319589
H	-4.735989	2.148810	2.585350
C	-0.737570	5.635572	1.106782
C	-0.545547	6.797349	1.856423

C	0.096920	6.742986	3.086698
C	0.537070	5.513477	3.576968
C	0.336417	4.357862	2.834178
H	0.657324	3.396819	3.230700
H	-1.255996	5.706074	0.155593
H	-0.904062	7.746673	1.470456
H	0.247241	7.648156	3.666611
H	1.026457	5.455178	4.544341
C	2.874476	1.252582	-1.035256
C	3.926059	0.453421	-1.455524
C	5.149544	0.462106	-0.797024
C	5.283303	1.251168	0.337213
Br	3.675646	-0.726844	-2.897180
H	5.961677	-0.165313	-1.141729
C	4.251827	2.062216	0.791734
H	4.381020	2.664046	1.685421
H	1.934367	1.244635	-1.576627
Br	6.892078	1.128109	1.327411
C	-4.905668	4.121498	-0.813465
C	-4.644726	5.439565	-1.091729
C	-3.821031	5.787105	-2.192546
C	-3.282629	4.808278	-2.989190
H	-5.532789	3.847235	0.032027
H	-5.069810	6.222676	-0.471384
H	-2.640791	5.065626	-3.827665
H	-3.621494	6.833381	-2.403178
C	4.266771	-4.113489	-1.948873
C	5.582416	-3.983300	-2.308985
C	6.470161	-3.220490	-1.509459
C	6.019918	-2.609697	-0.366918
H	3.579408	-4.693732	-2.559009
H	5.951815	-4.463646	-3.209676
H	7.511503	-3.128820	-1.802905
H	6.692383	-2.017481	0.252005
C	-1.359326	-3.954042	4.374559
C	-2.705208	-3.460403	4.898923
H	-0.538808	-3.576644	4.994746
H	-1.327829	-5.049527	4.458102
C	-3.806175	-3.849177	3.917162
H	-2.685876	-2.366920	5.007199
H	-2.896690	-3.877893	5.892670
C	-3.591217	-3.157313	2.572893
H	-3.795122	-4.938856	3.777812
H	-4.794172	-3.587244	4.309611
H	-3.813979	-2.084693	2.672024
H	-4.309567	-3.532266	1.840598
C	-3.912553	-4.856950	-0.342915
C	-5.272455	-5.544068	-0.439991
H	-3.458112	-5.030128	0.635982
H	-3.227955	-5.318820	-1.068893
C	-5.929738	-5.207269	-1.776072
H	-5.149211	-6.625794	-0.325555
H	-5.919877	-5.204384	0.380709
C	-6.202502	-3.706979	-1.858067
H	-5.257953	-5.506986	-2.590741
H	-6.863691	-5.763067	-1.907579
H	-7.048891	-3.464154	-1.199968
H	-6.514005	-3.427254	-2.870415

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M06-2X/6-31G* Energy = -8271.56275014

M06-2X/6-31G* Free Energy = -8270.680256

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.54336339

Lowest Frequency = 10.0167

M06-2X/6-31G* Geometry

C	0.996507	1.422425	-2.310870
C	0.605434	2.662921	-1.437346
C	-0.048579	1.018700	-3.316112
H	1.171526	0.597092	-1.614197
H	1.954703	1.629412	-2.796917
C	-1.043089	0.182469	-3.015988
H	0.002035	1.445771	-4.316132
N	-0.598775	2.239016	-0.712219
C	1.697305	2.952685	-0.398936
C	0.407426	3.947560	-2.252974
C	-1.755393	2.485438	-1.177503
C	-3.000322	2.006490	-0.546150
H	-1.886051	3.083228	-2.085297
H	-0.293405	0.970790	0.296579
H	-1.126794	-0.260397	-2.023959
H	-1.799933	-0.098339	-3.744842
C	3.414996	-3.432547	-1.226482
C	4.774619	-3.268217	-0.937325
C	2.512070	-2.401731	-0.881336
C	2.961897	-1.311504	-0.130089
C	4.316839	-1.136444	0.181774
C	5.194820	-2.120528	-0.268647
C	1.072152	-2.504887	-1.266401
C	0.664864	-2.639008	-2.611643
C	-0.679343	-2.917550	-2.888359
C	-1.598792	-2.986117	-1.839971
C	-1.250020	-2.736482	-0.513961
C	0.106590	-2.497829	-0.261162
O	2.040369	-0.342727	0.257508
O	0.520656	-2.225042	1.035321
P	0.894754	-0.684260	1.364830
O	-0.352469	0.113129	0.845541
O	1.302271	-0.521656	2.764496
C	4.867842	-0.012287	0.979807
C	-2.283448	-2.720076	0.548891
C	6.070577	0.614498	0.542955
C	6.697058	1.558234	1.312289
C	6.154321	1.946839	2.564927
C	4.943638	1.339919	2.996033
C	4.320526	0.357948	2.185960
C	-3.550000	-2.128583	0.274440
C	-4.555167	-2.156907	1.202556
C	-4.360034	-2.760802	2.471585
C	-3.092847	-3.332827	2.763888
C	-2.073411	-3.303347	1.778924
H	6.250071	-2.014342	-0.026655
H	-2.637909	-3.214579	-2.068439
H	6.486313	0.334678	-0.421336
H	7.614181	2.029698	0.967389
H	-1.114171	-3.756195	2.009978
H	-5.516445	-1.696945	0.983889
H	-3.703384	-1.628436	-0.679023
H	3.411995	-0.110534	2.552827
C	-0.123954	5.073305	-1.608648
C	-0.279228	6.277031	-2.281844
C	0.110869	6.387973	-3.616722
C	0.659238	5.286634	-4.260380
C	0.805062	4.074764	-3.582973
H	-0.406532	4.999697	-0.561148
H	-0.695187	7.134513	-1.762021
H	-0.005262	7.329433	-4.144241
H	1.248550	3.234876	-4.106826

H	0.978484	5.362094	-5.295315
C	3.001447	3.218029	-0.823387
C	3.981917	3.594511	0.087738
C	3.670204	3.724687	1.439340
C	2.380738	3.442591	1.873013
C	1.399511	3.060259	0.961426
H	0.393112	2.866272	1.317904
H	3.247739	3.166414	-1.881223
H	4.991387	3.794094	-0.258566
H	4.429229	4.030877	2.153149
H	2.134507	3.517756	2.927809
C	-3.043834	1.594942	0.789371
C	-4.259514	1.202569	1.330496
C	-5.428803	1.195796	0.573647
C	-5.359282	1.593606	-0.755475
Br	-4.345789	0.660956	3.131152
H	-6.370994	0.892280	1.014910
C	-4.162651	2.011715	-1.321609
H	-4.132740	2.336104	-2.356967
H	-2.148679	1.582341	1.399609
Br	-6.932499	1.580101	-1.802783
C	-2.881588	-3.920316	4.040295
C	-3.878867	-3.927976	4.980211
C	-5.138974	-3.347240	4.690644
C	-5.372164	-2.776882	3.466035
H	-1.909629	-4.354342	4.258815
H	-3.705958	-4.374363	5.954488
H	-6.332593	-2.320032	3.239839
H	-5.918420	-3.354199	5.446335
C	4.359179	1.753682	4.222612
C	4.947900	2.734400	4.979174
C	6.159177	3.336217	4.552605
C	6.750499	2.947249	3.377014
H	3.426244	1.287277	4.529976
H	4.490849	3.054062	5.910637
H	6.617815	4.107884	5.163454
H	7.677474	3.408255	3.044716
C	5.816754	-4.298784	-1.329464
C	5.227652	-5.683409	-1.582686
H	6.318744	-3.954564	-2.244871
H	6.590063	-4.342436	-0.554961
C	4.007990	-5.560321	-2.490560
H	4.923357	-6.137449	-0.630861
H	5.985859	-6.337456	-2.025072
C	2.914515	-4.749232	-1.799301
H	4.299704	-5.063953	-3.426965
H	3.616640	-6.546828	-2.759151
H	2.075191	-4.597089	-2.479744
H	2.508796	-5.335869	-0.962066
C	1.642607	-2.382655	-3.742910
C	1.200161	-2.999815	-5.067160
H	2.649522	-2.713964	-3.479562
H	1.707661	-1.290019	-3.864611
C	-0.238957	-2.594104	-5.372863
H	1.875333	-2.678976	-5.867020
H	1.268784	-4.095352	-5.008440
C	-1.173998	-3.154371	-4.303530
H	-0.302647	-1.498147	-5.380947
H	-0.549274	-2.947073	-6.361614
H	-1.282423	-4.237373	-4.456834
H	-2.179690	-2.731327	-4.410531

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M06-2X/6-31G* Energy = -8271.56676586

M06-2X/6-31G* Free Energy = -8270.683848

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.54361660

Lowest Frequency = 6.2016

M06-2X/6-31G* Geometry

C	0.803869	-0.819607	2.804454
C	0.403694	-2.247219	2.295991
C	-0.278543	-0.083918	3.546726
H	1.096209	-0.247124	1.916525
H	1.703887	-0.922265	3.419161
C	-1.151737	0.717433	2.937211
H	-0.354508	-0.229140	4.622715
N	-0.695727	-2.015597	1.353029
C	1.590972	-2.835942	1.521729
C	0.043520	-3.229075	3.416422
C	-1.913512	-2.091827	1.712934
C	-3.021247	-1.741321	0.802068
H	-2.194496	-2.411071	2.721949
H	-0.369372	-0.944688	0.183635
H	-1.110530	0.882634	1.861523
H	-1.928165	1.242049	3.489549
C	3.792058	3.438558	0.052093
C	5.078463	3.078255	-0.368128
C	2.786800	2.447364	0.109401
C	3.055581	1.166047	-0.380124
C	4.329361	0.792703	-0.828493
C	5.322963	1.767260	-0.773802
C	1.428620	2.777049	0.641225
C	1.237847	3.256173	1.954527
C	-0.029830	3.719961	2.327525
C	-1.092263	3.616362	1.430180
C	-0.975144	2.994514	0.187426
C	0.318082	2.605423	-0.184648
O	2.039483	0.217626	-0.355618
O	0.514752	1.963933	-1.401916
P	0.739283	0.364521	-1.324195
O	-0.431276	-0.101427	-0.394312
O	0.872845	-0.236271	-2.657035
C	4.659171	-0.542117	-1.388598
C	-2.186448	2.680628	-0.610584
C	5.850939	-1.200942	-0.972487
C	6.243525	-2.379943	-1.548616
C	5.464667	-2.983629	-2.571563
C	4.271346	-2.332852	-2.986311
C	3.893374	-1.109025	-2.380272
C	-3.385608	2.348563	0.087479
C	-4.549888	2.085252	-0.580410
C	-4.589492	2.098245	-1.998982
C	-3.392536	2.389011	-2.708646
C	-2.208377	2.691567	-1.988957
H	6.318722	1.504567	-1.124976
H	-2.069501	3.979179	1.740563
H	6.445199	-0.757411	-0.178044
H	7.152991	-2.876863	-1.219153
H	-1.311038	2.932478	-2.548974
H	-5.449498	1.818135	-0.029262
H	-3.365012	2.284717	1.171628
H	2.990341	-0.621319	-2.733241
C	-0.484906	-4.477699	3.060677
C	-0.786064	-5.428955	4.025416
C	-0.548290	-5.158195	5.373220
C	-0.002749	-3.934249	5.737156
C	0.289937	-2.976166	4.764923
H	-0.648263	-4.702506	2.009338

H	-1.196726	-6.388178	3.725842
H	-0.779241	-5.901707	6.129499
H	0.729806	-2.034653	5.075571
H	0.200076	-3.715639	6.781076
C	1.520149	-3.149551	0.164861
C	2.612006	-3.724062	-0.486023
C	3.786892	-3.982409	0.209325
C	3.867888	-3.663229	1.563509
C	2.776831	-3.102417	2.213767
H	2.836751	-2.894474	3.279621
H	0.607672	-2.965405	-0.393210
H	2.539968	-3.970457	-1.540959
H	4.631646	-4.431754	-0.302000
H	4.779739	-3.863964	2.117920
C	-2.839055	-1.705309	-0.583595
C	-3.891984	-1.316649	-1.396263
C	-5.140326	-1.007533	-0.865934
C	-5.301014	-1.050076	0.512060
Br	-3.620401	-1.132815	-3.248491
H	-5.953553	-0.705397	-1.515164
C	-4.262113	-1.416086	1.356573
H	-4.409028	-1.429328	2.431897
H	-1.884018	-1.959300	-1.025504
Br	-6.962000	-0.514301	1.241670
C	-3.415438	2.366670	-4.128985
C	-4.568611	2.064722	-4.806537
C	-5.762173	1.781486	-4.097680
C	-5.771892	1.802879	-2.726453
H	-2.496142	2.581996	-4.667039
H	-4.572461	2.042296	-5.891903
H	-6.685876	1.596524	-2.172692
H	-6.669640	1.549261	-4.646523
C	3.466359	-2.931548	-3.992601
C	3.827940	-4.131319	-4.550100
C	5.016093	-4.783452	-4.134158
C	5.815949	-4.221634	-3.171405
H	2.552389	-2.422970	-4.289615
H	3.205159	-4.588877	-5.312566
H	5.291147	-5.732684	-4.583744
H	6.728319	-4.718943	-2.850772
C	6.225688	4.070630	-0.401054
C	5.761097	5.523606	-0.438237
H	6.843721	3.919027	0.495302
H	6.870548	3.848033	-1.258037
C	4.697675	5.745463	0.632625
H	5.333693	5.751672	-1.423185
H	6.614648	6.193489	-0.292947
C	3.464039	4.895650	0.336978
H	5.108298	5.471231	1.614631
H	4.409891	6.800218	0.688908
H	2.741249	4.990035	1.149522
H	2.956947	5.297075	-0.552579
C	2.357677	3.163034	2.975333
C	2.136840	4.050064	4.198007
H	3.328426	3.370767	2.518687
H	2.402484	2.112396	3.301024
C	0.724276	3.851515	4.740758
H	2.887854	3.818090	4.960032
H	2.275123	5.104769	3.921459
C	-0.291970	4.311203	3.699312
H	0.567449	2.785976	4.955741
H	0.578816	4.400870	5.676454
H	-0.259658	5.407480	3.626484

H -1.309893 4.054634 4.013884

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M06-2X/6-31G* Energy = -8271.56917575

M06-2X/6-31G* Free Energy = -8270.686932

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.54283105

Lowest Frequency = 2.5086

M06-2X/6-31G* Geometry

C	3.147797	-0.384162	1.348148
C	2.540008	-1.821942	1.347686
C	2.701405	0.503219	2.478609
H	2.873198	0.065477	0.393115
H	4.238968	-0.461315	1.347802
C	1.650538	1.323292	2.427427
H	3.281025	0.466703	3.399871
N	1.088419	-1.643405	1.132516
C	3.111472	-2.629972	0.172237
C	2.855249	-2.625542	2.618529
C	0.335004	-1.459308	2.141107
C	-1.132164	-1.291506	2.074611
H	0.746221	-1.470800	3.154703
H	0.596784	-1.243729	-0.366493
H	1.026293	1.400169	1.540097
H	1.386948	1.949355	3.275926
C	0.168018	4.586208	-1.027959
C	1.412021	5.229732	-1.078171
C	0.128430	3.188282	-0.838560
C	1.321486	2.472424	-0.868405
C	2.574688	3.088918	-0.895540
C	2.584778	4.477773	-0.968630
C	-1.146867	2.451763	-0.580415
C	-1.947483	2.756596	0.541603
C	-3.185199	2.114751	0.687192
C	-3.596265	1.195340	-0.277961
C	-2.797004	0.817711	-1.358069
C	-1.540598	1.428249	-1.445868
O	1.247120	1.089533	-0.773139
O	-0.666795	1.044752	-2.453850
P	0.678272	0.245906	-2.042575
O	0.206992	-1.058127	-1.302117
O	1.575097	0.118881	-3.195787
C	3.830633	2.303712	-0.791342
C	-3.327795	-0.155359	-2.346438
C	4.715366	2.559826	0.292873
C	5.867867	1.833366	0.443916
C	6.211025	0.814530	-0.484573
C	5.334089	0.563303	-1.576924
C	4.142734	1.322337	-1.704222
C	-4.695644	-0.034581	-2.728779
C	-5.294404	-0.968483	-3.529453
C	-4.563893	-2.085371	-4.014463
C	-3.189639	-2.194939	-3.668922
C	-2.596528	-1.213954	-2.834769
H	3.545590	4.988442	-0.988669
H	-4.562083	0.705862	-0.159543
H	4.447888	3.325568	1.015867
H	6.536285	2.028870	1.279004
H	-1.564328	-1.354493	-2.540199
H	-6.339504	-0.863317	-3.809481
H	-5.264301	0.820531	-2.375034
H	3.474905	1.112541	-2.536201
C	2.152001	-3.812581	2.863171
C	2.448715	-4.607446	3.961910

C	3.470894	-4.239746	4.836502
C	4.191393	-3.077787	4.592157
C	3.885943	-2.277198	3.490677
H	1.367903	-4.117928	2.174819
H	1.887740	-5.521270	4.131647
H	3.706453	-4.860522	5.695128
H	4.474574	-1.383066	3.314045
H	4.997863	-2.785516	5.257669
C	4.497089	-2.726327	0.007024
C	5.039334	-3.525482	-0.992065
C	4.208129	-4.237354	-1.853229
C	2.830364	-4.151242	-1.694661
C	2.286148	-3.362435	-0.683212
H	1.208827	-3.321970	-0.568875
H	5.171122	-2.189156	0.669550
H	6.117887	-3.583095	-1.098185
H	4.632309	-4.856534	-2.637567
H	2.167952	-4.701439	-2.355753
C	-1.756723	-0.723215	3.190034
C	-3.141939	-0.677267	3.244160
C	-3.922333	-1.211364	2.227466
C	-3.284785	-1.769419	1.123569
Br	-4.001698	0.076047	4.746824
H	-5.004061	-1.205033	2.295529
C	-1.898657	-1.803530	1.021221
H	-1.425831	-2.251175	0.153304
H	-1.164190	-0.339097	4.014682
Br	-4.360700	-2.523735	-0.227335
C	-2.446362	-3.306674	-4.147886
C	-3.041158	-4.259113	-4.934175
C	-4.410436	-4.146472	-5.281037
C	-5.152757	-3.084260	-4.832678
H	-1.395463	-3.381752	-3.880341
H	-2.464535	-5.104050	-5.297530
H	-6.203038	-2.991168	-5.097221
H	-4.869116	-4.906568	-5.905960
C	5.676975	-0.436562	-2.525362
C	6.843747	-1.144571	-2.398858
C	7.711461	-0.905822	-1.303884
C	7.399550	0.046080	-0.366269
H	4.987871	-0.631254	-3.342810
H	7.100321	-1.905443	-3.129989
H	8.629326	-1.479106	-1.212140
H	8.065503	0.237190	0.471708
C	1.530569	6.736471	-1.215930
C	0.262228	7.395215	-1.752351
H	1.759219	7.158149	-0.226853
H	2.388200	6.974020	-1.854637
C	-0.953477	6.865188	-0.997359
H	0.148921	7.167078	-2.819934
H	0.340651	8.483258	-1.661424
C	-1.114453	5.368473	-1.251680
H	-0.821901	7.046227	0.078878
H	-1.864480	7.390135	-1.301946
H	-1.931061	4.963160	-0.649367
H	-1.415942	5.212964	-2.297533
C	-1.439275	3.694942	1.624097
C	-2.556454	4.255705	2.499791
H	-0.842922	4.504416	1.199071
H	-0.746921	3.123092	2.260020
C	-3.423604	3.111768	3.013075
H	-2.123578	4.824899	3.328739
H	-3.171887	4.953542	1.914887

C	-4.120113	2.427680	1.840608
H	-2.785148	2.388468	3.536295
H	-4.167521	3.459223	3.737481
H	-4.920160	3.084024	1.469883
H	-4.613990	1.508232	2.176208

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M06-2X/6-31G* Energy = -8271.56552894

M06-2X/6-31G* Free Energy = -8270.684036

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.54206442

Lowest Frequency = 7.1755

M06-2X/6-31G* Geometry

C	2.582465	2.459247	-0.793342
C	3.387491	1.125479	-0.909468
C	2.534613	3.037753	0.593087
H	1.567320	2.255612	-1.151637
H	3.007960	3.185462	-1.493835
C	1.450201	2.992222	1.364239
H	3.438530	3.508837	0.977429
N	2.695569	0.217294	0.022351
C	3.254535	0.544248	-2.323944
C	4.886564	1.280156	-0.618103
C	3.087544	0.104266	1.226680
C	2.351360	-0.673821	2.242716
H	4.021246	0.566479	1.564475
H	1.261696	-0.299378	-0.629753
H	0.524131	2.538782	1.012080
H	1.438484	3.433103	2.356904
C	-5.000579	1.163778	-0.790138
C	-5.208462	2.548712	-0.789881
C	-3.703240	0.662136	-0.548834
C	-2.630335	1.555076	-0.469353
C	-2.817267	2.940279	-0.472461
C	-4.122561	3.404592	-0.598905
C	-3.446784	-0.797463	-0.369461
C	-4.073481	-1.546809	0.650291
C	-3.832308	-2.925381	0.727666
C	-2.889930	-3.507665	-0.121550
C	-2.164089	-2.769304	-1.050282
C	-2.499356	-1.418982	-1.179956
O	-1.343093	1.048031	-0.321002
O	-1.836160	-0.647076	-2.126688
P	-0.653353	0.316172	-1.608911
O	0.352702	-0.667822	-0.920847
O	-0.164037	1.225742	-2.652408
C	-1.696243	3.907828	-0.331457
C	-1.015886	-3.370672	-1.769000
C	-0.704001	4.022189	-1.345186
C	0.281396	4.968226	-1.241339
C	0.356250	5.834797	-0.119616
C	-0.625336	5.715392	0.901878
C	-1.651439	4.745537	0.758969
C	-0.056641	-4.089245	-1.000340
C	1.033864	-4.661267	-1.597639
C	1.237892	-4.545846	-2.998622
C	0.293145	-3.811906	-3.769403
C	-0.828329	-3.231711	-3.124020
H	-4.287408	4.479963	-0.598003
H	-2.666887	-4.567338	-0.013491
H	-0.735399	3.350778	-2.197580
H	1.032121	5.058483	-2.023221
H	-1.541832	-2.667594	-3.717863
H	1.767031	-5.201780	-1.004348

H	-0.191125	-4.136155	0.077882
H	-2.406765	4.660352	1.537404
C	5.523716	2.517980	-0.540472
C	6.901820	2.601289	-0.334779
C	7.662581	1.447306	-0.201128
C	7.038588	0.202647	-0.287079
C	5.669381	0.123390	-0.500518
H	4.956160	3.436113	-0.648430
H	7.375395	3.576679	-0.279620
H	8.733821	1.512564	-0.038819
H	5.192805	-0.849952	-0.589652
H	7.623139	-0.707939	-0.198260
C	2.997544	-0.813340	-2.526643
C	2.915750	-1.338061	-3.814283
C	3.091794	-0.511901	-4.917784
C	3.369470	0.839259	-4.725650
C	3.458899	1.359419	-3.439922
H	3.697979	2.411077	-3.311861
H	2.843061	-1.474826	-1.678720
H	2.715978	-2.396123	-3.949806
H	3.016141	-0.921502	-5.920583
H	3.517807	1.493374	-5.579449
C	1.011027	-1.019407	2.062834
C	0.382155	-1.807774	3.012070
C	1.037268	-2.240162	4.160509
C	2.362115	-1.855603	4.337040
Br	-1.406463	-2.314341	2.664197
H	0.534117	-2.854606	4.897508
C	3.027787	-1.080284	3.395524
H	4.065788	-0.806164	3.554528
H	0.453891	-0.683183	1.198704
Br	3.278579	-2.413591	5.893522
C	0.504588	-3.674941	-5.167693
C	1.598285	-4.241626	-5.770828
C	2.536777	-4.975949	-5.003487
C	2.359753	-5.122558	-3.650869
H	-0.215268	-3.104596	-5.748498
H	1.750842	-4.128857	-6.839786
H	3.078478	-5.681109	-3.056551
H	3.399017	-5.419557	-5.491604
C	-0.543185	6.562462	2.038511
C	0.468375	7.480709	2.156184
C	1.446675	7.599214	1.138441
C	1.389106	6.796236	0.028167
H	-1.296748	6.466610	2.816204
H	0.523572	8.122117	3.030357
H	2.242633	8.330170	1.242796
H	2.137531	6.881007	-0.755938
C	-6.587095	3.157003	-0.968791
C	-7.588935	2.202709	-1.613563
H	-6.501872	4.079948	-1.552577
H	-6.965410	3.454066	0.019620
C	-7.517734	0.840974	-0.928496
H	-7.352807	2.080912	-2.678530
H	-8.597601	2.623727	-1.552810
C	-6.139110	0.220284	-1.140599
H	-7.707409	0.963344	0.147301
H	-8.288109	0.166262	-1.315392
H	-6.055977	-0.720915	-0.593126
H	-6.027682	-0.047134	-2.201419
C	-4.864903	-0.853547	1.745421
C	-5.797778	-1.795674	2.501860
H	-5.416889	0.005830	1.359971

H	-4.125230	-0.441338	2.449312
C	-5.030355	-3.028747	2.969634
H	-6.243521	-1.267563	3.350855
H	-6.623084	-2.105564	1.845467
C	-4.510707	-3.805983	1.761744
H	-4.184877	-2.709868	3.594254
H	-5.659546	-3.676949	3.587894
H	-5.351684	-4.325627	1.281960
H	-3.809802	-4.586060	2.081374

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M06-2X/6-31G* Energy = -8271.56552891

M06-2X/6-31G* Free Energy = -8270.684036

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.54206286

Lowest Frequency = 7.1719

M06-2X/6-31G* Geometry

C	2.582668	2.458703	-0.793410
C	3.387727	1.124961	-0.909638
C	2.534721	3.037014	0.593095
H	1.567535	2.255112	-1.151773
H	3.008190	3.185008	-1.493798
C	1.450193	2.991561	1.364085
H	3.438665	3.507891	0.977636
N	2.695784	0.216744	0.022120
C	3.254704	0.543855	-2.324151
C	4.886790	1.279617	-0.618277
C	3.087925	0.103288	1.226356
C	2.351630	-0.674738	2.242356
H	4.021813	0.565139	1.564136
H	1.261547	-0.299455	-0.630122
H	0.524083	2.538333	1.011750
H	1.438416	3.432313	2.356808
C	-4.073873	-1.546036	0.650574
C	-3.832917	-2.924641	0.727899
C	-3.447113	-0.796772	-0.369210
C	-2.499870	-1.418431	-1.179806
C	-2.164828	-2.768827	-1.050200
C	-2.890711	-3.507075	-0.121419
C	-3.703303	0.662885	-0.548506
C	-5.000524	1.164809	-0.789790
C	-5.208106	2.549802	-0.789553
C	-4.122015	3.405446	-0.598635
C	-2.816821	2.940836	-0.472192
C	-2.630202	1.555605	-0.469039
O	-1.836604	-0.646627	-2.126556
O	-1.343066	1.048241	-0.320764
P	-0.653633	0.316479	-1.608883
O	0.352442	-0.667691	-0.921080
O	-0.164407	1.226077	-2.652392
C	-1.016789	-3.370344	-1.769063
C	-1.695553	3.908108	-0.331129
C	-0.057538	-4.089082	-1.000565
C	1.032837	-4.661192	-1.598025
C	1.236714	-4.545725	-2.999026
C	0.291949	-3.811648	-3.769654
C	-0.829368	-3.231338	-3.124102
C	-0.703494	4.022490	-1.345040
C	0.282168	4.968244	-1.241146
C	0.357481	5.834482	-0.119194
C	-0.623907	5.715031	0.902486
C	-1.650303	4.745489	0.759524
H	-2.667845	-4.566789	-0.013388
H	-4.286616	4.480855	-0.597750

H	-0.191877	-4.136053	0.077671
H	1.766007	-5.201816	-1.004841
H	-2.405497	4.660304	1.538086
H	1.032755	5.058522	-2.023160
H	-0.735233	3.351289	-2.197586
H	-1.542868	-2.667100	-3.717835
C	5.669628	0.122831	-0.500971
C	7.038834	0.202063	-0.287514
C	7.662797	1.446719	-0.201270
C	6.902013	2.600722	-0.334638
C	5.523909	2.517439	-0.540341
H	5.193061	-0.850494	-0.590352
H	7.623408	-0.708530	-0.198914
H	8.734036	1.511969	-0.038949
H	4.956313	3.435579	-0.648063
H	7.375579	3.576104	-0.279246
C	2.997068	-0.813578	-2.527031
C	2.915119	-1.338092	-3.814752
C	3.091666	-0.511882	-4.918132
C	3.369988	0.839126	-4.725814
C	3.459555	1.359078	-3.440015
H	3.699175	2.410595	-3.311767
H	2.842233	-1.475094	-1.679196
H	2.714841	-2.396042	-3.950421
H	3.015897	-0.921322	-5.920988
H	3.518734	1.493269	-5.579521
C	3.027957	-1.081201	3.395222
C	2.362158	-1.856386	4.336768
C	1.037265	-2.240773	4.160211
C	0.382244	-1.808379	3.011716
Br	3.278510	-2.414423	5.893300
H	0.533991	-2.855085	4.897240
C	1.011264	-1.020192	2.062435
H	0.454217	-0.683962	1.198247
H	4.065980	-0.807176	3.554256
Br	-1.406481	-2.314633	2.663937
C	-0.541256	6.561719	2.039367
C	0.470596	7.479640	2.157101
C	1.448691	7.598195	1.139165
C	1.390634	6.795590	0.028646
H	-1.294675	6.465844	2.817196
H	0.526189	8.120748	3.031469
H	2.138892	6.880405	-0.755614
H	2.244876	8.328898	1.243571
C	0.503211	-3.674681	-5.167974
C	1.596746	-4.241493	-5.771278
C	2.535268	-4.975936	-5.004083
C	2.358423	-5.122546	-3.651443
H	-0.216662	-3.104239	-5.748665
H	1.749160	-4.128728	-6.840256
H	3.397385	-5.419636	-5.492333
H	3.077167	-5.681190	-3.057235
C	-4.511299	-3.805154	1.762068
C	-5.030660	-3.027829	2.970024
H	-3.810446	-4.585317	2.081606
H	-5.352413	-4.324693	1.282411
C	-5.797996	-1.794672	2.502342
H	-4.185042	-2.709052	3.594506
H	-5.659841	-3.675935	3.588397
C	-4.865152	-0.852653	1.745722
H	-6.623443	-2.104477	1.846086
H	-6.243540	-1.266480	3.351392
H	-5.417187	0.006677	1.360230

H	-4.125411	-0.440355	2.449487
C	-6.139244	0.221558	-1.140306
C	-7.517753	0.842523	-0.928258
H	-6.056309	-0.719683	-0.592875
H	-6.027824	-0.045824	-2.201138
C	-7.588621	2.204299	-1.613285
H	-8.288245	0.167983	-1.315223
H	-7.707473	0.964905	0.147530
C	-6.586633	3.158345	-0.968378
H	-7.352425	2.082495	-2.678237
H	-8.597204	2.625528	-1.552596
H	-6.964914	3.455290	0.020084
H	-6.501271	4.081381	-1.552002

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M06-2X/6-31G* Energy = -8271.56898034

M06-2X/6-31G* Free Energy = -8270.685314

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.54409237

Lowest Frequency = 10.4212

M06-2X/6-31G* Geometry

C	0.850213	-3.390798	-0.026999
C	0.214119	-2.970600	1.335075
C	-0.101813	-4.045869	-0.988761
H	1.264038	-2.483827	-0.485928
H	1.705643	-4.043016	0.176628
C	-0.501389	-3.463066	-2.117074
H	-0.481180	-5.035342	-0.736119
N	-0.937647	-2.151010	0.935193
C	-0.154578	-4.147521	2.244297
C	1.206870	-2.075553	2.088437
C	-2.147089	-2.531203	1.004425
C	-3.206736	-1.701952	0.387047
H	-2.439147	-3.457981	1.509478
H	-0.649395	-0.710705	0.330586
H	-0.145579	-2.472636	-2.402033
H	-1.183736	-3.960724	-2.800567
C	2.549534	3.189400	1.857988
C	1.512139	3.714477	2.642547
C	2.252699	2.716920	0.561966
C	0.932786	2.734804	0.115685
C	-0.119685	3.237676	0.884343
C	0.208234	3.735105	2.142554
C	3.286729	2.055514	-0.288482
C	4.444425	2.713856	-0.745200
C	5.443129	1.972604	-1.392857
C	5.248375	0.608653	-1.624485
C	4.063396	-0.036881	-1.287875
C	3.090826	0.714918	-0.629915
O	0.651690	2.137845	-1.111686
O	1.902508	0.100753	-0.272601
P	0.542493	0.527423	-1.062814
O	-0.551293	0.269759	0.022500
O	0.386048	-0.080431	-2.393786
C	-1.528066	3.195569	0.419519
C	3.825768	-1.471175	-1.609369
C	-2.525241	2.637065	1.267705
C	-3.839549	2.608921	0.884576
C	-4.238550	3.148725	-0.366872
C	-3.246688	3.691787	-1.228622
C	-1.893104	3.694456	-0.809147
C	4.418365	-2.483010	-0.806697
C	4.194928	-3.809038	-1.075731
C	3.373550	-4.201028	-2.166001

C	2.798216	-3.191425	-2.986141
C	3.030818	-1.827315	-2.673799
H	-0.589276	4.137689	2.764234
H	6.026296	0.038549	-2.128257
H	-2.218600	2.205551	2.216564
H	-4.595737	2.149192	1.518596
H	2.548428	-1.059535	-3.272697
H	4.642118	-4.580607	-0.452694
H	5.037533	-2.186096	0.035221
H	-1.137518	4.104281	-1.474214
C	2.506828	-2.540717	2.311886
C	3.430858	-1.763529	2.998756
C	3.069965	-0.504575	3.476639
C	1.780143	-0.033383	3.259436
C	0.850597	-0.819826	2.580154
H	2.798859	-3.525269	1.956451
H	4.433881	-2.144197	3.167478
H	3.789680	0.097298	4.024502
H	-0.149565	-0.430966	2.420296
H	1.485998	0.951937	3.611616
C	-0.770074	-3.870868	3.473044
C	-1.110197	-4.890975	4.351078
C	-0.825483	-6.216937	4.024463
C	-0.198389	-6.503406	2.818802
C	0.133257	-5.476260	1.933653
H	0.629879	-5.728195	1.002860
H	-0.969700	-2.835928	3.742625
H	-1.587005	-4.652187	5.296765
H	-1.084679	-7.016882	4.710819
H	0.038155	-7.530340	2.557803
C	-4.414574	-1.488400	1.055392
C	-5.352816	-0.642606	0.478572
C	-5.135848	-0.038729	-0.752376
C	-3.919464	-0.253205	-1.388779
Br	-6.936854	-0.209327	1.420091
H	-5.875874	0.617607	-1.192243
C	-2.959363	-1.092703	-0.846055
H	-2.023329	-1.260524	-1.367566
H	-4.606953	-1.942183	2.022181
Br	-3.545981	0.681793	-2.976565
C	1.994499	-3.575771	-4.092441
C	1.758143	-4.899244	-4.359299
C	2.307988	-5.904245	-3.526128
C	3.096056	-5.563304	-2.456838
H	1.560313	-2.795341	-4.712146
H	1.139468	-5.183168	-5.205045
H	3.529167	-6.331971	-1.821069
H	2.105711	-6.949001	-3.741876
C	-3.641313	4.212892	-2.490131
C	-4.955097	4.186183	-2.878917
C	-5.944242	3.646355	-2.019112
C	-5.594248	3.148823	-0.789841
H	-2.877133	4.623034	-3.145273
H	-5.245344	4.578745	-3.848514
H	-6.982620	3.636453	-2.336200
H	-6.345545	2.730643	-0.121503
C	1.760643	4.246724	4.041190
C	3.017632	3.662778	4.680634
H	0.880522	4.049651	4.663268
H	1.863898	5.339941	3.993650
C	4.188396	3.802624	3.712960
H	2.860621	2.599419	4.910008
H	3.226446	4.168359	5.628910

C	3.936446	2.989984	2.444506
H	4.313940	4.862769	3.453752
H	5.124443	3.474585	4.176742
H	4.038310	1.918383	2.666976
H	4.713292	3.203601	1.707496
C	4.559451	4.223916	-0.632768
C	6.000698	4.719181	-0.722781
H	4.077113	4.588451	0.277646
H	3.983098	4.657576	-1.462730
C	6.676123	4.125899	-1.956825
H	6.014524	5.813293	-0.756896
H	6.554900	4.417345	0.177188
C	6.751293	2.605815	-1.829956
H	6.093344	4.395017	-2.847179
H	7.681151	4.538003	-2.093107
H	7.523421	2.349976	-1.090479
H	7.074244	2.156245	-2.775281

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M06-2X/6-31G* Energy = -8271.56898023

M06-2X/6-31G* Free Energy = -8270.685311

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.54409230

Lowest Frequency = 10.4041

M06-2X/6-31G* Geometry

C	0.849507	-3.391076	-0.026949
C	0.213494	-2.970544	1.335084
C	-0.102771	-4.045952	-0.988595
H	1.263632	-2.484284	-0.485971
H	1.704718	-4.043580	0.176672
C	-0.502361	-3.463117	-2.116882
H	-0.482319	-5.035327	-0.735845
N	-0.938119	-2.150819	0.934990
C	-0.155431	-4.147231	2.244518
C	1.206329	-2.075521	2.088374
C	-2.147695	-2.530430	1.004782
C	-3.207105	-1.701146	0.387123
H	-2.439977	-3.456768	1.510494
H	-0.649434	-0.711204	0.330694
H	-0.146344	-2.472798	-2.401964
H	-1.184897	-3.960677	-2.800258
C	4.444973	2.712935	-0.745396
C	5.443446	1.971624	-1.393353
C	3.287260	2.054711	-0.288559
C	3.091092	0.714208	-0.630172
C	4.063422	-0.037653	-1.288410
C	5.248444	0.607736	-1.625147
C	2.253479	2.716181	0.562151
C	2.550539	3.188385	1.858207
C	1.513304	3.713475	2.642980
C	0.209360	3.734453	2.143132
C	-0.118780	3.237334	0.884858
C	0.933502	2.734347	0.116008
O	1.902747	0.100165	-0.272746
O	0.652165	2.137564	-1.111366
P	0.542627	0.527123	-1.062653
O	-0.550960	0.269406	0.022774
O	0.385824	-0.080551	-2.393677
C	3.825426	-1.471873	-1.609955
C	-1.527192	3.195600	0.420086
C	4.417663	-2.483954	-0.807345
C	4.193618	-3.809890	-1.076348
C	3.371908	-4.201536	-2.166484
C	2.796933	-3.191689	-2.986577

C	3.030213	-1.827687	-2.674298
C	-2.524558	2.637270	1.268128
C	-3.838851	2.609460	0.884877
C	-4.237630	3.149446	-0.366548
C	-3.245581	3.692444	-1.228128
C	-1.892047	3.694755	-0.808538
H	6.026196	0.037578	-2.129114
H	-0.588005	4.137116	2.764949
H	5.037039	-2.187324	0.034521
H	4.640582	-4.581647	-0.453381
H	-1.136316	4.104530	-1.473470
H	-4.595183	2.149883	1.518819
H	-2.218111	2.205532	2.216948
H	2.548096	-1.059710	-3.273159
C	2.506378	-2.540559	2.311469
C	3.430375	-1.763505	2.998551
C	3.069367	-0.504804	3.476953
C	1.779470	-0.033660	3.259996
C	0.849960	-0.819984	2.580555
H	2.798549	-3.524909	1.955602
H	4.433466	-2.144101	3.167032
H	3.789054	0.096914	4.025020
H	-0.150280	-0.431207	2.420949
H	1.485266	0.951519	3.612513
C	-0.770713	-3.870296	3.473300
C	-1.110967	-4.890221	4.351505
C	-0.826590	-6.216280	4.025032
C	-0.199679	-6.503039	2.819342
C	0.132091	-5.476084	1.934031
H	0.628567	-5.728257	1.003232
H	-0.970060	-2.835282	3.742805
H	-1.587617	-4.651197	5.297211
H	-1.085889	-7.016077	4.711521
H	0.036618	-7.530056	2.558452
C	-2.959400	-1.091935	-0.845943
C	-3.919260	-0.252296	-1.388837
C	-5.135744	-0.037638	-0.752673
C	-5.353056	-0.641481	0.478218
Br	-3.545237	0.682737	-2.976467
H	-5.875561	0.618838	-1.192696
C	-4.415041	-1.487423	1.055225
H	-4.607679	-1.941174	2.021978
H	-2.023346	-1.259960	-1.367358
Br	-6.937177	-0.207953	1.419452
C	-3.639943	4.213713	-2.489652
C	-4.953653	4.187118	-2.878684
C	-5.942982	3.647318	-2.019074
C	-5.593255	3.149724	-0.789748
H	-2.875600	4.623813	-3.144631
H	-5.243689	4.579711	-3.848332
H	-6.344755	2.731650	-0.121563
H	-6.981310	3.637500	-2.336331
C	1.992843	-3.575678	-4.092728
C	1.755799	-4.899048	-4.359495
C	2.305288	-5.904280	-3.526372
C	3.093697	-5.563684	-2.457222
H	1.558931	-2.795056	-4.712383
H	1.136824	-5.182699	-5.205113
H	2.102477	-6.948948	-3.742046
H	3.526529	-6.332549	-1.821503
C	6.751637	2.604682	-1.830585
C	6.676695	4.124798	-1.957229
H	7.074352	2.155197	-2.776032

H	7.523854	2.348614	-1.091280
C	6.001575	4.718011	-0.722985
H	6.093809	4.394135	-2.847447
H	7.681768	4.536762	-2.093616
C	4.560267	4.222956	-0.632782
H	6.555880	4.415961	0.176850
H	6.015565	5.812127	-0.756952
H	4.078157	4.587465	0.277765
H	3.983824	4.656812	-1.462585
C	3.937523	2.988757	2.444464
C	4.189713	3.801165	3.713023
H	4.714243	3.202475	1.707348
H	4.039381	1.917118	2.666739
C	3.019078	3.661150	4.680833
H	5.125812	3.473027	4.176629
H	4.315235	4.861356	3.453987
C	1.762008	4.245300	4.041748
H	2.862034	2.597740	4.909955
H	3.228053	4.166470	5.629214
H	1.865194	5.338539	3.994573
H	0.881997	4.047968	4.663909

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M06-2X/6-31G* Energy = -8271.56898032

M06-2X/6-31G* Free Energy = -8270.685306

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.54409227

Lowest Frequency = 10.4559

M06-2X/6-31G* Geometry

C	0.849880	-3.391232	-0.027107
C	0.213705	-2.970868	1.334875
C	-0.102223	-4.046031	-0.988994
H	1.264013	-2.484388	-0.486016
H	1.705097	-4.043697	0.176596
C	-0.501514	-3.463104	-2.117342
H	-0.481873	-5.035413	-0.736426
N	-0.937998	-2.151279	0.934760
C	-0.155173	-4.147688	2.244174
C	1.206333	-2.075762	2.088325
C	-2.147547	-2.530985	1.004649
C	-3.207062	-1.701654	0.387172
H	-2.439783	-3.457355	1.510337
H	-0.649313	-0.710966	0.330367
H	-0.145416	-2.472762	-2.402248
H	-1.183907	-3.960574	-2.800928
C	4.444736	2.713451	-0.745083
C	5.443365	1.972172	-1.392859
C	3.287035	2.055162	-0.288335
C	3.091026	0.714591	-0.629846
C	4.063487	-0.037211	-1.287923
C	5.248501	0.608263	-1.624570
C	2.253069	2.716575	0.562190
C	2.549948	3.188961	1.858236
C	1.512582	3.714036	2.642839
C	0.208681	3.734812	2.142840
C	-0.119273	3.237506	0.884591
C	0.933153	2.734562	0.115920
O	1.902675	0.100506	-0.272494
O	0.651999	2.137691	-1.111466
P	0.542717	0.527280	-1.062770
O	-0.551111	0.269528	0.022501
O	0.386274	-0.080408	-2.393808
C	3.825699	-1.471466	-1.609484
C	-1.527618	3.195665	0.419649

C	4.417968	-2.483430	-0.806751
C	4.194235	-3.809407	-1.075810
C	3.372856	-4.201201	-2.166142
C	2.797894	-3.191467	-2.986382
C	3.030807	-1.827420	-2.674024
C	-2.525034	2.637344	1.267646
C	-3.839281	2.609401	0.884250
C	-4.237947	3.149232	-0.367279
C	-3.245840	3.692201	-1.228814
C	-1.892356	3.694662	-0.809073
H	6.026343	0.038123	-2.128422
H	-0.588794	4.137441	2.764538
H	5.037122	-2.186676	0.035233
H	4.641167	-4.581084	-0.452719
H	-1.136570	4.104379	-1.473979
H	-4.595660	2.149795	1.518131
H	-2.218663	2.205771	2.216565
H	2.548676	-1.059520	-3.272975
C	0.849804	-0.820221	2.580340
C	1.779164	-0.033765	3.259851
C	3.069056	-0.504787	3.477027
C	3.430221	-1.763532	2.998812
C	2.506379	-2.540718	2.311679
H	-0.150430	-0.431520	2.420543
H	1.484834	0.951421	3.612247
H	3.788615	0.097061	4.025121
H	2.798647	-3.525099	1.955978
H	4.433312	-2.144045	3.167478
C	-0.770454	-3.870847	3.472983
C	-1.110794	-4.890838	4.351076
C	-0.826514	-6.216886	4.024456
C	-0.199622	-6.503554	2.818734
C	0.132233	-5.476526	1.933533
H	0.628686	-5.728647	1.002705
H	-0.969727	-2.835845	3.742588
H	-1.587434	-4.651880	5.296804
H	-1.085873	-7.016743	4.710852
H	0.036597	-7.530561	2.557731
C	-4.414873	-1.487858	1.055462
C	-5.352941	-0.641877	0.478604
C	-5.135804	-0.038067	-0.752338
C	-3.919434	-0.252790	-1.388713
Br	-6.936906	-0.208288	1.420084
H	-5.875682	0.618393	-1.192263
C	-2.959535	-1.092463	-0.845946
H	-2.023552	-1.260549	-1.367447
H	-4.607367	-1.941569	2.022262
Br	-3.545708	0.682188	-2.976445
C	-3.640121	4.213339	-2.490424
C	-4.953803	4.186684	-2.879543
C	-5.943191	3.646920	-2.019972
C	-5.593543	3.149428	-0.790593
H	-2.875746	4.623438	-3.145364
H	-5.243791	4.579232	-3.849224
H	-6.345052	2.731396	-0.122400
H	-6.981488	3.637063	-2.337326
C	1.994208	-3.575625	-4.092772
C	1.757502	-4.899039	-4.359602
C	2.306930	-5.904163	-3.526304
C	3.094975	-5.563409	-2.456940
H	1.560338	-2.795090	-4.712567
H	1.138853	-5.182823	-5.205415
H	2.104351	-6.948868	-3.742020

H	3.527780	-6.332179	-1.821087
C	6.751574	2.605305	-1.829940
C	6.676684	4.125437	-1.956428
H	7.074350	2.155935	-2.775420
H	7.523735	2.349120	-1.090620
C	6.001244	4.718574	-0.722323
H	6.094049	4.394888	-2.846773
H	7.681805	4.537378	-2.092516
C	4.559920	4.223489	-0.632569
H	6.555314	4.416491	0.177645
H	6.015230	5.812690	-0.756241
H	4.077448	4.588045	0.277762
H	3.983790	4.657260	-1.462629
C	3.936883	2.989476	2.444682
C	4.188821	3.801777	3.713361
H	4.713701	3.203391	1.707727
H	4.038834	1.917819	2.666822
C	3.017990	3.661851	4.680939
H	5.124810	3.473540	4.177120
H	4.314488	4.861971	3.454415
C	1.761116	4.246094	4.041548
H	2.860812	2.598467	4.910080
H	3.226819	4.167201	5.629335
H	1.864545	5.339300	3.994158
H	0.880947	4.049074	4.663573

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M06-2X/6-31G* Energy = -8271.56893766

M06-2X/6-31G* Free Energy = -8270.685551

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.54373574

Lowest Frequency = 8.9993

M06-2X/6-31G* Geometry

C	-1.583070	3.083104	-0.480548
C	-0.989227	2.919613	0.947695
C	-0.719212	3.851587	-1.438506
H	-1.781312	2.080469	-0.880043
H	-2.563118	3.559985	-0.369325
C	-0.193602	3.316014	-2.539276
H	-0.516568	4.896403	-1.202161
N	0.310668	2.261893	0.776255
C	-0.894991	4.237486	1.726240
C	-1.900305	1.958486	1.727554
C	1.407274	2.900734	0.719362
C	2.689642	2.175572	0.579806
H	1.451645	3.991586	0.811766
H	0.354177	0.901724	-0.062831
H	-0.368726	2.275865	-2.812010
H	0.423431	3.907441	-3.210449
C	-3.519731	-3.726236	-1.007234
C	-4.715769	-3.299221	-1.601979
C	-2.573037	-2.763865	-0.602458
C	-2.787305	-1.430958	-0.944467
C	-3.961557	-0.981620	-1.545908
C	-4.928998	-1.936460	-1.833211
C	-1.347592	-3.103666	0.183640
C	-1.445120	-3.646329	1.482864
C	-0.263636	-3.931596	2.180025
C	0.969269	-3.716430	1.563143
C	1.103847	-3.168891	0.286171
C	-0.091655	-2.809069	-0.351882
O	-1.786653	-0.512247	-0.659806
O	-0.049014	-2.147443	-1.573461
P	-0.453497	-0.581908	-1.582320

O	0.602359	0.085779	-0.636121
O	-0.600093	-0.082427	-2.956491
C	-4.125516	0.467542	-1.847263
C	2.461975	-3.050729	-0.310855
C	-3.492777	1.024651	-2.993134
C	-3.558976	2.371437	-3.235554
C	-4.243139	3.238610	-2.344333
C	-4.895345	2.682080	-1.208818
C	-4.823454	1.282002	-0.988295
C	3.397851	-4.092496	-0.033116
C	4.701475	-4.011476	-0.441184
C	5.164122	-2.889993	-1.178334
C	4.227885	-1.876821	-1.515612
C	2.887537	-1.977783	-1.062185
H	-5.860855	-1.613850	-2.292485
H	1.874737	-3.946627	2.120521
H	-2.918550	0.375175	-3.645060
H	-3.050737	2.799078	-4.095626
H	2.224390	-1.152417	-1.277952
H	5.399145	-4.812464	-0.210036
H	3.059014	-4.970238	0.509156
H	-5.281237	0.863985	-0.094688
C	-3.201811	2.367123	2.036916
C	-4.072742	1.516734	2.708049
C	-3.651608	0.245009	3.097128
C	-2.354123	-0.159835	2.807039
C	-1.485492	0.687551	2.122316
H	-3.534215	3.363190	1.752698
H	-5.080218	1.851911	2.938783
H	-4.327741	-0.417532	3.629567
H	-0.488693	0.333352	1.885806
H	-1.997754	-1.140029	3.110136
C	-0.242184	4.230375	2.966503
C	-0.160776	5.379717	3.740537
C	-0.746933	6.564498	3.294898
C	-1.416077	6.579358	2.078064
C	-1.490439	5.424192	1.297340
H	-2.033707	5.462522	0.358002
H	0.195969	3.303033	3.328399
H	0.351453	5.350149	4.697268
H	-0.687927	7.464557	3.898741
H	-1.887524	7.491784	1.726059
C	3.741204	2.741788	-0.143038
C	4.937755	2.043842	-0.247056
C	5.132737	0.826008	0.393754
C	4.079153	0.293397	1.129537
Br	6.334977	2.744648	-1.306325
H	6.072066	0.291951	0.304238
C	2.854870	0.940347	1.214642
H	2.041408	0.501264	1.781859
H	3.621431	3.698744	-0.640354
Br	4.336111	-1.347526	2.019812
C	4.668340	-0.753572	-2.266537
C	5.978742	-0.640497	-2.656754
C	6.913925	-1.646424	-2.306573
C	6.514600	-2.746457	-1.589634
H	3.945359	0.020416	-2.515170
H	6.306590	0.228990	-3.217490
H	7.227428	-3.523480	-1.325326
H	7.949908	-1.544956	-2.615276
C	-5.525673	3.554374	-0.281765
C	-5.482815	4.914566	-0.456444
C	-4.822999	5.468993	-1.582538

C	-4.227252	4.649122	-2.507494
H	-6.023432	3.121452	0.582980
H	-5.955441	5.572818	0.266157
H	-4.795586	6.546872	-1.710537
H	-3.713348	5.066346	-3.369581
C	-5.810184	-4.278528	-1.984791
C	-5.313449	-5.715045	-2.131575
H	-6.291008	-3.941327	-2.909503
H	-6.587446	-4.249503	-1.207984
C	-4.443826	-6.090073	-0.934244
H	-4.718550	-5.809303	-3.049099
H	-6.165668	-6.395265	-2.228672
C	-3.199095	-5.206885	-0.900359
H	-5.020661	-5.956420	-0.008172
H	-4.148418	-7.143169	-0.979609
H	-2.596878	-5.416021	-0.012671
H	-2.557530	-5.463386	-1.755652
C	-2.802292	-3.818037	2.146720
C	-2.754273	-4.673877	3.411561
H	-3.529044	-4.236229	1.446851
H	-3.189274	-2.818413	2.390932
C	-1.601012	-4.240557	4.311212
H	-3.712478	-4.603677	3.936339
H	-2.616215	-5.728613	3.136890
C	-0.278335	-4.487113	3.591361
H	-1.704013	-3.172902	4.548272
H	-1.617692	-4.782844	5.261987
H	0.557208	-4.057740	4.155055
H	-0.095662	-5.570099	3.548554

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M06-2X/6-31G* Energy = -8271.56237056

M06-2X/6-31G* Free Energy = -8270.680714

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.54138666

Lowest Frequency = 7.8992

M06-2X/6-31G* Geometry

C	2.926466	1.648004	-1.316176
C	3.560085	0.257181	-0.968029
C	2.830099	2.598845	-0.153963
H	1.933214	1.446738	-1.734264
H	3.512206	2.087461	-2.129618
C	1.738775	2.710806	0.604494
H	3.691309	3.226578	0.069229
N	2.695060	-0.260627	0.115277
C	3.467884	-0.691630	-2.167305
C	5.023275	0.320568	-0.522771
C	2.929288	-0.039475	1.354574
C	2.016777	-0.330887	2.461922
H	3.898866	0.382486	1.618783
H	1.677179	-0.578115	-0.248113
H	0.838944	2.130220	0.400070
H	1.690967	3.423263	1.423310
C	-4.682631	1.588072	-1.338331
C	-4.660586	2.948390	-1.670687
C	-3.493912	0.964668	-0.899935
C	-2.287160	1.672196	-0.959498
C	-2.246933	3.026784	-1.308682
C	-3.452355	3.645843	-1.620637
C	-3.486362	-0.435486	-0.380010
C	-4.275945	-0.832298	0.720972
C	-4.275859	-2.179138	1.111234
C	-3.401264	-3.073467	0.491772
C	-2.518250	-2.679976	-0.508582

C	-2.616554	-1.359721	-0.961470
O	-1.114811	1.035575	-0.604439
O	-1.816501	-0.942488	-2.002963
P	-0.471540	-0.094953	-1.629872
O	0.385462	-0.937582	-0.696939
O	0.093014	0.494021	-2.860929
C	-0.977387	3.802556	-1.373254
C	-1.460133	-3.598870	-0.991366
C	-0.020749	3.515685	-2.387916
C	1.105803	4.284640	-2.512643
C	1.364212	5.362192	-1.625330
C	0.419136	5.644530	-0.600934
C	-0.754253	4.849598	-0.509187
C	-0.684501	-4.291949	-0.018983
C	0.306703	-5.157876	-0.395504
C	0.588096	-5.384702	-1.769202
C	-0.170276	-4.680690	-2.746528
C	-1.189238	-3.788597	-2.326441
H	-3.436756	4.700706	-1.887192
H	-3.367677	-4.104334	0.839883
H	-0.192295	2.674037	-3.051174
H	1.827240	4.068355	-3.297735
H	-1.757664	-3.249490	-3.078358
H	0.897934	-5.679064	0.353375
H	-0.876455	-4.088291	1.032050
H	-1.483112	5.075209	0.266583
C	5.625820	-0.847840	-0.036281
C	6.960800	-0.856716	0.343282
C	7.728558	0.302403	0.226043
C	7.147529	1.459692	-0.275477
C	5.801509	1.470039	-0.645226
H	5.038215	-1.760979	0.027651
H	7.407939	-1.771944	0.718443
H	8.774360	0.296569	0.516270
H	5.373413	2.384124	-1.041311
H	7.737222	2.364769	-0.382000
C	2.923048	-1.972314	-2.068505
C	2.905694	-2.817828	-3.175743
C	3.431921	-2.394916	-4.389921
C	3.991525	-1.123245	-4.491350
C	4.015988	-0.282455	-3.385777
H	4.480647	0.696059	-3.471884
H	2.480220	-2.324619	-1.142509
H	2.477431	-3.810092	-3.080890
H	3.406922	-3.055164	-5.251526
H	4.413225	-0.783786	-5.432328
C	2.516055	-0.163946	3.758963
C	1.688214	-0.425199	4.841909
C	0.372440	-0.840763	4.662814
C	-0.101398	-0.990933	3.362828
Br	2.357867	-0.211029	6.594174
H	-0.265643	-1.038471	5.516315
C	0.696787	-0.744509	2.257242
H	0.285922	-0.867165	1.257577
H	3.537141	0.164544	3.923988
Br	-1.875681	-1.537282	3.029605
C	0.115798	-4.893548	-4.122170
C	1.101918	-5.765391	-4.507956
C	1.854865	-6.468266	-3.534226
C	1.603991	-6.279475	-2.198460
H	-0.459697	-4.344748	-4.862669
H	1.311373	-5.919632	-5.562048
H	2.180002	-6.813790	-1.446952

H	2.633242	-7.155681	-3.850880
C	0.683305	6.706439	0.303775
C	1.832378	7.448426	0.199876
C	2.773618	7.166705	-0.820355
C	2.541504	6.149619	-1.711115
H	-0.043323	6.919432	1.084005
H	2.024213	8.257148	0.898423
H	3.678319	7.762465	-0.894769
H	3.258372	5.929327	-2.498670
C	-5.915679	3.702308	-2.069940
C	-7.041409	2.789858	-2.549668
H	-6.269902	4.273571	-1.199960
H	-5.664839	4.441839	-2.838263
C	-7.214256	1.628969	-1.574281
H	-6.797161	2.389936	-3.542279
H	-7.969024	3.362533	-2.651583
C	-5.949371	0.774528	-1.548720
H	-7.414614	2.024728	-0.568376
H	-8.072432	1.008103	-1.851545
H	-6.040437	-0.019113	-0.804473
H	-5.848474	0.258787	-2.514745
C	-4.988226	0.201159	1.575918
C	-6.107934	-0.389697	2.428755
H	-5.360311	1.033014	0.975020
H	-4.223576	0.632976	2.240419
C	-5.591921	-1.595374	3.209063
H	-6.497680	0.376559	3.106757
H	-6.940602	-0.701715	1.782627
C	-5.153439	-2.691461	2.239687
H	-4.737128	-1.284048	3.824970
H	-6.355310	-1.983231	3.891304
H	-6.047170	-3.160140	1.804603
H	-4.622192	-3.486970	2.775962

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M06-2X/6-31G* Energy = -8271.56780128

M06-2X/6-31G* Free Energy = -8270.683336

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.54416200

Lowest Frequency = 12.8545

M06-2X/6-31G* Geometry

C	0.863821	-0.895805	2.478212
C	0.493224	-2.297314	1.884783
C	-0.238157	-0.219234	3.248390
H	1.155283	-0.270080	1.627125
H	1.759891	-1.020374	3.095141
C	-1.126934	0.590915	2.673992
H	-0.316241	-0.416211	4.315943
N	-0.605850	-2.036355	0.945295
C	1.699086	-2.825133	1.094100
C	0.142413	-3.349317	2.943963
C	-1.819907	-2.178410	1.299200
C	-2.961703	-1.849662	0.424429
H	-2.079936	-2.564256	2.290232
H	-0.310603	-0.905549	-0.171108
H	-1.088091	0.809905	1.607720
H	-1.917906	1.069346	3.246947
C	0.994707	3.300818	1.899906
C	-0.304075	3.690710	2.250335
C	1.245759	2.890955	0.574163
C	0.168669	2.695080	-0.291352
C	-1.154127	3.000410	0.057527
C	-1.332634	3.574891	1.316963
C	2.634243	2.660819	0.069624

C	3.591734	3.700404	0.095961
C	4.908536	3.423771	-0.292303
C	5.234164	2.146746	-0.749418
C	4.290778	1.132645	-0.884139
C	2.986222	1.422036	-0.471086
O	0.441080	2.138798	-1.533916
O	2.025537	0.419721	-0.534484
P	0.772602	0.556235	-1.564714
O	-0.408851	-0.059400	-0.742293
O	1.019600	0.084269	-2.931111
C	-2.332169	2.665855	-0.784021
C	4.700411	-0.170930	-1.467376
C	-2.285887	2.676361	-2.209998
C	-3.394415	2.362216	-2.948938
C	-4.636094	2.065290	-2.328528
C	-4.701400	2.069128	-0.909381
C	-3.524011	2.339322	-0.168768
C	4.072987	-0.666027	-2.644895
C	4.532919	-1.807486	-3.245125
C	5.615964	-2.541918	-2.695393
C	6.234883	-2.060969	-1.508461
C	5.760329	-0.859379	-0.924305
H	-2.330934	3.893876	1.605954
H	6.253770	1.943154	-1.069343
H	-1.361434	2.933208	-2.711085
H	-3.339557	2.356489	-4.034423
H	6.237949	-0.491783	-0.018563
H	4.056207	-2.174541	-4.150866
H	3.231372	-0.129534	-3.070458
H	-3.580820	2.278291	0.915247
C	-0.338036	-4.592435	2.508626
C	-0.628181	-5.604741	3.412290
C	-0.426854	-5.402308	4.778122
C	0.071302	-4.184285	5.220730
C	0.352586	-3.164545	4.309279
H	-0.472475	-4.762885	1.443037
H	-1.001366	-6.558123	3.051274
H	-0.648756	-6.193768	5.486959
H	0.756583	-2.229218	4.680951
H	0.246026	-4.018027	6.279282
C	2.859105	-3.170494	1.796255
C	3.958758	-3.701782	1.135862
C	3.915921	-3.908532	-0.241929
C	2.773404	-3.554008	-0.948631
C	1.670534	-3.013222	-0.287087
H	0.782256	-2.762273	-0.857762
H	2.887880	-3.052571	2.877136
H	4.848959	-3.969525	1.697469
H	4.768730	-4.341428	-0.756842
H	2.732240	-3.697348	-2.023692
C	-2.821183	-1.684822	-0.956869
C	-3.939189	-1.376907	-1.717418
C	-5.203333	-1.258557	-1.147911
C	-5.322575	-1.441513	0.224443
Br	-3.743980	-1.130580	-3.577024
H	-6.065530	-1.013956	-1.757273
C	-4.221978	-1.733820	1.017204
H	-4.343289	-1.872146	2.086925
H	-1.857714	-1.792556	-1.437469
Br	-7.025572	-1.293825	1.031694
C	7.285798	-2.816542	-0.925066
C	7.695257	-3.998955	-1.487117
C	7.080107	-4.477486	-2.670772

C	6.069609	-3.761666	-3.262073
H	7.751916	-2.445592	-0.015579
H	8.494006	-4.573578	-1.028323
H	5.592006	-4.124524	-4.168826
H	7.413403	-5.413900	-3.107395
C	-5.945714	1.806720	-0.276143
C	-7.071895	1.562174	-1.019791
C	-7.001459	1.538221	-2.435150
C	-5.808667	1.772678	-3.072480
H	-5.989871	1.789541	0.810504
H	-8.015743	1.358351	-0.524024
H	-7.896890	1.330871	-3.013254
H	-5.744496	1.747419	-4.157274
C	-0.631566	4.223516	3.632132
C	0.373903	3.774361	4.688778
H	-1.645874	3.913759	3.908089
H	-0.645172	5.321972	3.595132
C	1.791640	4.051128	4.195784
H	0.259199	2.696617	4.866055
H	0.177221	4.286128	5.636314
C	2.085559	3.216573	2.951691
H	1.892516	5.119641	3.958776
H	2.529406	3.824701	4.972258
H	2.159527	2.157385	3.243095
H	3.061035	3.476861	2.533973
C	3.183008	5.123955	0.439733
C	4.361910	6.013743	0.827033
H	2.426444	5.142236	1.226268
H	2.691112	5.546790	-0.448377
C	5.473050	5.899552	-0.211766
H	4.021020	7.049295	0.926498
H	4.749192	5.706655	1.808818
C	6.005986	4.469902	-0.232443
H	5.071079	6.160461	-1.199246
H	6.287373	6.599468	0.001174
H	6.599874	4.299842	0.676822
H	6.689686	4.323348	-1.075549

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M06-2X/6-31G* Energy = -8271.56780121

M06-2X/6-31G* Free Energy = -8270.683334

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.54415789

Lowest Frequency = 12.8614

M06-2X/6-31G* Geometry

C	0.864299	-0.895663	2.478688
C	0.493495	-2.297056	1.885065
C	-0.237647	-0.219032	3.248807
H	1.155909	-0.269943	1.627652
H	1.760320	-1.020437	3.095653
C	-1.125950	0.591638	2.674409
H	-0.316183	-0.416486	4.316238
N	-0.605340	-2.035855	0.945452
C	1.699361	-2.824978	1.094473
C	0.142299	-3.349055	2.944109
C	-1.819495	-2.177244	1.299304
C	-2.961255	-1.848599	0.424437
H	-2.079721	-2.562704	2.290439
H	-0.310737	-0.905197	-0.170835
H	-1.086640	0.810977	1.608233
H	-1.916982	1.070117	3.247238
C	3.591574	3.700476	0.095447
C	4.908432	3.423736	-0.292584
C	2.634091	2.660900	0.069294

C	2.986121	1.421968	-0.471060
C	4.290678	1.132488	-0.883983
C	5.234070	2.146627	-0.749412
C	1.245572	2.891153	0.573642
C	0.994422	3.301332	1.899299
C	-0.304389	3.691193	2.249529
C	-1.332890	3.575031	1.316100
C	-1.154290	3.000233	0.056844
C	0.168601	2.695009	-0.291927
O	2.025407	0.419595	-0.534279
O	0.441231	2.138596	-1.534375
P	0.772750	0.555994	-1.564875
O	-0.409058	-0.059474	-0.742792
O	1.020199	0.083846	-2.931131
C	4.700498	-0.171137	-1.466983
C	-2.332315	2.665248	-0.784561
C	4.073482	-0.666299	-2.644683
C	4.533795	-1.807660	-3.244828
C	5.616780	-2.541941	-2.694790
C	6.235219	-2.060973	-1.507612
C	5.760323	-0.859471	-0.923577
C	-2.286067	2.674946	-2.210540
C	-3.394657	2.360540	-2.949295
C	-4.636370	2.064143	-2.328720
C	-4.701613	2.068679	-0.909573
C	-3.524184	2.339114	-0.169136
H	6.253693	1.942945	-1.069221
H	-2.331216	3.894003	1.605007
H	3.231877	-0.129941	-3.070440
H	4.057428	-2.174745	-4.150738
H	-3.581010	2.278620	0.914905
H	-3.339786	2.354220	-4.034776
H	-1.361618	2.931428	-2.711817
H	6.237618	-0.491812	-0.017689
C	-0.338583	-4.591955	2.508652
C	-0.629049	-5.604254	3.412227
C	-0.427618	-5.402027	4.778070
C	0.070979	-4.184222	5.220792
C	0.352593	-3.164493	4.309438
H	-0.473111	-4.762258	1.443051
H	-1.002571	-6.557471	3.051124
H	-0.649780	-6.193481	5.486833
H	0.756946	-2.229342	4.681181
H	0.245790	-4.018132	6.279355
C	1.671014	-3.012570	-0.286785
C	2.773805	-3.553531	-0.948301
C	3.916081	-3.908661	-0.241506
C	3.958747	-3.702348	1.136353
C	2.859139	-3.170923	1.796724
H	2.887761	-3.053334	2.877646
H	0.782934	-2.761144	-0.857560
H	2.732743	-3.696527	-2.023407
H	4.768833	-4.341694	-0.756395
H	4.848767	-3.970537	1.698034
C	-2.821121	-1.684509	-0.957002
C	-3.939419	-1.377291	-1.717392
C	-5.203448	-1.258815	-1.147646
C	-5.322303	-1.440968	0.224833
Br	-3.744904	-1.132223	-3.577256
H	-6.065827	-1.014728	-1.756958
C	-4.221423	-1.732643	1.017441
H	-4.342453	-1.870485	2.087257
H	-1.857774	-1.792277	-1.437822

Br	-7.025101	-1.293171	1.032473
C	-5.945928	1.806731	-0.276136
C	-7.072175	1.561977	-1.019604
C	-7.001822	1.537395	-2.434964
C	-5.809040	1.771394	-3.072473
H	-5.990016	1.790103	0.810522
H	-8.016025	1.358493	-0.523699
H	-5.744939	1.745637	-4.157258
H	-7.897322	1.329933	-3.012920
C	7.286053	-2.816424	-0.923903
C	7.695898	-3.998725	-1.485896
C	7.081243	-4.477266	-2.669809
C	6.070835	-3.761573	-3.261406
H	7.751790	-2.445461	-0.014226
H	8.494579	-4.573255	-1.026867
H	7.414852	-5.413590	-3.106387
H	5.593608	-4.124442	-4.168352
C	6.005875	4.469861	-0.232657
C	5.472939	5.899519	-0.212700
H	6.599333	4.300145	0.676957
H	6.689969	4.322980	-1.075385
C	4.361592	6.014106	0.825846
H	5.071160	6.160011	-1.200367
H	6.287209	6.599532	0.000124
C	3.182782	5.124144	0.438671
H	4.748705	5.707421	1.807822
H	4.020664	7.049692	0.924839
H	2.426055	5.142702	1.225043
H	2.691063	5.546633	-0.449703
C	2.085208	3.217523	2.951182
C	1.791171	4.052699	4.194829
H	3.060716	3.477600	2.533416
H	2.159114	2.158473	3.243104
C	0.373500	3.775896	4.687992
H	2.528984	3.826852	4.971428
H	1.891832	5.121096	3.957208
C	-0.632126	4.224275	3.631168
H	0.259058	2.698216	4.865838
H	0.176729	4.288091	5.635280
H	-0.646262	5.322711	3.593805
H	-1.646289	3.914123	3.907217

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M06-2X/6-31G* Energy = -8271.57277421

M06-2X/6-31G* Free Energy = -8270.686886

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.54553525

Lowest Frequency = 11.5141

M06-2X/6-31G* Geometry

C	-0.715200	3.565658	1.227676
C	-0.936563	3.553847	-0.316405
C	-1.912959	3.125073	2.026145
H	0.122474	2.897508	1.449639
H	-0.390220	4.578336	1.498882
C	-1.910952	2.038472	2.796046
H	-2.828405	3.711255	1.938497
N	-1.471254	2.214155	-0.628788
C	-1.855945	4.675206	-0.817417
C	0.431893	3.697708	-1.002513
C	-2.712991	2.031637	-0.821166
C	-3.285706	0.705237	-1.128316
H	-3.428626	2.860014	-0.788350
H	-0.634008	0.908887	-0.052248
H	-1.015138	1.429117	2.901522

H	-2.791697	1.727641	3.352963
C	4.320818	-3.166617	0.547035
C	5.590451	-2.574461	0.536069
C	3.190266	-2.372120	0.258199
C	3.344704	-0.989838	0.111807
C	4.602126	-0.373191	0.121984
C	5.705399	-1.205037	0.300397
C	1.830175	-2.983844	0.150008
C	1.523131	-3.978030	-0.803895
C	0.258341	-4.578252	-0.768843
C	-0.694478	-4.136950	0.150609
C	-0.468944	-3.069411	1.014771
C	0.820538	-2.526800	0.992273
O	2.215465	-0.212678	-0.121451
O	1.100937	-1.423548	1.792100
P	1.099352	-0.000530	1.037155
O	-0.233778	0.008650	0.211960
O	1.343283	1.106364	1.977474
C	4.804218	1.091279	-0.022133
C	-1.573783	-2.471448	1.804401
C	5.804350	1.574983	-0.913569
C	6.082338	2.913876	-1.002608
C	5.372702	3.858411	-0.213949
C	4.357122	3.383418	0.659079
C	4.101735	1.992444	0.744021
C	-2.866798	-2.417079	1.209419
C	-3.921197	-1.821351	1.846225
C	-3.752275	-1.234004	3.127084
C	-2.473019	-1.304375	3.744831
C	-1.400619	-1.932330	3.060682
H	6.693909	-0.750446	0.316797
H	-1.673739	-4.610411	0.148504
H	6.345686	0.862799	-1.530913
H	6.850062	3.271041	-1.684911
H	-0.429160	-1.966304	3.543043
H	-4.896426	-1.767251	1.367966
H	-2.992547	-2.826060	0.212683
H	3.344578	1.655089	1.443868
C	1.129419	2.607130	-1.526222
C	2.369487	2.784880	-2.137938
C	2.926156	4.053895	-2.241185
C	2.248594	5.144634	-1.700771
C	1.014828	4.966536	-1.085986
H	0.715006	1.607358	-1.478583
H	2.900318	1.919392	-2.523376
H	3.890412	4.191447	-2.719968
H	0.486361	5.827153	-0.683327
H	2.686390	6.136791	-1.752193
C	-2.108743	4.750296	-2.195008
C	-2.920974	5.743725	-2.722559
C	-3.492980	6.698798	-1.880658
C	-3.238837	6.645835	-0.516942
C	-2.426992	5.639135	0.011751
H	-2.237832	5.628418	1.079580
H	-1.646050	4.019979	-2.854971
H	-3.100951	5.781735	-3.792509
H	-4.124674	7.480774	-2.290257
H	-3.668945	7.388641	0.147812
C	-2.520269	-0.299121	-1.729103
C	-3.127962	-1.505127	-2.041986
C	-4.471980	-1.745983	-1.768945
C	-5.202737	-0.740897	-1.149755
Br	-2.099235	-2.897068	-2.801831

H	-4.928436	-2.698940	-2.009478
C	-4.634266	0.487624	-0.842955
H	-5.230547	1.260393	-0.368633
H	-1.471092	-0.138138	-1.947736
Br	-6.996105	-1.079407	-0.662496
C	-2.297526	-0.718769	5.027583
C	-3.337997	-0.084994	5.656994
C	-4.609553	-0.007209	5.035413
C	-4.810518	-0.570315	3.800504
H	-1.317415	-0.771885	5.494191
H	-3.190644	0.364969	6.633810
H	-5.782439	-0.516819	3.315559
H	-5.424445	0.499377	5.543391
C	3.609653	4.314648	1.427326
C	3.869243	5.657988	1.336999
C	4.887289	6.132081	0.472525
C	5.619457	5.253972	-0.286463
H	2.824368	3.933758	2.075797
H	3.292125	6.366552	1.923454
H	5.084944	7.198339	0.412136
H	6.398013	5.614883	-0.954430
C	6.856265	-3.378303	0.768318
C	6.606457	-4.698997	1.491491
H	7.577338	-2.765539	1.320029
H	7.317002	-3.590202	-0.206982
C	5.441964	-5.432008	0.832298
H	6.360127	-4.505216	2.543428
H	7.515225	-5.309243	1.479620
C	4.159101	-4.616407	0.974521
H	5.665891	-5.587388	-0.232495
H	5.298257	-6.421770	1.277487
H	3.340615	-5.100820	0.438408
H	3.853967	-4.612724	2.031150
C	2.499231	-4.288538	-1.925934
C	2.169281	-5.572211	-2.685306
H	3.528341	-4.318878	-1.559422
H	2.463539	-3.439636	-2.624131
C	0.682674	-5.622312	-3.028222
H	2.784996	-5.630480	-3.588483
H	2.423103	-6.444358	-2.066977
C	-0.130420	-5.677004	-1.738137
H	0.408897	-4.720607	-3.594407
H	0.451416	-6.486260	-3.659295
H	0.024138	-6.653548	-1.258367
H	-1.203284	-5.604050	-1.950366

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M06-2X/6-31G* Energy = -8271.57277353

M06-2X/6-31G* Free Energy = -8270.686883

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.54552628

Lowest Frequency = 11.6264

M06-2X/6-31G* Geometry

C	-0.714087	3.565578	1.227048
C	-0.934701	3.553366	-0.317208
C	-1.912711	3.126541	2.025019
H	0.122715	2.896540	1.449570
H	-0.388134	4.578015	1.497968
C	-1.912668	2.039052	2.793674
H	-2.827068	3.714507	1.938009
N	-1.470276	2.213995	-0.629254
C	-1.853119	4.675165	-0.819100
C	0.434117	3.696113	-1.002780
C	-2.712286	2.032359	-0.820702

C	-3.286246	0.706365	-1.127275
H	-3.427243	2.861304	-0.787419
H	-0.633727	0.907179	-0.054858
H	-1.017924	1.428029	2.898520
H	-2.793927	1.729022	3.350244
C	1.523082	-3.978144	-0.804644
C	0.258284	-4.578371	-0.769630
C	1.830248	-2.984229	0.149498
C	0.820579	-2.527327	0.991828
C	-0.468919	-3.069896	1.014306
C	-0.694424	-4.137394	0.150067
C	3.190399	-2.372657	0.257865
C	4.320866	-3.167368	0.546629
C	5.590510	-2.575314	0.536046
C	5.705637	-1.205790	0.300795
C	4.602509	-0.373803	0.122385
C	3.345022	-0.990398	0.111811
O	1.100882	-1.424107	1.791752
O	2.215888	-0.213132	-0.121466
P	1.099506	-0.001092	1.036832
O	-0.233417	0.007609	0.211321
O	1.343031	1.105771	1.977275
C	-1.573895	-2.471885	1.803768
C	4.804595	1.090700	-0.021219
C	-2.866901	-2.418256	1.208639
C	-3.921527	-1.822482	1.845008
C	-3.752863	-1.234249	3.125475
C	-2.473693	-1.303975	3.743454
C	-1.401035	-1.932050	3.059796
C	5.805193	1.574735	-0.911956
C	6.083240	2.913655	-1.000389
C	5.373165	3.857935	-0.211819
C	4.357092	3.382632	0.660461
C	4.101672	1.991630	0.744812
H	-1.673636	-4.610939	0.147947
H	6.694209	-0.751345	0.317562
H	-2.992405	-2.827745	0.212082
H	-4.896787	-1.768917	1.366782
H	3.344151	1.654093	1.444170
H	6.851351	3.271027	-1.682149
H	6.346883	0.862785	-1.529263
H	-0.429644	-1.965524	3.542319
C	1.130803	2.605072	-1.526651
C	2.371174	2.781889	-2.138031
C	2.928955	4.050450	-2.240924
C	2.252159	5.141652	-1.700507
C	1.018151	4.964453	-1.085937
H	0.715541	1.605635	-1.479386
H	2.901345	1.916025	-2.523537
H	3.893445	4.187271	-2.719446
H	0.490383	5.825472	-0.683220
H	2.690769	6.133468	-1.751621
C	-2.423054	5.640433	0.009276
C	-3.233771	6.647621	-0.520221
C	-3.487912	6.699737	-1.883967
C	-2.917085	5.743265	-2.725078
C	-2.105965	4.749352	-2.196732
H	-1.644200	4.017926	-2.856116
H	-2.233941	5.630348	1.077116
H	-3.662999	7.391470	0.143935
H	-4.118695	7.482117	-2.294200
H	-3.097104	5.780543	-3.795048
C	-2.521811	-0.298771	-1.728085

C	-3.130496	-1.504415	-2.040356
C	-4.474639	-1.744122	-1.766902
C	-5.204392	-0.738268	-1.147780
Br	-2.102874	-2.897505	-2.799658
H	-4.931915	-2.696796	-2.007006
C	-4.634860	0.489870	-0.841389
H	-5.230350	1.263167	-0.366934
H	-1.472599	-0.138688	-1.947226
Br	-6.997915	-1.075179	-0.659932
C	3.609148	4.313568	1.428612
C	3.868726	5.656947	1.338862
C	4.887274	6.131349	0.475145
C	5.619920	5.253525	-0.283714
H	2.823501	3.932398	2.076483
H	3.291224	6.365312	1.925182
H	6.398852	5.614702	-0.951098
H	5.084935	7.197633	0.415229
C	-2.298587	-0.717531	5.025880
C	-3.339317	-0.083567	5.654676
C	-4.610768	-0.006349	5.032786
C	-4.811371	-0.570266	3.798192
H	-1.318563	-0.770136	5.492729
H	-3.192228	0.367042	6.631235
H	-5.425825	0.500459	5.540279
H	-5.783150	-0.517216	3.312887
C	-0.130604	-5.676786	-1.739248
C	0.682235	-5.621550	-3.029466
H	-1.203527	-5.603833	-1.951233
H	0.024097	-6.653499	-1.259866
C	2.168921	-5.571601	-2.686801
H	0.408302	-4.719598	-3.595181
H	0.450856	-6.485241	-3.660846
C	2.498974	-4.288220	-1.926983
H	2.422867	-6.444012	-2.068893
H	2.784456	-5.629479	-3.590127
H	2.463039	-3.439083	-2.624889
H	3.528167	-4.318565	-1.560704
C	4.158954	-4.617302	0.973514
C	5.441806	-5.432917	0.831231
H	3.340588	-5.101464	0.436981
H	3.853547	-4.614039	2.030065
C	6.606239	-4.700250	1.490910
H	5.297957	-6.422840	1.276019
H	5.665908	-5.587903	-0.233583
C	6.856255	-3.379253	0.768353
H	6.359777	-4.506918	2.542900
H	7.514968	-5.310554	1.478892
H	7.317324	-3.590726	-0.206885
H	7.577134	-2.766711	1.320566

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M06-2X/6-31G* Energy = -8271.57153530

M06-2X/6-31G* Free Energy = -8270.686744

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.54417891

Lowest Frequency = 8.1939

M06-2X/6-31G* Geometry

C	3.866257	-1.257011	1.365748
C	3.721362	-1.708209	-0.122351
C	3.418010	-2.284332	2.369906
H	3.269697	-0.343148	1.471704
H	4.907163	-0.961456	1.547589
C	2.264022	-2.230906	3.032711
H	4.085203	-3.123942	2.553585

N	2.272182	-1.730656	-0.379920
C	4.364448	-0.667770	-1.058518
C	4.418477	-3.040211	-0.444894
C	1.593478	-2.797197	-0.232265
C	0.151889	-2.897803	-0.534747
H	2.074274	-3.734174	0.065374
H	1.582555	-0.289904	-0.252003
H	1.549003	-1.425246	2.888182
H	2.004112	-3.006777	3.748342
C	-0.915090	4.553981	-1.225812
C	0.305095	5.143770	-1.584065
C	-0.940734	3.662731	-0.133565
C	0.261901	3.291133	0.461951
C	1.507137	3.802090	0.078338
C	1.476414	4.774061	-0.921436
C	-2.211027	3.078164	0.395583
C	-3.243800	3.912209	0.876734
C	-4.461939	3.337124	1.259556
C	-4.604062	1.950947	1.222968
C	-3.566849	1.092564	0.863680
C	-2.368316	1.688875	0.456347
O	0.202320	2.313306	1.448606
O	-1.319520	0.872669	0.050863
P	0.050363	0.800678	0.917676
O	1.134404	0.637525	-0.201816
O	0.057014	-0.166305	2.027032
C	2.791461	3.273477	0.605769
C	-3.789243	-0.374046	0.962968
C	3.916707	3.234931	-0.268273
C	5.117538	2.721326	0.136612
C	5.268338	2.154896	1.427519
C	4.157143	2.186240	2.312340
C	2.940193	2.777497	1.885555
C	-2.926275	-1.204390	1.732750
C	-3.241748	-2.521407	1.945041
C	-4.416171	-3.096531	1.391989
C	-5.251827	-2.285761	0.573494
C	-4.912951	-0.922591	0.386441
H	2.409117	5.244894	-1.222442
H	-5.543150	1.509251	1.548723
H	3.807726	3.585029	-1.289798
H	5.958393	2.696842	-0.548973
H	-5.558456	-0.302676	-0.232366
H	-2.588577	-3.145994	2.549798
H	-2.028484	-0.784853	2.174221
H	2.114752	2.806678	2.587327
C	4.106235	-3.703290	-1.638918
C	4.775647	-4.861455	-2.013113
C	5.791859	-5.374290	-1.208524
C	6.134285	-4.708870	-0.037889
C	5.453881	-3.551148	0.338964
H	3.335349	-3.296955	-2.288662
H	4.510538	-5.358867	-2.940977
H	6.317504	-6.278275	-1.499408
H	5.753810	-3.040014	1.248069
H	6.934667	-5.086642	0.590917
C	3.646835	-0.000274	-2.050072
C	4.295694	0.854120	-2.943217
C	5.669633	1.042169	-2.868218
C	6.395163	0.379805	-1.877753
C	5.747045	-0.458520	-0.980854
H	6.329977	-0.983168	-0.227964
H	2.577455	-0.147102	-2.145139

H	3.715614	1.361683	-3.708153
H	6.174916	1.693930	-3.574658
H	7.471083	0.513794	-1.806638
C	-0.472092	-4.122635	-0.287162
C	-1.793611	-4.308658	-0.669184
C	-2.527963	-3.294198	-1.272643
C	-1.891223	-2.077129	-1.502396
Br	-2.588022	-6.001110	-0.406605
H	-3.563196	-3.447190	-1.556825
C	-0.561216	-1.871370	-1.164226
H	-0.090809	-0.928842	-1.416312
H	0.076639	-4.936512	0.175720
Br	-2.839107	-0.689839	-2.359400
C	-6.405019	-2.863104	-0.021673
C	-6.722547	-4.178802	0.201185
C	-5.904015	-4.979483	1.034317
C	-4.779257	-4.449996	1.613984
H	-7.033268	-2.240186	-0.653362
H	-7.606597	-4.611219	-0.257275
H	-4.136553	-5.065529	2.237952
H	-6.166103	-6.019266	1.204353
C	4.281593	1.579292	3.591953
C	5.450234	0.967389	3.966015
C	6.560916	0.944888	3.084675
C	6.471089	1.527569	1.845660
H	3.423680	1.589661	4.259156
H	5.528901	0.494232	4.939772
H	7.482589	0.462384	3.396079
H	7.313905	1.509369	1.158460
C	0.393080	6.193134	-2.677063
C	-0.779563	6.145650	-3.653432
H	1.343850	6.083561	-3.210110
H	0.420136	7.184869	-2.203817
C	-2.093616	6.080234	-2.879982
H	-0.694616	5.256918	-4.292087
H	-0.752236	7.019990	-4.311660
C	-2.158530	4.790951	-2.064867
H	-2.164502	6.946996	-2.207787
H	-2.950907	6.129908	-3.558949
H	-2.254182	3.937112	-2.751649
H	-3.060791	4.771534	-1.449953
C	-3.006381	5.399017	1.087100
C	-4.298729	6.206813	1.178142
H	-2.354606	5.812707	0.315495
H	-2.449699	5.509239	2.029243
C	-5.246166	5.568987	2.189867
H	-4.066349	7.240181	1.455027
H	-4.785079	6.238991	0.192901
C	-5.643156	4.174483	1.713165
H	-4.739920	5.499183	3.161282
H	-6.140836	6.182805	2.335437
H	-6.341349	4.274076	0.869970
H	-6.186978	3.637419	2.497784

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M06-2X/6-31G* Energy = -8271.57295407

M06-2X/6-31G* Free Energy = -8270.688384

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.54391561

Lowest Frequency = 11.9162

M06-2X/6-31G* Geometry

C	-0.564868	3.533081	1.401988
C	-0.746029	3.564676	-0.153531
C	-1.824134	3.253000	2.180299

H	0.179234	2.761174	1.620967
H	-0.115121	4.488324	1.696003
C	-2.209405	2.025913	2.530743
H	-2.457923	4.095396	2.453006
N	-1.327067	2.258583	-0.505452
C	-1.598254	4.738035	-0.654158
C	0.640395	3.671072	-0.811241
C	-2.583126	2.137783	-0.655155
C	-3.245852	0.861027	-0.984983
H	-3.251544	3.000630	-0.573928
H	-0.480575	0.952666	0.027699
H	-1.615684	1.146224	2.282598
H	-3.128695	1.847892	3.082822
C	1.395774	-4.007478	-0.735330
C	0.114188	-4.557051	-0.605027
C	1.809401	-3.017540	0.182768
C	0.877386	-2.508892	1.082698
C	-0.426564	-3.000364	1.199671
C	-0.755632	-4.068243	0.371492
C	3.202814	-2.476861	0.206974
C	4.304279	-3.331229	0.433504
C	5.600800	-2.805956	0.357846
C	5.774179	-1.441778	0.128690
C	4.707968	-0.552753	0.014201
C	3.420879	-1.103476	0.057186
O	1.247570	-1.409620	1.851419
O	2.324665	-0.266861	-0.123865
P	1.271938	0.005344	1.080184
O	-0.101423	0.049323	0.319835
O	1.596635	1.115563	1.988934
C	-1.437023	-2.365621	2.080535
C	4.983083	0.902003	-0.103002
C	-1.106586	-1.896538	3.385474
C	-2.046371	-1.279240	4.166690
C	-3.376927	-1.095036	3.705912
C	-3.723560	-1.585305	2.417157
C	-2.727522	-2.209655	1.624025
C	5.963196	1.359926	-1.029232
C	6.318294	2.682461	-1.083684
C	5.710731	3.634965	-0.222613
C	4.715309	3.186869	0.686983
C	4.378163	1.811908	0.732627
H	-1.750131	-4.501842	0.451369
H	6.784220	-1.037890	0.101899
H	-0.095954	-2.027634	3.754251
H	-1.780187	-0.916570	5.156064
H	3.639076	1.493017	1.459561
H	7.069929	3.020418	-1.793144
H	6.427823	0.641684	-1.699828
H	-2.983180	-2.531490	0.616455
C	1.266402	2.589744	-1.434084
C	2.508425	2.745700	-2.048863
C	3.134068	3.985824	-2.063413
C	2.528135	5.065747	-1.424205
C	1.296028	4.907148	-0.801939
H	0.792146	1.616138	-1.467901
H	2.982617	1.886304	-2.513468
H	4.095500	4.108448	-2.551315
H	0.821233	5.762260	-0.326723
H	3.020862	6.033026	-1.406384
C	-1.866786	4.817974	-2.028403
C	-2.607528	5.866434	-2.554524
C	-3.087533	6.873418	-1.715614

C	-2.812750	6.816882	-0.356141
C	-2.074265	5.754673	0.171101
H	-1.862186	5.743281	1.234225
H	-1.474358	4.046563	-2.687043
H	-2.802658	5.906460	-3.621746
H	-3.663244	7.697825	-2.124487
H	-3.169641	7.599719	0.306059
C	-2.539225	-0.233474	-1.493664
C	-3.241932	-1.376874	-1.842198
C	-4.624339	-1.465936	-1.703265
C	-5.300180	-0.370544	-1.181141
Br	-2.299798	-2.885453	-2.481090
H	-5.155716	-2.369699	-1.977857
C	-4.632108	0.792810	-0.828149
H	-5.183383	1.634433	-0.421598
H	-1.463062	-0.195474	-1.613864
Br	-7.160785	-0.500661	-0.886967
C	4.070295	4.128068	1.531985
C	4.407825	5.455853	1.478361
C	5.403867	5.903711	0.574770
C	6.037929	5.015570	-0.257379
H	3.295416	3.768273	2.204424
H	3.909005	6.172980	2.123276
H	6.799492	5.356789	-0.954610
H	5.663271	6.957917	0.543202
C	-5.054047	-1.412568	1.953085
C	-5.985249	-0.751775	2.711507
C	-5.634986	-0.250498	3.989830
C	-4.364830	-0.428790	4.478132
H	-5.324442	-1.817494	0.983142
H	-6.991572	-0.612708	2.327687
H	-6.379835	0.268024	4.585725
H	-4.092485	-0.056171	5.462484
C	-0.376492	-5.660251	-1.522118
C	0.346796	-5.659361	-2.865634
H	-1.459157	-5.558453	-1.660542
H	-0.219773	-6.631388	-1.032138
C	1.854280	-5.655374	-2.625668
H	0.065606	-4.760137	-3.432174
H	0.043506	-6.527027	-3.460008
C	2.278668	-4.370355	-1.917731
H	2.120471	-6.524394	-2.008042
H	2.403894	-5.752082	-3.567392
H	2.218275	-3.533449	-2.628586
H	3.330107	-4.426898	-1.625322
C	4.092176	-4.772730	0.867901
C	5.321402	-5.652906	0.654238
H	3.222097	-5.214025	0.378281
H	3.846704	-4.756931	1.939913
C	6.556639	-4.984952	1.250559
H	5.150473	-6.636131	1.104290
H	5.478558	-5.814182	-0.421596
C	6.834173	-3.675109	0.518120
H	6.378437	-4.784495	2.314922
H	7.430587	-5.641162	1.187221
H	7.229172	-3.905152	-0.481615
H	7.614983	-3.103043	1.030821

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M06-2X/6-31G* Energy = -8271.57134467

M06-2X/6-31G* Free Energy = -8270.687172

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.54350270

Lowest Frequency = 13.7483

M06-2X/6-31G* Geometry

C	-0.561351	3.470576	1.725146
C	-0.634626	3.627608	0.168085
C	-1.884867	3.208875	2.395698
H	0.125498	2.644272	1.932581
H	-0.084205	4.374030	2.121116
C	-2.362754	1.985403	2.623861
H	-2.487950	4.065756	2.691973
N	-1.257720	2.386459	-0.318745
C	-1.389775	4.881329	-0.292976
C	0.794644	3.704774	-0.394887
C	-2.507209	2.347134	-0.546456
C	-3.215366	1.135559	-1.002668
H	-3.133605	3.238089	-0.438400
H	-0.507637	1.006450	0.169085
H	-1.805530	1.089967	2.347817
H	-3.326739	1.825833	3.100221
C	3.988528	-3.580664	0.569255
C	5.315187	-3.131746	0.595352
C	2.951324	-2.650322	0.335831
C	3.256677	-1.287019	0.283150
C	4.572666	-0.815440	0.340997
C	5.579889	-1.769014	0.460238
C	1.533330	-3.102449	0.200676
C	1.117485	-4.010848	-0.797261
C	-0.199725	-4.485791	-0.772502
C	-1.095386	-4.000666	0.182357
C	-0.752787	-3.005776	1.091852
C	0.581833	-2.588975	1.076858
O	2.228841	-0.370308	0.093660
O	0.970535	-1.562303	1.930888
P	1.125483	-0.106479	1.255377
O	-0.195981	0.067283	0.424236
O	1.464497	0.920802	2.250147
C	4.928745	0.627116	0.313069
C	-1.772728	-2.366173	1.957899
C	4.385220	1.521519	1.277949
C	4.798864	2.824947	1.325847
C	5.756734	3.324495	0.406491
C	6.281630	2.445226	-0.580254
C	5.857589	1.091167	-0.590627
C	-1.493937	-2.015672	3.311088
C	-2.441387	-1.400182	4.084522
C	-3.728458	-1.098418	3.565680
C	-4.023564	-1.465631	2.224245
C	-3.020583	-2.092833	1.442273
H	6.609910	-1.422435	0.509319
H	-2.116755	-4.375274	0.180962
H	3.643431	1.164826	1.983615
H	4.377283	3.502260	2.063921
H	-3.233194	-2.324127	0.400361
H	-2.214747	-1.129405	5.112395
H	-0.516278	-2.236864	3.723467
H	6.270136	0.417100	-1.338712
C	1.515539	4.894763	-0.237882
C	2.786049	5.034887	-0.781279
C	3.367434	3.984186	-1.490071
C	2.677209	2.786015	-1.616636
C	1.396325	2.648539	-1.079890
H	1.059099	5.732068	0.284711
H	3.325878	5.969711	-0.659987
H	4.358416	4.098620	-1.920187
H	0.873406	1.710258	-1.223902
H	3.128698	1.944955	-2.134220

C	-1.566407	5.074483	-1.670882
C	-2.215152	6.199055	-2.159989
C	-2.692158	7.169962	-1.278029
C	-2.506996	7.000842	0.087281
C	-1.861475	5.862582	0.576417
H	-1.718285	5.763045	1.646454
H	-1.175405	4.330370	-2.361021
H	-2.340292	6.326153	-3.230905
H	-3.195850	8.053460	-1.657473
H	-2.862300	7.753946	0.783912
C	-2.538716	0.036357	-1.540936
C	-3.279126	-1.041094	-2.003082
C	-4.670338	-1.059620	-1.948732
C	-5.316932	0.038298	-1.395682
Br	-2.381422	-2.558797	-2.682505
H	-5.231662	-1.913189	-2.310344
C	-4.610155	1.137367	-0.930081
H	-5.138907	1.981864	-0.500166
H	-1.456668	0.019744	-1.595070
Br	-7.195841	-0.003540	-1.213424
C	-5.309397	-1.171251	1.699734
C	-6.244306	-0.510590	2.453520
C	-5.944896	-0.132802	3.786176
C	-4.720866	-0.430655	4.330891
H	-5.542778	-1.482875	0.686883
H	-7.214362	-0.277577	2.024362
H	-4.488367	-0.152358	5.355791
H	-6.692620	0.386211	4.378044
C	7.194583	2.956636	-1.541063
C	7.560702	4.278487	-1.526823
C	7.040483	5.153154	-0.540172
C	6.164908	4.683672	0.405377
H	7.591377	2.281475	-2.295196
H	8.253008	4.660399	-2.270806
H	7.339440	6.196874	-0.538090
H	5.754815	5.349300	1.160909
C	6.485582	-4.082224	0.766701
C	6.092203	-5.413792	1.400248
H	7.267599	-3.589799	1.354693
H	6.922795	-4.276288	-0.223039
C	4.855920	-5.968858	0.699536
H	5.866508	-5.266275	2.464248
H	6.929004	-6.117190	1.341996
C	3.669660	-5.029402	0.902679
H	5.063474	-6.076041	-0.374478
H	4.603685	-6.964531	1.078328
H	2.803900	-5.387149	0.342423
H	3.366518	-5.060891	1.959448
C	2.046148	-4.360409	-1.948011
C	1.591388	-5.576978	-2.751601
H	3.073751	-4.495792	-1.601765
H	2.074937	-3.483778	-2.611425
C	0.103578	-5.474649	-3.077418
H	2.190477	-5.656703	-3.664281
H	1.768440	-6.492612	-2.170388
C	-0.699310	-5.502660	-1.780125
H	-0.088950	-4.530613	-3.606931
H	-0.213655	-6.288523	-3.737022
H	-0.632584	-6.507338	-1.339739
H	-1.763202	-5.323884	-1.974674

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M06-2X/6-31G* Energy = -8271.57119684

M06-2X/6-31G* Free Energy = -8270.685569

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.54493906

Lowest Frequency = 12.7820

M06-2X/6-31G* Geometry

C	-0.571172	3.551873	1.557291
C	-0.704238	3.674876	0.008089
C	-1.844515	3.152252	2.253836
H	0.199791	2.805120	1.771020
H	-0.187799	4.512081	1.925021
C	-1.967438	2.025183	2.952238
H	-2.709375	3.808563	2.150150
N	-1.325675	2.412369	-0.436373
C	-1.500586	4.904786	-0.447257
C	0.707845	3.752810	-0.595409
C	-2.562858	2.349864	-0.714863
C	-3.218189	1.102047	-1.156963
H	-3.211015	3.231013	-0.660727
H	-0.635412	1.003002	0.093967
H	-1.125488	1.345560	3.071209
H	-2.901387	1.750013	3.436492
C	3.881809	-3.560435	0.682629
C	5.197617	-3.089650	0.780317
C	2.844987	-2.649073	0.384642
C	3.131945	-1.281625	0.339942
C	4.436065	-0.788430	0.456058
C	5.449557	-1.724631	0.641334
C	1.445359	-3.121995	0.156707
C	1.110764	-4.022502	-0.877630
C	-0.204128	-4.497350	-0.958765
C	-1.170302	-4.021488	-0.070885
C	-0.902794	-3.037298	0.875925
C	0.429946	-2.621266	0.966361
O	2.099824	-0.382558	0.097770
O	0.759415	-1.603906	1.855415
P	0.939578	-0.139497	1.207838
O	-0.332415	0.054444	0.311492
O	1.230650	0.869520	2.238589
C	4.767920	0.659274	0.403023
C	-1.994684	-2.389362	1.643405
C	4.152572	1.576858	1.300615
C	4.527879	2.892930	1.312608
C	5.519470	3.381008	0.423396
C	6.119661	2.476431	-0.494962
C	5.731548	1.111884	-0.469801
C	-3.235513	-2.163802	0.981860
C	-4.267766	-1.514717	1.602830
C	-4.127340	-1.044542	2.934654
C	-2.902830	-1.286919	3.616631
C	-1.852137	-1.963978	2.946139
H	6.470785	-1.362233	0.737870
H	-2.187545	-4.395607	-0.163147
H	3.386969	1.227345	1.984341
H	4.051277	3.588064	1.999004
H	-0.920923	-2.129171	3.478328
H	-5.200563	-1.329800	1.074960
H	-3.334756	-2.485701	-0.049224
H	6.198298	0.420089	-1.168239
C	1.345250	2.648800	-1.163744
C	2.628709	2.765230	-1.697468
C	3.289690	3.986921	-1.679153
C	2.671278	5.088340	-1.089600
C	1.395116	4.971541	-0.552020
H	0.851431	1.685435	-1.209664
H	3.109099	1.887358	-2.119203

H	4.288793	4.080189	-2.096201
H	0.913139	5.843049	-0.115840
H	3.187630	6.043255	-1.052045
C	-1.665169	5.107733	-1.825372
C	-2.364049	6.203560	-2.311085
C	-2.907567	7.134443	-1.424502
C	-2.739353	6.954310	-0.058323
C	-2.041910	5.845452	0.427391
H	-1.917977	5.735676	1.499150
H	-1.223578	4.394935	-2.518172
H	-2.477167	6.339537	-3.382237
H	-3.450544	7.995728	-1.800861
H	-3.148205	7.676198	0.641940
C	-2.496524	0.080691	-1.782883
C	-3.176248	-1.043761	-2.224581
C	-4.551017	-1.187636	-2.055823
C	-5.239523	-0.169762	-1.409680
Br	-2.212427	-2.461424	-3.021188
H	-5.065019	-2.078820	-2.396325
C	-4.596496	0.981129	-0.975299
H	-5.160286	1.766664	-0.482537
H	-1.425118	0.166164	-1.921649
Br	-7.084256	-0.386536	-1.065934
C	-2.756042	-0.820407	4.950753
C	-3.770655	-0.136567	5.569725
C	-4.986527	0.112973	4.885251
C	-5.159620	-0.332630	3.599145
H	-1.817217	-1.005164	5.466144
H	-3.645034	0.221449	6.586769
H	-6.089514	-0.147464	3.066634
H	-5.781389	0.657428	5.385740
C	7.070724	2.972555	-1.426586
C	7.403160	4.303149	-1.448197
C	6.808198	5.203186	-0.528713
C	5.893305	4.749542	0.386641
H	7.525198	2.277885	-2.128679
H	8.126264	4.672635	-2.168823
H	7.081244	6.253698	-0.554338
H	5.424720	5.434478	1.088994
C	6.370415	-4.020042	1.028050
C	5.960602	-5.355090	1.643958
H	7.107051	-3.512397	1.660079
H	6.870510	-4.211385	0.068018
C	4.776833	-5.933233	0.874270
H	5.669804	-5.206777	2.691937
H	6.810376	-6.045211	1.639230
C	3.565952	-5.012321	1.003520
H	5.049033	-6.040580	-0.185206
H	4.519193	-6.931627	1.242046
H	2.739633	-5.383988	0.394314
H	3.201571	-5.045277	2.040662
C	2.125385	-4.358478	-1.957430
C	1.728519	-5.557458	-2.816579
H	3.121267	-4.509145	-1.533384
H	2.213698	-3.470466	-2.600102
C	0.270194	-5.441632	-3.252335
H	2.395258	-5.622988	-3.682264
H	1.857259	-6.484650	-2.241141
C	-0.629601	-5.491726	-2.020989
H	0.121577	-4.485890	-3.775035
H	0.001617	-6.240192	-3.951100
H	-0.602334	-6.505743	-1.598225
H	-1.673589	-5.298826	-2.293489

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M06-2X/6-31G* Energy = -8271.57134477

M06-2X/6-31G* Free Energy = -8270.687154

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.54350024

Lowest Frequency = 13.7608

M06-2X/6-31G* Geometry

C	-0.561397	3.470780	1.725235
C	-0.634632	3.627349	0.168129
C	-1.884805	3.209025	2.396019
H	0.125605	2.644642	1.932862
H	-0.084407	4.374437	2.120923
C	-2.363107	1.985551	2.623299
H	-2.487352	4.065849	2.693536
N	-1.257960	2.386170	-0.318366
C	-1.389563	4.881069	-0.293335
C	0.794672	3.704267	-0.394792
C	-2.507384	2.347148	-0.546614
C	-3.215694	1.135568	-1.002635
H	-3.133553	3.238312	-0.439123
H	-0.508757	1.006151	0.168563
H	-1.806421	1.090079	2.346268
H	-3.326925	1.825930	3.099980
C	1.117630	-4.010772	-0.797404
C	-0.199662	-4.485520	-0.772718
C	1.533509	-3.102338	0.200477
C	0.582007	-2.588653	1.076543
C	-0.752655	-3.005323	1.091514
C	-1.095320	-4.000229	0.182049
C	2.951542	-2.650356	0.335688
C	3.988633	-3.580764	0.569376
C	5.315336	-3.132003	0.595605
C	5.580226	-1.769306	0.460423
C	4.573114	-0.815669	0.340965
C	3.257054	-1.287094	0.282899
O	0.970761	-1.561801	1.930318
O	2.229481	-0.370232	0.093148
P	1.125553	-0.106154	1.254262
O	-0.195394	0.067027	0.422347
O	1.463936	0.921548	2.248807
C	-1.772544	-2.365672	1.957622
C	4.929191	0.626895	0.313128
C	-1.493617	-2.015174	3.310791
C	-2.440998	-1.399732	4.084346
C	-3.728145	-1.098015	3.565674
C	-4.023405	-1.465236	2.224277
C	-3.020485	-2.092376	1.442164
C	4.385415	1.521174	1.277988
C	4.798875	2.824653	1.326044
C	5.756841	3.324354	0.406879
C	6.282032	2.445201	-0.579814
C	5.858158	1.091089	-0.590353
H	-2.116713	-4.374764	0.180656
H	6.610279	-1.422836	0.509636
H	-0.515909	-2.236344	3.723052
H	-2.214251	-1.128970	5.112199
H	6.270927	0.417102	-1.338388
H	4.377088	3.501866	2.064091
H	3.643521	1.164374	1.983486
H	-3.233232	-2.323660	0.400283
C	1.396177	2.648128	-1.080053
C	2.677078	2.785555	-1.616858
C	3.367400	3.983629	-1.490183

C	2.786171	5.034260	-0.781125
C	1.515734	4.894153	-0.237612
H	0.873280	1.709861	-1.224207
H	3.128402	1.944512	-2.134600
H	4.358336	4.098126	-1.920391
H	1.059380	5.731391	0.285168
H	3.326135	5.968993	-0.659741
C	-1.565301	5.074300	-1.671349
C	-2.213922	6.198782	-2.160804
C	-2.691689	7.169541	-1.279085
C	-2.507417	7.000351	0.086330
C	-1.862020	5.862163	0.575814
H	-1.719533	5.762550	1.645930
H	-1.173699	4.330301	-2.361276
H	-2.338359	6.325950	-3.231793
H	-3.195271	8.052985	-1.658801
H	-2.863318	7.753343	0.782776
C	-2.539162	0.036387	-1.541099
C	-3.279678	-1.041096	-2.003007
C	-4.670864	-1.059630	-1.948273
C	-5.317341	0.038268	-1.395038
Br	-2.382166	-2.558854	-2.682556
H	-5.232266	-1.913239	-2.309672
C	-4.610469	1.137364	-0.929660
H	-5.139104	1.981852	-0.499584
H	-1.457134	0.019837	-1.595606
Br	-7.196172	-0.003672	-1.212142
C	7.195017	2.956807	-1.540491
C	7.560852	4.278736	-1.526204
C	7.040333	5.153288	-0.539604
C	6.164756	4.683611	0.405842
H	7.592034	2.281734	-2.294585
H	8.253148	4.660810	-2.270113
H	5.754447	5.349138	1.161346
H	7.339082	6.197068	-0.537482
C	-5.309346	-1.170964	1.699961
C	-6.244200	-0.510376	2.453882
C	-5.944616	-0.132547	3.786486
C	-4.720490	-0.430314	4.331021
H	-5.542864	-1.482623	0.687152
H	-7.214339	-0.277447	2.024867
H	-6.692290	0.386424	4.378455
H	-4.487860	-0.151998	5.355886
C	-0.699268	-5.502340	-1.780364
C	0.103448	-5.474012	-3.077755
H	-1.763221	-5.323713	-1.974705
H	-0.632276	-6.507087	-1.340169
C	1.591268	-5.576668	-2.752091
H	-0.089009	-4.529784	-3.606957
H	-0.213953	-6.287649	-3.737572
C	2.046344	-4.360490	-1.948074
H	1.768223	-6.492564	-2.171265
H	2.190281	-5.656129	-3.664846
H	2.075664	-3.483685	-2.611237
H	3.073824	-4.496430	-1.601674
C	3.669533	-5.029399	0.903038
C	4.855700	-5.969059	0.700295
H	2.803816	-5.387154	0.342718
H	3.366217	-5.060621	1.959767
C	6.091964	-5.413988	1.401031
H	4.603280	-6.964603	1.079308
H	5.063389	-6.076551	-0.373663
C	6.485581	-4.082615	0.767219

H	5.866167	-5.266194	2.464972
H	6.928681	-6.117509	1.343034
H	6.922810	-4.276968	-0.222460
H	7.267645	-3.590182	1.355141

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M06-2X/6-31G* Energy = -8271.57119679

M06-2X/6-31G* Free Energy = -8270.685571

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.54493398

Lowest Frequency = 12.7958

M06-2X/6-31G* Geometry

C	-0.571291	3.551554	1.557072
C	-0.704187	3.674462	0.007891
C	-1.844673	3.152041	2.253612
H	0.199678	2.804859	1.770985
H	-0.187975	4.511812	1.924753
C	-1.967719	2.025149	2.952277
H	-2.709484	3.808408	2.149808
N	-1.325799	2.412023	-0.436695
C	-1.500415	4.904425	-0.447563
C	0.707943	3.752267	-0.595490
C	-2.563083	2.349826	-0.714861
C	-3.218752	1.102177	-1.156946
H	-3.211086	3.231057	-0.660322
H	-0.635732	1.001957	0.092773
H	-1.125844	1.345484	3.071503
H	-2.901710	1.750223	3.436590
C	1.111380	-4.022494	-0.877714
C	-0.203515	-4.497316	-0.958983
C	1.445891	-3.121965	0.156638
C	0.430428	-2.621301	0.966275
C	-0.902270	-3.037452	0.875831
C	-1.169725	-4.021561	-0.071082
C	2.845478	-2.648926	0.384570
C	3.882396	-3.560150	0.682596
C	5.198168	-3.089228	0.780203
C	5.449952	-1.724183	0.641269
C	4.436349	-0.788087	0.456024
C	3.132298	-1.281437	0.339839
O	0.759781	-1.603803	1.855249
O	2.100101	-0.382512	0.097528
P	0.939634	-0.139473	1.207329
O	-0.332253	0.053736	0.310618
O	1.230185	0.869874	2.237895
C	-1.994216	-2.389702	1.643400
C	4.768015	0.659655	0.403112
C	-3.235078	-2.164190	0.981901
C	-4.267374	-1.515267	1.602960
C	-4.126943	-1.045167	2.934812
C	-2.902410	-1.287518	3.616756
C	-1.851679	-1.964445	2.946176
C	4.152312	1.577143	1.300549
C	4.527389	2.893280	1.312639
C	5.519128	3.381527	0.423686
C	6.119706	2.477040	-0.494510
C	5.731796	1.112438	-0.469466
H	-2.186946	-4.395726	-0.163371
H	6.471141	-1.361673	0.737799
H	-3.334291	-2.485995	-0.049215
H	-5.200237	-1.330413	1.075189
H	6.198822	0.420734	-1.167809
H	4.050476	3.588322	1.998912
H	3.386627	1.227520	1.984125

H	-0.920462	-2.129657	3.478354
C	1.345387	2.648205	-1.163669
C	2.628950	2.764509	-1.697178
C	3.290003	3.986158	-1.678843
C	2.671542	5.087653	-1.089473
C	1.395309	4.970951	-0.552048
H	0.851504	1.684881	-1.209690
H	3.109363	1.886551	-2.118710
H	4.289189	4.079335	-2.095709
H	0.913354	5.842504	-0.115935
H	3.187909	6.042559	-1.051923
C	-1.664728	5.107413	-1.825706
C	-2.363589	6.203208	-2.311514
C	-2.907388	7.133998	-1.425000
C	-2.739453	6.953810	-0.058795
C	-2.042010	5.844991	0.427017
H	-1.918296	5.735180	1.498801
H	-1.222933	4.394677	-2.518440
H	-2.476490	6.339239	-3.382683
H	-3.450367	7.995246	-1.801439
H	-3.148534	7.675615	0.641421
C	-2.497404	0.080650	-1.782963
C	-3.177424	-1.043702	-2.224428
C	-4.552202	-1.187295	-2.055444
C	-5.240393	-0.169259	-1.409237
Br	-2.213983	-2.461715	-3.020890
H	-5.066399	-2.078438	-2.395763
C	-4.597042	0.981515	-0.974998
H	-5.160574	1.767174	-0.482135
H	-1.426009	0.165899	-1.921959
Br	-7.085070	-0.385674	-1.065015
C	7.070932	2.973314	-1.425891
C	7.403136	4.303965	-1.447440
C	6.807781	5.203912	-0.528124
C	5.892739	4.750124	0.387011
H	7.525712	2.278713	-2.127854
H	8.126366	4.673564	-2.167881
H	5.423863	5.434991	1.089236
H	7.080641	6.254473	-0.553700
C	-2.755657	-0.821125	4.950919
C	-3.770315	-0.137386	5.569944
C	-4.986186	0.112172	4.885481
C	-5.159255	-0.333339	3.599336
H	-1.816835	-1.005882	5.466315
H	-3.644702	0.220564	6.587013
H	-5.781074	0.656558	5.386006
H	-6.089151	-0.148177	3.066822
C	-0.628945	-5.491498	-2.021389
C	0.270814	-5.440998	-3.252745
H	-1.672967	-5.298632	-2.293789
H	-0.601568	-6.505630	-1.598903
C	1.729119	-5.557088	-2.817010
H	0.122227	-4.485065	-3.775097
H	0.002206	-6.239309	-3.951782
C	2.126160	-4.358521	-1.957354
H	1.857749	-6.484526	-2.241946
H	2.395875	-5.622350	-3.682704
H	3.121848	-4.509806	-1.533065
H	2.215096	-3.470317	-2.599667
C	3.566837	-5.012071	1.003543
C	4.777672	-5.932853	0.872990
H	2.739867	-5.383616	0.395151
H	3.203584	-5.045228	2.041080

C	5.961726	-5.355106	1.642550
H	4.520322	-6.931519	1.240228
H	5.049350	-6.039442	-0.186700
C	6.371146	-4.019507	1.027556
H	5.671361	-5.207696	2.690776
H	6.811605	-6.045093	1.636918
H	6.871409	-4.210024	0.067448
H	7.107579	-3.512092	1.660011

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M06-2X/6-31G* Energy = -8271.57134455

M06-2X/6-31G* Free Energy = -8270.687142

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.54350613

Lowest Frequency = 13.7928

M06-2X/6-31G* Geometry

C	-0.562590	3.470486	1.724733
C	-0.635437	3.627386	0.167650
C	-1.886153	3.208361	2.395050
H	0.124576	2.644479	1.932385
H	-0.085937	4.374151	2.120817
C	-2.364534	1.984834	2.621869
H	-2.488809	4.065101	2.692616
N	-1.258249	2.386011	-0.319131
C	-1.390630	4.880927	-0.293733
C	0.794001	3.704804	-0.394849
C	-2.507622	2.346673	-0.547473
C	-3.215733	1.134931	-1.003324
H	-3.133975	3.237730	-0.440088
H	-0.507220	1.007085	0.168837
H	-1.807826	1.089402	2.344745
H	-3.328472	1.825165	3.098296
C	1.117848	-4.010754	-0.796824
C	-0.199336	-4.485762	-0.771677
C	1.533862	-3.102032	0.200748
C	0.582445	-2.588303	1.076902
C	-0.752161	-3.005124	1.092230
C	-1.094878	-4.000317	0.183112
C	2.951878	-2.649944	0.335666
C	3.989067	-3.580334	0.569052
C	5.315758	-3.131536	0.595098
C	5.580578	-1.768812	0.459989
C	4.573395	-0.815238	0.340778
C	3.257320	-1.286659	0.282888
O	0.971236	-1.561337	1.930525
O	2.229791	-0.369775	0.093274
P	1.125942	-0.105729	1.254502
O	-0.195217	0.067652	0.422775
O	1.464401	0.922089	2.248899
C	-1.771987	-2.365348	1.958281
C	4.929341	0.627368	0.313000
C	-1.493053	-2.014732	3.311419
C	-2.440479	-1.399317	4.084948
C	-3.727633	-1.097682	3.566234
C	-4.022825	-1.464915	2.224831
C	-3.019912	-2.092136	1.442788
C	4.385838	1.521466	1.278171
C	4.799197	2.824979	1.326252
C	5.756776	3.324888	0.406797
C	6.281681	2.445914	-0.580206
C	5.857943	1.091756	-0.590757
H	-2.116241	-4.374951	0.181983
H	6.610618	-1.422290	0.509069
H	-0.515315	-2.235797	3.723675

H	-2.213752	-1.128493	5.112787
H	6.270512	0.417903	-1.339021
H	4.377608	3.502046	2.064544
H	3.644203	1.164519	1.983874
H	-3.232660	-2.323622	0.400949
C	1.395750	2.649106	-1.080739
C	2.676693	2.787003	-1.617086
C	3.367025	3.985047	-1.489278
C	2.785598	5.035105	-0.779699
C	1.514908	4.894554	-0.236677
H	0.872757	1.711001	-1.225667
H	3.128272	1.946488	-2.135463
H	4.358082	4.099714	-1.919168
H	1.058429	5.731490	0.286477
H	3.325371	5.969830	-0.657429
C	-1.566461	5.074210	-1.671717
C	-2.215392	6.198578	-2.161044
C	-2.693390	7.169130	-1.279229
C	-2.509083	6.999842	0.086177
C	-1.863381	5.861779	0.575533
H	-1.720910	5.762042	1.645644
H	-1.174702	4.330376	-2.361730
H	-2.339894	6.325800	-3.232020
H	-3.197199	8.052478	-1.658866
H	-2.865195	7.752654	0.782710
C	-4.610503	1.136622	-0.930371
C	-5.317247	0.037321	-1.395460
C	-4.670637	-1.060594	-1.948501
C	-3.279443	-1.041907	-2.003276
Br	-7.196062	-0.004815	-1.212354
H	-5.231945	-1.914331	-2.309743
C	-2.539036	0.035692	-1.541454
H	-1.456979	0.019262	-1.595634
H	-5.139216	1.981169	-0.500508
Br	-2.381840	-2.559615	-2.682793
C	7.194299	2.957720	-1.541127
C	7.560085	4.279660	-1.526757
C	7.039864	5.154033	-0.539837
C	6.164622	4.684169	0.405823
H	7.591085	2.282778	-2.295461
H	8.252107	4.661883	-2.270844
H	5.754547	5.349558	1.161578
H	7.338579	6.197823	-0.537641
C	-5.308668	-1.170517	1.700360
C	-6.243529	-0.509797	2.454140
C	-5.944061	-0.132028	3.786800
C	-4.720026	-0.429921	4.331475
H	-5.542069	-1.482177	0.687534
H	-7.213584	-0.276765	2.024981
H	-6.691749	0.387016	4.378687
H	-4.487480	-0.151594	5.356356
C	-0.698911	-5.503259	-1.778661
C	0.103898	-5.476240	-3.076014
H	-1.762821	-5.324681	-1.973297
H	-0.632121	-6.507629	-1.337564
C	1.591770	-5.577991	-2.750254
H	-0.088806	-4.532747	-3.606428
H	-0.213245	-6.290795	-3.734829
C	2.046237	-4.360650	-1.947690
H	1.769149	-6.493136	-2.168374
H	2.190758	-5.658231	-3.662962
H	3.074064	-4.495156	-1.601774
H	2.074198	-3.484480	-2.611763

C	3.670154	-5.029060	0.902497
C	4.856327	-5.968612	0.699292
H	2.804358	-5.386800	0.342291
H	3.367064	-5.060531	1.959286
C	6.092708	-5.413665	1.399906
H	4.604009	-6.964249	1.078140
H	5.063786	-6.075858	-0.374734
C	6.486102	-4.082089	0.766394
H	5.867146	-5.266218	2.463944
H	6.929461	-6.117115	1.341504
H	6.923272	-4.276132	-0.223373
H	7.268164	-3.589715	1.354372

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M06-2X/6-31G* Energy = -8271.56656703

M06-2X/6-31G* Free Energy = -8270.681490

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.54420031

Lowest Frequency = 10.3570

M06-2X/6-31G* Geometry

C	0.966818	-1.213740	2.462275
C	0.605011	-2.561111	1.749362
C	-0.110596	-0.656338	3.353066
H	1.192489	-0.496260	1.665029
H	1.898658	-1.368215	3.016313
C	-1.044572	0.186803	2.913699
H	-0.131783	-0.971642	4.394516
N	-0.546334	-2.241751	0.896007
C	1.783708	-2.964292	0.851199
C	0.337266	-3.723288	2.712886
C	-1.738255	-2.451095	1.289186
C	-2.914384	-2.051268	0.491719
H	-1.947977	-2.937113	2.247665
H	-0.362387	-0.956404	-0.110781
H	-1.062537	0.522907	1.877788
H	-1.816748	0.577824	3.572400
C	3.363626	3.760150	0.416955
C	4.664884	3.578106	-0.067802
C	2.443419	2.690509	0.335453
C	2.806825	1.528113	-0.348352
C	4.095320	1.334574	-0.857048
C	5.008741	2.367568	-0.669933
C	1.079504	2.809482	0.935906
C	0.890687	3.065176	2.310438
C	-0.400580	3.345597	2.774340
C	-1.478903	3.274811	1.892996
C	-1.348064	2.860058	0.567630
C	-0.037748	2.657301	0.114994
O	1.880835	0.498500	-0.463212
O	0.177178	2.241017	-1.192579
P	0.559695	0.683707	-1.396788
O	-0.540111	-0.058109	-0.561810
O	0.732638	0.348894	-2.814007
C	4.513529	0.112355	-1.590711
C	-2.553736	2.564652	-0.245887
C	3.829061	-0.290929	-2.771526
C	4.287139	-1.350184	-3.508196
C	5.427296	-2.090636	-3.100351
C	6.105004	-1.702432	-1.911902
C	5.628328	-0.583261	-1.183313
C	-3.700612	2.036340	0.418358
C	-4.863254	1.785621	-0.256905
C	-4.949807	2.005266	-1.656352
C	-3.801205	2.490652	-2.338927

C	-2.621140	2.778279	-1.606203
H	6.015042	2.238770	-1.062650
H	-2.473619	3.494970	2.273503
H	2.944730	0.250556	-3.090924
H	3.765856	-1.646655	-4.415257
H	-1.764469	3.172735	-2.142049
H	-5.721865	1.370169	0.267033
H	-3.638949	1.809937	1.478910
H	6.150042	-0.286786	-0.275813
C	-0.139936	-4.929195	2.180501
C	-0.357363	-6.034114	2.991593
C	-0.084569	-5.963504	4.358100
C	0.411784	-4.782830	4.894232
C	0.620008	-3.670283	4.076700
H	-0.330288	-4.996207	1.111950
H	-0.729796	-6.956393	2.556615
H	-0.249941	-6.827265	4.994264
H	1.024615	-2.766297	4.518705
H	0.641889	-4.718325	5.953281
C	1.693986	-2.996272	-0.539825
C	2.779546	-3.418314	-1.307619
C	3.966639	-3.806032	-0.698433
C	4.069151	-3.756901	0.690769
C	2.986098	-3.345940	1.456473
H	3.063832	-3.349820	2.541359
H	0.772497	-2.712129	-1.037536
H	2.690372	-3.441076	-2.389021
H	4.807523	-4.142578	-1.298200
H	4.993484	-4.053132	1.177978
C	-2.815296	-1.803339	-0.880392
C	-3.939423	-1.389571	-1.577590
C	-5.174902	-1.262839	-0.950827
C	-5.252582	-1.515375	0.411807
Br	-3.790013	-0.924060	-3.394156
H	-6.044547	-0.939198	-1.510626
C	-4.142336	-1.911422	1.144197
H	-4.226161	-2.092183	2.211130
H	-1.870916	-1.914936	-1.397695
Br	-6.904169	-1.232593	1.289522
C	-3.867348	2.675419	-3.745897
C	-5.015583	2.386055	-4.437349
C	-6.161293	1.908370	-3.754544
C	-6.128966	1.726938	-2.395537
H	-2.984218	3.038939	-4.264458
H	-5.052094	2.522909	-5.513672
H	-7.006644	1.369016	-1.860683
H	-7.065574	1.687863	-4.313382
C	7.218217	-2.466553	-1.473226
C	7.632567	-3.569706	-2.175707
C	6.957946	-3.956230	-3.360567
C	5.885086	-3.229630	-3.812751
H	7.729460	-2.167051	-0.561655
H	8.480305	-4.151695	-1.827411
H	7.295067	-4.830530	-3.908768
H	5.361848	-3.522055	-4.719801
C	5.726096	4.657162	0.040393
C	5.144877	6.054101	0.238640
H	6.377924	4.420071	0.893222
H	6.364091	4.625809	-0.849415
C	4.091919	6.016481	1.341775
H	4.677813	6.397758	-0.693313
H	5.944858	6.761504	0.479366
C	2.924863	5.123388	0.927509

H	4.545488	5.627264	2.264239
H	3.721269	7.021811	1.566245
H	2.213648	5.030028	1.750333
H	2.368804	5.613783	0.115233
C	2.046110	2.921629	3.284224
C	1.790183	3.595255	4.629960
H	2.981345	3.278773	2.846485
H	2.187236	1.841993	3.447475
C	0.419351	3.190730	5.165557
H	2.583517	3.322933	5.333484
H	1.826769	4.687353	4.511588
C	-0.667853	3.701792	4.224217
H	0.365313	2.095348	5.223988
H	0.257111	3.582337	6.174902
H	-0.734783	4.795160	4.314822
H	-1.648363	3.309863	4.517530

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M06-2X/6-31G* Energy = -8271.56656564

M06-2X/6-31G* Free Energy = -8270.681494

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.54418801

Lowest Frequency = 10.3141

M06-2X/6-31G* Geometry

C	0.969365	-1.205155	2.463088
C	0.608403	-2.553921	1.752459
C	-0.108270	-0.647511	3.353503
H	1.193965	-0.488715	1.664566
H	1.901597	-1.357830	3.016932
C	-1.045006	0.191719	2.912549
H	-0.127349	-0.959427	4.396007
N	-0.543462	-2.236793	0.898887
C	1.786991	-2.958156	0.854633
C	0.341768	-3.714709	2.718049
C	-1.734962	-2.446456	1.293295
C	-2.912359	-2.049802	0.496180
H	-1.943355	-2.930803	2.252903
H	-0.359986	-0.954731	-0.112361
H	-1.065028	0.524536	1.875591
H	-1.817452	0.582935	3.570811
C	3.361030	3.759989	0.413837
C	4.662844	3.577720	-0.069383
C	2.441012	2.690202	0.332042
C	2.805200	1.527462	-0.350838
C	4.094308	1.333628	-0.857880
C	5.007452	2.366809	-0.670261
C	1.076602	2.809383	0.931420
C	0.886933	3.066550	2.305559
C	-0.404595	3.347762	2.768240
C	-1.482361	3.275694	1.886340
C	-1.350772	2.859062	0.561618
C	-0.040108	2.656315	0.109877
O	1.879063	0.497980	-0.466531
O	0.175907	2.240395	-1.197439
P	0.559900	0.683580	-1.402874
O	-0.540637	-0.061299	-0.571958
O	0.735863	0.352189	-2.820516
C	4.513646	0.111173	-1.590497
C	-2.556076	2.561855	-0.251866
C	3.830392	-0.293150	-2.771681
C	4.289620	-1.352616	-3.507307
C	5.429859	-2.092211	-3.098114
C	6.106497	-1.702841	-1.909460
C	5.628548	-0.583561	-1.181854

C	-3.703361	2.035509	0.413298
C	-4.865801	1.783185	-0.261692
C	-4.951791	1.998904	-1.661764
C	-3.802793	2.482123	-2.345203
C	-2.622966	2.771705	-1.612815
H	6.014204	2.237828	-1.061763
H	-2.477270	3.496415	2.265986
H	2.946231	0.247879	-3.092322
H	3.769262	-1.649898	-4.414631
H	-1.766171	3.164748	-2.149475
H	-5.724699	1.369526	0.263190
H	-3.642267	1.811841	1.474453
H	6.149370	-0.286326	-0.274085
C	-0.134414	-4.921953	2.187784
C	-0.350787	-6.025670	3.000792
C	-0.077924	-5.952480	4.367147
C	0.417476	-4.770462	4.901193
C	0.624634	-3.659137	4.081732
H	-0.324821	-4.990978	1.119370
H	-0.722448	-6.949020	2.567429
H	-0.242484	-6.815283	5.004819
H	1.028544	-2.754071	4.522154
H	0.647651	-4.703950	5.960102
C	2.989799	-3.338049	1.460170
C	4.072456	-3.750868	0.694899
C	3.969113	-3.803665	-0.694096
C	2.781670	-3.417491	-1.303595
C	1.696497	-2.993629	-0.536257
H	0.774671	-2.710892	-1.034137
H	3.068133	-3.339325	2.545020
H	4.997088	-4.045787	1.182344
H	4.809635	-4.141761	-1.293488
H	2.691913	-3.443040	-2.384894
C	-2.815469	-1.806415	-0.876876
C	-3.940875	-1.395540	-1.573763
C	-5.175468	-1.267369	-0.945577
C	-5.250977	-1.515494	0.418006
Br	-3.794339	-0.935919	-3.392074
H	-6.046100	-0.945952	-1.505141
C	-4.139449	-1.908542	1.150035
H	-4.221567	-2.085782	2.217691
H	-1.871815	-1.919310	-1.395165
Br	-6.901389	-1.230808	1.297324
C	-3.868330	2.662921	-3.752713
C	-5.016376	2.371886	-4.443789
C	-6.162470	1.896386	-3.760111
C	-6.130714	1.718722	-2.400594
H	-2.984930	3.024813	-4.271947
H	-5.052423	2.505715	-5.520509
H	-7.008645	1.362412	-1.865082
H	-7.066540	1.674412	-4.318713
C	7.219816	-2.466062	-1.469466
C	7.635205	-3.569512	-2.170864
C	6.961605	-3.957226	-3.355923
C	5.888727	-3.231467	-3.809393
H	7.730250	-2.165653	-0.557737
H	8.482991	-4.150829	-1.821565
H	7.299553	-4.831758	-3.903244
H	5.366277	-3.524762	-4.716615
C	5.723884	4.656930	0.039155
C	5.142433	6.053932	0.236279
H	6.375071	4.420256	0.892586
H	6.362556	4.625206	-0.850153

C	4.088329	6.016734	1.338328
H	4.676292	6.397191	-0.696285
H	5.942165	6.761450	0.477484
C	2.921703	5.123574	0.923002
H	4.540872	5.627728	2.261392
H	3.717497	7.022144	1.562125
H	2.209304	5.030777	1.744851
H	2.366884	5.613591	0.109650
C	2.041635	2.924120	3.280352
C	1.784982	3.600033	4.624804
H	2.977315	3.280148	2.842679
H	2.182178	1.844680	3.445511
C	0.413823	3.196401	5.160228
H	2.577908	3.328913	5.329246
H	1.821661	4.691933	4.504580
C	-0.672835	3.705987	4.217453
H	0.359759	2.101099	5.220252
H	0.250950	3.589505	6.168885
H	-0.740001	4.799470	4.306441
H	-1.653482	3.314336	4.510692

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M06-2X/6-31G* Energy = -8271.57119372

M06-2X/6-31G* Free Energy = -8270.684433

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.54569553

Lowest Frequency = 10.4065

M06-2X/6-31G* Geometry

C	0.208202	3.593503	-1.201712
C	0.507589	3.571609	0.327674
C	1.404426	3.400414	-2.093527
H	-0.510192	2.789908	-1.402378
H	-0.306546	4.541464	-1.403892
C	1.527682	2.342506	-2.895350
H	2.189706	4.156607	-2.079142
N	1.257211	2.302219	0.552835
C	1.331940	4.758794	0.833102
C	-0.830599	3.547081	1.078865
C	2.537711	2.260157	0.571041
C	3.377472	1.067836	0.672057
H	3.070321	3.209373	0.519999
H	0.703261	1.354540	0.381014
H	0.752787	1.577503	-2.932678
H	2.388388	2.229350	-3.549661
C	-2.172452	-3.914760	1.248267
C	-1.001666	-4.619793	1.549953
C	-2.161295	-3.007612	0.167927
C	-0.961317	-2.729441	-0.490338
C	0.208311	-3.466188	-0.247205
C	0.140134	-4.409766	0.778789
C	-3.412011	-2.324281	-0.282185
C	-4.523779	-3.063142	-0.740283
C	-5.720893	-2.389960	-1.014279
C	-5.775994	-1.004289	-0.863429
C	-4.665559	-0.238597	-0.516944
C	-3.475630	-0.929925	-0.253951
O	-0.961309	-1.715215	-1.427528
O	-2.345514	-0.232123	0.123935
P	-1.046019	-0.176412	-0.875599
O	0.118959	0.060088	0.077337
O	-1.232912	0.723447	-2.041103
C	1.485439	-3.304340	-0.989219
C	-4.792260	1.238955	-0.436857
C	2.303004	-4.458634	-1.190385

C	3.575634	-4.357610	-1.680249
C	4.118101	-3.094022	-2.038295
C	3.277223	-1.954126	-1.940911
C	1.972457	-2.084729	-1.401093
C	-5.873680	1.799497	0.299765
C	-6.075251	3.154500	0.342069
C	-5.208237	4.036904	-0.353070
C	-4.126314	3.482259	-1.090417
C	-3.935734	2.078034	-1.113088
H	1.037988	-4.971501	1.027420
H	-6.709619	-0.488643	-1.080459
H	1.902313	-5.435472	-0.936811
H	4.189220	-5.246618	-1.802528
H	-3.114100	1.669903	-1.696429
H	-6.902371	3.570885	0.912376
H	-6.539318	1.131069	0.839755
H	1.398919	-1.180656	-1.245129
C	-1.403015	2.387146	1.597068
C	-2.661334	2.433810	2.200020
C	-3.343510	3.636018	2.318205
C	-2.772127	4.801672	1.808185
C	-1.533536	4.754659	1.185388
H	-0.907784	1.426406	1.529789
H	-3.102089	1.510538	2.562947
H	-4.323450	3.666378	2.783949
H	-1.104817	5.668051	0.781341
H	-3.302612	5.746138	1.874199
C	1.689602	5.839099	0.029110
C	2.405008	6.914483	0.560977
C	2.774068	6.918019	1.899421
C	2.410990	5.845949	2.716085
C	1.690665	4.783940	2.188431
H	1.383032	3.962816	2.832059
H	1.400364	5.867004	-1.015638
H	2.668878	7.749306	-0.080576
H	3.331996	7.753132	2.310798
H	2.678694	5.845871	3.767986
C	2.914412	-0.176618	1.118753
C	3.824733	-1.220944	1.211439
C	5.156634	-1.076095	0.830428
C	5.587855	0.164926	0.380807
Br	3.249477	-2.893749	1.849732
H	5.836983	-1.918735	0.870530
C	4.723207	1.246597	0.326377
H	5.084420	2.212271	-0.012670
H	1.869731	-0.337612	1.364205
Br	7.368280	0.370207	-0.198084
C	-3.263803	4.353247	-1.808260
C	-3.446614	5.711854	-1.767794
C	-4.511315	6.265441	-1.013351
C	-5.374691	5.446574	-0.330011
H	-2.463524	3.911709	-2.396704
H	-2.783419	6.370016	-2.321889
H	-6.200948	5.866310	0.239199
H	-4.648915	7.342471	-0.989992
C	3.790423	-0.684766	-2.319097
C	5.086537	-0.552408	-2.746961
C	5.934199	-1.685860	-2.816774
C	5.456205	-2.928183	-2.481768
H	3.135872	0.181201	-2.240488
H	5.479475	0.425190	-3.013442
H	6.963815	-1.564773	-3.139507
H	6.098077	-3.803345	-2.546476

C	-0.935661	-5.630293	2.679990
C	-2.053214	-5.457002	3.704977
H	0.045391	-5.566544	3.164313
H	-1.000919	-6.640831	2.252244
C	-3.390839	-5.315479	2.984384
H	-1.870894	-4.555268	4.303950
H	-2.063302	-6.306890	4.395131
C	-3.399345	-4.047024	2.134533
H	-3.551127	-6.192072	2.340962
H	-4.220635	-5.285728	3.697990
H	-3.423421	-3.170199	2.798031
H	-4.317985	-3.991134	1.546385
C	-4.399357	-4.551248	-1.022475
C	-5.747990	-5.263285	-1.096139
H	-3.752527	-5.039611	-0.290192
H	-3.883037	-4.660376	-1.987243
C	-6.690906	-4.507801	-2.028039
H	-5.601523	-6.293674	-1.436115
H	-6.194019	-5.315704	-0.092753
C	-6.974841	-3.121577	-1.455866
H	-6.219957	-4.412349	-3.014929
H	-7.629402	-5.053822	-2.168985
H	-7.642687	-3.226455	-0.588865
H	-7.514551	-2.506515	-2.184268

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M06-2X/6-31G* Energy = -8271.57119378

M06-2X/6-31G* Free Energy = -8270.684424

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.54569048

Lowest Frequency = 10.4091

M06-2X/6-31G* Geometry

C	0.208663	3.593498	-1.201620
C	0.507900	3.571633	0.327761
C	1.404915	3.400310	-2.093370
H	-0.509773	2.789946	-1.402313
H	-0.306010	4.541483	-1.403903
C	1.528194	2.342288	-2.895038
H	2.190176	4.156526	-2.079077
N	1.257345	2.302182	0.553113
C	1.332404	4.758686	0.833229
C	-0.830367	3.547371	1.078833
C	2.537876	2.259946	0.570937
C	3.377505	1.067542	0.671925
H	3.070575	3.209098	0.519593
H	0.703433	1.354633	0.381376
H	0.753270	1.577308	-2.932275
H	2.388899	2.229026	-3.549331
C	-4.523996	-3.062898	-0.740366
C	-5.721023	-2.389632	-1.014469
C	-3.412222	-2.324125	-0.282097
C	-3.475763	-0.929774	-0.253789
C	-4.665631	-0.238361	-0.516900
C	-5.776062	-1.003948	-0.863561
C	-2.161593	-3.007553	0.168071
C	-2.172859	-3.914776	1.248355
C	-1.002116	-4.619836	1.550117
C	0.139781	-4.409756	0.779099
C	0.208064	-3.466141	-0.246843
C	-0.961546	-2.729379	-0.490065
O	-2.345671	-0.232029	0.124250
O	-0.961478	-1.715103	-1.427212
P	-1.046040	-0.176352	-0.875148
O	0.118812	0.059943	0.077964

O	-1.232673	0.723631	-2.040613
C	-4.792148	1.239206	-0.436798
C	1.485228	-3.304346	-0.988813
C	-5.873522	1.799892	0.299766
C	-6.074944	3.154923	0.342017
C	-5.207815	4.037205	-0.353124
C	-4.125902	3.482415	-1.090387
C	-3.935481	2.078164	-1.113005
C	2.302741	-4.458651	-1.190009
C	3.575318	-4.357678	-1.680055
C	4.117751	-3.094130	-2.038271
C	3.276928	-1.954197	-1.940764
C	1.972249	-2.084751	-1.400762
H	-6.709629	-0.488243	-1.080699
H	1.037613	-4.971488	1.027821
H	-6.539277	1.131562	0.839733
H	-6.902059	3.571405	0.912262
H	1.398783	-1.180652	-1.244706
H	4.188859	-5.246712	-1.802357
H	1.902096	-5.435476	-0.936307
H	-3.113859	1.669922	-1.696288
C	-1.403055	2.387540	1.597016
C	-2.661396	2.434466	2.199866
C	-3.343353	3.636824	2.317976
C	-2.771718	4.802339	1.807965
C	-1.533075	4.755065	1.185251
H	-0.908014	1.426703	1.529732
H	-3.102371	1.511291	2.562774
H	-4.323316	3.667371	2.783663
H	-1.104186	5.668376	0.781191
H	-3.302007	5.746922	1.873871
C	1.691219	4.783727	2.188530
C	2.411661	5.845664	2.716185
C	2.774752	6.917750	1.899553
C	2.405591	6.914318	0.561133
C	1.690078	5.839010	0.029262
H	1.400767	5.866966	-1.015467
H	1.383572	3.962594	2.832140
H	2.679451	5.845504	3.768064
H	3.332758	7.752807	2.310941
H	2.669465	7.749163	-0.080390
C	4.723233	1.246149	0.326097
C	5.587798	0.164413	0.380498
C	5.156488	-1.076551	0.830218
C	3.824622	-1.221254	1.211405
Br	7.368191	0.369518	-0.198523
H	5.836752	-1.919265	0.870260
C	2.914392	-0.176842	1.118770
H	1.869723	-0.337733	1.364336
H	5.084496	2.211781	-0.013024
Br	3.249281	-2.893951	1.849910
C	3.790108	-0.684857	-2.319054
C	5.086144	-0.552540	-2.747160
C	5.933744	-1.686032	-2.817139
C	5.455776	-2.928332	-2.482013
H	3.135607	0.181141	-2.240332
H	5.479060	0.425064	-3.013660
H	6.097611	-3.803512	-2.546838
H	6.963298	-1.565014	-3.140096
C	-3.263271	4.353272	-1.808249
C	-3.445979	5.711899	-1.767917
C	-4.510676	6.265627	-1.013577
C	-5.374146	5.446892	-0.330195

H	-2.462994	3.911603	-2.396599
H	-2.782701	6.369966	-2.322027
H	-4.648212	7.342669	-0.990322
H	-6.200389	5.866763	0.238937
C	-6.974914	-3.121155	-1.456357
C	-6.690796	-4.507137	-2.029021
H	-7.514635	-2.505861	-2.184553
H	-7.642800	-3.226438	-0.589436
C	-5.748163	-5.262961	-1.097114
H	-6.219552	-4.411265	-3.015728
H	-7.629231	-5.053138	-2.170454
C	-4.399541	-4.550979	-1.022669
H	-6.194546	-5.315775	-0.093908
H	-5.601568	-6.293219	-1.437436
H	-3.753154	-5.039490	-0.290086
H	-3.882675	-4.660022	-1.987153
C	-3.399840	-4.047004	2.134517
C	-3.391424	-5.315385	2.984476
H	-3.423978	-3.170117	2.797930
H	-4.318427	-3.991161	1.546280
C	-2.053803	-5.456981	3.705074
H	-4.221207	-5.285500	3.698093
H	-3.551790	-6.192025	2.341142
C	-0.936284	-5.630421	2.680079
H	-1.871401	-4.555234	4.304000
H	-2.063967	-6.306842	4.395262
H	-1.001751	-6.640923	2.252278
H	0.044785	-5.566905	3.164397

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M06-2X/6-31G* Energy = -8271.56527689

M06-2X/6-31G* Free Energy = -8270.683666

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.54018398

Lowest Frequency = 11.5783

M06-2X/6-31G* Geometry

C	-1.147384	0.443118	4.032521
C	-1.834808	-0.724161	3.257187
C	-1.873381	1.759710	3.958105
H	-0.153220	0.566071	3.589576
H	-0.998384	0.132750	5.072738
C	-1.397150	2.811964	3.296740
H	-2.839793	1.839134	4.453904
N	-2.066307	-0.141834	1.924242
C	-0.825157	-1.870058	3.123082
C	-3.094737	-1.275756	3.930674
C	-3.216785	0.007387	1.407140
C	-3.352940	0.747183	0.136181
H	-4.123145	-0.396726	1.868675
H	-0.667733	0.439401	1.176698
H	-0.449049	2.767643	2.763688
H	-1.940938	3.751367	3.251326
C	4.428640	-1.714557	-1.886509
C	4.138953	-2.819851	-2.697900
C	3.426672	-1.211078	-1.031046
C	2.131459	-1.723686	-1.122616
C	1.820792	-2.833289	-1.917694
C	2.859187	-3.376359	-2.669717
C	3.711205	-0.145244	-0.022566
C	4.647628	-0.334211	1.016881
C	4.908219	0.722978	1.899987
C	4.212563	1.925852	1.763663
C	3.224272	2.111209	0.801971
C	2.985365	1.042611	-0.066323

O	1.145824	-1.163018	-0.329105
O	1.945322	1.147470	-0.984870
P	0.596246	0.336452	-0.637096
O	0.199691	0.827661	0.803595
O	-0.397561	0.423417	-1.716403
C	0.467215	-3.444791	-1.942637
C	2.441349	3.367312	0.724306
C	0.337442	-4.843454	-1.707842
C	-0.892369	-5.447541	-1.710565
C	-2.069128	-4.696709	-1.969035
C	-1.943376	-3.304559	-2.232524
C	-0.660751	-2.699910	-2.204276
C	1.911669	3.940012	1.913464
C	1.163851	5.087415	1.869774
C	0.907124	5.740882	0.636410
C	1.467675	5.196814	-0.551658
C	2.221314	4.000654	-0.478095
H	2.644880	-4.238665	-3.298283
H	4.435302	2.744081	2.445885
H	1.232610	-5.424544	-1.500365
H	-0.982269	-6.512705	-1.513178
H	2.615457	3.574583	-1.396381
H	0.741037	5.502034	2.781793
H	2.080802	3.431711	2.859235
H	-0.584287	-1.634702	-2.404826
C	-3.729390	-2.381439	3.346124
C	-4.872455	-2.932613	3.909424
C	-5.397795	-2.400172	5.086783
C	-4.766614	-1.319190	5.688407
C	-3.624762	-0.759365	5.112802
H	-3.307285	-2.817582	2.443157
H	-5.347143	-3.786788	3.436637
H	-6.286920	-2.833389	5.533978
H	-3.146350	0.075656	5.612617
H	-5.157316	-0.904214	6.612404
C	-0.280836	-2.431927	4.284248
C	0.646828	-3.461508	4.203915
C	1.042398	-3.951876	2.958700
C	0.491012	-3.413162	1.803584
C	-0.445387	-2.381947	1.885446
H	-0.869222	-1.986616	0.967733
H	-0.599741	-2.071509	5.259182
H	1.059903	-3.885558	5.114207
H	1.770107	-4.755210	2.895173
H	0.778898	-3.785205	0.824616
C	-2.555406	1.868546	-0.082477
C	-2.582568	2.492762	-1.319258
C	-3.415842	2.044513	-2.336339
C	-4.237167	0.952348	-2.076386
Br	-1.388974	3.919557	-1.614318
H	-3.418948	2.522182	-3.308668
C	-4.229601	0.297927	-0.852379
H	-4.853397	-0.575994	-0.693449
H	-1.895318	2.231478	0.697111
Br	-5.354591	0.299925	-3.457227
C	1.211638	5.840969	-1.792763
C	0.417070	6.957168	-1.850382
C	-0.150196	7.492319	-0.666616
C	0.095511	6.902040	0.546039
H	1.639610	5.416541	-2.697330
H	0.214819	7.433410	-2.804667
H	-0.336116	7.309226	1.456817
H	-0.781358	8.373364	-0.726355

C	-3.109837	-2.548742	-2.529596
C	-4.343940	-3.146892	-2.540921
C	-4.471079	-4.529964	-2.256987
C	-3.360770	-5.286304	-1.982022
H	-3.000908	-1.490560	-2.755407
H	-5.224393	-2.557848	-2.780049
H	-5.454264	-4.990745	-2.268804
H	-3.451891	-6.349639	-1.774839
C	5.185711	-3.454141	-3.595008
C	6.364709	-2.530886	-3.891424
H	4.711697	-3.785417	-4.525347
H	5.561513	-4.362242	-3.102527
C	6.862017	-1.897336	-2.595140
H	6.049900	-1.737042	-4.580998
H	7.162334	-3.092326	-4.388380
C	5.772157	-1.013573	-1.993357
H	7.132070	-2.689575	-1.882696
H	7.763832	-1.301849	-2.769805
H	6.089503	-0.621095	-1.024407
H	5.632477	-0.131702	-2.635289
C	5.267502	-1.701076	1.253710
C	6.525815	-1.650119	2.116569
H	5.475885	-2.210301	0.310431
H	4.508364	-2.317346	1.757990
C	6.265691	-0.833969	3.379342
H	6.841777	-2.668332	2.365467
H	7.345360	-1.188771	1.547935
C	5.946961	0.609858	3.000280
H	5.417196	-1.271009	3.921510
H	7.128816	-0.861414	4.052244
H	6.870281	1.099473	2.659721
H	5.607938	1.173663	3.876247

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M06-2X/6-31G* Energy = -8271.56669779

M06-2X/6-31G* Free Energy = -8270.681918

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.54328255

Lowest Frequency = 9.7571

M06-2X/6-31G* Geometry

C	-3.540061	-0.403202	-1.467948
C	-3.705800	0.505349	-0.209538
C	-3.881527	-1.842901	-1.220107
H	-2.500630	-0.313605	-1.806991
H	-4.161833	-0.004569	-2.275579
C	-2.964175	-2.787636	-1.015948
H	-4.938784	-2.103784	-1.189438
N	-2.644036	0.053007	0.710498
C	-3.373330	1.976367	-0.516665
C	-5.127992	0.432765	0.370018
C	-2.818842	-0.958960	1.462325
C	-1.744136	-1.524787	2.300289
H	-3.787286	-1.461484	1.529047
H	-1.240203	0.812454	0.280040
H	-1.898504	-2.560130	-1.050414
H	-3.240148	-3.823816	-0.841500
C	4.250178	0.160233	0.746122
C	4.375410	1.123924	1.756516
C	3.376385	0.409236	-0.334111
C	2.579712	1.552675	-0.308807
C	2.638149	2.495773	0.720465
C	3.572184	2.264939	1.726420
C	3.233812	-0.544782	-1.474720
C	4.340657	-0.918918	-2.266437

C	4.186946	-1.933539	-3.220279
C	2.929579	-2.505511	-3.413833
C	1.794154	-2.066885	-2.738603
C	1.972263	-1.074144	-1.769349
O	1.672525	1.744945	-1.344075
O	0.875381	-0.633281	-1.036175
P	0.318448	0.873942	-1.311797
O	-0.338687	1.245749	0.060571
O	-0.463413	1.029690	-2.547814
C	1.732572	3.669070	0.774644
C	0.467807	-2.646013	-3.080335
C	1.064531	3.962602	1.996475
C	0.248235	5.055841	2.106132
C	0.050803	5.928673	1.003834
C	0.703183	5.634298	-0.225170
C	1.535609	4.489985	-0.311855
C	0.252571	-4.044682	-2.937533
C	-0.942558	-4.611852	-3.298207
C	-1.994680	-3.816925	-3.823486
C	-1.777250	-2.420921	-3.984351
C	-0.532383	-1.859818	-3.605193
H	3.661891	2.994748	2.528824
H	2.812473	-3.284606	-4.164627
H	1.196064	3.283863	2.835148
H	-0.265850	5.267740	3.040429
H	-0.381205	-0.791524	-3.726875
H	-1.103516	-5.679988	-3.174933
H	1.049777	-4.657567	-2.525585
H	2.029738	4.272334	-1.254405
C	-6.228536	0.324208	-0.486452
C	-7.530009	0.339733	0.005554
C	-7.763946	0.470112	1.370949
C	-6.681259	0.591846	2.235169
C	-5.380361	0.575541	1.739289
H	-6.077038	0.234745	-1.557360
H	-8.363097	0.251659	-0.685027
H	-8.778541	0.480424	1.756282
H	-4.554760	0.675240	2.437250
H	-6.844126	0.701872	3.302969
C	-3.308745	2.872411	0.557479
C	-2.917856	4.189310	0.367134
C	-2.584098	4.640696	-0.909320
C	-2.650133	3.760876	-1.981141
C	-3.043428	2.435371	-1.788802
H	-3.029459	1.763476	-2.638365
H	-3.549595	2.526939	1.558986
H	-2.858487	4.866459	1.214303
H	-2.261391	5.667298	-1.056006
H	-2.371080	4.091278	-2.976791
C	-1.994856	-2.712033	2.991364
C	-0.993050	-3.266375	3.778362
C	0.255117	-2.666174	3.896807
C	0.477154	-1.482106	3.200060
Br	-1.330966	-4.875239	4.711912
H	1.029164	-3.108514	4.512516
C	-0.498982	-0.901636	2.408340
H	-0.281433	0.020183	1.883399
H	-2.958823	-3.204408	2.911635
Br	2.157870	-0.622634	3.284095
C	-2.827573	-1.610554	-4.490523
C	-4.046839	-2.158865	-4.794874
C	-4.267103	-3.549117	-4.625399
C	-3.263236	-4.358491	-4.159870

H	-2.644451	-0.544796	-4.609581
H	-4.849281	-1.531853	-5.172375
H	-3.427058	-5.425712	-4.031829
H	-5.236478	-3.971377	-4.872339
C	0.510756	6.504565	-1.331634
C	-0.288740	7.613433	-1.221886
C	-0.944287	7.902652	0.001320
C	-0.779205	7.077729	1.085215
H	1.010743	6.272496	-2.268289
H	-0.426770	8.273026	-2.073047
H	-1.577579	8.781284	0.076024
H	-1.277844	7.295624	2.026768
C	5.346319	0.959450	2.913478
C	5.807165	-0.480689	3.136067
H	4.888550	1.359635	3.826063
H	6.225653	1.587626	2.714097
C	6.164556	-1.129459	1.801826
H	5.003650	-1.059560	3.609367
H	6.658698	-0.494406	3.823958
C	4.932590	-1.186530	0.901990
H	6.956132	-0.547047	1.309315
H	6.556858	-2.140121	1.954140
H	5.183518	-1.624198	-0.065685
H	4.190155	-1.862546	1.353021
C	5.657297	-0.166918	-2.161147
C	6.843551	-0.957168	-2.707807
H	5.851477	0.153196	-1.135743
H	5.549746	0.760682	-2.742085
C	6.525854	-1.474086	-4.108033
H	7.735310	-0.322200	-2.717196
H	7.059983	-1.806869	-2.044794
C	5.352321	-2.448276	-4.044688
H	6.268412	-0.624415	-4.753450
H	7.395587	-1.966527	-4.554700
H	5.699024	-3.392198	-3.600624
H	5.001430	-2.696163	-5.052318

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M06-2X/6-31G* Energy = -8271.56439596

M06-2X/6-31G* Free Energy = -8270.680870

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.54182647

Lowest Frequency = 7.3018

M06-2X/6-31G* Geometry

C	-3.251101	-1.266041	-1.768139
C	-3.676809	-0.027906	-0.918239
C	-3.456282	-2.575068	-1.064387
H	-2.195537	-1.138717	-2.036942
H	-3.812454	-1.253451	-2.707725
C	-2.464330	-3.272237	-0.511669
H	-4.478410	-2.947080	-0.998076
N	-2.710035	-0.000689	0.195567
C	-3.462594	1.291621	-1.679774
C	-5.149253	-0.103702	-0.481456
C	-2.879022	-0.727826	1.226469
C	-1.870313	-0.835545	2.298068
H	-3.792926	-1.310156	1.371889
H	-1.357808	0.773167	-0.332587
H	-1.432009	-2.926081	-0.566424
H	-2.637019	-4.225675	-0.019129
C	4.094315	1.096599	0.782493
C	3.985904	2.331210	1.437546
C	3.333821	0.870206	-0.385163
C	2.415206	1.836111	-0.790166

C	2.242398	3.047329	-0.116052
C	3.068685	3.279020	0.979131
C	3.431659	-0.401285	-1.161743
C	4.655838	-0.842306	-1.708544
C	4.725039	-2.113583	-2.291920
C	3.569721	-2.891731	-2.376077
C	2.325292	-2.432708	-1.954936
C	2.279750	-1.170748	-1.355990
O	1.621951	1.569668	-1.899914
O	1.062204	-0.683294	-0.892488
P	0.383141	0.557240	-1.706497
O	-0.489814	1.244923	-0.603669
O	-0.234338	0.186469	-2.987839
C	1.203355	4.025223	-0.519893
C	1.121496	-3.282093	-2.168093
C	1.102193	4.468246	-1.868791
C	0.165209	5.397935	-2.228213
C	-0.739751	5.930284	-1.272104
C	-0.664049	5.470715	0.071625
C	0.328367	4.518637	0.419396
C	0.123527	-2.890060	-3.105398
C	-0.926176	-3.724189	-3.385386
C	-1.060813	-4.980874	-2.738326
C	-0.080163	-5.366579	-1.784074
C	1.012760	-4.496225	-1.530674
H	2.975327	4.226160	1.506627
H	3.624623	-3.875537	-2.837260
H	1.783567	4.060093	-2.607929
H	0.097937	5.739188	-3.258194
H	1.771849	-4.800040	-0.813023
H	-1.684998	-3.423279	-4.103956
H	0.204549	-1.923035	-3.590376
H	0.376979	4.151776	1.442858
C	-5.593223	0.460195	0.720182
C	-6.942641	0.458300	1.062040
C	-7.883575	-0.104312	0.206011
C	-7.459473	-0.657196	-0.998108
C	-6.109706	-0.653176	-1.336695
H	-4.881329	0.908865	1.406147
H	-7.255742	0.901696	2.002335
H	-8.935744	-0.108245	0.472230
H	-5.810718	-1.078643	-2.289147
H	-8.180509	-1.093323	-1.682653
C	-3.563552	2.488061	-0.959225
C	-3.313199	3.711776	-1.562021
C	-2.961612	3.759135	-2.910874
C	-2.860147	2.579714	-3.635763
C	-3.106693	1.349616	-3.024134
H	-2.962452	0.445821	-3.603589
H	-3.819806	2.457984	0.096467
H	-3.379217	4.627803	-0.981192
H	-2.755591	4.715544	-3.383015
H	-2.564107	2.602155	-4.679787
C	-0.711550	-0.056481	2.285543
C	0.212451	-0.206244	3.305184
C	0.019792	-1.106603	4.348631
C	-1.143148	-1.868249	4.344107
Br	1.782252	0.841545	3.214728
H	0.751837	-1.214072	5.140066
C	-2.090098	-1.745120	3.334660
H	-2.985832	-2.357737	3.351919
H	-0.517849	0.655752	1.493515
Br	-1.437432	-3.102539	5.745504

C	-0.230139	-6.604626	-1.104726
C	-1.305185	-7.417283	-1.358834
C	-2.281874	-7.032796	-2.310622
C	-2.159923	-5.844186	-2.983406
H	0.522047	-6.893920	-0.375150
H	-1.412209	-8.360269	-0.831574
H	-2.909511	-5.538609	-3.708947
H	-3.128856	-7.684339	-2.502459
C	-1.592605	5.972131	1.021840
C	-2.544738	6.890298	0.657135
C	-2.611641	7.357092	-0.679147
C	-1.728295	6.887820	-1.618595
H	-1.534928	5.612719	2.046130
H	-3.250064	7.265748	1.392079
H	-3.366318	8.086802	-0.955725
H	-1.774837	7.240859	-2.646160
C	4.818303	2.670966	2.662245
C	5.393736	1.448205	3.375727
H	4.211543	3.267137	3.354116
H	5.646028	3.320813	2.345712
C	5.988810	0.480315	2.356977
H	4.599428	0.935337	3.933454
H	6.144527	1.765054	4.106751
C	4.898292	-0.024565	1.415479
H	6.770728	0.991376	1.777586
H	6.464084	-0.368782	2.858654
H	4.183946	-0.635452	1.988414
H	5.321116	-0.691092	0.661791
C	5.859054	0.084949	-1.757115
C	7.180514	-0.657848	-1.937742
H	5.899892	0.728900	-0.876434
H	5.712601	0.763743	-2.609864
C	7.080724	-1.623326	-3.115393
H	7.989909	0.063441	-2.089664
H	7.417585	-1.220167	-1.023441
C	6.025702	-2.687176	-2.822718
H	6.801540	-1.061913	-4.016308
H	8.044949	-2.100270	-3.318381
H	6.425585	-3.386535	-2.074828
H	5.819573	-3.283505	-3.718136

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M06-2X/6-31G* Energy = -8271.57336975

M06-2X/6-31G* Free Energy = -8270.687231

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.54434214

Lowest Frequency = 12.3605

M06-2X/6-31G* Geometry

C	-0.453946	3.555428	1.443937
C	-0.758554	3.588867	-0.083575
C	-1.613794	3.095138	2.286470
H	0.390030	2.878346	1.606520
H	-0.110148	4.558285	1.728343
C	-1.556003	2.028025	3.080087
H	-2.551107	3.646910	2.206579
N	-1.359671	2.275235	-0.396225
C	-1.655093	4.760041	-0.506101
C	0.575708	3.691372	-0.841810
C	-2.598956	2.153318	-0.644593
C	-3.232002	0.865125	-0.993690
H	-3.271921	3.016929	-0.642516
H	-0.531925	0.951411	0.184526
H	-0.641442	1.446683	3.175291
H	-2.417536	1.704133	3.657606

C	1.478492	-4.007441	-0.732645
C	0.209745	-4.591321	-0.630297
C	1.852084	-3.021635	0.206918
C	0.895003	-2.552297	1.101679
C	-0.398082	-3.077722	1.190308
C	-0.685250	-4.142046	0.342096
C	3.227089	-2.436430	0.247304
C	4.355581	-3.255021	0.469848
C	5.634007	-2.687586	0.393194
C	5.762725	-1.319381	0.158148
C	4.668376	-0.464542	0.044802
C	3.400273	-1.056308	0.101669
O	1.231696	-1.462087	1.898292
O	2.273471	-0.256926	-0.061636
P	1.239754	-0.027147	1.167575
O	-0.141697	0.042189	0.429251
O	1.583156	1.051694	2.109263
C	-1.443983	-2.474668	2.051665
C	4.896538	0.995623	-0.104934
C	-1.157039	-1.996628	3.363433
C	-2.128863	-1.394635	4.116445
C	-3.449988	-1.235614	3.619662
C	-3.754662	-1.741500	2.326458
C	-2.725525	-2.347913	1.562546
C	5.858397	1.457470	-1.048711
C	6.169575	2.788363	-1.145623
C	5.533653	3.746573	-0.311981
C	4.555320	3.294201	0.614042
C	4.263217	1.910623	0.703856
H	-1.670209	-4.600319	0.398304
H	6.759498	-0.884424	0.122434
H	-0.154742	-2.109102	3.760232
H	-1.896719	-1.025350	5.112382
H	3.537536	1.589100	1.443414
H	6.907497	3.128572	-1.868314
H	6.343690	0.734724	-1.699472
H	-2.948055	-2.674361	0.548718
C	1.199934	2.582774	-1.417535
C	2.408337	2.722896	-2.098790
C	3.005081	3.971762	-2.220446
C	2.403338	5.079063	-1.626228
C	1.202104	4.938293	-0.941459
H	0.750945	1.598592	-1.356702
H	2.881928	1.844005	-2.526077
H	3.943534	4.080300	-2.754755
H	0.732297	5.811797	-0.496203
H	2.875644	6.054504	-1.689973
C	-2.190240	5.687183	0.386751
C	-2.988897	6.739252	-0.068445
C	-3.267013	6.874740	-1.421755
C	-2.733077	5.956316	-2.326905
C	-1.933097	4.917766	-1.872001
H	-1.499830	4.215739	-2.580931
H	-1.982791	5.612304	1.448494
H	-3.389520	7.452470	0.645312
H	-3.888140	7.692137	-1.774432
H	-2.932876	6.057680	-3.389172
C	-2.487095	-0.213072	-1.481424
C	-3.153203	-1.370264	-1.855557
C	-4.536537	-1.488893	-1.760277
C	-5.251846	-0.409504	-1.257124
Br	-2.157922	-2.854228	-2.471949
H	-5.040066	-2.402707	-2.053736

C	-4.621226	0.768523	-0.884429
H	-5.204570	1.598148	-0.498489
H	-1.408935	-0.151082	-1.567774
Br	-7.117236	-0.583139	-1.023007
C	3.883910	4.240517	1.432400
C	4.178455	5.576324	1.336956
C	5.157569	6.027683	0.417196
C	5.817563	5.134752	-0.389282
H	3.128095	3.877658	2.124741
H	3.659459	6.296247	1.962542
H	6.566860	5.477992	-1.098736
H	5.383521	7.088073	0.352894
C	-5.076694	-1.599843	1.829025
C	-6.040570	-0.957142	2.562309
C	-5.732166	-0.441121	3.845048
C	-4.469871	-0.586136	4.363348
H	-5.314773	-2.013076	0.853622
H	-7.040187	-0.841585	2.154135
H	-6.502331	0.063863	4.419997
H	-4.229981	-0.202833	5.352243
C	-0.246861	-5.680682	-1.581031
C	0.496745	-5.633864	-2.912623
H	-1.328772	-5.591992	-1.735001
H	-0.082263	-6.661178	-1.112859
C	1.999822	-5.605891	-2.648728
H	0.206352	-4.727115	-3.462340
H	0.219732	-6.492822	-3.531918
C	2.388059	-4.328546	-1.906744
H	2.273357	-6.482668	-2.045508
H	2.565923	-5.671587	-3.583318
H	3.435112	-4.373626	-1.597070
H	2.325653	-3.477715	-2.600734
C	4.189348	-4.704378	0.897002
C	5.445979	-5.543454	0.677748
H	3.332605	-5.169110	0.405155
H	3.944453	-4.702261	1.969221
C	6.659213	-4.838767	1.277185
H	5.307504	-6.534033	1.122758
H	5.607611	-5.693931	-0.398993
C	6.894838	-3.516733	0.551619
H	6.474864	-4.649632	2.342570
H	7.553878	-5.466068	1.210529
H	7.298791	-3.728679	-0.448539
H	7.655743	-2.922127	1.068602

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M06-2X/6-31G* Energy = -8271.56753099

M06-2X/6-31G* Free Energy = -8270.682529

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.54309142

Lowest Frequency = 11.3845

M06-2X/6-31G* Geometry

C	1.105871	-3.599131	-1.258208
C	0.685873	-3.628759	0.246982
C	0.052770	-4.042602	-2.234228
H	1.392647	-2.567465	-1.486078
H	2.010249	-4.210895	-1.355179
C	-0.574759	-3.197452	-3.051950
H	-0.206342	-5.101036	-2.258864
N	-0.470405	-2.720721	0.366277
C	0.357120	-5.033337	0.771303
C	1.859238	-3.077948	1.070838
C	-1.624538	-3.162061	0.062894
C	-2.831933	-2.317055	0.141462

H	-1.781687	-4.202940	-0.236878
H	-0.368787	-1.067798	0.236684
H	-0.337022	-2.135684	-3.046628
H	-1.325058	-3.547164	-3.756229
C	1.098965	4.379477	1.216242
C	-0.162863	4.827667	1.626309
C	1.177738	3.471536	0.139464
C	0.003248	2.922383	-0.375888
C	-1.274686	3.340954	0.020634
C	-1.305770	4.335414	0.999434
C	2.493642	3.085196	-0.455713
C	3.361732	4.060032	-0.996702
C	4.647774	3.677825	-1.396873
C	5.027858	2.339004	-1.294603
C	4.156863	1.339057	-0.871509
C	2.876068	1.743310	-0.479363
O	0.129348	1.934129	-1.344827
O	1.970033	0.791139	-0.027981
P	0.658293	0.472207	-0.925056
O	-0.362583	-0.049425	0.144108
O	0.884635	-0.364316	-2.116583
C	-2.544816	2.804868	-0.538361
C	4.621063	-0.072953	-0.858142
C	-2.642576	2.318656	-1.877595
C	-3.834630	1.868785	-2.377855
C	-5.021988	1.904180	-1.600775
C	-4.946573	2.417926	-0.277975
C	-3.689708	2.830133	0.230862
C	3.945706	-1.068574	-1.618975
C	4.454238	-2.336992	-1.702128
C	5.635323	-2.704734	-1.006789
C	6.296586	-1.722927	-0.220005
C	5.772924	-0.404910	-0.182749
H	-2.267905	4.742226	1.298347
H	6.027265	2.047286	-1.610125
H	-1.762321	2.309483	-2.506887
H	-3.888605	1.493023	-3.396263
H	6.288946	0.348254	0.409247
H	3.950328	-3.085733	-2.308685
H	3.040058	-0.804025	-2.156235
H	-3.645184	3.152716	1.266766
C	3.055645	-3.804664	1.097838
C	4.167991	-3.326457	1.776763
C	4.105553	-2.105558	2.446655
C	2.917691	-1.388095	2.445311
C	1.797516	-1.873624	1.769828
H	3.119870	-4.758840	0.578932
H	5.095550	-3.892888	1.759336
H	4.983362	-1.720379	2.957097
H	0.885709	-1.291447	1.796460
H	2.850645	-0.434575	2.960273
C	-0.237961	-5.148741	2.034889
C	-0.513271	-6.392626	2.585555
C	-0.187869	-7.555301	1.886505
C	0.418640	-7.455164	0.641406
C	0.689418	-6.202335	0.087825
H	1.173358	-6.152633	-0.882203
H	-0.477349	-4.245603	2.590778
H	-0.975492	-6.457046	3.565775
H	-0.400767	-8.529369	2.315493
H	0.685629	-8.351767	0.090415
C	-2.959563	-1.367112	1.156323
C	-4.144766	-0.654627	1.262689

C	-5.191565	-0.832117	0.363740
C	-5.029278	-1.769468	-0.651017
Br	-4.361218	0.534134	2.715262
H	-6.109229	-0.261392	0.454158
C	-3.874623	-2.531273	-0.761538
H	-3.780267	-3.274812	-1.546351
H	-2.158125	-1.214060	1.870693
Br	-6.434741	-2.042441	-1.885119
C	7.444306	-2.099555	0.525601
C	7.912221	-3.389094	0.490706
C	7.259488	-4.364252	-0.303354
C	6.149815	-4.026264	-1.036476
H	7.943226	-1.347137	1.131544
H	8.787862	-3.667174	1.069156
H	5.639221	-4.770503	-1.643089
H	7.641747	-5.380158	-0.326934
C	-6.133796	2.495010	0.499360
C	-7.333315	2.066570	-0.011688
C	-7.401667	1.528838	-1.321123
C	-6.272131	1.453510	-2.097135
H	-6.072645	2.892789	1.508506
H	-8.235797	2.133457	0.588247
H	-8.351891	1.172821	-1.707143
H	-6.316673	1.034723	-3.099006
C	-0.330429	5.878270	2.708827
C	0.891883	6.011995	3.613260
H	-1.224163	5.650142	3.299708
H	-0.521931	6.846446	2.225035
C	2.155385	6.097655	2.761985
H	0.962597	5.137944	4.273540
H	0.786713	6.893049	4.254355
C	2.345622	4.804334	1.973008
H	2.070637	6.945455	2.067500
H	3.036676	6.280661	3.385086
H	2.595631	3.992901	2.672131
H	3.205338	4.888628	1.305370
C	2.880962	5.483027	-1.229417
C	4.022934	6.483078	-1.392914
H	2.204117	5.807962	-0.436795
H	2.275419	5.478115	-2.147357
C	5.024406	5.972246	-2.424395
H	3.618312	7.456858	-1.686922
H	4.532219	6.623777	-0.428931
C	5.659832	4.677412	-1.925386
H	4.501622	5.788242	-3.371812
H	5.801578	6.716933	-2.623825
H	6.365495	4.916733	-1.117257
H	6.251780	4.206833	-2.717852

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M06-2X/6-31G* Energy = -8271.57199323

M06-2X/6-31G* Free Energy = -8270.687071

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.54270027

Lowest Frequency = 11.5465

M06-2X/6-31G* Geometry

C	1.427083	-3.290116	-0.492422
C	0.714248	-3.153314	0.888962
C	0.632465	-4.015307	-1.541135
H	1.653385	-2.274277	-0.842406
H	2.391390	-3.785458	-0.335586
C	0.166813	-3.421019	-2.638857
H	0.431610	-5.074187	-1.377548
N	-0.548941	-2.488670	0.549641

C	0.539245	-4.478372	1.634224
C	1.545109	-2.199837	1.761655
C	-1.673243	-3.069943	0.435875
C	-2.798849	-2.293389	-0.137553
H	-1.833022	-4.107221	0.749252
H	-0.537269	-0.948247	0.225747
H	0.344415	-2.361785	-2.825603
H	-0.402860	-3.971548	-3.382574
C	3.552964	3.713750	-0.737203
C	4.637808	3.293189	-1.520022
C	2.630661	2.757042	-0.271914
C	2.749068	1.436555	-0.704270
C	3.820666	0.995965	-1.479200
C	4.767207	1.941688	-1.854451
C	1.527983	3.074839	0.683581
C	1.799111	3.494906	2.001025
C	0.724103	3.726004	2.870636
C	-0.578581	3.487958	2.432729
C	-0.874886	2.992066	1.162786
C	0.212565	2.805480	0.304038
O	1.779004	0.525940	-0.323371
O	0.009148	2.238730	-0.953530
P	0.312233	0.652205	-1.021474
O	-0.624013	0.073143	0.083856
O	0.245352	0.099525	-2.384405
C	3.911514	-0.441666	-1.856706
C	-2.281443	2.664910	0.814811
C	3.222083	-0.919299	-3.004671
C	3.248628	-2.251533	-3.324501
C	3.930988	-3.184600	-2.501202
C	4.629850	-2.709237	-1.357163
C	4.610893	-1.321149	-1.065659
C	-3.100188	2.051696	1.809066
C	-4.440290	1.861387	1.609847
C	-5.056661	2.279579	0.401113
C	-4.236931	2.819751	-0.627900
C	-2.846464	2.994158	-0.396936
H	5.616961	1.620852	-2.453279
H	-1.401523	3.674824	3.119229
H	2.644043	-0.219201	-3.598999
H	2.706816	-2.619315	-4.191717
H	-2.236693	3.429139	-1.184102
H	-5.052429	1.381686	2.369970
H	-2.635386	1.723205	2.734231
H	5.117034	-0.961732	-0.172767
C	2.907609	-2.460349	1.944411
C	3.704600	-1.588409	2.675673
C	3.153157	-0.439039	3.241740
C	1.794454	-0.188697	3.091630
C	0.992267	-1.073976	2.371630
H	3.351629	-3.354072	1.512932
H	4.761319	-1.806462	2.803778
H	3.778528	0.246139	3.807222
H	-0.064313	-0.854145	2.267677
H	1.346957	0.702991	3.523577
C	1.151848	-5.665542	1.231520
C	0.996048	-6.834015	1.978627
C	0.225953	-6.832426	3.134841
C	-0.380330	-5.648318	3.553769
C	-0.216838	-4.484766	2.813852
H	-0.669975	-3.557019	3.156737
H	1.770240	-5.691807	0.339405
H	1.482813	-7.746977	1.649594

H	0.103975	-7.743126	3.712747
H	-0.971970	-5.630382	4.463892
C	-2.546060	-1.495477	-1.254544
C	-3.522756	-0.619706	-1.701706
C	-4.771628	-0.551314	-1.094425
C	-5.010771	-1.383883	-0.005150
Br	-3.091804	0.539776	-3.120374
H	-5.526356	0.144144	-1.446472
C	-4.049387	-2.261174	0.481054
H	-4.261423	-2.873111	1.351669
H	-1.580721	-1.526310	-1.748597
Br	-6.677714	-1.275108	0.884757
C	-4.841937	3.188480	-1.859618
C	-6.191433	3.039902	-2.051971
C	-7.009568	2.524720	-1.015330
C	-6.454597	2.157178	0.184192
H	-4.209944	3.582678	-2.650834
H	-6.640149	3.321055	-2.999588
H	-7.072054	1.751427	0.980012
H	-8.078818	2.424776	-1.174940
C	5.258323	-3.647559	-0.495340
C	5.165132	-4.994898	-0.737795
C	4.457101	-5.468781	-1.871757
C	3.865659	-4.583284	-2.736823
H	5.795848	-3.276679	0.374623
H	5.635589	-5.704346	-0.063832
H	4.389599	-6.537118	-2.053307
H	3.312059	-4.938470	-3.602023
C	5.703082	4.263949	-1.995227
C	5.246584	5.720979	-1.969717
H	6.028958	3.979973	-3.001879
H	6.584601	4.157339	-1.347197
C	4.580931	6.032653	-0.631658
H	4.525510	5.897732	-2.778208
H	6.100616	6.381940	-2.149184
C	3.318317	5.189901	-0.470230
H	5.282666	5.810286	0.184470
H	4.328044	7.095154	-0.557451
H	2.874565	5.341773	0.517356
H	2.561933	5.538800	-1.187897
C	3.229260	3.544488	2.510393
C	3.383122	4.317118	3.818657
H	3.906437	3.948224	1.754279
H	3.550235	2.502381	2.660471
C	2.325921	3.876400	4.826642
H	4.392336	4.167250	4.215763
H	3.270401	5.393043	3.627145
C	0.938294	4.217163	4.289492
H	2.406919	2.792095	4.985968
H	2.481684	4.357405	5.797611
H	0.808662	5.308388	4.311449
H	0.158153	3.803065	4.937520

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M06-2X/6-31G* Energy = -8271.57042876

M06-2X/6-31G* Free Energy = -8270.685803

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.54235793

Lowest Frequency = 12.7953

M06-2X/6-31G* Geometry

C	3.169538	-0.861158	0.835172
C	2.532329	-2.255854	0.514501
C	2.787241	-0.245071	2.152476
H	2.865696	-0.199714	0.020974

H	4.257918	-0.966026	0.759098
C	1.782655	0.619410	2.305330
H	3.364824	-0.528475	3.031134
N	1.067364	-2.030038	0.480848
C	3.053661	-2.678214	-0.868939
C	2.909171	-3.358428	1.512650
C	0.450280	-2.055124	1.595591
C	-0.989208	-1.777846	1.792558
H	0.981853	-2.311839	2.516134
H	0.291390	-1.271825	-0.700679
H	1.164411	0.929948	1.464645
H	1.549374	1.045205	3.278206
C	0.377851	4.656249	-0.611369
C	1.658789	5.189703	-0.807553
C	0.220872	3.255416	-0.561321
C	1.312549	2.446097	-0.861087
C	2.605384	2.948197	-1.025206
C	2.749381	4.330419	-0.967923
C	-1.066320	2.604153	-0.168493
C	-1.617771	2.796124	1.116183
C	-2.847351	2.195003	1.418976
C	-3.509191	1.454086	0.439499
C	-2.967999	1.204367	-0.822422
C	-1.700498	1.745003	-1.065923
O	1.112727	1.071906	-0.904346
O	-1.035767	1.434623	-2.246659
P	0.237348	0.447877	-2.127706
O	-0.313609	-0.846822	-1.424571
O	0.928209	0.314567	-3.414920
C	3.771020	2.036746	-1.145634
C	-3.765437	0.442778	-1.817860
C	3.830971	1.037585	-2.158922
C	4.879849	0.157359	-2.199629
C	5.927819	0.220066	-1.241777
C	5.877815	1.223161	-0.234256
C	4.781702	2.123333	-0.215449
C	-5.164766	0.710319	-1.882219
C	-5.993065	-0.019609	-2.689745
C	-5.479382	-1.064601	-3.502111
C	-4.080707	-1.315267	-3.474009
C	-3.246780	-0.544994	-2.624350
H	3.744509	4.752146	-1.093300
H	-4.468593	1.000464	0.684104
H	3.031084	0.966349	-2.890361
H	4.909416	-0.617995	-2.961287
H	-2.195940	-0.799122	-2.582856
H	-7.057682	0.197350	-2.724294
H	-5.570923	1.516831	-1.278812
H	4.724252	2.865708	0.577712
C	2.238511	-4.586426	1.432058
C	2.569580	-5.638402	2.274527
C	3.592060	-5.489071	3.212107
C	4.277970	-4.284057	3.287844
C	3.938391	-3.225232	2.443257
H	1.452184	-4.711871	0.691844
H	2.035662	-6.580330	2.195237
H	3.854031	-6.310864	3.871004
H	4.503017	-2.300948	2.508107
H	5.083881	-4.158487	4.004345
C	2.272654	-2.671238	-2.023554
C	2.824721	-3.013355	-3.259124
C	4.155588	-3.398604	-3.355689
C	4.939883	-3.426959	-2.202899

C	4.397652	-3.059383	-0.978137
H	5.027393	-3.080393	-0.092144
H	1.224224	-2.410625	-1.990249
H	2.196835	-2.975371	-4.143494
H	4.579387	-3.677695	-4.315447
H	5.979458	-3.737751	-2.255902
C	-1.360482	-1.324326	3.063081
C	-2.702776	-1.137015	3.355275
C	-3.690583	-1.420858	2.421669
C	-3.304280	-1.876168	1.164289
Br	-3.212601	-0.532958	5.070749
H	-4.739640	-1.305212	2.668797
C	-1.965600	-2.046922	0.827465
H	-1.692642	-2.411166	-0.156526
H	-0.604649	-1.129461	3.817581
Br	-4.659069	-2.302403	-0.074633
C	-3.553053	-2.357214	-4.282431
C	-4.375982	-3.108436	-5.080963
C	-5.769610	-2.854381	-5.110824
C	-6.307318	-1.855481	-4.340500
H	-2.482453	-2.542760	-4.256392
H	-3.962856	-3.901394	-5.696556
H	-7.375375	-1.654093	-4.360431
H	-6.410284	-3.455502	-5.748687
C	6.906667	1.271211	0.744014
C	7.937089	0.366891	0.721878
C	7.991943	-0.627898	-0.285728
C	7.012298	-0.696532	-1.243500
H	6.859423	2.038382	1.512807
H	8.718105	0.411356	1.474739
H	8.816201	-1.334490	-0.296706
H	7.046442	-1.454447	-2.021329
C	1.909638	6.686296	-0.815047
C	0.647412	7.508139	-1.065016
H	2.333058	6.972181	0.158263
H	2.676112	6.920312	-1.561807
C	-0.483435	7.004182	-0.172275
H	0.344736	7.412248	-2.115669
H	0.851319	8.568205	-0.883485
C	-0.836390	5.565034	-0.540165
H	-0.166043	7.051731	0.878977
H	-1.371208	7.637279	-0.268422
H	-1.585454	5.163508	0.147162
H	-1.312752	5.555467	-1.531037
C	-0.833939	3.547152	2.180731
C	-1.666973	3.908950	3.408842
H	-0.369238	4.444608	1.765580
H	0.004272	2.906380	2.490470
C	-2.478602	2.702182	3.867203
H	-1.006332	4.268662	4.204211
H	-2.351066	4.732566	3.162682
C	-3.489165	2.338910	2.784409
H	-1.803629	1.852925	4.040243
H	-2.993914	2.897455	4.813307
H	-4.258884	3.122371	2.738099
H	-4.012325	1.411384	3.042797

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M06-2X/6-31G* Energy = -8271.56411996

M06-2X/6-31G* Free Energy = -8270.681689

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.53886605

Lowest Frequency = 11.4332

M06-2X/6-31G* Geometry

C	-1.208148	1.509905	3.595059
C	-1.884668	0.160380	3.194635
C	-1.940227	2.744111	3.139254
H	-0.213654	1.503971	3.136130
H	-1.059275	1.516728	4.680658
C	-1.480559	3.546164	2.181150
H	-2.896786	2.973451	3.606628
N	-2.116067	0.323860	1.750165
C	-0.861149	-0.962241	3.402669
C	-3.142090	-0.181726	3.998026
C	-3.264289	0.300847	1.207097
C	-3.380708	0.636059	-0.227130
H	-4.171793	0.039103	1.759819
H	-0.704919	0.686937	0.862272
H	-0.543223	3.335499	1.667662
H	-2.022785	4.431297	1.860800
C	4.509592	-2.091025	-1.404390
C	4.267045	-3.395151	-1.856518
C	3.478139	-1.392775	-0.742560
C	2.201183	-1.953600	-0.688921
C	1.936677	-3.256750	-1.126935
C	3.003878	-3.961319	-1.677395
C	3.711905	-0.068838	-0.089544
C	4.634436	0.087538	0.968306
C	4.847929	1.365128	1.504349
C	4.124763	2.453161	1.010761
C	3.148637	2.313185	0.030063
C	2.952424	1.029685	-0.484051
O	1.187419	-1.218649	-0.099028
O	1.918351	0.834232	-1.395013
P	0.594453	0.104657	-0.833822
O	0.157046	0.975388	0.401614
O	-0.383170	-0.163323	-1.897807
C	0.600366	-3.890172	-0.988699
C	2.338536	3.464687	-0.434797
C	0.498040	-5.164369	-0.360938
C	-0.717719	-5.776975	-0.204240
C	-1.906211	-5.165070	-0.682580
C	-1.806592	-3.905479	-1.335375
C	-0.538864	-3.284729	-1.468811
C	2.208230	3.737158	-1.826221
C	1.491354	4.818224	-2.261397
C	0.828623	5.675257	-1.342163
C	0.954241	5.411183	0.049240
C	1.729208	4.300080	0.472294
H	2.826244	-4.976278	-2.027881
H	4.313229	3.444463	1.418043
H	1.401791	-5.636040	0.016984
H	-0.787206	-6.741968	0.291346
H	1.815612	4.094474	1.537567
H	1.403488	5.025112	-3.325827
H	2.687861	3.073153	-2.538133
H	-0.483294	-2.322418	-1.969752
C	-3.763232	-1.416914	3.762974
C	-4.904868	-1.789305	4.459941
C	-5.441920	-0.938977	5.426500
C	-4.823917	0.277614	5.685114
C	-3.683636	0.654661	4.973699
H	-3.331225	-2.095158	3.030093
H	-5.369272	-2.749599	4.258371
H	-6.329937	-1.230245	5.978584
H	-3.215147	1.604581	5.206236
H	-5.223887	0.942208	6.444689

C	-0.335869	-1.167692	4.684141
C	0.609192	-2.158955	4.910641
C	1.041798	-2.967220	3.858503
C	0.509660	-2.782599	2.589117
C	-0.444170	-1.789543	2.363384
H	-0.852751	-1.674798	1.364426
H	-0.683562	-0.556899	5.513808
H	1.006836	-2.304656	5.910516
H	1.782992	-3.740909	4.034383
H	0.826117	-3.405986	1.757967
C	-2.579324	1.655217	-0.735195
C	-2.537036	1.872100	-2.101875
C	-3.321638	1.133192	-2.977142
C	-4.162384	0.164469	-2.437438
Br	-1.273350	3.116332	-2.731712
H	-3.268778	1.289756	-4.047622
C	-4.210280	-0.099161	-1.074821
H	-4.836849	-0.898915	-0.693044
H	-1.957737	2.245688	-0.072661
Br	-5.218071	-0.882699	-3.608210
C	0.287810	6.258649	0.973753
C	-0.473684	7.311496	0.534572
C	-0.603658	7.569695	-0.852097
C	0.033557	6.770792	-1.766786
H	0.386529	6.050550	2.036628
H	-0.981280	7.952261	1.249041
H	-0.065372	6.961450	-2.832429
H	-1.212815	8.403270	-1.187389
C	-2.982806	-3.297223	-1.851239
C	-4.203246	-3.905208	-1.704859
C	-4.305332	-5.151110	-1.035964
C	-3.184452	-5.767022	-0.540907
H	-2.891268	-2.346079	-2.370362
H	-5.091302	-3.433094	-2.114780
H	-5.277703	-5.621856	-0.926460
H	-3.257009	-6.727594	-0.036961
C	5.347855	-4.229876	-2.518245
C	6.503512	-3.395670	-3.064645
H	4.900398	-4.836553	-3.313015
H	5.742115	-4.939180	-1.776727
C	6.959191	-2.392341	-2.008758
H	6.177018	-2.850975	-3.959916
H	7.326101	-4.051218	-3.367886
C	5.833190	-1.407699	-1.702554
H	7.240234	-2.930375	-1.092408
H	7.845807	-1.844692	-2.343950
H	6.121608	-0.736836	-0.889872
H	5.678452	-0.759126	-2.577029
C	5.288520	-1.128906	1.602003
C	6.523598	-0.786065	2.431612
H	5.535045	-1.882359	0.850912
H	4.535354	-1.598623	2.251995
C	6.212037	0.355975	3.394254
H	6.859853	-1.675888	2.973504
H	7.344408	-0.485782	1.765357
C	5.866026	1.613528	2.601689
H	5.361904	0.071215	4.027563
H	7.059006	0.554464	4.058900
H	6.783889	2.008375	2.143620
H	5.494344	2.400266	3.267233

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M06-2X/6-31G* Energy = -8271.56950558

M06-2X/6-31G* Free Energy = -8270.680986

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.54472211

Lowest Frequency = 18.0372

M06-2X/6-31G* Geometry

C	0.052017	0.899004	2.829262
C	-0.044371	-0.655466	2.714267
C	-1.161622	1.543145	3.443074
H	0.215001	1.272685	1.812334
H	0.935927	1.171763	3.411351
C	-2.216899	1.966601	2.748667
H	-1.177128	1.636814	4.527326
N	-0.995705	-0.870505	1.605842
C	1.290211	-1.284235	2.287455
C	-0.434260	-1.331884	4.037994
C	-2.245952	-0.925315	1.838894
C	-3.285337	-1.064794	0.798707
H	-2.626094	-0.888111	2.864192
H	-0.213568	-0.806052	0.094201
H	-2.242888	1.872219	1.666971
H	-3.081587	2.409724	3.235106
C	4.083166	3.007822	-1.060215
C	5.386427	2.569502	-1.322141
C	3.104555	2.057323	-0.695485
C	3.412115	0.695190	-0.733898
C	4.714410	0.235853	-0.979989
C	5.677171	1.208803	-1.242847
C	1.733707	2.495949	-0.295465
C	1.530837	3.358601	0.800777
C	0.249737	3.881980	1.012860
C	-0.797836	3.491432	0.180697
C	-0.672638	2.517307	-0.813057
C	0.634154	2.042916	-1.027870
O	2.384266	-0.209838	-0.481512
O	0.881745	1.119650	-2.027321
P	1.262586	-0.409250	-1.636469
O	0.045072	-1.015557	-0.863770
O	1.663892	-1.147556	-2.837529
C	5.125396	-1.190473	-0.952797
C	-1.876486	2.043041	-1.553703
C	6.326909	-1.536794	-0.268949
C	6.774362	-2.831181	-0.231129
C	6.041527	-3.870159	-0.864963
C	4.842906	-3.529944	-1.550777
C	4.413399	-2.179161	-1.591383
C	-1.798185	1.483931	-2.866304
C	-2.925541	1.081167	-3.530356
C	-4.215373	1.227302	-2.958992
C	-4.314121	1.791897	-1.659841
C	-3.129087	2.173726	-0.983721
H	6.692255	0.879641	-1.454783
H	-1.768444	3.951742	0.343342
H	6.880960	-0.756150	0.245601
H	7.689974	-3.081735	0.298851
H	-3.246175	2.587554	0.013057
H	-2.840708	0.650063	-4.524249
H	-0.836755	1.385866	-3.350378
H	3.514212	-1.940616	-2.151177
C	-1.031626	-2.597510	4.043967
C	-1.300127	-3.257846	5.237814
C	-0.960955	-2.673299	6.455329
C	-0.341394	-1.428597	6.462958
C	-0.079336	-0.767620	5.265303
H	-1.284807	-3.079013	3.103745
H	-1.769278	-4.236554	5.214212

H	-1.169275	-3.188193	7.387729
H	0.424095	0.193870	5.298421
H	-0.056118	-0.966196	7.402888
C	2.523088	-0.779559	2.701222
C	3.706054	-1.427001	2.352359
C	3.672514	-2.597097	1.602824
C	2.448030	-3.111944	1.189632
C	1.269196	-2.462363	1.533551
H	0.319237	-2.867244	1.195856
H	2.583350	0.118261	3.308264
H	4.659258	-1.012812	2.668409
H	4.595177	-3.098960	1.329374
H	2.414561	-4.015801	0.588033
C	-3.004551	-1.473763	-0.509980
C	-4.060331	-1.659689	-1.391194
C	-5.383340	-1.439887	-1.019634
C	-5.633257	-1.005954	0.275084
Br	-3.702897	-2.253127	-3.145814
H	-6.191036	-1.584730	-1.726606
C	-4.605848	-0.825326	1.189960
H	-4.830483	-0.506416	2.203192
H	-1.989229	-1.660188	-0.838754
Br	-7.412599	-0.653915	0.800592
C	-5.599472	1.964409	-1.078981
C	-6.730338	1.597736	-1.762397
C	-6.627965	1.013577	-3.049648
C	-5.398732	0.826746	-3.631256
H	-5.672131	2.388556	-0.079831
H	-7.706904	1.729901	-1.308003
H	-5.311562	0.373580	-4.615300
H	-7.530359	0.715322	-3.574954
C	4.090186	-4.558591	-2.179627
C	4.509834	-5.862753	-2.123550
C	5.705305	-6.200830	-1.441145
C	6.452776	-5.228365	-0.827694
H	3.176190	-4.283059	-2.699830
H	3.928571	-6.643775	-2.603804
H	6.026960	-7.237209	-1.406177
H	7.369663	-5.483514	-0.302245
C	6.505535	3.529060	-1.680795
C	5.999937	4.871015	-2.202378
H	7.116311	3.704379	-0.783775
H	7.167074	3.053362	-2.412800
C	4.914573	5.403325	-1.271842
H	5.581062	4.744012	-3.208896
H	6.831619	5.577961	-2.284912
C	3.709329	4.465669	-1.275072
H	5.317684	5.483574	-0.252361
H	4.597393	6.407464	-1.570979
H	2.972391	4.800223	-0.542048
H	3.203975	4.534292	-2.249358
C	2.652584	3.627882	1.787877
C	2.390301	4.831689	2.689877
H	3.612022	3.735784	1.276512
H	2.755436	2.724469	2.409403
C	0.977822	4.769016	3.264779
H	3.140170	4.862882	3.486819
H	2.501521	5.758030	2.109202
C	-0.040426	4.861915	2.132621
H	0.842389	3.817378	3.798533
H	0.810287	5.572695	3.988860
H	-0.032193	5.882938	1.725785
H	-1.052294	4.681683	2.511210

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M06-2X/6-31G* Energy = -8271.58107919

M06-2X/6-31G* Free Energy = -8270.692715

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.54451325

Lowest Frequency = 15.6098

M06-2X/6-31G* Geometry

C	4.175311	-1.170017	-1.621692
C	4.212998	-0.317789	-0.307554
C	3.980494	-2.644441	-1.412262
H	3.349254	-0.778266	-2.223009
H	5.094994	-0.957567	-2.177532
C	2.792575	-3.243308	-1.495444
H	4.856661	-3.240588	-1.162979
N	2.871511	-0.458905	0.280699
C	5.323093	-0.738514	0.655798
C	4.373818	1.160374	-0.709144
C	2.585809	-1.408024	1.078336
C	1.205683	-1.496606	1.607211
H	3.318520	-2.149201	1.411678
H	1.469698	-0.195035	-0.635627
H	1.886838	-2.685794	-1.736233
H	2.683169	-4.314284	-1.342522
C	-4.090168	-0.480069	0.463894
C	-4.089704	-1.876572	0.599231
C	-3.249436	0.104481	-0.508401
C	-2.402590	-0.709658	-1.265667
C	-2.357853	-2.100292	-1.119810
C	-3.245542	-2.650048	-0.194804
C	-3.175628	1.584366	-0.703160
C	-4.285050	2.359238	-1.089460
C	-4.158360	3.755894	-1.120123
C	-2.925218	4.342553	-0.838690
C	-1.776745	3.596971	-0.570198
C	-1.940519	2.210814	-0.513517
O	-1.581543	-0.097408	-2.207115
O	-0.827536	1.392606	-0.322700
P	-0.281638	0.709404	-1.695682
O	0.642717	-0.444464	-1.161337
O	0.247192	1.638936	-2.699045
C	-1.406398	-2.978891	-1.845507
C	-0.463009	4.262479	-0.390164
C	-1.025809	-2.753742	-3.200853
C	-0.164600	-3.609450	-3.836269
C	0.375844	-4.742467	-3.171546
C	-0.005684	-4.979399	-1.823594
C	-0.892452	-4.077169	-1.190618
C	-0.141741	5.387186	-1.202731
C	1.024807	6.080333	-1.021525
C	1.963773	5.680053	-0.035283
C	1.675415	4.528628	0.747894
C	0.442643	3.853292	0.564351
H	-3.274350	-3.730927	-0.080555
H	-2.847860	5.427631	-0.853630
H	-1.429213	-1.899107	-3.730558
H	0.118625	-3.426553	-4.869477
H	0.199403	3.021626	1.219717
H	1.252915	6.942506	-1.643145
H	-0.834130	5.682997	-1.985104
H	-1.151103	-4.260956	-0.152542
C	5.527908	1.894278	-0.430148
C	5.637306	3.221385	-0.844630
C	4.599017	3.834303	-1.537058

C	3.444835	3.109096	-1.823738
C	3.344276	1.783530	-1.421820
H	6.348913	1.439396	0.114286
H	6.540916	3.778433	-0.614004
H	4.684036	4.871889	-1.843677
H	2.446656	1.242818	-1.695861
H	2.611353	3.559856	-2.355342
C	5.276156	-0.290878	1.983013
C	6.299269	-0.583480	2.876078
C	7.403575	-1.323710	2.456192
C	7.473382	-1.755713	1.137384
C	6.441848	-1.462992	0.244901
H	6.530555	-1.795344	-0.783956
H	4.430500	0.308241	2.310933
H	6.239030	-0.226266	3.899549
H	8.204983	-1.553512	3.151253
H	8.333333	-2.322059	0.793428
C	0.521868	-0.307858	1.863418
C	-0.783587	-0.357121	2.323511
C	-1.432411	-1.567847	2.534268
C	-0.731463	-2.738302	2.266125
Br	-1.675111	1.260004	2.693879
H	-2.454635	-1.600600	2.892838
C	0.583600	-2.728032	1.818409
H	1.102475	-3.657942	1.606283
H	1.011722	0.644163	1.686446
Br	-1.614999	-4.392967	2.518195
C	2.635536	4.087405	1.697204
C	3.812015	4.767843	1.872987
C	4.081728	5.935435	1.117010
C	3.179443	6.378492	0.184714
H	2.419017	3.194351	2.278845
H	4.544130	4.414575	2.592547
H	3.385935	7.266158	-0.408565
H	5.013026	6.471558	1.273236
C	0.537172	-6.094921	-1.131742
C	1.426343	-6.934116	-1.753632
C	1.811384	-6.696104	-3.097137
C	1.296889	-5.628238	-3.788409
H	0.233601	-6.261675	-0.100118
H	1.839687	-7.784764	-1.220461
H	2.518397	-7.365474	-3.577256
H	1.593076	-5.441226	-4.817267
C	-4.982782	-2.603074	1.589417
C	-5.596270	-1.689708	2.648132
H	-4.399077	-3.403905	2.058991
H	-5.789979	-3.096842	1.031243
C	-6.109670	-0.409824	1.995313
H	-4.840929	-1.421826	3.400523
H	-6.395597	-2.217863	3.177549
C	-4.937363	0.365495	1.399767
H	-6.832102	-0.663206	1.206987
H	-6.632838	0.218036	2.723577
H	-5.287805	1.273757	0.906749
H	-4.290715	0.708602	2.216367
C	-5.557355	1.695754	-1.586312
C	-6.776878	2.609791	-1.498820
H	-5.740343	0.750516	-1.070357
H	-5.391175	1.426676	-2.639558
C	-6.470427	3.948221	-2.166574
H	-7.636801	2.125036	-1.972058
H	-7.040800	2.778119	-0.445145
C	-5.341264	4.657516	-1.421910

H	-6.172054	3.767943	-3.207323
H	-7.358078	4.588440	-2.192314
H	-5.732121	5.042581	-0.469418
H	-4.997529	5.531499	-1.985788

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M06-2X/6-31G* Energy = -8271.57140510

M06-2X/6-31G* Free Energy = -8270.685433

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.54207026

Lowest Frequency = 12.1384

M06-2X/6-31G* Geometry

C	-1.648628	3.081770	-2.230848
C	-1.192287	3.685660	-0.863939
C	-3.093467	2.687216	-2.264496
H	-1.028750	2.199942	-2.423053
H	-1.422247	3.808894	-3.017798
C	-3.485521	1.414970	-2.209420
H	-3.834344	3.485707	-2.302649
N	-1.270787	2.550975	0.081097
C	0.288719	4.107342	-0.919283
C	-2.044094	4.900892	-0.463055
C	-2.390090	2.215478	0.588610
C	-2.593834	0.979470	1.371355
H	-3.283054	2.830674	0.450484
H	0.131004	1.715019	0.060799
H	-2.753121	0.609084	-2.167048
H	-4.533476	1.125285	-2.214671
C	2.729938	-3.172215	1.367468
C	3.349139	-2.552374	2.461212
C	2.553298	-2.427762	0.183631
C	2.961144	-1.098643	0.129731
C	3.619919	-0.472791	1.191680
C	3.800590	-1.237003	2.343382
C	1.787038	-2.978535	-0.969015
C	2.233632	-4.069981	-1.733861
C	1.385322	-4.605649	-2.712312
C	0.126325	-4.038475	-2.909427
C	-0.309971	-2.910771	-2.215373
C	0.569004	-2.368583	-1.275793
O	2.639984	-0.374497	-1.016506
O	0.259605	-1.170897	-0.638706
P	1.110653	0.136166	-1.137849
O	0.963347	1.113631	0.077230
O	0.759851	0.609997	-2.483912
C	4.118088	0.922174	1.132508
C	-1.678479	-2.387277	-2.441179
C	3.958800	1.769067	2.265397
C	4.508483	3.021781	2.292313
C	5.258251	3.509404	1.190305
C	5.395053	2.683379	0.040498
C	4.806028	1.393789	0.037489
C	-2.143137	-2.171800	-3.768203
C	-3.442390	-1.812041	-4.008722
C	-4.361474	-1.655246	-2.938788
C	-3.901376	-1.858442	-1.607659
C	-2.545906	-2.213452	-1.385401
H	4.307412	-0.781573	3.191589
H	-0.546839	-4.488335	-3.636826
H	3.377381	1.408546	3.108962
H	4.377335	3.661898	3.161160
H	-2.196418	-2.374445	-0.366176
H	-3.785686	-1.636400	-5.024843
H	-1.441427	-2.283246	-4.589603

H	4.928280	0.764348	-0.839550
C	-2.334461	5.197647	0.873565
C	-3.041308	6.346206	1.220674
C	-3.472559	7.229051	0.236587
C	-3.180490	6.954629	-1.096109
C	-2.472735	5.806806	-1.438849
H	-2.002696	4.528139	1.661540
H	-3.251621	6.548385	2.266513
H	-4.026124	8.123241	0.504926
H	-2.246932	5.625300	-2.484648
H	-3.501532	7.637273	-1.876863
C	1.114820	3.789956	-1.999109
C	2.462028	4.148770	-1.987962
C	3.004279	4.822901	-0.901747
C	2.193312	5.120914	0.190667
C	0.849701	4.768705	0.178642
H	0.227931	5.017638	1.033291
H	0.738298	3.230479	-2.846393
H	3.090007	3.887385	-2.834465
H	4.052470	5.104763	-0.898485
H	2.612311	5.630019	1.054176
C	-3.881271	0.696466	1.833579
C	-4.112180	-0.491719	2.514069
C	-3.101683	-1.421655	2.732530
C	-1.832059	-1.121893	2.247413
Br	-5.875618	-0.924481	3.036545
H	-3.306751	-2.360698	3.233039
C	-1.559221	0.068470	1.595183
H	-0.553194	0.257842	1.250270
H	-4.702952	1.378237	1.638762
Br	-0.431525	-2.382862	2.390150
C	-4.817038	-1.694665	-0.535763
C	-6.114541	-1.316214	-0.765677
C	-6.568593	-1.102282	-2.091174
C	-5.713897	-1.277257	-3.150387
H	-4.469487	-1.882184	0.474218
H	-6.791147	-1.184223	0.073585
H	-6.056965	-1.120490	-4.169934
H	-7.598745	-0.806843	-2.265133
C	6.136235	3.169841	-1.069610
C	6.717402	4.412060	-1.036054
C	6.581571	5.233695	0.111017
C	5.865426	4.792324	1.195256
H	6.234550	2.536027	-1.947132
H	7.283601	4.772432	-1.889340
H	7.045510	6.215091	0.125982
H	5.755262	5.418415	2.077399
C	3.520684	-3.267904	3.786448
C	2.501939	-4.389918	3.966165
H	3.443672	-2.537902	4.599382
H	4.532985	-3.692101	3.844866
C	2.558719	-5.312038	2.752210
H	1.494757	-3.960080	4.056290
H	2.704066	-4.941870	4.889530
C	2.138240	-4.568443	1.484295
H	3.585759	-5.683945	2.638206
H	1.916237	-6.187655	2.888868
H	1.043031	-4.474010	1.457305
H	2.385813	-5.170752	0.606079
C	3.654274	-4.580512	-1.579249
C	3.835573	-5.997359	-2.118156
H	3.984618	-4.511339	-0.539575
H	4.310901	-3.899960	-2.140326

C	3.280809	-6.086493	-3.538141
H	4.895552	-6.269763	-2.094607
H	3.304113	-6.711382	-1.473491
C	1.776138	-5.823171	-3.528918
H	3.783958	-5.339587	-4.165662
H	3.483671	-7.067422	-3.979763
H	1.264675	-6.700472	-3.108371
H	1.398384	-5.711223	-4.551165

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M06-2X/6-31G* Energy = -8271.56606032

M06-2X/6-31G* Free Energy = -8270.681636

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.53966235

Lowest Frequency = 10.9533

M06-2X/6-31G* Geometry

C	3.325263	-0.955541	0.736322
C	2.682947	-2.326777	0.347948
C	3.015739	-0.442249	2.114403
H	2.970542	-0.237835	-0.006074
H	4.408652	-1.043482	0.590949
C	2.090871	0.484199	2.369213
H	3.581643	-0.854698	2.948629
N	1.217927	-2.124582	0.376891
C	3.141348	-2.644798	-1.086027
C	3.103625	-3.489351	1.256953
C	0.633653	-2.197051	1.505509
C	-0.828602	-2.036723	1.653504
H	1.180530	-2.432174	2.423421
H	0.235564	-1.230183	-0.730230
H	1.489605	0.920173	1.574310
H	1.912061	0.839105	3.381015
C	0.545534	4.684442	-0.201533
C	1.838933	5.186316	-0.396766
C	0.337348	3.288502	-0.252294
C	1.389821	2.462344	-0.638791
C	2.694629	2.934685	-0.809213
C	2.889349	4.303475	-0.657640
C	-0.984637	2.681317	0.093764
C	-1.559042	2.838894	1.372661
C	-2.857781	2.361202	1.592117
C	-3.549721	1.740757	0.551933
C	-2.979774	1.486672	-0.694803
C	-1.664573	1.935584	-0.868141
O	1.142730	1.099865	-0.761511
O	-0.993593	1.635815	-2.049337
P	0.209205	0.564628	-1.986389
O	-0.413394	-0.717993	-1.315231
O	0.874343	0.437026	-3.287206
C	3.834313	2.015468	-1.052916
C	-3.766699	0.831429	-1.770244
C	3.825229	1.095145	-2.139302
C	4.865261	0.220155	-2.310807
C	5.970575	0.209988	-1.418564
C	5.988530	1.132618	-0.336065
C	4.900846	2.029963	-0.182143
C	-3.601598	1.212429	-3.135525
C	-4.385381	0.667945	-4.115467
C	-5.395997	-0.280155	-3.807576
C	-5.580878	-0.657095	-2.450101
C	-4.740571	-0.091535	-1.457457
H	3.894537	4.698348	-0.789606
H	-4.582102	1.444576	0.722537
H	2.981682	1.078490	-2.823389

H	4.844377	-0.495679	-3.128769
H	-4.876875	-0.409395	-0.426807
H	-4.248887	0.968732	-5.150885
H	-2.850439	1.948311	-3.394752
H	4.897386	2.711825	0.665588
C	2.411069	-4.703381	1.154899
C	2.781783	-5.804810	1.914066
C	3.865989	-5.720082	2.787670
C	4.574301	-4.529196	2.882252
C	4.195828	-3.421639	2.121277
H	1.575648	-4.779780	0.463583
H	2.229501	-6.734637	1.818936
H	4.158474	-6.580235	3.381585
H	4.779369	-2.509758	2.196693
H	5.428330	-4.453148	3.548233
C	4.451116	-3.097828	-1.286792
C	4.927590	-3.364277	-2.564964
C	4.111310	-3.160596	-3.676830
C	2.815875	-2.693722	-3.489385
C	2.331129	-2.450507	-2.204081
H	1.307742	-2.118746	-2.103966
H	5.105534	-3.255479	-0.433390
H	5.941368	-3.734027	-2.690794
H	4.483811	-3.363944	-4.676213
H	2.164293	-2.511066	-4.337837
C	-1.340530	-1.471755	2.824188
C	-2.716127	-1.405971	2.993761
C	-3.593905	-1.919444	2.044779
C	-3.058720	-2.497055	0.897564
Br	-3.422037	-0.677072	4.589396
H	-4.664857	-1.897923	2.209634
C	-1.688981	-2.546711	0.680202
H	-1.291242	-3.007034	-0.217482
H	-0.673118	-1.093269	3.591970
Br	-4.217659	-3.294531	-0.357181
C	-6.606405	-1.587466	-2.130181
C	-7.399055	-2.121333	-3.113338
C	-7.207588	-1.750992	-4.467246
C	-6.229941	-0.850480	-4.803961
H	-6.748719	-1.869684	-1.090558
H	-8.181163	-2.829441	-2.857229
H	-6.079158	-0.557782	-5.839830
H	-7.840913	-2.182313	-5.236222
C	7.076487	1.103575	0.577131
C	8.098218	0.202596	0.420632
C	8.084763	-0.711572	-0.662177
C	7.047041	-0.705275	-1.558935
H	7.081528	1.808584	1.404645
H	8.924517	0.187752	1.124781
H	8.902296	-1.416506	-0.778265
H	7.026051	-1.402678	-2.391825
C	2.148480	6.669067	-0.305112
C	0.913942	7.552894	-0.461171
H	2.606782	6.868343	0.673944
H	2.905077	6.926274	-1.054300
C	-0.208981	7.028175	0.428723
H	0.579132	7.541600	-1.506401
H	1.163436	8.589508	-0.213315
C	-0.628794	5.632109	-0.024858
H	0.139933	6.989262	1.470284
H	-1.074805	7.697543	0.405212
H	-1.370032	5.216249	0.661385
H	-1.139405	5.708797	-0.995738

C	-0.755168	3.436994	2.514660
C	-1.627021	3.924651	3.669524
H	-0.103748	4.239261	2.160585
H	-0.078841	2.653389	2.887632
C	-2.613930	2.833411	4.072389
H	-0.991309	4.212460	4.513058
H	-2.180140	4.823031	3.361723
C	-3.569643	2.550647	2.917642
H	-2.063171	1.916844	4.320342
H	-3.180602	3.117754	4.965300
H	-4.273568	3.389048	2.819458
H	-4.173356	1.662945	3.133136

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M06-2X/6-31G* Energy = -8271.56375104

M06-2X/6-31G* Free Energy = -8270.680316

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.53844454

Lowest Frequency = 9.5714

M06-2X/6-31G* Geometry

C	-3.382869	-2.779093	0.158732
C	-3.759002	-1.262308	0.201898
C	-2.925372	-3.293890	-1.181818
H	-2.566883	-2.911104	0.876522
H	-4.242783	-3.343231	0.535964
C	-1.649570	-3.580456	-1.434907
H	-3.668176	-3.426831	-1.967334
N	-2.602649	-0.611213	-0.470877
C	-5.074305	-0.887810	-0.476409
C	-3.817546	-0.815444	1.663072
C	-2.649576	0.022157	-1.579019
C	-1.481627	0.473531	-2.334325
H	-3.629948	0.243604	-1.999995
H	-1.630690	-0.881134	0.001375
H	-0.875821	-3.442836	-0.681292
H	-1.335891	-3.959390	-2.403901
C	4.718604	-0.051282	-0.130823
C	5.118148	-1.228979	-0.783772
C	3.638827	-0.101281	0.773147
C	2.917364	-1.293298	0.927338
C	3.230612	-2.443347	0.191872
C	4.370015	-2.392062	-0.610860
C	3.123880	1.145258	1.416226
C	3.888440	1.955888	2.278186
C	3.346216	3.163501	2.741565
C	2.040209	3.517584	2.392218
C	1.232829	2.691342	1.618050
C	1.805649	1.510978	1.138134
O	1.865726	-1.332587	1.810675
O	0.997849	0.607764	0.475971
P	0.444431	-0.569089	1.508458
O	-0.412798	-1.440835	0.601313
O	-0.073603	-0.003489	2.767912
C	2.335535	-3.625525	0.137348
C	-0.200933	2.981048	1.371243
C	2.103687	-4.223242	-1.136759
C	1.293429	-5.318405	-1.270783
C	0.635037	-5.875894	-0.143666
C	0.839697	-5.272640	1.128433
C	1.702110	-4.152182	1.241295
C	-0.751785	2.882029	0.059676
C	-2.078179	3.141633	-0.164818
C	-2.947268	3.497344	0.900368
C	-2.408670	3.592482	2.212788

C	-1.028284	3.331505	2.413970
H	4.658253	-3.285161	-1.161281
H	1.628556	4.454227	2.763735
H	2.557241	-3.768135	-2.013152
H	1.122169	-5.760007	-2.249719
H	-0.627036	3.368272	3.424233
H	-2.484199	3.090364	-1.173151
H	-0.099587	2.604942	-0.764588
H	1.851572	-3.705242	2.218531
C	-2.959969	0.138976	2.195357
C	-3.023935	0.457853	3.552636
C	-3.972274	-0.139072	4.369495
C	-4.861689	-1.070816	3.829978
C	-4.781015	-1.410791	2.488173
H	-2.211939	0.637198	1.586175
H	-2.296720	1.155889	3.952279
H	-4.019939	0.110300	5.424979
H	-5.479547	-2.132156	2.070833
H	-5.613641	-1.537505	4.458944
C	-5.864121	-1.798603	-1.174751
C	-7.066592	-1.392402	-1.756944
C	-7.486261	-0.072199	-1.653039
C	-6.706434	0.844989	-0.946869
C	-5.518575	0.437348	-0.355964
H	-4.928475	1.144668	0.224861
H	-5.563824	-2.837151	-1.257018
H	-7.673824	-2.117248	-2.289941
H	-8.420971	0.240883	-2.107438
H	-7.034004	1.874894	-0.838748
C	-0.210682	-0.064603	-2.121666
C	0.854857	0.442148	-2.852749
C	0.682310	1.455564	-3.790955
C	-0.599306	1.955034	-4.006734
Br	2.569336	-0.251377	-2.510092
H	1.526248	1.844254	-4.349043
C	-1.687155	1.468499	-3.298327
H	-2.679630	1.867750	-3.483565
H	-0.045394	-0.850632	-1.390437
Br	-0.858725	3.313580	-5.291101
C	-3.278688	3.915400	3.287868
C	-4.614819	4.132176	3.070390
C	-5.148198	4.049179	1.760814
C	-4.330921	3.745642	0.701596
H	-2.864886	3.976783	4.291325
H	-5.271029	4.369122	3.901803
H	-4.730962	3.688714	-0.309166
H	-6.206527	4.231052	1.600122
C	0.164849	-5.809153	2.258023
C	-0.672226	-6.886802	2.127827
C	-0.876870	-7.484436	0.859447
C	-0.238694	-6.989285	-0.248439
H	0.321363	-5.341752	3.226481
H	-1.185055	-7.286192	2.997358
H	-1.543792	-8.336443	0.769450
H	-0.394075	-7.440278	-1.225439
C	6.292178	-1.246583	-1.742695
C	6.490213	0.104548	-2.424621
H	6.141501	-2.039082	-2.483867
H	7.208220	-1.505572	-1.193380
C	6.585237	1.192462	-1.359096
H	5.633037	0.309389	-3.081207
H	7.387124	0.086873	-3.052236
C	5.281510	1.291025	-0.569355

H	7.414136	0.954670	-0.678419
H	6.811075	2.165144	-1.808331
H	4.506861	1.746732	-1.206140
H	5.405708	1.974997	0.272450
C	5.228150	1.466157	2.798928
C	6.109549	2.592226	3.333425
H	5.757279	0.886200	2.038865
H	5.020656	0.758738	3.614667
C	5.319120	3.446406	4.321435
H	7.001874	2.170205	3.807064
H	6.453654	3.222386	2.501123
C	4.148842	4.117897	3.606492
H	4.941194	2.804028	5.127217
H	5.957332	4.205337	4.785720
H	4.539596	4.922623	2.967422
H	3.481769	4.600161	4.329634

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M06-2X/6-31G* Energy = -8271.57104811

M06-2X/6-31G* Free Energy = -8270.684752

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.54076407

Lowest Frequency = 15.3989

M06-2X/6-31G* Geometry

C	3.411058	2.145294	-1.615561
C	3.954181	1.411241	-0.342870
C	2.804699	3.483071	-1.313207
H	2.659551	1.488190	-2.069029
H	4.228473	2.241545	-2.336804
C	1.493636	3.709057	-1.250806
H	3.485482	4.302869	-1.090002
N	2.749236	1.088745	0.430538
C	4.649751	0.104946	-0.751853
C	4.982508	2.228288	0.452258
C	2.237199	1.942355	1.225317
C	0.952685	1.644583	1.896552
H	2.711106	2.905786	1.432504
H	1.697758	-0.072997	-0.157526
H	0.762135	2.930538	-1.474129
H	1.114277	4.694772	-0.997458
C	-3.274537	-2.837897	0.691541
C	-2.679995	-4.014778	1.164938
C	-2.656266	-2.137314	-0.360743
C	-1.401954	-2.545066	-0.817471
C	-0.761944	-3.684517	-0.320852
C	-1.454817	-4.421978	0.639424
C	-3.281864	-0.942452	-0.994400
C	-4.519960	-1.031194	-1.662355
C	-5.059343	0.121652	-2.249841
C	-4.331406	1.309282	-2.214201
C	-3.072937	1.406141	-1.624539
C	-2.570282	0.261261	-1.007515
O	-0.779289	-1.782130	-1.799191
O	-1.297337	0.275504	-0.437561
P	-0.129875	-0.360560	-1.381425
O	0.990370	-0.775723	-0.368214
O	0.239884	0.472555	-2.534137
C	0.595334	-4.101691	-0.745171
C	-2.323807	2.684280	-1.766878
C	0.994955	-4.066636	-2.111835
C	2.236799	-4.502482	-2.486895
C	3.157653	-5.005030	-1.530412
C	2.769056	-5.040464	-0.162758
C	1.482047	-4.570526	0.198713

C	-1.891498	3.055190	-3.070790
C	-1.331657	4.282357	-3.299833
C	-1.160369	5.208809	-2.239112
C	-1.559302	4.832320	-0.925864
C	-2.145775	3.554191	-0.717986
H	-1.001744	-5.338266	1.011251
H	-4.741002	2.195190	-2.695192
H	0.300551	-3.692038	-2.855075
H	2.534251	-4.471254	-3.531595
H	-2.480806	3.283444	0.280466
H	-0.998402	4.558749	-4.296574
H	-2.003340	2.337188	-3.876978
H	1.203124	-4.564265	1.250179
C	5.267247	1.864646	1.774179
C	6.248085	2.525228	2.503583
C	6.979598	3.557642	1.919296
C	6.723953	3.912035	0.600077
C	5.734380	3.251408	-0.126946
H	4.718395	1.045132	2.230825
H	6.448205	2.226906	3.528116
H	7.747140	4.074349	2.486761
H	5.560986	3.540670	-1.158771
H	7.293558	4.706601	0.127943
C	5.711603	0.155214	-1.661515
C	6.399430	-0.996834	-2.021206
C	6.049940	-2.222913	-1.459334
C	5.011931	-2.280625	-0.537687
C	4.311954	-1.125988	-0.189678
H	3.500180	-1.196232	0.526459
H	6.022946	1.108791	-2.079653
H	7.216090	-0.933614	-2.734067
H	6.584133	-3.128679	-1.730064
H	4.746210	-3.227186	-0.078915
C	0.643444	0.322510	2.215933
C	-0.610254	0.018982	2.718364
C	-1.546343	1.010889	2.979690
C	-1.192314	2.328655	2.713358
Br	-1.065795	-1.793134	2.961876
H	-2.524563	0.769563	3.378218
C	0.037305	2.666902	2.161598
H	0.267909	3.698703	1.911887
H	1.360595	-0.467817	2.034030
Br	-2.459032	3.679499	3.103192
C	-1.339153	5.743841	0.142181
C	-0.740800	6.958004	-0.082538
C	-0.345150	7.331040	-1.390615
C	-0.556636	6.477189	-2.442542
H	-1.648994	5.458233	1.143004
H	-0.572463	7.641496	0.744139
H	-0.250334	6.751482	-3.448724
H	0.125609	8.295295	-1.555410
C	3.689103	-5.532629	0.801930
C	4.935908	-5.963791	0.425600
C	5.323663	-5.924696	-0.937037
C	4.453611	-5.457688	-1.889975
H	3.387156	-5.557148	1.845944
H	5.632234	-6.335740	1.170744
H	6.313604	-6.267281	-1.222693
H	4.746329	-5.420666	-2.936237
C	-3.316371	-4.840565	2.267225
C	-4.247847	-4.016986	3.153882
H	-2.528971	-5.311870	2.866141
H	-3.889259	-5.660993	1.812641

C	-5.222897	-3.231782	2.280714
H	-3.654828	-3.313178	3.753228
H	-4.779855	-4.672113	3.851045
C	-4.462474	-2.230918	1.414447
H	-5.780727	-3.929506	1.640566
H	-5.959025	-2.701557	2.893447
H	-5.139239	-1.726052	0.720988
H	-4.052545	-1.439172	2.061234
C	-5.198308	-2.376801	-1.864424
C	-6.675654	-2.257635	-2.231960
H	-5.079334	-3.018540	-0.989507
H	-4.666626	-2.891465	-2.678018
C	-6.856980	-1.269817	-3.380439
H	-7.067234	-3.244928	-2.497196
H	-7.246204	-1.908791	-1.359907
C	-6.413852	0.120136	-2.932484
H	-6.250369	-1.595586	-4.235277
H	-7.898750	-1.240497	-3.715473
H	-7.158455	0.520136	-2.229801
H	-6.391360	0.812930	-3.780670

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M06-2X/6-31G* Energy = -8271.56754535

M06-2X/6-31G* Free Energy = -8270.679521

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.54226705

Lowest Frequency = 11.6626

M06-2X/6-31G* Geometry

C	1.290260	2.099828	2.901386
C	1.335398	3.089208	1.686297
C	2.592554	1.398904	3.173182
H	0.525225	1.355669	2.661127
H	0.932322	2.666291	3.766951
C	2.895118	0.220227	2.625676
H	3.318153	1.893559	3.816346
N	1.686805	2.207190	0.531986
C	-0.069364	3.682022	1.472632
C	2.371303	4.200158	1.830270
C	2.899915	1.982581	0.171868
C	3.337525	0.994781	-0.808079
H	3.677018	2.590270	0.630159
H	0.954586	1.455581	0.287812
H	2.188820	-0.298789	1.976023
H	3.848285	-0.268401	2.809755
C	-4.605878	-2.795594	-0.612486
C	-5.599788	-2.117679	-1.329430
C	-3.517202	-2.067229	-0.087056
C	-3.366341	-0.719109	-0.423089
C	-4.358651	-0.023225	-1.126127
C	-5.475015	-0.743225	-1.538691
C	-2.515258	-2.699589	0.822508
C	-2.881238	-3.263024	2.062847
C	-1.899081	-3.898386	2.835497
C	-0.576873	-3.914587	2.391683
C	-0.169488	-3.281200	1.219664
C	-1.170967	-2.675271	0.451914
O	-2.250857	-0.039050	0.023671
O	-0.834745	-2.010191	-0.708656
P	-0.776204	-0.374971	-0.638576
O	0.218361	0.058090	0.420957
O	-0.632936	0.136157	-2.025298
C	-4.267759	1.438173	-1.375495
C	1.261343	-3.243742	0.833315
C	-3.154203	1.996647	-2.064819

C	-3.080879	3.347708	-2.275551
C	-4.089605	4.224924	-1.798366
C	-5.205229	3.672637	-1.110143
C	-5.273412	2.266367	-0.929090
C	1.664824	-3.410560	-0.524128
C	2.990417	-3.419311	-0.863342
C	4.002620	-3.240796	0.115929
C	3.612056	-3.074474	1.472916
C	2.231960	-3.085426	1.798720
H	-6.254119	-0.217079	-2.086887
H	0.169936	-4.432481	2.989923
H	-2.362594	1.340169	-2.413764
H	-2.227414	3.770518	-2.799472
H	1.942645	-2.929535	2.835900
H	3.280202	-3.551985	-1.903493
H	0.908807	-3.523627	-1.292615
H	-6.120292	1.846642	-0.389893
C	2.901696	4.562941	3.066863
C	3.779541	5.641779	3.177487
C	4.138907	6.372212	2.051728
C	3.603309	6.028509	0.810765
C	2.723348	4.959280	0.704948
H	2.622462	4.020414	3.963271
H	4.178825	5.907573	4.151086
H	4.824449	7.209110	2.138074
H	2.284737	4.717407	-0.260260
H	3.862269	6.601414	-0.073996
C	-0.313950	5.053350	1.593244
C	-1.604794	5.557911	1.442643
C	-2.669320	4.705973	1.171998
C	-2.434484	3.337294	1.065495
C	-1.150628	2.828661	1.222877
H	-1.007194	1.756289	1.142609
H	0.494218	5.742590	1.809631
H	-1.770982	6.627011	1.534794
H	-3.673061	5.100746	1.035908
H	-3.247989	2.652026	0.847171
C	2.456360	0.353234	-1.685045
C	2.967445	-0.606697	-2.546754
C	4.329895	-0.891587	-2.598287
C	5.190882	-0.215668	-1.740501
Br	1.786547	-1.572706	-3.643576
H	4.711912	-1.627700	-3.297030
C	4.711287	0.717789	-0.836166
H	5.394286	1.218973	-0.157978
H	1.395316	0.582789	-1.723568
Br	7.040736	-0.578145	-1.815384
C	4.618199	-2.886908	2.458288
C	5.944568	-2.844594	2.109085
C	6.331202	-2.999107	0.755492
C	5.381599	-3.203955	-0.213267
H	4.314665	-2.772427	3.496549
H	6.704338	-2.696561	2.870505
H	5.675915	-3.324695	-1.253760
H	7.381632	-2.952443	0.485143
C	-6.197298	4.548636	-0.593854
C	-6.083767	5.907100	-0.749425
C	-4.973677	6.456415	-1.437990
C	-4.003997	5.633292	-1.951593
H	-7.046577	4.121593	-0.066287
H	-6.845930	6.567289	-0.346828
H	-4.895055	7.532869	-1.555780
H	-3.146083	6.047765	-2.474838

C	-6.830353	-2.824929	-1.866648
C	-6.652557	-4.336439	-1.985476
H	-7.102983	-2.391520	-2.835181
H	-7.673521	-2.619851	-1.191571
C	-6.048047	-4.886696	-0.696680
H	-5.980633	-4.565878	-2.822635
H	-7.615067	-4.810006	-2.204768
C	-4.650581	-4.309289	-0.486237
H	-6.692301	-4.616196	0.151982
H	-5.994960	-5.979974	-0.723447
H	-4.241801	-4.638140	0.471886
H	-3.975005	-4.722309	-1.249362
C	-4.289380	-3.091822	2.607296
C	-4.637513	-4.099688	3.700196
H	-5.030876	-3.128032	1.806627
H	-4.357754	-2.075645	3.022577
C	-3.541426	-4.123475	4.761663
H	-5.606065	-3.843611	4.141890
H	-4.739234	-5.101665	3.260062
C	-2.232875	-4.601914	4.138058
H	-3.411442	-3.111156	5.165990
H	-3.816064	-4.773214	5.599073
H	-2.308069	-5.681077	3.942692
H	-1.401937	-4.476699	4.841138

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M06-2X/6-31G* Energy = -8271.57258576

M06-2X/6-31G* Free Energy = -8270.687539

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.53891074

Lowest Frequency = 13.2122

M06-2X/6-31G* Geometry

C	3.406705	2.487704	-0.543367
C	4.003559	1.258023	0.223759
C	2.717039	3.485472	0.343110
H	2.693091	2.087685	-1.273706
H	4.214893	2.956390	-1.114403
C	1.399545	3.493201	0.537050
H	3.329815	4.217212	0.865729
N	2.834474	0.579400	0.786392
C	4.670979	0.314578	-0.786358
C	5.048622	1.631890	1.280945
C	2.375698	0.879002	1.932327
C	1.104381	0.228863	2.350663
H	2.866436	1.592730	2.601028
H	1.593340	-0.070133	-0.157905
H	0.742944	2.795967	0.017716
H	0.918422	4.225681	1.180057
C	-4.744704	0.254547	-1.498002
C	-5.233383	1.561715	-1.622046
C	-3.446846	0.052042	-0.987317
C	-2.612086	1.153804	-0.784931
C	-3.070252	2.463288	-0.933007
C	-4.399282	2.635550	-1.307628
C	-2.926405	-1.304457	-0.654027
C	-3.542307	-2.130024	0.314330
C	-2.983293	-3.386836	0.583947
C	-1.823691	-3.785925	-0.083610
C	-1.164310	-2.970199	-0.996295
C	-1.747246	-1.728598	-1.260996
O	-1.305872	0.938691	-0.360208
O	-1.097750	-0.848015	-2.125352
P	-0.227227	0.307865	-1.408048
O	0.734399	-0.505015	-0.475803

O	0.357669	1.277731	-2.345211
C	-2.196745	3.645325	-0.713159
C	0.104915	-3.408838	-1.622719
C	-2.459201	4.521138	0.375681
C	-1.709670	5.654839	0.557169
C	-0.647339	5.972748	-0.330215
C	-0.376582	5.093780	-1.415319
C	-1.174533	3.934082	-1.586256
C	0.294189	-3.312971	-3.029985
C	1.430448	-3.801968	-3.615096
C	2.453272	-4.403219	-2.834597
C	2.289616	-4.463272	-1.422024
C	1.096023	-3.960193	-0.843326
H	-4.777688	3.650419	-1.412622
H	-1.403302	-4.766079	0.130441
H	-3.260584	4.271036	1.065555
H	-1.912773	6.321484	1.391696
H	0.966533	-4.003425	0.236727
H	1.563248	-3.740215	-4.691911
H	-0.482620	-2.856736	-3.634642
H	-0.949836	3.257723	-2.406425
C	5.454492	0.652687	2.197410
C	6.440902	0.916549	3.138181
C	7.057824	2.166797	3.173183
C	6.681638	3.138908	2.255028
C	5.684265	2.872786	1.316169
H	4.994497	-0.331841	2.158896
H	6.736954	0.142562	3.839596
H	7.831038	2.375101	3.905889
H	5.418203	3.644974	0.601854
H	7.162137	4.112423	2.262990
C	4.219032	-0.986391	-1.008191
C	4.872395	-1.814530	-1.920125
C	5.976497	-1.352289	-2.625183
C	6.435763	-0.054236	-2.407843
C	5.791792	0.766738	-1.491071
H	6.177170	1.766585	-1.305133
H	3.355386	-1.371039	-0.476026
H	4.511283	-2.825807	-2.072002
H	6.479603	-2.001083	-3.335821
H	7.302335	0.317355	-2.946375
C	-0.057194	0.989734	2.451926
C	-1.270808	0.336766	2.615864
C	-1.350461	-1.044192	2.745036
C	-0.168062	-1.772971	2.685658
Br	-2.853513	1.365781	2.584155
H	-2.302798	-1.543131	2.876464
C	1.057151	-1.160237	2.471839
H	1.960623	-1.752253	2.371576
H	-0.033154	2.066520	2.323736
Br	-0.230122	-3.650599	2.906011
C	3.325833	-5.033282	-0.634665
C	4.458170	-5.537234	-1.222447
C	4.611175	-5.495746	-2.630545
C	3.632823	-4.938954	-3.415443
H	3.200199	-5.066288	0.444781
H	5.242974	-5.970840	-0.610591
H	3.747980	-4.894679	-4.495413
H	5.509756	-5.901969	-3.084492
C	0.713402	5.375929	-2.280423
C	1.497320	6.481342	-2.075895
C	1.225405	7.360955	-0.998076
C	0.178187	7.113780	-0.148158

H	0.922039	4.682449	-3.090893
H	2.334082	6.686709	-2.736475
H	1.853244	8.234060	-0.847856
H	-0.031359	7.783905	0.681985
C	-6.653710	1.848266	-2.072609
C	-7.293264	0.687757	-2.831596
H	-6.665023	2.759299	-2.680695
H	-7.260988	2.066942	-1.182780
C	-7.057770	-0.619036	-2.078347
H	-6.848015	0.609038	-3.831757
H	-8.362745	0.876930	-2.969004
C	-5.562222	-0.918445	-2.011798
H	-7.465554	-0.532994	-1.061187
H	-7.579189	-1.450063	-2.564101
H	-5.372755	-1.821534	-1.427317
H	-5.201089	-1.145229	-3.025464
C	-4.718288	-1.624714	1.134224
C	-5.486834	-2.739121	1.840890
H	-5.400479	-1.031225	0.522260
H	-4.327832	-0.916796	1.878453
C	-4.527217	-3.666762	2.580005
H	-6.216687	-2.299780	2.528406
H	-6.052350	-3.322965	1.101445
C	-3.599448	-4.349865	1.580340
H	-3.933578	-3.083853	3.298392
H	-5.072519	-4.418730	3.159356
H	-4.167619	-5.110792	1.027507
H	-2.796379	-4.880468	2.102932

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M06-2X/6-31G* Energy = -8271.57176154

M06-2X/6-31G* Free Energy = -8270.684941

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.54037422

Lowest Frequency = 15.2554

M06-2X/6-31G* Geometry

C	3.872304	1.536323	-1.432608
C	4.154480	0.813160	-0.068345
C	3.483396	2.976421	-1.287691
H	3.059178	0.993789	-1.925244
H	4.763840	1.419101	-2.058260
C	2.224418	3.405639	-1.366091
H	4.272843	3.693418	-1.067389
N	2.839517	0.710450	0.599565
C	4.648556	-0.612186	-0.379490
C	5.187199	1.553280	0.787557
C	2.378470	1.714490	1.236647
C	1.033499	1.668517	1.850244
H	2.949802	2.637672	1.357842
H	1.697094	-0.443464	0.200119
H	1.401413	2.723979	-1.587797
H	1.979911	4.455723	-1.229429
C	-3.620651	-2.208457	0.977980
C	-3.224998	-3.373320	1.648859
C	-2.867555	-1.765252	-0.124979
C	-1.677462	-2.416923	-0.448037
C	-1.232426	-3.545579	0.242561
C	-2.050928	-4.021086	1.265064
C	-3.269087	-0.598221	-0.960590
C	-4.470759	-0.600722	-1.696898
C	-4.786947	0.513318	-2.487313
C	-3.881628	1.569398	-2.571144
C	-2.656884	1.566595	-1.907604
C	-2.373231	0.467126	-1.098637

O	-0.902215	-1.896882	-1.480851
O	-1.146033	0.385968	-0.442134
P	-0.034037	-0.573826	-1.149226
O	0.878246	-1.032380	0.038302
O	0.623230	0.007497	-2.330235
C	0.063917	-4.197215	-0.055573
C	-1.715815	2.694448	-2.146957
C	0.946841	-4.490649	1.020568
C	2.139162	-5.124339	0.796236
C	2.523526	-5.502785	-0.516720
C	1.653303	-5.197027	-1.599952
C	0.426223	-4.538710	-1.337781
C	-1.127659	2.821758	-3.435864
C	-0.376565	3.920489	-3.755750
C	-0.160425	4.952231	-2.805835
C	-0.718331	4.815678	-1.503683
C	-1.500454	3.668513	-1.201999
H	-1.739094	-4.913915	1.803727
H	-4.120792	2.423037	-3.202067
H	0.666873	-4.171184	2.021011
H	2.816559	-5.332893	1.620096
H	-1.958242	3.583277	-0.219762
H	0.074140	4.011861	-4.740362
H	-1.278948	2.024431	-4.156702
H	-0.233918	-4.306895	-2.168999
C	5.219970	1.359240	2.173742
C	6.210958	1.940640	2.957547
C	7.201038	2.723032	2.368165
C	7.193194	2.906775	0.989690
C	6.197596	2.323717	0.208372
H	4.468227	0.731652	2.643586
H	6.212728	1.774940	4.030524
H	7.975093	3.178554	2.977669
H	6.225486	2.464582	-0.867367
H	7.965382	3.503678	0.514244
C	3.862852	-1.450697	-1.182306
C	4.299637	-2.727186	-1.518458
C	5.533698	-3.189166	-1.063948
C	6.321083	-2.365384	-0.270525
C	5.883310	-1.085896	0.068957
H	6.520395	-0.460336	0.683985
H	2.904554	-1.107638	-1.563557
H	3.679231	-3.363369	-2.143410
H	5.870224	-4.185433	-1.332961
H	7.286191	-2.710500	0.088645
C	0.240409	2.818995	1.883659
C	-1.041425	2.726305	2.410165
C	-1.563435	1.524843	2.876153
C	-0.744991	0.403146	2.844580
Br	-2.139666	4.265486	2.498852
H	-2.576463	1.470977	3.256792
C	0.555070	0.467241	2.372078
H	1.179373	-0.417310	2.374608
H	0.608608	3.758499	1.480483
Br	-1.421727	-1.268338	3.392703
C	-0.463265	5.828498	-0.539608
C	0.315844	6.913946	-0.852201
C	0.868995	7.049436	-2.149510
C	0.631288	6.092462	-3.102564
H	-0.894233	5.723534	0.452024
H	0.507714	7.677921	-0.104968
H	1.057850	6.184494	-4.098041
H	1.482167	7.913942	-2.384391

C	2.044976	-5.550794	-2.919467
C	3.245264	-6.172160	-3.151229
C	4.110374	-6.479213	-2.071236
C	3.755657	-6.153002	-0.786890
H	1.377127	-5.310597	-3.742559
H	3.537946	-6.432931	-4.163531
H	5.057316	-6.973462	-2.266880
H	4.419273	-6.377330	0.044593
C	-4.016905	-3.928397	2.818037
C	-4.891267	-2.878464	3.501487
H	-3.326163	-4.381816	3.538460
H	-4.657223	-4.744152	2.454016
C	-5.687926	-2.106225	2.452828
H	-4.254813	-2.175823	4.055210
H	-5.554414	-3.359211	4.227737
C	-4.736592	-1.344712	1.533603
H	-6.292969	-2.808564	1.862486
H	-6.382204	-1.405089	2.927094
H	-5.286208	-0.839177	0.735848
H	-4.247948	-0.545254	2.112759
C	-5.346022	-1.842653	-1.745840
C	-6.764451	-1.561542	-2.237186
H	-5.376127	-2.346758	-0.778024
H	-4.863765	-2.555230	-2.430887
C	-6.725859	-0.751503	-3.529624
H	-7.295486	-2.507812	-2.382204
H	-7.315328	-0.997377	-1.471776
C	-6.087913	0.608737	-3.260978
H	-6.137387	-1.296238	-4.279212
H	-7.731118	-0.618270	-3.942089
H	-6.792885	1.222668	-2.682805
H	-5.911850	1.147132	-4.198542

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M06-2X/6-31G* Energy = -8271.58187917

M06-2X/6-31G* Free Energy = -8270.691697

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.54356173

Lowest Frequency = 18.5976

M06-2X/6-31G* Geometry

C	-3.380584	-2.721734	1.612501
C	-3.687884	-2.009637	0.251161
C	-2.637799	-4.021504	1.489790
H	-2.781413	-2.024183	2.204206
H	-4.331118	-2.844427	2.142474
C	-1.314417	-4.114089	1.621854
H	-3.214525	-4.916713	1.262760
N	-2.368049	-1.671406	-0.310877
C	-4.528839	-2.865819	-0.695958
C	-4.391013	-0.672373	0.553699
C	-1.721560	-2.490568	-1.038476
C	-0.383589	-2.106654	-1.542374
H	-2.119082	-3.467002	-1.331299
H	-1.247315	-0.812418	0.581839
H	-0.702958	-3.238256	1.840726
H	-0.793173	-5.064379	1.532202
C	3.966511	1.283348	-0.356034
C	4.486906	-0.009709	-0.512768
C	2.938035	1.480387	0.590016
C	2.468146	0.400781	1.338942
C	2.994177	-0.890239	1.222509
C	4.018856	-1.049795	0.289194
C	2.210687	2.781927	0.685063
C	2.809959	3.985904	1.092825

C	2.075538	5.177904	0.998066
C	0.751195	5.140901	0.559739
C	0.094918	3.947874	0.259205
C	0.855646	2.781546	0.341895
O	1.413227	0.637283	2.213917
O	0.228843	1.546902	0.175022
P	-0.069273	0.802040	1.595419
O	-0.416044	-0.661494	1.145719
O	-0.979714	1.511202	2.501236
C	2.466634	-2.063347	1.963941
C	-1.337372	3.922579	-0.127020
C	1.990374	-1.978708	3.305220
C	1.533584	-3.094478	3.956885
C	1.514765	-4.365766	3.322606
C	1.992421	-4.459432	1.988172
C	2.458346	-3.291622	1.341116
C	-1.756710	3.181974	-1.269986
C	-3.062843	3.203348	-1.676650
C	-4.034569	3.966172	-0.975971
C	-3.629622	4.690473	0.178749
C	-2.268333	4.648056	0.579597
H	4.455791	-2.037209	0.156730
H	0.196273	6.072809	0.472256
H	1.996894	-1.020674	3.811370
H	1.174327	-3.016592	4.979683
H	-1.965376	5.193148	1.470679
H	-3.372791	2.646143	-2.557032
H	-1.011719	2.627225	-1.832494
H	2.801148	-3.383464	0.317082
C	-3.709187	0.282479	1.315961
C	-4.273136	1.517865	1.601611
C	-5.554818	1.816765	1.144129
C	-6.253466	0.868142	0.405883
C	-5.678655	-0.369369	0.109998
H	-2.721998	0.080674	1.712052
H	-3.692932	2.237379	2.171795
H	-5.995977	2.787479	1.351107
H	-6.242206	-1.089581	-0.474023
H	-7.253311	1.090678	0.044067
C	-4.586797	-2.527745	-2.054822
C	-5.398393	-3.231455	-2.936149
C	-6.182109	-4.287583	-2.473965
C	-6.149031	-4.621578	-1.125490
C	-5.330624	-3.914512	-0.244723
H	-5.337077	-4.185320	0.805780
H	-3.997131	-1.690762	-2.419305
H	-5.425182	-2.950054	-3.984388
H	-6.817361	-4.839147	-3.159823
H	-6.762527	-5.434440	-0.749353
C	-0.146794	-0.767055	-1.859117
C	1.105130	-0.391563	-2.317616
C	2.132847	-1.315406	-2.462445
C	1.874840	-2.639202	-2.130981
Br	1.416870	1.405215	-2.791744
H	3.107954	-1.014663	-2.825826
C	0.627633	-3.058676	-1.685807
H	0.454405	-4.097697	-1.421669
H	-0.937312	-0.032850	-1.739342
Br	3.297471	-3.881210	-2.266236
C	-4.600539	5.443554	0.891436
C	-5.902905	5.494542	0.461917
C	-6.301196	4.784604	-0.697726
C	-5.388630	4.033262	-1.393681

H	-4.289477	5.987543	1.779661
H	-6.634296	6.080822	1.009834
H	-5.689712	3.473408	-2.275413
H	-7.334371	4.832830	-1.027916
C	1.965017	-5.713578	1.321501
C	1.479399	-6.827503	1.958109
C	1.000226	-6.735867	3.289398
C	1.018536	-5.535346	3.954449
H	2.335608	-5.762065	0.299128
H	1.459754	-7.784787	1.446299
H	0.615811	-7.623994	3.781253
H	0.647388	-5.462380	4.973385
C	5.504957	-0.338514	-1.588149
C	5.494649	0.694024	-2.712465
H	5.295040	-1.347044	-1.968676
H	6.512022	-0.379148	-1.150502
C	5.648726	2.083645	-2.102570
H	4.540346	0.652615	-3.257222
H	6.292640	0.483003	-3.431069
C	4.435678	2.429173	-1.237228
H	6.561074	2.104309	-1.491756
H	5.767688	2.846045	-2.878858
H	4.661304	3.313017	-0.635676
H	3.597489	2.723082	-1.879198
C	4.172056	3.976412	1.761336
C	4.874209	5.329956	1.690433
H	4.802336	3.177648	1.363128
H	4.009763	3.719187	2.818074
C	3.939368	6.420176	2.210650
H	5.799912	5.299554	2.273938
H	5.153722	5.552075	0.650940
C	2.700788	6.522364	1.321776
H	3.639027	6.171398	3.236574
H	4.447795	7.388870	2.250359
H	2.982615	7.006194	0.375875
H	1.949166	7.171794	1.783615

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M06-2X/6-31G* Energy = -8271.56622946

M06-2X/6-31G* Free Energy = -8270.681658

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.53737615

Lowest Frequency = 11.3760

M06-2X/6-31G* Geometry

C	3.522775	-2.680457	0.049885
C	3.825601	-1.205398	-0.371303
C	3.236226	-2.886299	1.514199
H	2.640625	-2.983896	-0.524116
H	4.358975	-3.299634	-0.292333
C	1.997956	-3.058897	1.973410
H	4.072492	-2.883812	2.211842
N	2.687671	-0.448501	0.216509
C	5.162263	-0.641590	0.100825
C	3.769903	-1.125429	-1.897158
C	2.778441	0.389508	1.177370
C	1.648770	0.966918	1.900770
H	3.773152	0.710085	1.482751
H	1.699374	-0.822999	-0.111328
H	1.139619	-3.055777	1.302266
H	1.799719	-3.212660	3.030702
C	-4.704449	-0.287658	0.473072
C	-4.940562	-1.318954	1.396821
C	-3.705877	-0.462336	-0.505200
C	-2.901369	-1.609573	-0.481549

C	-3.043501	-2.588932	0.510302
C	-4.110461	-2.438346	1.396671
C	-3.348306	0.645331	-1.441071
C	-4.243273	1.200318	-2.376016
C	-3.838609	2.305228	-3.139585
C	-2.538066	2.799219	-3.008709
C	-1.610579	2.215813	-2.153278
C	-2.043159	1.140702	-1.376172
O	-1.935272	-1.764915	-1.447520
O	-1.111228	0.455104	-0.621161
P	-0.553376	-0.879385	-1.433141
O	0.430253	-1.506675	-0.457106
O	-0.170805	-0.558805	-2.823079
C	-2.044721	-3.665738	0.724876
C	-0.182363	2.628385	-2.131861
C	-1.689131	-3.982729	2.069858
C	-0.773067	-4.959570	2.352969
C	-0.120487	-5.666508	1.309555
C	-0.448289	-5.341986	-0.035965
C	-1.423034	-4.345911	-0.299506
C	0.587909	2.484491	-3.319511
C	1.917948	2.810789	-3.339326
C	2.557991	3.320378	-2.179123
C	1.787023	3.501827	-0.996182
C	0.419738	3.117435	-0.994847
H	-4.273248	-3.206613	2.149328
H	-2.227886	3.642488	-3.623209
H	-2.135352	-3.405850	2.875115
H	-0.510142	-5.185104	3.383828
H	-0.155734	3.221254	-0.076365
H	2.508446	2.666007	-4.240397
H	0.105130	2.061144	-4.195009
H	-1.665831	-4.116467	-1.331310
C	2.787305	-0.420671	-2.580230
C	2.734705	-0.462943	-3.974218
C	3.689695	-1.169405	-4.691064
C	4.704115	-1.845580	-4.009708
C	4.740067	-1.828976	-2.623278
H	2.028227	0.153394	-2.061356
H	1.913463	0.041856	-4.471451
H	3.646770	-1.203277	-5.775324
H	5.533244	-2.354715	-2.096753
H	5.462561	-2.393148	-4.560851
C	5.490902	0.669492	-0.275106
C	6.694314	1.238745	0.116051
C	7.606541	0.497282	0.868619
C	7.300535	-0.810253	1.223824
C	6.080807	-1.376286	0.846982
H	5.865488	-2.401176	1.128621
H	4.792550	1.244542	-0.882088
H	6.923653	2.258318	-0.178391
H	8.553101	0.936688	1.167195
H	8.008585	-1.399545	1.797955
C	0.380675	0.381351	1.914124
C	-0.641231	1.028566	2.594537
C	-0.434362	2.242815	3.243583
C	0.844417	2.791407	3.234054
Br	-2.350118	0.241671	2.576673
H	-1.249446	2.749605	3.747354
C	1.896772	2.154051	2.597419
H	2.886000	2.599785	2.596659
H	0.184676	-0.551426	1.393868
Br	1.153037	4.464349	4.051544

C	2.409571	4.084110	0.141562
C	3.742304	4.410934	0.126192
C	4.519066	4.188974	-1.038587
C	3.936394	3.664737	-2.165485
H	1.805591	4.285101	1.023022
H	4.201029	4.862972	1.001206
H	4.519151	3.511570	-3.070398
H	5.570598	4.461234	-1.043924
C	0.222178	-6.022621	-1.087912
C	1.171913	-6.972709	-0.814641
C	1.498084	-7.293028	0.526591
C	0.866516	-6.654149	1.562426
H	-0.028496	-5.767414	-2.114049
H	1.680638	-7.483324	-1.626498
H	2.252809	-8.046694	0.729643
H	1.115059	-6.891054	2.594029
C	-6.020485	-1.204541	2.454383
C	-6.272239	0.247176	2.853671
H	-5.738516	-1.805466	3.325795
H	-6.955904	-1.634813	2.069933
C	-6.557901	1.067420	1.599137
H	-5.380129	0.646087	3.356681
H	-7.103608	0.308658	3.563386
C	-5.344963	1.076830	0.670729
H	-7.421126	0.632137	1.077377
H	-6.826601	2.097677	1.854694
H	-5.606876	1.544598	-0.280323
H	-4.561183	1.716658	1.105622
C	-5.576820	0.527074	-2.650041
C	-6.586369	1.453555	-3.323105
H	-5.994289	0.094292	-1.737713
H	-5.379103	-0.326474	-3.314329
C	-5.951034	2.114943	-4.543569
H	-7.478672	0.885565	-3.605717
H	-6.908884	2.229661	-2.614676
C	-4.782173	2.995326	-4.107169
H	-5.591945	1.334539	-5.226771
H	-6.683772	2.714020	-5.094085
H	-5.181284	3.896919	-3.620839
H	-4.216756	3.344433	-4.978320

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M06-2X/6-31G* Energy = -8271.56793096

M06-2X/6-31G* Free Energy = -8270.679504

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.54111488

Lowest Frequency = 11.3905

M06-2X/6-31G* Geometry

C	1.719964	2.385719	2.965925
C	1.775690	3.108243	1.574614
C	2.937860	1.584669	3.318190
H	0.863136	1.708853	2.932515
H	1.508992	3.155357	3.715319
C	2.977024	0.261765	3.149866
H	3.813060	2.109549	3.699350
N	1.860082	2.006297	0.562961
C	0.465755	3.898643	1.401423
C	2.988853	4.027010	1.420461
C	2.966471	1.377367	0.373338
C	3.225286	0.188108	-0.438154
H	3.843597	1.798204	0.857671
H	0.951501	1.644049	0.113498
H	2.110706	-0.269870	2.757199
H	3.862060	-0.317224	3.400596

C	-4.949705	-1.621967	-0.921027
C	-5.670303	-0.688936	-1.676957
C	-3.906462	-1.170379	-0.084721
C	-3.506681	0.170043	-0.131554
C	-4.189321	1.107030	-0.920686
C	-5.288853	0.651060	-1.644233
C	-3.177694	-2.119251	0.807570
C	-3.824053	-2.859367	1.819502
C	-3.093341	-3.812580	2.541656
C	-1.733873	-3.988399	2.271358
C	-1.058198	-3.208889	1.340398
C	-1.801201	-2.263513	0.635473
O	-2.469150	0.588942	0.678094
O	-1.146517	-1.389602	-0.217515
P	-0.920689	0.086709	0.458773
O	-0.266208	0.937961	-0.610972
O	-0.249397	0.007731	1.787498
C	-3.776437	2.525884	-1.074280
C	0.405655	-3.374314	1.123516
C	-4.740925	3.563215	-0.926989
C	-4.418825	4.869367	-1.189461
C	-3.110165	5.224012	-1.613481
C	-2.137056	4.195235	-1.736437
C	-2.499663	2.851730	-1.467942
C	1.324346	-2.823913	2.058874
C	2.671081	-3.040388	1.923476
C	3.180710	-3.825112	0.854677
C	2.266317	-4.365344	-0.091532
C	0.878827	-4.110546	0.064831
H	-5.829703	1.366670	-2.260675
H	-1.173809	-4.735560	2.830318
H	-5.744603	3.302165	-0.601438
H	-5.164580	5.652929	-1.077550
H	0.182865	-4.525569	-0.660138
H	3.371195	-2.627687	2.645801
H	0.927923	-2.223121	2.871731
H	-1.747776	2.077698	-1.582698
C	3.440319	4.384670	0.143633
C	4.484893	5.287587	-0.018290
C	5.094624	5.859206	1.096718
C	4.643174	5.525168	2.368448
C	3.596930	4.618005	2.528231
H	2.954985	3.965066	-0.733825
H	4.817115	5.550617	-1.017656
H	5.910438	6.564135	0.972822
H	3.249743	4.387277	3.529837
H	5.102140	5.971216	3.245120
C	-0.759079	3.269390	1.660721
C	-1.950232	3.983389	1.617637
C	-1.940367	5.346133	1.333308
C	-0.732198	5.979786	1.069226
C	0.462716	5.263566	1.100922
H	1.390205	5.788025	0.901141
H	-0.795113	2.218332	1.923496
H	-2.885036	3.460933	1.795875
H	-2.870648	5.904665	1.300274
H	-0.712831	7.037489	0.825685
C	2.261106	-0.490698	-1.194201
C	2.657644	-1.591242	-1.939118
C	3.977934	-2.031418	-1.965585
C	4.915239	-1.350917	-1.196719
Br	1.363958	-2.499888	-2.961076
H	4.262999	-2.895788	-2.553451

C	4.556945	-0.252311	-0.432362
H	5.307984	0.262126	0.158775
H	1.227292	-0.159771	-1.218924
Br	6.711835	-1.928084	-1.198531
C	2.768014	-5.150253	-1.163704
C	4.112235	-5.401752	-1.279050
C	5.022855	-4.867011	-0.334195
C	4.566848	-4.092444	0.702361
H	2.064555	-5.548765	-1.890041
H	4.484501	-6.012080	-2.096544
H	5.265335	-3.664059	1.417785
H	6.085793	-5.058579	-0.443157
C	-0.814715	4.537624	-2.123322
C	-0.478653	5.840550	-2.387729
C	-1.451003	6.864815	-2.274056
C	-2.734616	6.563540	-1.893373
H	-0.078931	3.739831	-2.193413
H	0.536209	6.095802	-2.678695
H	-1.174362	7.892886	-2.488918
H	-3.482534	7.347567	-1.800321
C	-6.856483	-1.087023	-2.535313
C	-6.863751	-2.569069	-2.900242
H	-6.875119	-0.466439	-3.437912
H	-7.779281	-0.854558	-1.984769
C	-6.610407	-3.405701	-1.649576
H	-6.074364	-2.774008	-3.635048
H	-7.817452	-2.835071	-3.367729
C	-5.221605	-3.108302	-1.089409
H	-7.372206	-3.169012	-0.893320
H	-6.697165	-4.475061	-1.868308
H	-4.464789	-3.501651	-1.783990
H	-5.066948	-3.651052	-0.155042
C	-5.262445	-2.548547	2.198449
C	-5.935173	-3.678525	2.973932
H	-5.853447	-2.283600	1.318891
H	-5.247726	-1.644561	2.824305
C	-5.048838	-4.114554	4.137256
H	-6.916101	-3.347737	3.330496
H	-6.107095	-4.534774	2.306403
C	-3.739156	-4.686603	3.600845
H	-4.840262	-3.245269	4.774268
H	-5.553705	-4.858963	4.761582
H	-3.937416	-5.675746	3.163959
H	-3.027152	-4.851379	4.417122

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M06-2X/6-31G* Energy = -8271.56793094

M06-2X/6-31G* Free Energy = -8270.679500

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.54111796

Lowest Frequency = 11.4132

M06-2X/6-31G* Geometry

C	1.719205	2.385295	2.966389
C	1.775923	3.107642	1.575008
C	2.936857	1.584308	3.319599
H	0.862389	1.708455	2.932482
H	1.507768	3.155052	3.715522
C	2.976008	0.261339	3.151880
H	3.811873	2.109292	3.701038
N	1.860254	2.005598	0.563404
C	0.466474	3.898676	1.401071
C	2.989578	4.025849	1.421392
C	2.966400	1.376050	0.374409
C	3.225120	0.187085	-0.437536

H	3.843428	1.796165	0.859532
H	0.951634	1.644118	0.113220
H	2.109842	-0.270324	2.758965
H	3.860842	-0.317616	3.403396
C	-3.824217	-2.859110	1.819765
C	-3.093625	-3.812471	2.541833
C	-3.177760	-2.118939	0.807932
C	-1.801261	-2.263188	0.635946
C	-1.058396	-3.208751	1.340766
C	-1.734155	-3.988374	2.271558
C	-3.906446	-1.170139	-0.084499
C	-4.949514	-1.621882	-0.920951
C	-5.669986	-0.688975	-1.677148
C	-5.288612	0.651038	-1.644477
C	-4.189235	1.107134	-0.920777
C	-3.506688	0.170286	-0.131442
O	-1.146437	-1.389268	-0.216870
O	-2.469282	0.589293	0.678344
P	-0.920798	0.087222	0.459143
O	-0.266312	0.938151	-0.610864
O	-0.249540	0.008511	1.787896
C	0.405479	-3.374073	1.123966
C	-3.776511	2.526032	-1.074465
C	1.324044	-2.823609	2.059359
C	2.670822	-3.039918	1.923967
C	3.180554	-3.824488	0.855127
C	2.266251	-4.364835	-0.091112
C	0.878745	-4.110236	0.065262
C	-4.741105	3.563217	-0.926953
C	-4.419244	4.869404	-1.189556
C	-3.110760	5.224173	-1.613979
C	-2.137531	4.195529	-1.737175
C	-2.499868	2.851998	-1.468466
H	-1.174166	-4.735667	2.830416
H	-5.829391	1.366563	-2.261079
H	0.927524	-2.222968	2.872276
H	3.370864	-2.627254	2.646379
H	-1.747921	2.078025	-1.583293
H	-5.165054	5.652884	-1.077455
H	-5.744656	3.302033	-0.601126
H	0.182810	-4.525322	-0.659703
C	3.596614	4.617395	2.529453
C	4.643241	5.524214	2.370261
C	5.096135	5.857384	1.098818
C	4.487450	5.285243	-0.016491
C	3.442485	4.382669	0.144843
H	3.248285	4.387365	3.530819
H	5.101372	5.970667	3.247164
H	5.912246	6.562045	0.975357
H	2.958037	3.962664	-0.732905
H	4.820805	5.547603	-1.015655
C	-0.758772	3.270162	1.660298
C	-1.949510	3.984803	1.616740
C	-1.938833	5.347463	1.331958
C	-0.730274	5.980343	1.067840
C	0.464243	5.263465	1.100021
H	1.392063	5.787335	0.900220
H	-0.795420	2.219200	1.923362
H	-2.884653	3.462937	1.794945
H	-2.868800	5.906495	1.298586
H	-0.710256	7.037952	0.823951
C	2.260738	-0.491626	-1.193437
C	2.657144	-1.591777	-1.938961

C	3.977553	-2.031568	-1.966332
C	4.915084	-1.351165	-1.197664
Br	1.363274	-2.500429	-2.960654
H	4.262553	-2.895527	-2.554814
C	4.556873	-0.253050	-0.432543
H	5.308097	0.261311	0.158426
H	1.226863	-0.160883	-1.217639
Br	6.711856	-1.927721	-1.201149
C	-0.815365	4.538125	-2.124477
C	-0.479601	5.841086	-2.389057
C	-1.452067	6.865221	-2.275121
C	-2.735505	6.563759	-1.894033
H	-0.079436	3.740485	-2.194723
H	0.535121	6.096477	-2.680377
H	-3.483531	7.347656	-1.800767
H	-1.175634	7.893323	-2.490101
C	2.768122	-5.149596	-1.163329
C	4.112384	-5.400877	-1.278630
C	5.022908	-4.866122	-0.333663
C	4.566758	-4.091609	0.702847
H	2.064776	-5.548122	-1.889777
H	4.484737	-6.011046	-2.096207
H	6.085869	-5.057566	-0.442582
H	5.265100	-3.663266	1.418434
C	-3.739544	-4.686538	3.600926
C	-5.049227	-4.114453	4.137299
H	-3.027595	-4.851377	4.417235
H	-3.937817	-5.675651	3.163986
C	-5.935458	-3.678240	2.973966
H	-4.840625	-3.245241	4.774400
H	-5.554185	-4.858880	4.761526
C	-5.262607	-2.548215	2.198655
H	-6.107380	-4.534403	2.306326
H	-6.916390	-3.347436	3.330496
H	-5.853519	-2.283126	1.319079
H	-5.247877	-1.644302	2.824609
C	-5.221302	-3.108262	-1.089219
C	-6.609896	-3.405799	-1.649835
H	-5.066970	-3.650870	-0.154726
H	-4.464217	-3.501688	-1.783459
C	-6.862896	-2.569281	-2.900641
H	-6.696500	-4.475180	-1.868504
H	-7.371960	-3.169101	-0.893849
C	-6.855900	-1.087216	-2.535803
H	-6.073230	-2.774176	-3.635159
H	-7.816405	-2.835409	-3.368441
H	-7.778882	-0.854802	-1.985552
H	-6.874317	-0.466691	-3.438444

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M06-2X/6-31G* Energy = -8271.56204534

M06-2X/6-31G* Free Energy = -8270.675894

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.53770070

Lowest Frequency = 13.9416

M06-2X/6-31G* Geometry

C	1.414529	1.169809	3.188833
C	1.151439	-0.364723	3.372769
C	2.839902	1.532161	2.888986
H	0.775844	1.504526	2.365699
H	1.054189	1.667786	4.094973
C	3.276845	1.796524	1.657124
H	3.540747	1.558556	3.721447
N	1.373313	-0.964542	2.025533

C	2.082799	-1.013677	4.396286
C	-0.320702	-0.566363	3.763289
C	2.554366	-1.184393	1.567820
C	2.848453	-1.663840	0.219093
H	3.395267	-1.002978	2.232680
H	0.518001	-1.042988	1.342100
H	2.603384	1.780908	0.800576
H	4.313465	2.060068	1.461121
C	-2.718196	3.684055	-1.634594
C	-1.818657	4.617289	-2.165058
C	-2.216557	2.573712	-0.915685
C	-0.837934	2.349095	-0.878162
C	0.074235	3.268997	-1.412581
C	-0.447389	4.406935	-2.018127
C	-3.150904	1.613967	-0.248511
C	-4.098261	2.042600	0.708695
C	-5.108987	1.159908	1.108316
C	-5.132980	-0.136436	0.587727
C	-4.137753	-0.628314	-0.252051
C	-3.127032	0.270298	-0.630888
O	-0.366071	1.224195	-0.230994
O	-2.128954	-0.149854	-1.478378
P	-0.598927	-0.272527	-0.916198
O	-0.578161	-1.175778	0.305063
O	0.291094	-0.522061	-2.070411
C	1.546905	3.081532	-1.346178
C	-4.214377	-2.019607	-0.765961
C	2.160600	1.922911	-1.903727
C	3.524163	1.784925	-1.879965
C	4.354825	2.766896	-1.278491
C	3.748576	3.929939	-0.727871
C	2.337007	4.063213	-0.789593
C	-5.463770	-2.496713	-1.256164
C	-5.596022	-3.772174	-1.736709
C	-4.485815	-4.655889	-1.762787
C	-3.236499	-4.188552	-1.270609
C	-3.128750	-2.866159	-0.771219
H	0.247305	5.129386	-2.441750
H	-5.926671	-0.812517	0.900116
H	1.538644	1.152067	-2.349136
H	3.993273	0.910964	-2.323629
H	-2.175220	-2.532722	-0.372513
H	-6.552870	-4.119872	-2.117957
H	-6.314149	-1.820332	-1.267031
H	1.874720	4.948644	-0.358156
C	-0.686266	-1.229083	4.937882
C	-2.028209	-1.355105	5.290935
C	-3.019820	-0.824186	4.474657
C	-2.663013	-0.161465	3.303260
C	-1.325226	-0.024408	2.952950
H	0.070329	-1.649613	5.590639
H	-2.291561	-1.873820	6.207520
H	-4.066497	-0.928055	4.744999
H	-1.082931	0.484071	2.024116
H	-3.423490	0.249119	2.648305
C	2.339277	-2.388950	4.347454
C	3.104117	-3.008252	5.330303
C	3.617244	-2.264555	6.390144
C	3.349357	-0.901659	6.461509
C	2.585979	-0.282871	5.473999
H	2.372644	0.777359	5.562349
H	1.920872	-2.987886	3.543298
H	3.290392	-4.075874	5.270983

H	4.214236	-2.746072	7.157896
H	3.732131	-0.312532	7.288822
C	4.084774	-1.306556	-0.335823
C	4.359716	-1.690839	-1.637522
C	3.448007	-2.424226	-2.393189
C	2.241182	-2.788977	-1.809323
Br	5.991425	-1.164273	-2.431712
H	3.672121	-2.694727	-3.418295
C	1.934748	-2.429752	-0.504909
H	0.974338	-2.698381	-0.082999
H	4.795432	-0.704367	0.222247
Br	0.956033	-3.726923	-2.802860
C	-2.116969	-5.063036	-1.294823
C	-2.230852	-6.333629	-1.796455
C	-3.476897	-6.798647	-2.286478
C	-4.576361	-5.979335	-2.268513
H	-1.162823	-4.693062	-0.930853
H	-1.365785	-6.989719	-1.819791
H	-5.534113	-6.330162	-2.644860
H	-3.555938	-7.807920	-2.678974
C	4.571932	4.899009	-0.095233
C	5.927754	4.714239	-0.002971
C	6.529496	3.550570	-0.543904
C	5.761272	2.602387	-1.171138
H	4.104744	5.786138	0.324843
H	6.546926	5.458745	0.487975
H	7.603480	3.414529	-0.460611
H	6.208879	1.700102	-1.581042
C	-2.281188	5.864053	-2.896284
C	-3.705134	5.752210	-3.432748
H	-1.579088	6.087848	-3.706794
H	-2.230275	6.715699	-2.202839
C	-4.622059	5.225016	-2.333789
H	-3.727810	5.059189	-4.283594
H	-4.045255	6.726237	-3.799236
C	-4.204783	3.813196	-1.928952
H	-4.564414	5.891718	-1.461618
H	-5.666331	5.217380	-2.662666
H	-4.810163	3.471981	-1.087588
H	-4.434045	3.121143	-2.752356
C	-3.960986	3.406221	1.364528
C	-5.237416	3.871750	2.060618
H	-3.620996	4.155757	0.645788
H	-3.156063	3.327356	2.110925
C	-5.780106	2.762507	2.957579
H	-5.032091	4.779226	2.637608
H	-5.995167	4.133437	1.308537
C	-6.182424	1.563797	2.102276
H	-5.000215	2.462819	3.671006
H	-6.637419	3.110310	3.542939
H	-7.100481	1.812047	1.551043
H	-6.430293	0.703969	2.735455

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M06-2X/6-31G* Energy = -8271.56367555

M06-2X/6-31G* Free Energy = -8270.678522

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.53615688

Lowest Frequency = 11.9504

M06-2X/6-31G* Geometry

C	2.217330	1.220361	2.891130
C	1.704903	-0.196397	3.328696
C	3.627548	1.256135	2.377306
H	1.541257	1.568591	2.104376

H	2.088036	1.896222	3.743478
C	3.931898	1.258335	1.080075
H	4.431838	1.261428	3.110784
N	1.580197	-0.978350	2.075769
C	2.628624	-0.869095	4.348036
C	0.298673	-0.018203	3.928663
C	2.630465	-1.512802	1.586300
C	2.601806	-2.221381	0.291724
H	3.594979	-1.454046	2.095862
H	0.202706	-0.940562	1.091078
H	3.155893	1.245463	0.314809
H	4.962219	1.286869	0.733112
C	-2.055821	3.930206	-1.747190
C	-1.088739	4.679074	-2.430650
C	-1.650749	2.796246	-1.004361
C	-0.325434	2.370673	-1.093008
C	0.652535	3.091497	-1.787841
C	0.243369	4.262120	-2.416132
C	-2.634740	2.033379	-0.172816
C	-3.384458	2.659243	0.848827
C	-4.448942	1.962785	1.433785
C	-4.727651	0.657074	1.022536
C	-3.937034	-0.028898	0.104367
C	-2.862335	0.683730	-0.443493
O	0.047957	1.221789	-0.403389
O	-2.023220	0.040199	-1.341872
P	-0.495614	-0.230530	-0.906769
O	-0.608741	-0.983431	0.468614
O	0.256655	-0.847787	-2.005515
C	2.064307	2.638865	-1.876085
C	-4.303078	-1.408619	-0.314330
C	2.363218	1.354440	-2.410417
C	3.659154	0.923870	-2.501635
C	4.733221	1.737379	-2.056484
C	4.445236	3.035109	-1.549234
C	3.093009	3.462904	-1.478763
C	-3.350917	-2.464675	-0.403507
C	-3.740165	-3.723443	-0.775498
C	-5.093565	-4.017073	-1.085565
C	-6.051423	-2.970195	-1.001434
C	-5.621817	-1.676266	-0.612925
H	0.985907	4.838460	-2.963927
H	-5.560541	0.128120	1.480555
H	1.557227	0.711941	-2.745808
H	3.878506	-0.057648	-2.911304
H	-6.357087	-0.875513	-0.574359
H	-3.003371	-4.520786	-0.833422
H	-2.315118	-2.279525	-0.146821
H	2.873652	4.444909	-1.064858
C	-0.710461	0.557890	3.147782
C	-1.986275	0.752522	3.663184
C	-2.276913	0.395550	4.977780
C	-1.278949	-0.161223	5.767613
C	-0.001963	-0.368073	5.247301
H	-0.515459	0.852051	2.120101
H	-2.754181	1.177047	3.025540
H	-3.274779	0.548869	5.378466
H	0.757861	-0.807548	5.883712
H	-1.487500	-0.443943	6.795005
C	3.418343	-0.123264	5.224905
C	4.172587	-0.746302	6.217753
C	4.144009	-2.129508	6.355706
C	3.345434	-2.884772	5.499666

C	2.593207	-2.259372	4.511597
H	1.957552	-2.857527	3.865070
H	3.439896	0.959363	5.153028
H	4.780787	-0.143475	6.885016
H	4.732636	-2.615745	7.127167
H	3.301225	-3.964342	5.605072
C	3.693680	-2.103768	-0.572475
C	3.614805	-2.691756	-1.826773
C	2.474794	-3.363350	-2.255976
C	1.413225	-3.478424	-1.367419
Br	5.089524	-2.544345	-3.006867
H	2.413169	-3.772739	-3.256922
C	1.478327	-2.953324	-0.086907
H	0.641973	-3.069502	0.591195
H	4.573686	-1.536446	-0.283687
Br	-0.204228	-4.262774	-1.929547
C	-7.408085	-3.251125	-1.313914
C	-7.793227	-4.512680	-1.687466
C	-6.838630	-5.556445	-1.768430
C	-5.521505	-5.312868	-1.474857
H	-8.135794	-2.446003	-1.251107
H	-8.832783	-4.717707	-1.923821
H	-4.783814	-6.108805	-1.536402
H	-7.156162	-6.551008	-2.066011
C	5.516777	3.838119	-1.076604
C	6.805050	3.367508	-1.092999
C	7.087864	2.069046	-1.586065
C	6.075318	1.274513	-2.061382
H	5.295153	4.828609	-0.687457
H	7.615552	3.987263	-0.721977
H	8.111259	1.706586	-1.584940
H	6.272157	0.269937	-2.429004
C	-1.436747	5.943852	-3.193700
C	-2.913135	6.034922	-3.567887
H	-0.806172	6.010231	-4.086812
H	-1.175115	6.809468	-2.568690
C	-3.768631	5.716160	-2.346015
H	-3.139753	5.314370	-4.364179
H	-3.138560	7.031802	-3.959941
C	-3.528832	4.277592	-1.894196
H	-3.510955	6.407150	-1.530954
H	-4.832254	5.858329	-2.562530
H	-4.079681	4.078258	-0.973460
H	-3.951910	3.591209	-2.642076
C	-2.969836	4.020864	1.379182
C	-4.070993	4.716201	2.175603
H	-2.612923	4.665807	0.572688
H	-2.101417	3.860610	2.036160
C	-4.644314	3.760536	3.218157
H	-3.668735	5.617798	2.648316
H	-4.872853	5.038798	1.496520
C	-5.312769	2.579057	2.519365
H	-3.829811	3.399749	3.861041
H	-5.366037	4.268040	3.866063
H	-6.255767	2.918127	2.067908
H	-5.583842	1.804064	3.245636

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M06-2X/6-31G* Energy = -8271.55707982

M06-2X/6-31G* Free Energy = -8270.669969

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.53324260

Lowest Frequency = 13.3706

M06-2X/6-31G* Geometry

C	-2.170898	0.467316	-3.299845
C	-2.498980	1.705588	-2.403204
C	-3.207381	-0.618736	-3.201090
H	-1.204708	0.081695	-2.960815
H	-2.038431	0.829346	-4.324415
C	-3.114292	-1.629566	-2.335751
H	-4.084461	-0.543795	-3.841078
N	-2.465252	1.170183	-1.021350
C	-1.366161	2.750349	-2.473672
C	-3.853949	2.341299	-2.698402
C	-3.453440	0.757380	-0.319515
C	-3.223329	0.332151	1.064674
H	-4.461659	0.808177	-0.726989
H	-1.507545	0.776635	-0.700611
H	-2.247396	-1.742962	-1.682527
H	-3.890832	-2.386607	-2.266027
C	3.995859	-2.610797	-1.716520
C	3.476592	-3.634692	-2.520088
C	3.211389	-2.119500	-0.651864
C	1.888018	-2.550810	-0.512501
C	1.316987	-3.512789	-1.361026
C	2.169260	-4.068899	-2.317248
C	3.746716	-1.077784	0.278335
C	4.928539	-1.269977	1.027054
C	5.497823	-0.181631	1.699710
C	4.868984	1.065394	1.647007
C	3.641866	1.249278	1.021662
C	3.079739	0.145436	0.369058
O	1.150037	-2.026973	0.521717
O	1.854328	0.282684	-0.250980
P	0.583216	-0.491843	0.465752
O	-0.518851	-0.396900	-0.570343
O	0.359768	-0.058663	1.864253
C	-0.115736	-3.913174	-1.326349
C	2.973463	2.576904	0.997122
C	-0.714738	-4.360384	-2.543842
C	-2.010082	-4.794194	-2.594447
C	-2.828528	-4.770444	-1.437092
C	-2.268965	-4.274563	-0.227539
C	-0.904649	-3.879103	-0.192760
C	1.680362	2.743825	1.570471
C	1.050256	3.958210	1.518660
C	1.654290	5.072603	0.876148
C	2.957273	4.918808	0.325508
C	3.599700	3.654586	0.415273
H	1.798166	-4.872644	-2.947544
H	5.324580	1.912504	2.156165
H	-0.134013	-4.330525	-3.459291
H	-2.439340	-5.129896	-3.535161
H	4.588479	3.534651	-0.023122
H	0.072485	4.079552	1.981362
H	1.210325	1.892924	2.054983
H	-0.492944	-3.540360	0.750450
C	-4.428456	3.216852	-1.766470
C	-5.622278	3.872727	-2.041189
C	-6.259048	3.680302	-3.265973
C	-5.684924	2.836747	-4.209458
C	-4.491289	2.173424	-3.927351
H	-3.921024	3.406280	-0.823558
H	-6.048825	4.544187	-1.302746
H	-7.190253	4.193055	-3.484486
H	-4.055086	1.533621	-4.686451
H	-6.162412	2.690229	-5.173054

C	-1.587194	4.053327	-2.926060
C	-0.555645	4.991557	-2.905244
C	0.704447	4.646659	-2.428984
C	0.939912	3.338880	-2.011426
C	-0.080313	2.396250	-2.044123
H	0.143848	1.388877	-1.706067
H	-2.565393	4.353121	-3.285877
H	-0.751217	6.003289	-3.247524
H	1.495871	5.389341	-2.370861
H	1.914394	3.042508	-1.634739
C	-3.949264	-0.716344	1.643856
C	-3.694555	-1.028022	2.970271
C	-2.778150	-0.308296	3.737101
C	-2.091262	0.739877	3.144288
Br	-4.614025	-2.460322	3.792074
H	-2.607978	-0.565091	4.775829
C	-2.293404	1.059116	1.809208
H	-1.734153	1.872835	1.358493
H	-4.660199	-1.297734	1.065682
Br	-0.865420	1.752214	4.139577
C	3.562781	6.024669	-0.328131
C	2.903322	7.223437	-0.437236
C	1.604847	7.374682	0.107883
C	0.999809	6.325060	0.751928
H	4.559127	5.901661	-0.745553
H	3.375358	8.061495	-0.940989
H	0.002880	6.434517	1.171207
H	1.091645	8.326920	0.014879
C	-3.109357	-4.163684	0.914486
C	-4.429901	-4.533617	0.852273
C	-4.977160	-5.045344	-0.349956
C	-4.191961	-5.161779	-1.468256
H	-2.694678	-3.765900	1.838274
H	-5.061376	-4.427786	1.728077
H	-6.021083	-5.342336	-0.380970
H	-4.603441	-5.544751	-2.399086
C	4.300838	-4.303763	-3.604862
C	5.463927	-3.444112	-4.092202
H	3.647745	-4.578895	-4.440408
H	4.701763	-5.246614	-3.206367
C	6.233052	-2.896175	-2.893818
H	5.081283	-2.604700	-4.687318
H	6.116371	-4.032736	-4.745483
C	5.335163	-1.981743	-2.063810
H	6.583309	-3.732563	-2.272512
H	7.121193	-2.343386	-3.217180
H	5.124478	-1.069129	-2.640857
H	5.863395	-1.643860	-1.171117
C	5.527244	-2.658830	1.171723
C	6.993103	-2.637048	1.597401
H	5.401850	-3.238674	0.254303
H	4.941784	-3.189707	1.936175
C	7.166716	-1.740202	2.820169
H	7.331906	-3.656783	1.807541
H	7.613220	-2.254980	0.773781
C	6.805100	-0.300927	2.461584
H	6.508845	-2.098604	3.622409
H	8.192579	-1.783678	3.200395
H	7.609088	0.122186	1.842401
H	6.756820	0.319428	3.363332

B-1

M06-2X/6-31G* Energy = -8271.58987569

M06-2X/6-31G* Free Energy = -8270.703401

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.56731784

Lowest Frequency = 13.4590

M06-2X/6-31G* Geometry

C	-0.995751	1.729912	3.705835
C	-1.560976	3.535909	0.127188
C	-2.214700	1.747301	3.171278
H	-0.226808	1.032694	3.377952
H	-0.715301	2.426115	4.491162
C	-2.659452	0.822296	2.075727
H	-2.949135	2.476527	3.518202
N	-1.690105	2.272365	0.383883
C	-2.741512	4.390593	-0.139408
C	-0.216758	4.122379	0.103433
C	-2.925701	1.571363	0.753694
C	-3.391492	0.603020	-0.315380
H	-3.701096	2.324822	0.918042
H	-0.814015	1.648534	0.452565
H	-1.904752	0.048036	1.893083
H	-3.597697	0.320595	2.342346
C	2.037293	-3.686261	-1.088345
C	0.787457	-4.309353	-1.190831
C	2.259445	-2.776707	-0.036184
C	1.200939	-2.405675	0.795045
C	-0.047717	-3.039011	0.726958
C	-0.203313	-4.012834	-0.256671
C	3.588764	-2.140761	0.198986
C	4.715735	-2.895079	0.579386
C	5.940267	-2.238938	0.765448
C	6.009086	-0.856810	0.593834
C	4.895891	-0.079947	0.278237
C	3.680201	-0.750942	0.106804
O	1.411521	-1.382948	1.693362
O	2.527871	-0.043785	-0.156290
P	1.470514	0.154785	1.094394
O	0.152857	0.450843	0.412045
O	1.997560	1.032849	2.164547
C	-1.178802	-2.697316	1.621848
C	5.046210	1.384220	0.100436
C	-0.974379	-2.385323	2.998570
C	-2.034892	-2.107676	3.820266
C	-3.366702	-2.107791	3.326430
C	-3.582131	-2.421506	1.955917
C	-2.467896	-2.718901	1.132903
C	5.846515	2.121670	1.018504
C	6.124428	3.446415	0.811172
C	5.628476	4.120320	-0.335778
C	4.799627	3.401059	-1.242375
C	4.514939	2.035028	-0.991121
H	-1.154380	-4.536680	-0.324344
H	6.971259	-0.361878	0.712392
H	0.037129	-2.365309	3.387463
H	-1.865286	-1.864077	4.865920
H	3.889401	1.490537	-1.692689
H	6.735897	3.998251	1.520553
H	6.226610	1.614243	1.900226
H	-2.639683	-2.919600	0.077986
C	0.059542	5.229770	-0.715045
C	1.343481	5.753083	-0.747610
C	2.353210	5.181669	0.028880
C	2.084540	4.081356	0.840920
C	0.797977	3.561836	0.893371
H	-0.723246	5.655149	-1.335713
H	1.568981	6.598735	-1.389585

H	3.355964	5.596439	-0.009127
H	0.597905	2.735789	1.567776
H	2.863650	3.609678	1.433307
C	-3.728527	3.973911	-1.040912
C	-4.820843	4.793391	-1.300658
C	-4.939227	6.022400	-0.653907
C	-3.957742	6.440849	0.242225
C	-2.851936	5.635069	0.490035
H	-2.075482	5.957490	1.177105
H	-3.627441	3.016656	-1.545720
H	-5.578078	4.472652	-2.008461
H	-5.796229	6.657966	-0.853384
H	-4.049819	7.398463	0.743901
C	-2.486514	-0.185646	-1.029790
C	-2.985394	-1.140559	-1.907797
C	-4.349289	-1.347501	-2.086542
C	-5.222439	-0.562165	-1.344848
Br	-1.767905	-2.282549	-2.797629
H	-4.716972	-2.119285	-2.752086
C	-4.764736	0.418653	-0.476031
H	-5.474159	0.999734	0.105807
H	-1.414168	-0.103609	-0.862322
Br	-7.075964	-0.925960	-1.421165
C	4.295030	4.072579	-2.388604
C	4.603191	5.387791	-2.626353
C	5.432188	6.101971	-1.725322
C	5.929774	5.481838	-0.606316
H	3.655785	3.521171	-3.073045
H	4.213773	5.887814	-3.508044
H	6.566649	6.022973	0.089149
H	5.674036	7.141273	-1.926080
C	-4.902505	-2.363855	1.435554
C	-5.954749	-1.982805	2.228306
C	-5.739754	-1.672485	3.594807
C	-4.478274	-1.745401	4.131593
H	-5.063715	-2.606972	0.388545
H	-6.952256	-1.915589	1.803577
H	-6.579912	-1.379084	4.216907
H	-4.307419	-1.506320	5.178216
C	0.465338	-5.291559	-2.300115
C	1.388439	-5.129937	-3.504785
H	-0.583027	-5.162028	-2.596081
H	0.552593	-6.317531	-1.915741
C	2.840720	-5.113859	-3.034324
H	1.162444	-4.182867	-4.014032
H	1.214589	-5.935869	-4.225108
C	3.099107	-3.892601	-2.154171
H	3.042988	-6.031100	-2.463996
H	3.530418	-5.106764	-3.884589
H	4.096331	-3.947375	-1.708673
H	3.110696	-2.990843	-2.783393
C	4.579068	-4.374559	0.895360
C	5.915237	-5.113804	0.899593
H	3.878314	-4.859675	0.211485
H	4.119107	-4.457657	1.890851
C	6.933125	-4.357715	1.748904
H	5.770819	-6.132643	1.273605
H	6.293948	-5.198953	-0.128553
C	7.207489	-2.991925	1.124678
H	6.530913	-4.228112	2.762069
H	7.867101	-4.921718	1.841196
H	7.803932	-3.133558	0.212112
H	7.817036	-2.376076	1.795267

B-2

M06-2X/6-31G* Energy = -8271.59099885

M06-2X/6-31G* Free Energy = -8270.702473

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.56812714

Lowest Frequency = 14.4805

M06-2X/6-31G* Geometry

C	-0.695433	-0.453466	3.010570
C	1.104567	2.905482	1.592428
C	0.616802	-0.345328	3.209188
H	-1.095437	-0.716628	2.032082
H	-1.408263	-0.276967	3.811925
C	1.623847	-0.569654	2.117192
H	1.002607	-0.064639	4.190316
N	1.257205	1.667839	1.248308
C	-0.154914	3.580418	1.249716
C	2.162147	3.646646	2.317271
C	2.312051	0.737127	1.672396
C	3.316752	0.498187	0.558741
H	2.827639	1.188233	2.526046
H	0.522108	1.201900	0.620366
H	1.137917	-1.013459	1.243762
H	2.421159	-1.248348	2.445474
C	-4.839257	-2.893587	-0.162596
C	-6.053675	-2.298409	-0.527048
C	-3.712209	-2.074473	0.054708
C	-3.778784	-0.706391	-0.227702
C	-4.988849	-0.096363	-0.588753
C	-6.109420	-0.915861	-0.698916
C	-2.429910	-2.643279	0.567325
C	-2.346428	-3.256487	1.833124
C	-1.132404	-3.837164	2.220336
C	-0.038619	-3.780287	1.358209
C	-0.054419	-3.089649	0.144786
C	-1.280803	-2.504564	-0.215664
O	-2.639656	0.054660	-0.068980
O	-1.390627	-1.747230	-1.359238
P	-1.386297	-0.110903	-1.151611
O	-0.169447	0.231153	-0.324146
O	-1.674837	0.523596	-2.452606
C	-5.122114	1.363897	-0.818155
C	1.183331	-2.988334	-0.674743
C	-6.161247	2.072058	-0.148921
C	-6.334234	3.419022	-0.334159
C	-5.474035	4.146361	-1.198372
C	-4.434802	3.443750	-1.869653
C	-4.285270	2.047190	-1.671744
C	1.135443	-2.866833	-2.096577
C	2.284858	-2.836402	-2.839073
C	3.563423	-2.937927	-2.230651
C	3.628965	-3.051232	-0.816275
C	2.423234	-3.065699	-0.071405
H	-7.055668	-0.459205	-0.983599
H	0.874509	-4.287607	1.659282
H	-6.810769	1.526875	0.530832
H	-7.126941	3.949697	0.187425
H	2.502510	-3.140893	1.009587
H	2.228679	-2.739382	-3.920038
H	0.174519	-2.802443	-2.589976
H	-3.486948	1.525649	-2.194969
C	3.487558	3.615824	1.867692
C	4.465827	4.333740	2.546478
C	4.128868	5.072465	3.678945

C	2.809183	5.109539	4.125452
C	1.822316	4.411578	3.438823
H	3.743158	3.047479	0.977834
H	5.489962	4.316226	2.188615
H	4.895565	5.626880	4.210912
H	0.789006	4.445704	3.770658
H	2.546914	5.688697	5.004627
C	-0.159231	4.959853	0.995205
C	-1.339812	5.587686	0.622280
C	-2.521389	4.853788	0.529594
C	-2.526942	3.487202	0.810338
C	-1.347250	2.844269	1.157953
H	-1.357235	1.778612	1.369323
H	0.765749	5.524552	1.059767
H	-1.339296	6.648871	0.395786
H	-3.442538	5.345732	0.229501
H	-3.447712	2.916187	0.744965
C	2.927100	0.464297	-0.782687
C	3.904649	0.284738	-1.755134
C	5.244877	0.102531	-1.434734
C	5.594099	0.095093	-0.091942
Br	3.412966	0.305478	-3.575767
H	5.987488	-0.049832	-2.207803
C	4.653328	0.303209	0.907964
H	4.964434	0.323277	1.948563
H	1.882214	0.561741	-1.067769
Br	7.398128	-0.207585	0.382813
C	4.901114	-3.160312	-0.192299
C	6.050819	-3.170003	-0.940277
C	5.983657	-3.039820	-2.349750
C	4.768956	-2.920468	-2.978537
H	4.946719	-3.242674	0.891517
H	7.017290	-3.251942	-0.453378
H	4.710135	-2.813214	-4.058724
H	6.901023	-3.036364	-2.931074
C	-3.535170	4.166415	-2.698955
C	-3.668599	5.522138	-2.858038
C	-4.715484	6.219977	-2.203815
C	-5.597736	5.548177	-1.395112
H	-2.733097	3.616697	-3.184804
H	-2.973191	6.068288	-3.487911
H	-4.816565	7.291779	-2.346862
H	-6.400523	6.079108	-0.889018
C	-7.321442	-3.108154	-0.724928
C	-7.053151	-4.589566	-0.976583
H	-7.944852	-3.009649	0.175330
H	-7.902159	-2.675940	-1.547218
C	-6.060190	-5.113339	0.057046
H	-6.631016	-4.724646	-1.980778
H	-7.992400	-5.151217	-0.942402
C	-4.715599	-4.406947	-0.099864
H	-6.457825	-4.932724	1.065846
H	-5.921466	-6.194684	-0.043991
H	-4.030458	-4.714841	0.693504
H	-4.244415	-4.737467	-1.036888
C	-3.511544	-3.176647	2.803950
C	-3.396862	-4.157917	3.968317
H	-4.465249	-3.309162	2.287482
H	-3.535688	-2.149882	3.199817
C	-2.002375	-4.086312	4.583978
H	-4.168734	-3.936562	4.712610
H	-3.580721	-5.180089	3.609250
C	-0.968012	-4.536140	3.556082

H	-1.792235	-3.050833	4.884197
H	-1.934631	-4.706959	5.483413
H	-1.060881	-5.621319	3.407567
H	0.046977	-4.361479	3.930048

B-3

M06-2X/6-31G* Energy = -8271.59003488

M06-2X/6-31G* Free Energy = -8270.704361

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.56471388

Lowest Frequency = 12.3986

M06-2X/6-31G* Geometry

C	0.959027	-0.786803	3.894359
C	1.770546	2.591588	1.625637
C	2.216553	-0.546584	3.528474
H	0.237365	-1.174669	3.177891
H	0.616620	-0.595975	4.907420
C	2.723284	-0.800148	2.138390
H	2.927176	-0.136894	4.248092
N	1.853860	1.327643	1.358525
C	0.455752	3.227280	1.806893
C	3.002206	3.410150	1.755526
C	3.065461	0.496778	1.373594
C	3.527013	0.128802	-0.023070
H	3.852316	1.048327	1.897119
H	0.962001	0.739053	1.171279
H	1.969215	-1.340266	1.557133
H	3.632045	-1.414985	2.151439
C	-5.267723	-1.432191	-1.068365
C	-6.031573	-0.371283	-1.571334
C	-4.083492	-1.150493	-0.354730
C	-3.606619	0.165213	-0.298966
C	-4.354535	1.237673	-0.807163
C	-5.576672	0.936014	-1.403217
C	-3.312787	-2.233802	0.328526
C	-3.876074	-3.032514	1.345536
C	-3.110207	-4.071638	1.892762
C	-1.789747	-4.248582	1.478803
C	-1.171516	-3.408542	0.554607
C	-1.974491	-2.415398	-0.019495
O	-2.410203	0.418708	0.338869
O	-1.427737	-1.534241	-0.931052
P	-0.978785	-0.089749	-0.308696
O	-0.091477	-0.325848	0.897118
O	-0.492980	0.776346	-1.412793
C	-3.897343	2.649624	-0.749938
C	0.278397	-3.529115	0.261904
C	-4.801593	3.661993	-0.319087
C	-4.443541	4.985486	-0.333049
C	-3.152026	5.382468	-0.770671
C	-2.241062	4.374112	-1.189576
C	-2.640042	3.014730	-1.175341
C	0.801663	-3.316236	-1.048555
C	2.144190	-3.425867	-1.292272
C	3.060361	-3.729374	-0.250178
C	2.549309	-3.957169	1.056923
C	1.152178	-3.853931	1.278077
H	-6.168539	1.754111	-1.809639
H	-1.211811	-5.063383	1.909801
H	-5.789238	3.368318	0.027205
H	-5.145355	5.748994	-0.005332
H	0.780213	-3.982316	2.292175
H	2.525793	-3.255571	-2.296116
H	0.127827	-3.055105	-1.856293

H	-1.936084	2.264941	-1.525590
C	3.960681	3.399103	0.736211
C	5.107337	4.176560	0.855991
C	5.307928	4.952533	1.995719
C	4.354892	4.964380	3.012324
C	3.195649	4.206411	2.888975
H	3.796670	2.792927	-0.150766
H	5.843442	4.174757	0.058935
H	6.207064	5.553195	2.090038
H	2.440647	4.220661	3.669392
H	4.510764	5.569890	3.899092
C	0.327539	4.616834	1.643655
C	-0.905697	5.227876	1.816812
C	-2.024602	4.459904	2.134760
C	-1.909408	3.079407	2.282729
C	-0.674806	2.461709	2.137989
H	-0.596054	1.388934	2.281512
H	1.187277	5.211603	1.353221
H	-1.004270	6.296929	1.661051
H	-2.993970	4.936250	2.242790
H	-2.782444	2.474062	2.501691
C	2.628648	0.072959	-1.086842
C	3.059065	-0.443857	-2.303205
C	4.366069	-0.872372	-2.501144
C	5.242863	-0.791031	-1.425422
Br	1.791395	-0.674396	-3.677888
H	4.683196	-1.284314	-3.451951
C	4.844533	-0.301163	-0.190484
H	5.545081	-0.290314	0.639225
H	1.594048	0.391635	-0.992679
Br	6.997951	-1.467604	-1.625100
C	3.460330	-4.225370	2.113737
C	4.813241	-4.248694	1.883932
C	5.322132	-4.020195	0.580887
C	4.462376	-3.782907	-0.461621
H	3.064593	-4.392154	3.112786
H	5.500685	-4.444463	2.701500
H	4.849177	-3.609823	-1.462908
H	6.393976	-4.028660	0.406433
C	-0.938040	4.749167	-1.613558
C	-0.559050	6.067296	-1.620097
C	-1.467565	7.073619	-1.204476
C	-2.732299	6.738951	-0.788956
H	-0.254548	3.960986	-1.920312
H	0.437846	6.348339	-1.946673
H	-1.158514	8.114749	-1.221208
H	-3.432473	7.508654	-0.472427
C	-7.351686	-0.595333	-2.285409
C	-7.507770	-2.012315	-2.831221
H	-7.458446	0.141537	-3.089059
H	-8.169595	-0.397317	-1.577874
C	-7.129533	-3.023354	-1.752514
H	-6.848931	-2.150269	-3.698284
H	-8.534606	-2.168765	-3.177570
C	-5.656717	-2.867673	-1.381706
H	-7.754949	-2.858269	-0.863614
H	-7.317532	-4.047413	-2.091258
H	-5.397880	-3.537921	-0.559347
H	-5.038721	-3.195278	-2.230375
C	-5.244675	-2.708680	1.920525
C	-5.882970	-3.888102	2.650360
H	-5.918203	-2.326942	1.150621
H	-5.112952	-1.878941	2.630567

C	-4.897415	-4.479132	3.654508
H	-6.801166	-3.560031	3.148556
H	-6.169689	-4.661063	1.923461
C	-3.681636	-5.034718	2.917210
H	-4.580942	-3.692255	4.351621
H	-5.366292	-5.268991	4.250448
H	-3.974342	-5.959595	2.400138
H	-2.896507	-5.318224	3.626888

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M06-2X/6-31G* Energy = -8271.58417840

M06-2X/6-31G* Free Energy = -8270.700312

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.56287650

Lowest Frequency = 7.6749

M06-2X/6-31G* Geometry

C	-2.038179	0.952043	-3.883201
C	-2.299679	3.033162	-0.828266
C	-3.062954	0.686589	-3.075311
H	-1.040235	0.581713	-3.655634
H	-2.176885	1.533069	-4.791249
C	-2.941726	-0.107534	-1.806216
H	-4.059607	1.066554	-3.310266
N	-2.168520	1.789843	-0.491688
C	-1.107380	3.848577	-1.110206
C	-3.635950	3.667523	-0.938074
C	-3.230890	0.774163	-0.570598
C	-3.368683	-0.052963	0.689760
H	-4.174714	1.292854	-0.746173
H	-1.176206	1.417558	-0.266736
H	-1.944470	-0.561170	-1.726154
H	-3.682050	-0.916325	-1.779738
C	4.523159	-1.820851	1.395005
C	5.126624	-0.905289	2.266003
C	3.705318	-1.343034	0.349064
C	3.381491	0.016727	0.294313
C	3.973774	0.944562	1.161312
C	4.864816	0.456502	2.112188
C	3.160841	-2.261645	-0.695161
C	3.995889	-3.003037	-1.557248
C	3.410765	-3.871847	-2.489055
C	2.019910	-3.952317	-2.579643
C	1.174341	-3.176043	-1.793196
C	1.778688	-2.332140	-0.857726
O	2.532180	0.475558	-0.690326
O	0.997847	-1.464956	-0.114497
P	0.947321	0.051644	-0.742201
O	0.159823	0.853110	0.272944
O	0.509805	0.067039	-2.162943
C	3.684389	2.399906	1.093727
C	-0.296014	-3.221139	-1.977681
C	2.347053	2.873100	1.213205
C	2.085544	4.216207	1.223271
C	3.129041	5.169748	1.090392
C	4.466461	4.703947	0.958225
C	4.713049	3.306095	0.974799
C	-0.832969	-3.125148	-3.292032
C	-2.183179	-3.196968	-3.511169
C	-3.084689	-3.372621	-2.429172
C	-2.556648	-3.468057	-1.111625
C	-1.155081	-3.380090	-0.912741
H	5.329278	1.165902	2.794302
H	1.577669	-4.631029	-3.306754
H	1.537454	2.155474	1.297779

H	1.061173	4.571608	1.315047
H	-0.766550	-3.425814	0.102836
H	-2.583260	-3.096577	-4.516826
H	-0.149736	-2.958381	-4.119513
H	5.736918	2.952245	0.873834
C	-4.547618	3.575780	0.119983
C	-5.783626	4.204940	0.024468
C	-6.117220	4.912271	-1.129574
C	-5.211045	5.002887	-2.184145
C	-3.964157	4.394720	-2.085436
H	-4.277349	3.019757	1.014828
H	-6.485168	4.143915	0.849930
H	-7.085077	5.397715	-1.204737
H	-3.244790	4.463807	-2.896169
H	-5.472820	5.553279	-3.081777
C	0.004152	3.264614	-1.733824
C	1.120567	4.043235	-2.016171
C	1.129950	5.398182	-1.694647
C	0.015017	5.986801	-1.095035
C	-1.105723	5.219511	-0.808216
H	-1.974605	5.671229	-0.338609
H	-0.016156	2.218679	-2.030626
H	1.984659	3.580272	-2.481072
H	2.010217	5.999678	-1.900488
H	0.024025	7.044011	-0.849049
C	-4.650401	-0.271247	1.194094
C	-4.825021	-1.136343	2.268093
C	-3.752899	-1.782327	2.866068
C	-2.487492	-1.555726	2.334781
Br	-6.575074	-1.506266	2.883266
H	-3.899695	-2.468586	3.691456
C	-2.273585	-0.704906	1.260752
H	-1.266855	-0.564370	0.879960
H	-5.514614	0.203192	0.738648
Br	-1.026674	-2.545775	3.004428
C	-3.454306	-3.607160	-0.019235
C	-4.811304	-3.589035	-0.216003
C	-5.336923	-3.480733	-1.528910
C	-4.493697	-3.394238	-2.608267
H	-3.035631	-3.705228	0.978023
H	-5.487619	-3.641355	0.633434
H	-4.891840	-3.318605	-3.617211
H	-6.412739	-3.476029	-1.676104
C	5.512274	5.653387	0.809557
C	5.243874	6.998182	0.790312
C	3.911948	7.462097	0.923768
C	2.882222	6.567719	1.072101
H	6.532787	5.292434	0.708750
H	6.051982	7.713889	0.674449
H	3.712106	8.529342	0.911992
H	1.856676	6.913626	1.180590
C	6.073559	-1.344445	3.367365
C	5.913281	-2.814232	3.747285
H	5.933098	-0.701976	4.243616
H	7.105885	-1.177650	3.028007
C	5.883603	-3.671693	2.485157
H	4.973940	-2.954253	4.297862
H	6.726791	-3.119415	4.413568
C	4.665394	-3.314484	1.637042
H	6.801637	-3.498188	1.906001
H	5.858729	-4.737417	2.735109
H	3.756600	-3.649030	2.158575
H	4.679786	-3.868436	0.695797

C	5.497671	-2.772253	-1.563813
C	6.277227	-3.908358	-2.221647
H	5.874027	-2.587549	-0.555358
H	5.682909	-1.841340	-2.119284
C	5.674188	-4.239667	-3.583738
H	7.330494	-3.624812	-2.317086
H	6.240825	-4.800938	-1.581329
C	4.246519	-4.748590	-3.403063
H	5.669262	-3.334072	-4.204117
H	6.274492	-4.989043	-4.110039
H	4.283220	-5.761789	-2.978072
H	3.744479	-4.842682	-4.372365

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M06-2X/6-31G* Energy = -8271.57838120

M06-2X/6-31G* Free Energy = -8270.696016

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.56118246

Lowest Frequency = 8.4749

M06-2X/6-31G* Geometry

C	0.214254	-3.286244	1.862666
C	-1.665833	0.062979	2.847963
C	-1.096926	-3.326779	1.641282
H	0.883739	-2.733639	1.205522
H	0.665469	-3.833365	2.685306
C	-1.791627	-2.586208	0.533613
H	-1.741393	-3.906371	2.303834
N	-1.672719	-0.444168	1.660284
C	-2.804875	-0.083054	3.782087
C	-0.473106	0.824404	3.266138
C	-2.621541	-1.412438	1.098107
C	-3.504734	-0.769872	0.046250
H	-3.250412	-1.786424	1.911951
H	-0.864881	-0.143371	0.973072
H	-1.076889	-2.206477	-0.210166
H	-2.482457	-3.249134	-0.000134
C	4.628635	1.610317	0.881980
C	4.238361	2.871140	1.358799
C	3.878755	1.008107	-0.151638
C	2.719914	1.635037	-0.613043
C	2.278453	2.858418	-0.100362
C	3.076457	3.465811	0.864626
C	4.218445	-0.338633	-0.699271
C	5.461456	-0.612207	-1.305343
C	5.782549	-1.934199	-1.639861
C	4.845490	-2.943239	-1.413413
C	3.565449	-2.681928	-0.933553
C	3.261643	-1.356102	-0.597017
O	1.969164	0.985697	-1.570442
O	2.016438	-1.051247	-0.083712
P	0.948904	-0.162178	-1.001310
O	0.052298	0.478602	0.037227
O	0.379199	-0.931194	-2.127461
C	0.987584	3.461281	-0.509492
C	2.583437	-3.784405	-0.765487
C	0.068394	3.857273	0.501301
C	-1.123091	4.446632	0.173254
C	-1.468024	4.683528	-1.183523
C	-0.559701	4.275629	-2.199552
C	0.660577	3.655724	-1.831108
C	2.911453	-4.892514	0.064371
C	2.020884	-5.917452	0.255416
C	0.748774	-5.899386	-0.373598
C	0.425452	-4.803092	-1.219824

C	1.363920	-3.756633	-1.402385
H	2.763502	4.428027	1.266451
H	5.099701	-3.969268	-1.673400
H	0.321500	3.656680	1.540186
H	-1.825510	4.739678	0.949857
H	1.098206	-2.917248	-2.039764
H	2.275292	-6.754933	0.900547
H	3.877968	-4.905497	0.561606
H	1.345820	3.336803	-2.611634
C	-0.607868	1.944510	4.097306
C	0.512528	2.697208	4.429623
C	1.767825	2.325363	3.947814
C	1.907577	1.194730	3.145344
C	0.793568	0.442523	2.803023
H	-1.590301	2.235679	4.456991
H	0.405634	3.575629	5.057682
H	2.643850	2.916194	4.201905
H	0.907703	-0.437502	2.179204
H	2.882122	0.906134	2.765170
C	-4.116112	0.142876	3.345786
C	-5.173520	0.028112	4.240978
C	-4.929040	-0.322330	5.567467
C	-3.624690	-0.542154	6.006205
C	-2.561177	-0.408187	5.121130
H	-1.540366	-0.565373	5.456223
H	-4.300206	0.426795	2.312954
H	-6.187295	0.214266	3.902057
H	-5.756895	-0.417555	6.262980
H	-3.435099	-0.811385	7.040002
C	-4.839520	-1.169472	-0.035623
C	-5.652547	-0.622023	-1.019943
C	-5.173248	0.321119	-1.919789
C	-3.840574	0.706965	-1.814510
Br	-7.464272	-1.160337	-1.126151
H	-5.819273	0.747600	-2.677499
C	-2.995820	0.172316	-0.847995
H	-1.958539	0.495388	-0.800434
H	-5.245745	-1.897795	0.660149
Br	-3.156224	2.012405	-2.989160
C	-0.847417	-4.767258	-1.850544
C	-1.759222	-5.770011	-1.639211
C	-1.438443	-6.860082	-0.791236
C	-0.213795	-6.923873	-0.177055
H	-1.080133	-3.918989	-2.490388
H	-2.730856	-5.735280	-2.123145
H	0.036574	-7.759487	0.472030
H	-2.168119	-7.648793	-0.633923
C	-0.899336	4.510117	-3.559377
C	-2.080100	5.124960	-3.891761
C	-2.982808	5.533618	-2.878120
C	-2.683814	5.313469	-1.558460
H	-0.205027	4.188908	-4.331396
H	-2.328853	5.299947	-4.934068
H	-3.915946	6.015103	-3.153791
H	-3.375073	5.619189	-0.776968
C	5.033519	3.602463	2.423365
C	5.844769	2.656970	3.304533
H	4.355163	4.217866	3.026147
H	5.723143	4.304869	1.934190
C	6.662301	1.721578	2.418077
H	5.169212	2.059569	3.934114
H	6.491744	3.228503	3.977969
C	5.741264	0.839758	1.577414

H	7.301477	2.322782	1.756922
H	7.326082	1.090660	3.018027
H	5.264204	0.094611	2.233089
H	6.327479	0.255975	0.865076
C	6.395341	0.522852	-1.690074
C	7.836494	0.065400	-1.901945
H	6.351450	1.336436	-0.962152
H	6.017271	0.951372	-2.629543
C	7.868913	-1.130084	-2.850606
H	8.433074	0.894599	-2.296065
H	8.281138	-0.222111	-0.938466
C	7.132484	-2.310691	-2.221954
H	7.382933	-0.850610	-3.794277
H	8.898163	-1.416562	-3.090131
H	7.754786	-2.727870	-1.417261
H	7.000461	-3.115422	-2.953420

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M06-2X/6-31G* Energy = -8271.58803610

M06-2X/6-31G* Free Energy = -8270.702904

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.56391986

Lowest Frequency = 12.2550

M06-2X/6-31G* Geometry

C	1.142106	-0.376348	3.830229
C	1.481807	2.933686	1.374836
C	2.355846	0.021167	3.453684
H	0.493512	-0.909433	3.137624
H	0.763364	-0.174897	4.828212
C	2.910445	-0.241601	2.083783
H	2.990821	0.573821	4.148045
N	1.748482	1.684739	1.167108
C	0.087742	3.389731	1.503901
C	2.584002	3.922153	1.492857
C	3.067419	1.041038	1.239026
C	3.593854	0.658062	-0.130112
H	3.760025	1.731854	1.728770
H	0.954587	0.961334	1.003225
H	2.251233	-0.922779	1.536967
H	3.900383	-0.712031	2.138109
C	-4.825969	-2.336796	-1.070178
C	-5.736075	-1.446724	-1.654366
C	-3.712968	-1.824842	-0.369717
C	-3.449375	-0.450553	-0.406712
C	-4.349886	0.452464	-0.986521
C	-5.497187	-0.074783	-1.572765
C	-2.798361	-2.719253	0.402848
C	-3.251604	-3.513539	1.476345
C	-2.343357	-4.370397	2.114433
C	-1.003198	-4.368998	1.726834
C	-0.504493	-3.518986	0.741258
C	-1.441152	-2.712893	0.082337
O	-2.318084	0.038330	0.212000
O	-1.024440	-1.834296	-0.896580
P	-0.821554	-0.285688	-0.409939
O	0.085959	-0.266502	0.804441
O	-0.484736	0.542767	-1.592983
C	-4.132185	1.922346	-0.983196
C	0.951869	-3.434964	0.467809
C	-2.937181	2.487677	-1.515088
C	-2.789444	3.847072	-1.586764
C	-3.800032	4.725264	-1.114391
C	-4.984376	4.167221	-0.559043
C	-5.124982	2.755994	-0.518754

C	1.458654	-3.234509	-0.851220
C	2.805696	-3.146212	-1.077567
C	3.739482	-3.228003	-0.010529
C	3.247827	-3.446407	1.305557
C	1.848046	-3.549526	1.509823
H	-6.203245	0.613514	-2.033109
H	-0.314347	-5.045928	2.227715
H	-2.149099	1.831349	-1.872567
H	-1.878207	4.273101	-1.999643
H	1.483526	-3.664174	2.528217
H	3.173090	-2.986854	-2.088487
H	0.767347	-3.139748	-1.680353
H	-6.034835	2.331450	-0.099100
C	2.640806	4.771048	2.602862
C	3.677605	5.690232	2.718757
C	4.641721	5.784181	1.716946
C	4.576095	4.952703	0.600726
C	3.554301	4.015898	0.489232
H	1.876732	4.700542	3.371375
H	3.728760	6.338002	3.587699
H	5.444048	6.509949	1.804387
H	3.496534	3.363631	-0.378323
H	5.320813	5.031450	-0.184369
C	-0.219251	4.744852	1.289003
C	-1.524668	5.192603	1.422448
C	-2.540243	4.296653	1.756667
C	-2.247445	2.949061	1.950857
C	-0.939113	2.493767	1.841888
H	-0.723907	1.445365	2.023161
H	0.564277	5.439107	1.004051
H	-1.762970	6.235906	1.242565
H	-3.563112	4.652138	1.842090
H	-3.036835	2.241187	2.179901
C	2.725595	0.380804	-1.184540
C	3.243675	-0.153275	-2.358385
C	4.603941	-0.383842	-2.526209
C	5.446797	-0.082407	-1.462744
Br	2.041652	-0.692157	-3.705327
H	4.990612	-0.813428	-3.442863
C	4.964247	0.431410	-0.268129
H	5.645936	0.614519	0.557147
H	1.652733	0.536053	-1.112434
Br	7.288153	-0.488985	-1.612361
C	4.171094	-3.493113	2.384550
C	5.514012	-3.311773	2.166416
C	6.002891	-3.090319	0.854432
C	5.135249	-3.066946	-0.208106
H	3.789583	-3.654525	3.389944
H	6.209041	-3.338193	3.000411
H	5.507023	-2.900964	-1.216164
H	7.064929	-2.935586	0.688322
C	-5.976760	5.039681	-0.036431
C	-5.797420	6.399586	-0.055833
C	-4.619160	6.955747	-0.613538
C	-3.649709	6.136553	-1.134763
H	-6.880485	4.607504	0.386261
H	-6.560132	7.056288	0.351229
H	-4.490916	8.033844	-0.629978
H	-2.742413	6.555577	-1.563877
C	-6.990793	-1.924676	-2.361563
C	-6.915494	-3.384712	-2.800782
H	-7.193318	-1.273948	-3.219339
H	-7.843797	-1.804662	-1.678356

C	-6.405424	-4.243785	-1.647145
H	-6.227301	-3.481134	-3.650475
H	-7.899145	-3.723816	-3.141764
C	-4.981435	-3.834056	-1.279374
H	-7.064928	-4.113993	-0.777216
H	-6.426632	-5.306441	-1.909982
H	-4.635763	-4.393998	-0.407752
H	-4.305006	-4.121226	-2.097525
C	-4.666735	-3.365752	2.009430
C	-5.124989	-4.564842	2.836159
H	-5.375549	-3.165804	1.203314
H	-4.685098	-2.467109	2.643536
C	-4.078079	-4.904845	3.893072
H	-6.092751	-4.345070	3.298778
H	-5.272522	-5.432628	2.178010
C	-2.777566	-5.323878	3.212558
H	-3.900885	-4.021025	4.519806
H	-4.428965	-5.704310	4.553835
H	-2.914444	-6.322441	2.773753
H	-1.971407	-5.422224	3.947987

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M06-2X/6-31G* Energy = -8271.57838142

M06-2X/6-31G* Free Energy = -8270.695992

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.56117585

Lowest Frequency = 8.5213

M06-2X/6-31G* Geometry

C	0.213779	-3.285600	1.863792
C	-1.666207	0.063945	2.848111
C	-1.097375	-3.326191	1.642293
H	0.883350	-2.733096	1.206652
H	0.664890	-3.832607	2.686566
C	-1.791981	-2.585797	0.534455
H	-1.741869	-3.905744	2.304848
N	-1.673088	-0.443399	1.660528
C	-2.805148	-0.082231	3.782370
C	-0.473725	0.825834	3.266140
C	-2.621850	-1.411826	1.098576
C	-3.504772	-0.769568	0.046311
H	-3.250836	-1.785565	1.912439
H	-0.865534	-0.142420	0.972930
H	-1.077213	-2.206324	-0.209435
H	-2.482907	-3.248761	0.000889
C	5.461536	-0.612671	-1.305432
C	5.782560	-1.934749	-1.639707
C	4.218596	-0.338907	-0.699302
C	3.261800	-1.356352	-0.596671
C	3.565522	-2.682253	-0.933003
C	4.845486	-2.943717	-1.412978
C	3.878961	1.007962	-0.151984
C	4.628939	1.610473	0.881395
C	4.238632	2.871366	1.358006
C	3.076616	3.465846	0.863861
C	2.278540	2.858170	-0.100894
C	2.720019	1.634722	-0.613352
O	2.016698	-1.051481	-0.083208
O	1.969070	0.985058	-1.570409
P	0.948860	-0.162414	-1.000399
O	0.053119	0.478943	0.038556
O	0.378176	-0.931629	-2.125916
C	2.583412	-3.784597	-0.764631
C	0.987562	3.460838	-0.509941
C	2.911438	-4.892636	0.065319

C	2.020803	-5.917479	0.256595
C	0.748633	-5.899397	-0.372298
C	0.425290	-4.803165	-1.218596
C	1.363805	-3.756781	-1.401351
C	0.068338	3.856646	0.500910
C	-1.123240	4.445826	0.172904
C	-1.468247	4.682694	-1.183873
C	-0.559902	4.274964	-2.199939
C	0.660494	3.655238	-1.831538
H	5.099611	-3.969804	-1.672818
H	2.763606	4.428099	1.265548
H	3.878013	-4.905642	0.562435
H	2.275224	-6.754909	0.901786
H	1.345774	3.336441	-2.612087
H	-1.825686	4.738781	0.949519
H	0.321528	3.656019	1.539770
H	1.098042	-2.917439	-2.038765
C	0.793155	0.443906	2.803655
C	1.906915	1.196558	3.145845
C	1.766714	2.327688	3.947533
C	0.511197	2.699577	4.428750
C	-0.608940	1.946420	4.096602
H	0.907561	-0.436413	2.180316
H	2.881638	0.907911	2.766170
H	2.642561	2.918867	4.201441
H	-1.591531	2.237608	4.455841
H	0.403937	3.578387	5.056203
C	-4.116492	0.143201	3.346096
C	-5.173786	0.028395	4.241418
C	-4.929084	-0.321637	5.567979
C	-3.624643	-0.541023	6.006656
C	-2.561237	-0.406991	5.121452
H	-1.540352	-0.563823	5.456484
H	-4.300756	0.426762	2.313194
H	-6.187646	0.214202	3.902559
H	-5.756852	-0.416906	6.263592
H	-3.434902	-0.809965	7.040501
C	-4.839553	-1.169084	-0.035771
C	-5.652227	-0.622049	-1.020635
C	-5.172557	0.320573	-1.920813
C	-3.839875	0.706385	-1.815310
Br	-7.463972	-1.160249	-1.127139
H	-5.818298	0.746705	-2.678965
C	-2.995500	0.172169	-0.848236
H	-1.958222	0.495222	-0.800544
H	-5.246088	-1.896975	0.660275
Br	-3.155040	2.011143	-2.990423
C	-0.899631	4.509395	-3.559750
C	-2.080526	5.124024	-3.892087
C	-2.983261	5.532517	-2.878409
C	-2.684162	5.312427	-1.558760
H	-0.205279	4.188338	-4.331796
H	-2.329356	5.298962	-4.934385
H	-3.375433	5.618043	-0.777239
H	-3.916502	6.013828	-3.154032
C	-0.847607	-4.767357	-1.849263
C	-1.759434	-5.770062	-1.637788
C	-1.438649	-6.860055	-0.789716
C	-0.213965	-6.923827	-0.175596
H	-1.080319	-3.919150	-2.489189
H	-2.731090	-5.735347	-2.121677
H	-2.168341	-7.648725	-0.632280
H	0.036412	-7.759402	0.473537

C	7.132432	-2.311414	-2.221818
C	7.868900	-1.130969	-2.850727
H	7.000328	-3.116281	-2.953121
H	7.754764	-2.728478	-1.417086
C	7.836573	0.064698	-1.902276
H	7.382888	-0.851634	-3.794423
H	8.898121	-1.417548	-3.090252
C	6.395443	0.522259	-1.690489
H	8.281198	-0.222676	-0.938747
H	8.433197	0.893796	-2.296539
H	6.351582	1.336043	-0.962789
H	6.017377	0.950534	-2.630073
C	5.741625	0.840082	1.576925
C	6.662624	1.722053	2.417464
H	6.327868	0.256207	0.864685
H	5.264567	0.095024	2.232706
C	5.845058	2.657587	3.303760
H	7.326408	1.091240	3.017518
H	7.301794	2.323180	1.756232
C	5.033829	3.602911	2.422385
H	5.169488	2.060294	3.933428
H	6.492020	3.229236	3.977112
H	5.723503	4.305150	1.933037
H	4.355509	4.218508	3.025013

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M06-2X/6-31G* Energy = -8271.58928740

M06-2X/6-31G* Free Energy = -8270.701363

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.56666132

Lowest Frequency = 13.9855

M06-2X/6-31G* Geometry

C	-0.641961	-0.196569	2.880977
C	0.876155	3.099834	1.256709
C	0.652562	0.033335	3.090987
H	-0.993573	-0.594394	1.929668
H	-1.388119	0.008150	3.644318
C	1.701300	-0.224054	2.046545
H	0.990163	0.446375	4.042821
N	1.178360	1.878663	0.949946
C	-0.445171	3.631382	0.896039
C	1.843901	3.959260	1.978520
C	2.296257	1.081754	1.479305
C	3.350805	0.814691	0.421206
H	2.749626	1.653044	2.294191
H	0.520601	1.301181	0.337108
H	1.275606	-0.795790	1.217504
H	2.542349	-0.795035	2.459564
C	-4.551954	-3.201487	-0.078061
C	-5.781935	-2.709472	-0.533469
C	-3.463351	-2.314230	0.059459
C	-3.584058	-0.998290	-0.396150
C	-4.809104	-0.491424	-0.850896
C	-5.893978	-1.361564	-0.878326
C	-2.173569	-2.750114	0.675977
C	-2.104969	-3.201735	2.009473
C	-0.876519	-3.659480	2.502963
C	0.247679	-3.636717	1.678755
C	0.240592	-3.098577	0.390882
C	-1.002375	-2.640075	-0.078996
O	-2.492171	-0.162304	-0.314779
O	-1.105082	-2.043074	-1.312692
P	-1.193575	-0.397239	-1.332675
O	-0.037976	0.138458	-0.520090

O	-1.467454	0.025190	-2.718679
C	-4.969103	0.927666	-1.259654
C	1.501924	-3.008247	-0.393762
C	-4.152398	1.482168	-2.286150
C	-4.306011	2.790696	-2.659661
C	-5.261683	3.630056	-2.029396
C	-6.077063	3.084168	-0.998484
C	-5.917001	1.717398	-0.646697
C	1.507774	-3.068366	-1.820258
C	2.682973	-3.031146	-2.521060
C	3.936994	-2.942640	-1.861635
C	3.948349	-2.875240	-0.442896
C	2.716032	-2.908065	0.256448
H	-6.851021	-0.982602	-1.231787
H	1.176365	-4.044581	2.070199
H	-3.397491	0.862097	-2.760429
H	-3.677839	3.207639	-3.442589
H	2.751683	-2.846372	1.340551
H	2.667333	-3.074052	-3.606854
H	0.567934	-3.148001	-2.350632
H	-6.535034	1.303606	0.147680
C	3.161823	4.067999	1.518708
C	4.063347	4.887180	2.188501
C	3.658169	5.587542	3.323314
C	2.346781	5.481361	3.782595
C	1.434306	4.680101	3.105209
H	3.469625	3.520815	0.631501
H	5.081090	4.977720	1.823537
H	4.365380	6.221787	3.848363
H	0.407331	4.599839	3.448729
H	2.032315	6.027842	4.665573
C	-1.534000	2.759987	0.730639
C	-2.785783	3.270609	0.417322
C	-2.965278	4.646070	0.271115
C	-1.884603	5.514532	0.423652
C	-0.628502	5.014384	0.739295
H	0.214846	5.688674	0.849362
H	-1.416028	1.688670	0.862852
H	-3.620890	2.588916	0.293043
H	-3.951110	5.037984	0.034919
H	-2.021520	6.583319	0.295538
C	3.008691	0.571374	-0.911530
C	4.028276	0.349164	-1.830133
C	5.368102	0.327451	-1.460736
C	5.673869	0.531411	-0.123000
Br	3.593356	0.076496	-3.644918
H	6.144858	0.135423	-2.190160
C	4.687600	0.789116	0.819881
H	4.962416	0.970857	1.854979
H	1.969035	0.535828	-1.227910
Br	7.480596	0.445759	0.425354
C	5.195579	-2.785494	0.232401
C	6.374309	-2.779979	-0.468885
C	6.359914	-2.835646	-1.884845
C	5.169217	-2.908950	-2.564393
H	5.199002	-2.728266	1.318788
H	7.321163	-2.707754	0.056543
H	5.150129	-2.942888	-3.650783
H	7.298961	-2.819465	-2.430278
C	-7.003394	3.932230	-0.334287
C	-7.115496	5.255736	-0.677285
C	-6.310813	5.796433	-1.711280
C	-5.409284	5.000424	-2.371598

H	-7.620698	3.512210	0.455930
H	-7.825264	5.894343	-0.160457
H	-6.413396	6.843737	-1.978707
H	-4.785752	5.407757	-3.163496
C	-7.010368	-3.592830	-0.648750
C	-6.676221	-5.081004	-0.709316
H	-7.656378	-3.410476	0.222031
H	-7.591007	-3.291955	-1.527683
C	-5.682853	-5.429366	0.395462
H	-6.229147	-5.321078	-1.682620
H	-7.592117	-5.674129	-0.619123
C	-4.366491	-4.689276	0.170033
H	-6.106925	-5.143096	1.368418
H	-5.497297	-6.507796	0.431325
H	-3.681810	-4.868483	1.002320
H	-3.866683	-5.109648	-0.714659
C	-3.307286	-3.073683	2.928908
C	-3.187313	-3.909920	4.200682
H	-4.234568	-3.312440	2.403019
H	-3.394653	-2.011516	3.204235
C	-1.824666	-3.688234	4.850896
H	-3.999297	-3.651741	4.888292
H	-3.301206	-4.974826	3.954506
C	-0.726614	-4.188147	3.916562
H	-1.684238	-2.615102	5.038535
H	-1.758971	-4.199456	5.816883
H	-0.751339	-5.286845	3.892807
H	0.261126	-3.910126	4.300690

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M06-2X/6-31G* Energy = -8271.58928741

M06-2X/6-31G* Free Energy = -8270.701355

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.56665884

Lowest Frequency = 13.9883

M06-2X/6-31G* Geometry

C	-0.641865	-0.196469	2.880583
C	0.876155	3.099766	1.256550
C	0.652676	0.033269	3.090729
H	-0.993433	-0.594101	1.929180
H	-1.388021	0.008165	3.643946
C	1.701436	-0.224025	2.046278
H	0.990235	0.446079	4.042673
N	1.178529	1.878666	0.949635
C	-0.445288	3.631158	0.896098
C	1.843866	3.959237	1.978355
C	2.296409	1.081824	1.479101
C	3.351103	0.814741	0.421129
H	2.749693	1.653091	2.294042
H	0.520780	1.301183	0.336855
H	1.275734	-0.795681	1.217179
H	2.542477	-0.795049	2.459257
C	-2.105453	-3.201563	2.009430
C	-0.877045	-3.659313	2.503008
C	-2.173977	-2.750021	0.675897
C	-1.002747	-2.640149	-0.079044
C	0.240192	-3.098663	0.390929
C	0.247199	-3.636672	1.678851
C	-3.463696	-2.314051	0.059313
C	-4.552412	-3.201188	-0.078109
C	-5.782345	-2.709088	-0.533541
C	-5.894241	-1.361201	-0.878554
C	-4.809259	-0.491203	-0.851263
C	-3.584246	-0.998140	-0.396446

O	-1.105390	-2.043231	-1.312789
O	-2.492337	-0.162244	-0.315200
P	-1.193564	-0.397396	-1.332802
O	-0.038024	0.138069	-0.519978
O	-1.467087	0.025144	-2.718847
C	1.501554	-3.008439	-0.393669
C	-4.969013	0.927893	-1.260091
C	1.507508	-3.068681	-1.820160
C	2.682761	-3.031527	-2.520878
C	3.936737	-2.942958	-1.861374
C	3.947987	-2.875457	-0.442632
C	2.715620	-2.908262	0.256620
C	-4.151976	1.482281	-2.286395
C	-4.305203	2.790873	-2.659844
C	-5.260770	3.630423	-2.029668
C	-6.076531	3.084627	-0.999004
C	-5.916896	1.717781	-0.647316
H	1.175852	-4.044517	2.070397
H	-6.851245	-0.982169	-1.232049
H	0.567714	-3.148369	-2.350609
H	2.667195	-3.074545	-3.606669
H	-6.535184	1.304074	0.146906
H	-3.676778	3.207717	-3.442622
H	-3.397144	0.862076	-2.760625
H	2.751182	-2.846534	1.340723
C	3.161691	4.068274	1.518332
C	4.063215	4.887449	2.188127
C	3.658149	5.587513	3.323167
C	2.346868	5.481009	3.782675
C	1.434386	4.679753	3.105289
H	3.469429	3.521255	0.630994
H	5.080880	4.978188	1.822992
H	4.365353	6.221761	3.848218
H	0.407494	4.599245	3.449010
H	2.032464	6.027241	4.665832
C	-0.628932	5.014178	0.739786
C	-1.885187	5.514155	0.424468
C	-2.965706	4.645505	0.271844
C	-2.785886	3.270043	0.417608
C	-1.533951	2.759581	0.730564
H	-1.415742	1.688240	0.862396
H	0.214294	5.688602	0.849927
H	-2.022357	6.582945	0.296659
H	-3.951672	5.037272	0.035930
H	-3.620867	2.588214	0.293248
C	3.009080	0.571260	-0.911609
C	4.028719	0.348909	-1.830115
C	5.368511	0.327216	-1.460594
C	5.674191	0.531342	-0.122865
Br	3.593944	0.076007	-3.644898
H	6.145328	0.135032	-2.189917
C	4.687857	0.789213	0.819912
H	4.962580	0.971063	1.855016
H	1.969449	0.535658	-1.228065
Br	7.480868	0.445570	0.425627
C	-7.002719	3.932884	-0.334863
C	-7.114321	5.256492	-0.677664
C	-6.309264	5.797094	-1.711411
C	-5.407865	5.000888	-2.371677
H	-7.620318	3.512948	0.455170
H	-7.823983	5.895235	-0.160857
H	-4.784036	5.408146	-3.163379
H	-6.411443	6.844474	-1.978692

C	5.195162	-2.785621	0.232749
C	6.373952	-2.780127	-0.468445
C	6.359664	-2.835938	-1.884393
C	5.169015	-2.909328	-2.564028
H	5.198501	-2.728305	1.319131
H	7.320757	-2.707805	0.057060
H	7.298745	-2.819790	-2.429771
H	5.150030	-2.943359	-3.650418
C	-0.727200	-4.187812	3.916676
C	-1.825240	-3.687710	4.850921
H	0.260550	-3.909801	4.300793
H	-0.751996	-5.286514	3.893062
C	-3.187886	-3.909436	4.200715
H	-1.684766	-2.614559	5.038409
H	-1.759596	-4.198802	5.816984
C	-3.307813	-3.073412	2.928794
H	-3.301831	-4.974377	3.954728
H	-3.999867	-3.651091	4.888273
H	-3.395251	-2.011201	3.203929
H	-4.235063	-3.312318	2.402906
C	-4.367127	-4.688979	0.170107
C	-5.683561	-5.428849	0.395822
H	-3.682310	-4.868207	1.002280
H	-3.867558	-5.109502	-0.714652
C	-6.676995	-5.080538	-0.708923
H	-5.498156	-6.507303	0.431837
H	-6.107491	-5.142359	1.368774
C	-7.010900	-3.592298	-0.648627
H	-6.230064	-5.320897	-1.682222
H	-7.592980	-5.673496	-0.618501
H	-7.656843	-3.409681	0.222153
H	-7.591545	-3.291504	-1.527587

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M06-2X/6-31G* Energy = -8271.58722609

M06-2X/6-31G* Free Energy = -8270.699485

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.56632561

Lowest Frequency = 14.6259

M06-2X/6-31G* Geometry

C	-0.745541	-0.133735	3.158432
C	1.056658	3.113903	1.533928
C	0.555499	0.005340	3.405663
H	-1.098476	-0.481270	2.187990
H	-1.495103	0.099462	3.910195
C	1.611579	-0.293031	2.380049
H	0.894736	0.369602	4.376376
N	1.242540	1.853114	1.311741
C	-0.201574	3.725481	1.083468
C	2.073402	3.941751	2.221667
C	2.296836	0.984577	1.847744
C	3.330269	0.648425	0.786826
H	2.782528	1.514559	2.673318
H	0.540992	1.317125	0.697114
H	1.169064	-0.818771	1.528593
H	2.402622	-0.926967	2.799793
C	-4.625498	-2.987237	0.081937
C	-5.854202	-2.468861	-0.346800
C	-3.532896	-2.111868	0.250048
C	-3.644102	-0.774081	-0.142330
C	-4.868302	-0.240977	-0.571570
C	-5.956693	-1.107762	-0.631732
C	-2.238551	-2.590852	0.821189
C	-2.150124	-3.100327	2.132805

C	-0.920131	-3.596358	2.580756
C	0.183608	-3.568309	1.728098
C	0.154383	-2.988182	0.459305
C	-1.085103	-2.472649	0.042599
O	-2.538507	0.040667	-0.024549
O	-1.198580	-1.804916	-1.155370
P	-1.247615	-0.158772	-1.057668
O	-0.070943	0.280403	-0.217929
O	-1.514716	0.378952	-2.406087
C	-5.045404	1.189162	-0.926897
C	1.388644	-2.931258	-0.366738
C	-6.122239	1.916802	-0.343826
C	-6.332462	3.236819	-0.647945
C	-5.474803	3.916149	-1.552972
C	-4.398663	3.193433	-2.139245
C	-4.210463	1.824938	-1.818285
C	2.662188	-2.878248	0.276772
C	3.829488	-2.910819	-0.436556
C	3.810177	-2.990171	-1.852990
C	2.551069	-3.023351	-2.511050
C	1.358154	-2.994341	-1.744751
H	-6.913233	-0.711622	-0.968073
H	1.113455	-4.007178	2.082233
H	-6.770924	1.410500	0.366170
H	-7.153893	3.783313	-0.191178
H	0.408394	-3.033029	-2.266663
H	4.789144	-2.845985	0.072894
H	2.706547	-2.798728	1.358374
H	-3.382767	1.289080	-2.277137
C	3.418529	3.882882	1.837409
C	4.356661	4.685653	2.476393
C	3.960745	5.536867	3.506139
C	2.622066	5.600286	3.888467
C	1.675289	4.817005	3.238730
H	3.720624	3.226379	1.025854
H	5.396039	4.647023	2.167703
H	4.696428	6.157937	4.007307
H	0.627726	4.870282	3.519314
H	2.313892	6.266307	4.687572
C	-1.374992	2.956812	1.018472
C	-2.552174	3.535147	0.565138
C	-2.562302	4.868070	0.153469
C	-1.399661	5.634606	0.219105
C	-0.222711	5.073364	0.695405
H	0.687834	5.663053	0.738479
H	-1.372896	1.916649	1.331817
H	-3.458127	2.939000	0.520709
H	-3.480563	5.307251	-0.226866
H	-1.410687	6.668728	-0.109289
C	3.002262	0.634279	-0.570415
C	3.985706	0.305994	-1.495958
C	5.275862	-0.036364	-1.108006
C	5.558663	-0.065565	0.249902
Br	3.550991	0.259019	-3.325122
H	6.020603	-0.313926	-1.844215
C	4.613064	0.290578	1.203249
H	4.872696	0.274266	2.257844
H	1.989386	0.833383	-0.907455
Br	7.259744	-0.675892	0.810266
C	2.521455	-3.094334	-3.930351
C	3.684923	-3.118532	-4.654593
C	4.939337	-3.074359	-3.996163
C	4.999182	-3.014407	-2.627490

H	1.556081	-3.117398	-4.428804
H	3.651003	-3.166625	-5.738648
H	5.956797	-2.984703	-2.110942
H	5.853111	-3.090952	-4.582437
C	-3.502737	3.870727	-3.009873
C	-3.675409	5.202158	-3.290172
C	-4.758542	5.918768	-2.720638
C	-5.637368	5.290928	-1.873594
H	-2.672468	3.307590	-3.428405
H	-2.983383	5.714414	-3.951490
H	-4.890151	6.970095	-2.959026
H	-6.467752	5.836981	-1.432269
C	-7.087801	-3.339269	-0.497462
C	-6.760382	-4.824274	-0.629790
H	-7.728695	-3.195801	0.384310
H	-7.671160	-2.994380	-1.358244
C	-5.767051	-5.228724	0.455759
H	-6.315796	-5.019489	-1.614243
H	-7.678590	-5.417314	-0.566273
C	-4.447087	-4.485314	0.264558
H	-6.188958	-4.986809	1.441582
H	-5.586521	-6.308522	0.440661
H	-3.765003	-4.704372	1.089412
H	-3.947319	-4.868946	-0.636761
C	-3.332160	-2.989075	3.079937
C	-3.194002	-3.863242	4.324252
H	-4.271427	-3.206101	2.565410
H	-3.406507	-1.934774	3.387390
C	-1.813258	-3.679182	4.947667
H	-3.985850	-3.614189	5.038213
H	-3.328567	-4.919009	4.050701
C	-0.745498	-4.169391	3.973857
H	-1.651523	-2.613685	5.160047
H	-1.732841	-4.217525	5.897716
H	-0.788140	-5.266463	3.919448
H	0.255427	-3.917701	4.342141

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M06-2X/6-31G* Energy = -8271.58549863

M06-2X/6-31G* Free Energy = -8270.699447

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.56450138

Lowest Frequency = 7.2520

M06-2X/6-31G* Geometry

C	-2.008741	1.144782	3.733896
C	-2.465834	2.879458	0.250279
C	-3.125890	0.827640	3.083511
H	-1.053433	0.707853	3.447341
H	-2.010771	1.835163	4.572087
C	-3.144334	-0.121278	1.919559
H	-4.077116	1.273665	3.376732
N	-2.310786	1.603236	0.414616
C	-3.792969	3.437903	-0.107186
C	-1.323633	3.785048	0.412370
C	-3.377207	0.597986	0.574667
C	-3.391791	-0.385047	-0.581414
H	-4.331231	1.129936	0.606726
H	-1.338038	1.195240	0.596519
H	-2.195925	-0.666586	1.869547
H	-3.947262	-0.860068	2.024566
C	2.739139	-3.472944	-0.850492
C	1.797804	-4.488350	-0.637876
C	2.782021	-2.385260	0.044627
C	1.796676	-2.256490	1.026874

C	0.797593	-3.224799	1.204043
C	0.871919	-4.356471	0.395529
C	3.794182	-1.295756	-0.089235
C	5.177951	-1.523860	0.045248
C	6.066583	-0.460256	-0.165128
C	5.565207	0.804481	-0.476083
C	4.200349	1.074435	-0.538142
C	3.330506	0.001019	-0.318897
O	1.824153	-1.138339	1.826707
O	1.969803	0.220477	-0.297129
P	1.294514	0.292578	1.208835
O	-0.191694	0.174837	0.947561
O	1.845051	1.384247	2.041029
C	-0.352228	-3.043292	2.122935
C	3.707858	2.436817	-0.853206
C	-1.634405	-3.500670	1.695215
C	-2.735323	-3.380394	2.500373
C	-2.638786	-2.768088	3.777580
C	-1.368134	-2.297090	4.209475
C	-0.240274	-2.453333	3.364089
C	2.669084	2.621513	-1.812388
C	2.293833	3.875940	-2.208638
C	2.914411	5.030491	-1.663137
C	3.914739	4.859105	-0.666930
C	4.297033	3.545834	-0.289851
H	0.129773	-5.140895	0.528213
H	6.264895	1.614909	-0.671247
H	-1.733039	-3.911379	0.693121
H	-3.708023	-3.722305	2.153800
H	5.065265	3.420725	0.469636
H	1.510875	4.006079	-2.951643
H	2.189513	1.745823	-2.235736
H	0.723363	-2.091563	3.707655
C	-0.231869	3.403491	1.204574
C	0.872011	4.237655	1.322983
C	0.873398	5.475912	0.685832
C	-0.218919	5.872463	-0.089949
C	-1.313237	5.033617	-0.234547
H	-0.231599	2.465347	1.746826
H	1.719540	3.887655	1.902712
H	1.734085	6.134008	0.774708
H	-2.149997	5.328996	-0.859896
H	-0.198916	6.831479	-0.597969
C	-4.336768	4.476479	0.654172
C	-5.583298	4.996659	0.322138
C	-6.274086	4.503824	-0.783095
C	-5.722282	3.485120	-1.558096
C	-4.485629	2.947055	-1.219055
H	-4.045459	2.154891	-1.819056
H	-3.784084	4.861981	1.505776
H	-6.012370	5.791764	0.922931
H	-7.242312	4.918514	-1.045023
H	-6.252859	3.109111	-2.426939
C	-2.264093	-1.162579	-0.858720
C	-2.328033	-2.091645	-1.888346
C	-3.476889	-2.274656	-2.652247
C	-4.582710	-1.489345	-2.354634
Br	-0.799299	-3.156290	-2.219760
H	-3.509300	-3.005484	-3.451307
C	-4.556848	-0.550039	-1.329150
H	-5.441231	0.044353	-1.118379
H	-1.347705	-1.041198	-0.282309
Br	-6.165819	-1.701058	-3.370150

C	4.495886	6.012368	-0.074116
C	4.108049	7.271847	-0.457427
C	3.123733	7.440748	-1.463345
C	2.545430	6.344289	-2.051854
H	5.254776	5.877482	0.692448
H	4.558962	8.145029	0.004097
H	1.783962	6.464549	-2.819002
H	2.832101	8.441921	-1.766083
C	-1.265305	-1.666046	5.478886
C	-2.372736	-1.492650	6.267863
C	-3.641060	-1.944092	5.827486
C	-3.768792	-2.568952	4.613056
H	-0.290449	-1.312170	5.804603
H	-2.283332	-1.002722	7.232582
H	-4.512044	-1.796199	6.458705
H	-4.738873	-2.923176	4.271724
C	1.694465	-5.693575	-1.553135
C	2.275778	-5.420462	-2.938069
H	0.642181	-5.992743	-1.630498
H	2.226511	-6.543032	-1.102475
C	3.674705	-4.828023	-2.793363
H	1.632376	-4.705356	-3.470727
H	2.293942	-6.341651	-3.529361
C	3.606470	-3.470349	-2.097614
H	4.296116	-5.515994	-2.203423
H	4.158537	-4.716134	-3.769086
H	3.169744	-2.734061	-2.788663
H	4.612885	-3.103285	-1.881240
C	5.690157	-2.871617	0.522382
C	7.169743	-3.092503	0.216764
H	5.088369	-3.687757	0.115021
H	5.539419	-2.913262	1.610891
C	7.986165	-1.890866	0.684999
H	7.512935	-4.012744	0.700669
H	7.308710	-3.226178	-0.865300
C	7.570912	-0.648585	-0.099302
H	7.806096	-1.730291	1.755899
H	9.059234	-2.069931	0.560886
H	7.959430	-0.730971	-1.124426
H	8.030069	0.249034	0.329617

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M06-2X/6-31G* Energy = -8271.57864402

M06-2X/6-31G* Free Energy = -8270.694557

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.56238521

Lowest Frequency = 8.1659

M06-2X/6-31G* Geometry

C	-0.521979	-0.352526	3.018612
C	1.018260	3.054879	1.596264
C	0.795011	-0.273406	3.195321
H	-0.947155	-0.550503	2.035295
H	-1.215508	-0.229727	3.846497
C	1.779830	-0.404068	2.067038
H	1.204309	-0.068547	4.185445
N	1.244682	1.826363	1.256844
C	-0.256803	3.673479	1.212145
C	2.014314	3.847162	2.354686
C	2.363393	0.970425	1.675949
C	3.401540	0.855892	0.575484
H	2.824445	1.433715	2.554074
H	0.546673	1.321210	0.625114
H	1.295733	-0.837624	1.186676
H	2.622677	-1.050166	2.339458

C	-4.739090	-2.880212	-0.066807
C	-5.937917	-2.335292	-0.543828
C	-3.633052	-2.028744	0.132810
C	-3.698906	-0.693535	-0.270098
C	-4.895766	-0.128918	-0.733829
C	-5.999945	-0.972170	-0.831356
C	-2.369824	-2.530708	0.749635
C	-2.342870	-3.032566	2.067730
C	-1.152022	-3.578536	2.558739
C	-0.036776	-3.642453	1.723651
C	-0.014557	-3.104332	0.437150
C	-1.192145	-2.473733	-0.000647
O	-2.565643	0.081817	-0.128371
O	-1.228402	-1.816643	-1.208531
P	-1.290725	-0.166571	-1.166282
O	-0.100033	0.315974	-0.364446
O	-1.569254	0.322228	-2.531005
C	-5.037363	1.310947	-1.063530
C	1.195135	-3.289713	-0.408106
C	-6.121194	2.038088	-0.492057
C	-6.295791	3.372213	-0.752535
C	-5.390233	4.068504	-1.595558
C	-4.307363	3.346687	-2.170641
C	-4.160112	1.961680	-1.901996
C	1.722304	-2.263563	-1.243816
C	2.850614	-2.481988	-1.989351
C	3.529686	-3.726302	-1.956109
C	3.011150	-4.760056	-1.130428
C	1.840252	-4.509479	-0.373050
H	-6.936141	-0.554716	-1.197685
H	0.878141	-4.087553	2.109706
H	-6.803494	1.519014	0.175851
H	-7.123086	3.917446	-0.304909
H	1.433350	-5.317659	0.230281
H	3.238214	-1.694901	-2.629433
H	1.227659	-1.300091	-1.274990
H	-3.331750	1.422665	-2.356546
C	3.346548	3.919420	1.931720
C	4.258917	4.687256	2.646908
C	3.850153	5.372378	3.789260
C	2.522820	5.306982	4.209051
C	1.600345	4.559958	3.485686
H	3.658609	3.394079	1.033737
H	5.288224	4.750521	2.309697
H	4.566195	5.965220	4.349520
H	0.560614	4.515516	3.795529
H	2.203837	5.845015	5.095543
C	-0.304460	5.053394	0.961414
C	-1.488174	5.634418	0.528504
C	-2.631974	4.853147	0.373140
C	-2.597084	3.486709	0.653123
C	-1.411860	2.889907	1.059347
H	-1.391227	1.823490	1.265170
H	0.592228	5.654879	1.073438
H	-1.518833	6.695446	0.303589
H	-3.554741	5.307365	0.023255
H	-3.489282	2.879395	0.539501
C	3.042298	0.920473	-0.771315
C	4.039041	0.811931	-1.734511
C	5.374152	0.619313	-1.400125
C	5.702075	0.546996	-0.051620
Br	3.561198	0.911941	-3.556961
H	6.134708	0.533230	-2.166589

C	4.735738	0.669360	0.938475
H	5.024435	0.625884	1.984539
H	2.003771	1.035509	-1.072402
Br	7.509583	0.302715	0.444121
C	3.679886	-6.013092	-1.096262
C	4.811079	-6.223131	-1.841641
C	5.329711	-5.189961	-2.661567
C	4.702220	-3.972125	-2.716895
H	3.276975	-6.802915	-0.467174
H	5.314935	-7.184257	-1.808217
H	5.090654	-3.174295	-3.345250
H	6.225690	-5.369855	-3.247682
C	-3.362154	4.041825	-2.972322
C	-3.490446	5.389339	-3.192698
C	-4.579462	6.105459	-2.634190
C	-5.508857	5.459974	-1.857722
H	-2.530441	3.478595	-3.387711
H	-2.759534	5.914645	-3.799681
H	-4.675996	7.169936	-2.826434
H	-6.345225	6.004668	-1.426028
C	-7.183516	-3.178393	-0.742694
C	-6.883285	-4.670687	-0.855829
H	-7.857860	-3.016577	0.110488
H	-7.721628	-2.824614	-1.628939
C	-5.947371	-5.091517	0.273612
H	-6.400735	-4.879523	-1.819301
H	-7.816132	-5.243349	-0.830207
C	-4.603322	-4.379761	0.137158
H	-6.406212	-4.834473	1.238880
H	-5.791269	-6.175200	0.271489
H	-3.966305	-4.604580	0.996014
H	-4.069784	-4.783223	-0.735558
C	-3.549100	-2.865774	2.975776
C	-3.481107	-3.736522	4.227957
H	-4.478325	-3.053771	2.432142
H	-3.596299	-1.807443	3.274535
C	-2.120913	-3.582336	4.902234
H	-4.292713	-3.464489	4.910650
H	-3.631238	-4.789920	3.953339
C	-1.026710	-4.104721	3.975388
H	-1.944453	-2.519605	5.116364
H	-2.089658	-4.114511	5.858591
H	-1.071186	-5.202827	3.954534
H	-0.036229	-3.843703	4.365324

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M06-2X/6-31G* Energy = -8271.57618922

M06-2X/6-31G* Free Energy = -8270.694389

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.56003756

Lowest Frequency = 9.9300

M06-2X/6-31G* Geometry

C	-0.440823	3.373968	1.347419
C	1.743577	0.400323	2.734605
C	0.859361	3.508118	1.101235
H	-1.056560	2.681117	0.776839
H	-0.938258	3.979375	2.099731
C	1.615981	2.699740	0.084670
H	1.448567	4.225630	1.674319
N	1.708406	0.728538	1.486079
C	2.860689	0.784683	3.626372
C	0.624010	-0.398550	3.269235
C	2.559553	1.695744	0.784558
C	3.499391	1.003750	-0.183586

H	3.151478	2.234741	1.530753
H	0.936570	0.253481	0.854730
H	0.939581	2.158971	-0.591203
H	2.241794	3.347625	-0.541386
C	-5.360793	-0.096756	-1.454747
C	-5.769595	1.135188	-1.980776
C	-4.109941	-0.189160	-0.810393
C	-3.230793	0.899107	-0.854846
C	-3.625762	2.138199	-1.374455
C	-4.911446	2.233374	-1.897539
C	-3.683773	-1.412150	-0.067476
C	-4.401097	-1.905858	1.043449
C	-3.927783	-3.050226	1.703923
C	-2.720766	-3.627032	1.305273
C	-1.956399	-3.114654	0.260709
C	-2.478577	-2.016090	-0.428740
O	-1.971302	0.766938	-0.304293
O	-1.768595	-1.463254	-1.473236
P	-0.838960	-0.171951	-1.088293
O	0.095772	-0.584218	0.030141
O	-0.327397	0.462287	-2.319760
C	-2.732920	3.326777	-1.339707
C	-0.621191	-3.674863	-0.056632
C	-1.478076	3.313670	-2.012837
C	-0.666434	4.416509	-1.979155
C	-1.040884	5.587547	-1.268691
C	-2.295617	5.607837	-0.599926
C	-3.126157	4.458125	-0.661960
C	0.309967	-3.866953	1.001557
C	1.546094	-4.403542	0.759093
C	1.928154	-4.786777	-0.553588
C	1.006953	-4.583438	-1.618409
C	-0.261495	-4.015893	-1.339700
H	-5.233750	3.190729	-2.302245
H	-2.345644	-4.493970	1.846563
H	-1.169240	2.417226	-2.542272
H	0.288984	4.403000	-2.499159
H	-0.956248	-3.853753	-2.158992
H	2.256509	-4.539890	1.570912
H	0.028874	-3.551992	2.004180
H	-4.081559	4.471704	-0.141087
C	-0.669940	-0.204620	2.766141
C	-1.713498	-0.994154	3.226263
C	-1.476415	-1.975858	4.186410
C	-0.194581	-2.158959	4.705819
C	0.855247	-1.366941	4.255346
H	-0.860645	0.559677	2.020341
H	-2.708389	-0.852852	2.816632
H	-2.297048	-2.597750	4.534172
H	1.858327	-1.512683	4.645133
H	-0.011990	-2.921355	5.456108
C	4.188464	0.623340	3.211446
C	5.228257	0.962815	4.069420
C	4.948673	1.473919	5.335494
C	3.628446	1.631068	5.753158
C	2.584259	1.273234	4.908120
H	1.552377	1.380519	5.228672
H	4.400488	0.214385	2.226878
H	6.255889	0.826289	3.749174
H	5.762336	1.744189	6.001121
H	3.412172	2.026232	6.740194
C	4.772043	1.545067	-0.372373
C	5.635303	0.948404	-1.282314

C	5.268943	-0.181981	-2.001848
C	3.997798	-0.706599	-1.791225
Br	7.362636	1.681535	-1.531869
H	5.954993	-0.644374	-2.701126
C	3.103516	-0.127504	-0.897291
H	2.115747	-0.562932	-0.767411
H	5.092211	2.421012	0.184229
Br	3.468862	-2.265515	-2.709509
C	1.383153	-4.963886	-2.934884
C	2.611525	-5.524236	-3.179284
C	3.527250	-5.729370	-2.116659
C	3.193166	-5.365089	-0.837906
H	0.678474	-4.797670	-3.745442
H	2.888250	-5.811796	-4.189072
H	3.893879	-5.514172	-0.020128
H	4.497959	-6.169425	-2.323180
C	-2.670957	6.770911	0.122936
C	-1.839025	7.859714	0.181517
C	-0.588881	7.838860	-0.483953
C	-0.202309	6.729483	-1.192005
H	-3.632080	6.781363	0.631158
H	-2.136168	8.743763	0.737439
H	0.060927	8.707142	-0.431763
H	0.755284	6.707137	-1.706531
C	-7.133097	1.323612	-2.619715
C	-7.773965	0.013342	-3.071193
H	-7.046106	2.019493	-3.461282
H	-7.796395	1.808680	-1.889284
C	-7.672516	-1.024247	-1.956196
H	-7.254333	-0.365783	-3.960581
H	-8.816877	0.186436	-3.356010
C	-6.206341	-1.340408	-1.670917
H	-8.151720	-0.631012	-1.048247
H	-8.202640	-1.943276	-2.226669
H	-6.117092	-2.031318	-0.829154
H	-5.783838	-1.875705	-2.533508
C	-5.574702	-1.122926	1.613391
C	-6.441818	-1.935202	2.572677
H	-6.190902	-0.694816	0.820342
H	-5.160506	-0.256783	2.152711
C	-5.571487	-2.664471	3.592093
H	-7.158508	-1.272831	3.068880
H	-7.025738	-2.673920	2.006594
C	-4.681676	-3.669226	2.865790
H	-4.949391	-1.931899	4.126660
H	-6.184663	-3.174892	4.341901
H	-5.311351	-4.486771	2.487135
H	-3.968224	-4.134386	3.556336

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M06-2X/6-31G* Energy = -8271.57618927

M06-2X/6-31G* Free Energy = -8270.694353

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.56003994

Lowest Frequency = 9.9526

M06-2X/6-31G* Geometry

C	-0.441171	3.374250	1.346792
C	1.744015	0.401196	2.734666
C	0.859062	3.508158	1.100758
H	-1.057030	2.681605	0.776092
H	-0.938570	3.979747	2.099062
C	1.615656	2.699805	0.084183
H	1.448347	4.225526	1.673956
N	1.708842	0.728924	1.486003

C	2.861120	0.785940	3.626277
C	0.624465	-0.397505	3.269485
C	2.559606	1.696173	0.784104
C	3.499365	1.004147	-0.184076
H	3.151562	2.235503	1.530048
H	0.936902	0.253579	0.854968
H	0.939274	2.158797	-0.591512
H	2.241283	3.347732	-0.542033
C	-4.400309	-1.906561	1.044064
C	-3.926387	-3.050305	1.705167
C	-3.683275	-1.413101	-0.067151
C	-2.477824	-2.016647	-0.428190
C	-1.955121	-3.114641	0.261777
C	-2.719138	-3.626785	1.306714
C	-4.109998	-0.190582	-0.810518
C	-5.360814	-0.098928	-1.454999
C	-5.770070	1.132659	-1.981515
C	-4.912432	2.231261	-1.898528
C	-3.626793	2.136842	-1.375201
C	-3.231335	0.898072	-0.855210
O	-1.768081	-1.463897	-1.472904
O	-1.971865	0.766539	-0.304477
P	-0.839103	-0.171965	-1.088275
O	0.095783	-0.583504	0.030274
O	-0.327815	0.462201	-2.319888
C	-0.619758	-3.674491	-0.055486
C	-2.734493	3.325829	-1.340427
C	0.311852	-3.865284	1.002536
C	1.548190	-4.401377	0.760050
C	1.930010	-4.785414	-0.552475
C	1.008316	-4.583425	-1.617128
C	-0.260321	-4.016307	-1.338413
C	-1.479538	3.313270	-2.013352
C	-0.668343	4.416432	-1.979469
C	-1.043404	5.587298	-1.269041
C	-2.298268	5.607055	-0.600504
C	-3.128312	4.456990	-0.662703
H	-2.343552	-4.493242	1.848450
H	-5.235148	3.188352	-2.303530
H	0.030910	-3.549725	2.005018
H	2.258950	-4.536751	1.571733
H	-4.083812	4.470149	-0.142000
H	0.287194	4.403320	-2.499265
H	-1.170226	2.416939	-2.542693
H	-0.955430	-3.855112	-2.157595
C	-0.669486	-0.203623	2.766361
C	-1.713095	-0.992980	3.226693
C	-1.476070	-1.974416	4.187130
C	-0.194244	-2.157405	4.706620
C	0.855634	-1.365575	4.255927
H	-0.860161	0.560456	2.020324
H	-2.707968	-0.851741	2.816974
H	-2.296739	-2.596160	4.535090
H	1.858698	-1.511250	4.645788
H	-0.011688	-2.919578	5.457146
C	2.584775	1.274828	4.907909
C	3.629025	1.633033	5.752719
C	4.949216	1.475944	5.334926
C	5.228717	0.964488	4.068969
C	4.188863	0.624613	3.211235
H	4.400797	0.215356	2.226772
H	1.552913	1.382054	5.228556
H	3.412841	2.028457	6.739672

H	5.762926	1.746549	6.000362
H	6.256327	0.828002	3.748638
C	3.103338	-0.127016	-0.897846
C	3.997484	-0.706091	-1.791939
C	5.268654	-0.181571	-2.002610
C	5.635194	0.948709	-1.282978
Br	3.468309	-2.264858	-2.710330
H	5.954598	-0.643946	-2.702009
C	4.772074	1.545353	-0.372902
H	5.092343	2.421237	0.183741
H	2.115521	-0.562341	-0.767913
Br	7.362531	1.681759	-1.532721
C	-2.674215	6.769948	0.122338
C	-1.842728	7.859079	0.181127
C	-0.592447	7.838750	-0.484104
C	-0.205294	6.729562	-1.192135
H	-3.635436	6.779987	0.630382
H	-2.140322	8.742989	0.737032
H	0.752413	6.707620	-1.706465
H	0.057005	8.707288	-0.431745
C	1.384232	-4.964745	-2.933431
C	2.612811	-5.524647	-3.177824
C	3.529049	-5.728389	-2.115378
C	3.195246	-5.363240	-0.836797
H	0.679149	-4.799607	-3.743858
H	2.889316	-5.812896	-4.187476
H	4.499933	-6.168056	-2.321906
H	3.896344	-5.511286	-0.019162
C	-4.679815	-3.668898	2.867543
C	-5.569720	-2.663942	3.593456
H	-3.966056	-4.133465	3.558170
H	-5.309377	-4.486826	2.489523
C	-6.440686	-1.935768	2.573798
H	-4.947690	-1.930755	4.127261
H	-6.182452	-3.174024	4.343860
C	-5.574291	-1.123862	1.613530
H	-7.024523	-2.675150	2.008496
H	-7.157469	-1.273305	3.069747
H	-5.160553	-0.256876	2.151842
H	-6.190995	-0.696981	0.820191
C	-6.205795	-1.343022	-1.670761
C	-7.672099	-1.027570	-1.956167
H	-6.116204	-2.033594	-0.828750
H	-5.783061	-1.878433	-2.533168
C	-7.773913	0.009530	-3.071593
H	-8.201880	-1.946904	-2.226277
H	-8.151461	-0.634146	-1.048381
C	-7.133594	1.320259	-2.620654
H	-7.254084	-0.369761	-3.960797
H	-8.816879	0.182082	-3.356549
H	-7.797138	1.805415	-1.890504
H	-7.046812	2.015779	-3.462546

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M06-2X/6-31G* Energy = -8271.58498592

M06-2X/6-31G* Free Energy = -8270.699252

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.56360677

Lowest Frequency = 6.5300

M06-2X/6-31G* Geometry

C	2.201387	0.275420	-3.907842
C	2.994311	2.212440	-0.574061
C	3.199282	-0.227220	-3.184522
H	1.165147	0.111202	-3.616994

H	2.382505	0.851678	-4.810237
C	2.970788	-1.023766	-1.931872
H	4.234321	-0.054771	-3.482305
N	2.546970	0.997854	-0.641130
C	4.405572	2.474846	-0.198717
C	2.102918	3.340591	-0.863864
C	3.347006	-0.240592	-0.656830
C	3.103902	-1.069137	0.591099
H	4.400816	0.045742	-0.700865
H	1.510006	0.812812	-0.833733
H	1.918467	-1.319708	-1.866779
H	3.573693	-1.939457	-1.929658
C	-3.547251	-2.554815	1.012859
C	-2.903342	-3.793375	0.894404
C	-3.331677	-1.576578	0.020820
C	-2.367890	-1.793700	-0.967130
C	-1.643046	-2.992043	-1.043748
C	-1.988639	-3.992078	-0.138354
C	-4.035675	-0.259626	0.048598
C	-5.436883	-0.150593	-0.049754
C	-6.028981	1.113740	0.070250
C	-5.221421	2.237015	0.249549
C	-3.829344	2.170442	0.266637
C	-3.258646	0.897564	0.145268
O	-2.137028	-0.790107	-1.877767
O	-1.888097	0.762239	0.096245
P	-1.257749	0.520059	-1.411287
O	0.161080	0.066720	-1.140441
O	-1.546148	1.626121	-2.349422
C	-0.487976	-3.181775	-1.954546
C	-3.023041	3.402900	0.445440
C	0.647417	-3.889421	-1.458298
C	1.745160	-4.111544	-2.246000
C	1.798423	-3.615649	-3.575150
C	0.677642	-2.897395	-4.076169
C	-0.455243	-2.700701	-3.246113
C	-3.463482	4.619861	-0.150745
C	-2.836577	5.808458	0.111609
C	-1.718551	5.863247	0.984760
C	-1.233117	4.646707	1.539260
C	-1.905651	3.431959	1.252415
H	-1.469323	-4.946545	-0.193439
H	-5.700084	3.206054	0.375944
H	0.644193	-4.215435	-0.420866
H	2.607366	-4.642016	-1.848102
H	-1.542427	2.515005	1.705668
H	-3.192170	6.729565	-0.344221
H	-4.310321	4.590863	-0.829939
H	-1.303652	-2.152681	-3.642677
C	2.378871	4.613103	-0.335502
C	1.522808	5.670552	-0.605146
C	0.380841	5.465586	-1.381184
C	0.093687	4.204218	-1.898957
C	0.965101	3.150419	-1.661815
H	3.245900	4.763379	0.300088
H	1.724840	6.649624	-0.184559
H	-0.294094	6.294666	-1.570469
H	0.752498	2.190663	-2.117438
H	-0.803526	4.008505	-2.476120
C	4.926660	1.941087	0.984626
C	6.245717	2.200292	1.340532
C	7.048935	2.982282	0.512270
C	6.529843	3.518798	-0.664338

C	5.205401	3.279304	-1.015505
H	4.787383	3.703046	-1.923782
H	4.291630	1.335610	1.625849
H	6.644094	1.792193	2.263882
H	8.080257	3.178816	0.787584
H	7.155062	4.130104	-1.306747
C	1.814339	-1.510256	0.898973
C	1.628086	-2.305206	2.021608
C	2.683343	-2.679762	2.847831
C	3.954708	-2.229938	2.516901
Br	-0.123917	-2.911755	2.395999
H	2.520450	-3.301965	3.719560
C	4.179971	-1.432086	1.399938
H	5.187360	-1.098752	1.167364
H	0.966122	-1.233136	0.274018
Br	5.417957	-2.711806	3.616708
C	-0.101286	4.689766	2.397124
C	0.507456	5.880822	2.699896
C	0.016272	7.092801	2.153953
C	-1.066456	7.080994	1.311120
H	0.267932	3.756567	2.814971
H	1.366977	5.901092	3.363328
H	-1.447986	8.007147	0.887221
H	0.500739	8.031350	2.407067
C	0.729583	-2.380421	-5.399136
C	1.846368	-2.550701	-6.175590
C	2.968856	-3.250183	-5.668552
C	2.942917	-3.771558	-4.400113
H	-0.131664	-1.835343	-5.777018
H	1.877100	-2.145298	-7.182294
H	3.849626	-3.374663	-6.291156
H	3.799376	-4.314484	-4.006784
C	-3.099634	-4.902774	1.910142
C	-3.572152	-4.376870	3.263312
H	-2.158930	-5.455328	2.020793
H	-3.838500	-5.620879	1.527809
C	-4.767507	-3.450036	3.060603
H	-2.757331	-3.816550	3.744095
H	-3.824239	-5.211185	3.925849
C	-4.352895	-2.220004	2.256454
H	-5.557459	-3.994312	2.524503
H	-5.189595	-3.135717	4.020653
H	-5.227256	-1.611585	2.012993
H	-3.716158	-1.578834	2.884390
C	-6.281580	-1.365768	-0.390877
C	-7.757284	-1.186176	-0.042527
H	-5.883359	-2.267157	0.081048
H	-6.187526	-1.537094	-1.473042
C	-8.272403	0.133885	-0.609739
H	-8.333747	-2.031847	-0.431530
H	-7.882766	-1.185695	1.049430
C	-7.534965	1.299119	0.045468
H	-8.100987	0.149510	-1.693888
H	-9.350887	0.237702	-0.451505
H	-7.891834	1.407007	1.079695
H	-7.776284	2.240692	-0.460216

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M06-2X/6-31G* Energy = -8271.58529719

M06-2X/6-31G* Free Energy = -8270.698250

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.56488807

Lowest Frequency = 13.6451

M06-2X/6-31G* Geometry

C	-0.730745	0.159299	2.988375
C	0.750583	3.328435	1.136937
C	0.544778	0.445592	3.241077
H	-1.021527	-0.333877	2.061311
H	-1.520801	0.409624	3.691561
C	1.652337	0.129636	2.276856
H	0.821444	0.952778	4.166605
N	1.110494	2.096595	0.965674
C	-0.572847	3.764204	0.670234
C	1.652873	4.294703	1.805932
C	2.230687	1.398458	1.611238
C	3.327988	1.050316	0.622818
H	2.635887	2.059481	2.382750
H	0.503472	1.435486	0.381082
H	1.286335	-0.531589	1.486045
H	2.487499	-0.369783	2.783404
C	-4.256269	-3.352840	0.212437
C	-5.503415	-2.979855	-0.305241
C	-3.226633	-2.391286	0.288568
C	-3.416676	-1.130117	-0.283552
C	-4.659696	-0.741753	-0.801298
C	-5.689059	-1.676895	-0.770072
C	-1.924225	-2.691879	0.957188
C	-1.850470	-3.016353	2.327672
C	-0.604134	-3.341959	2.876561
C	0.530863	-3.327715	2.065301
C	0.508799	-2.924405	0.730003
C	-0.750206	-2.580076	0.208456
O	-2.380772	-0.223516	-0.257621
O	-0.862872	-2.094678	-1.072870
P	-1.040379	-0.462309	-1.221053
O	0.055651	0.202450	-0.421377
O	-1.297521	-0.160679	-2.641488
C	-4.896239	0.623536	-1.336501
C	1.767411	-2.858198	-0.058525
C	-4.087628	1.140607	-2.388705
C	-4.316735	2.397635	-2.881792
C	-5.345361	3.221112	-2.353335
C	-6.152430	2.713573	-1.296757
C	-5.910997	1.398272	-0.818564
C	3.001604	-2.591971	0.608039
C	4.194645	-2.588711	-0.062667
C	4.242147	-2.850017	-1.456383
C	3.021620	-3.103370	-2.138386
C	1.801273	-3.102183	-1.416235
H	-6.659061	-1.390737	-1.172132
H	1.477982	-3.630597	2.505840
H	-3.278753	0.535221	-2.787178
H	-3.694426	2.786179	-3.683829
H	0.883056	-3.306164	-1.955679
H	5.120945	-2.357359	0.460037
H	2.992762	-2.373563	1.671177
H	-6.523714	1.014564	-0.005206
C	2.988417	4.402265	1.399330
C	3.827155	5.324094	2.014957
C	3.342399	6.128237	3.044962
C	2.014010	6.022163	3.452414
C	1.163788	5.117572	2.826172
H	3.358218	3.773696	0.593071
H	4.858290	5.414080	1.689805
H	4.000951	6.842959	3.528282
H	0.123996	5.036132	3.128293
H	1.637698	6.648997	4.254066

C	-0.801162	5.114512	0.361583
C	-2.059178	5.525037	-0.058496
C	-3.097524	4.599940	-0.165229
C	-2.873446	3.255959	0.132819
C	-1.618846	2.834517	0.550648
H	-1.466101	1.788358	0.798237
H	0.009808	5.832032	0.435504
H	-2.230425	6.567948	-0.304363
H	-4.085004	4.922293	-0.484748
H	-3.675898	2.530521	0.045492
C	3.053152	0.828076	-0.727837
C	4.095977	0.477488	-1.576823
C	5.397807	0.317289	-1.116552
C	5.632740	0.496901	0.238853
Br	3.731433	0.140173	-3.390835
H	6.191116	0.018053	-1.790878
C	4.623511	0.880371	1.112849
H	4.844652	1.026374	2.166199
H	2.039106	0.878161	-1.112230
Br	7.362012	0.135904	0.916940
C	3.057939	-3.361570	-3.535694
C	4.246690	-3.355836	-4.217922
C	5.461604	-3.091536	-3.537239
C	5.458431	-2.847264	-2.187867
H	2.121383	-3.552490	-4.052712
H	4.262763	-3.548266	-5.286255
H	6.385659	-2.647691	-1.653833
H	6.395776	-3.086326	-4.090674
C	-7.156374	3.548818	-0.737302
C	-7.349921	4.824023	-1.203956
C	-6.552255	5.326114	-2.262534
C	-5.577028	4.541023	-2.823859
H	-7.767790	3.158021	0.072249
H	-8.118898	5.453462	-0.766765
H	-6.719436	6.334643	-2.628329
H	-4.959332	4.918971	-3.634758
C	-6.672721	-3.945264	-0.363497
C	-6.246450	-5.409104	-0.289064
H	-7.347564	-3.730311	0.477466
H	-7.251478	-3.757984	-1.274633
C	-5.259035	-5.598450	0.858987
H	-5.763274	-5.702698	-1.229919
H	-7.125907	-6.049143	-0.163737
C	-3.985717	-4.798945	0.593249
H	-5.722038	-5.257434	1.795852
H	-5.008666	-6.656049	0.991423
H	-3.310517	-4.861810	1.449902
H	-3.440550	-5.261566	-0.242221
C	-3.075363	-2.880757	3.215922
C	-2.920457	-3.570838	4.569105
H	-3.973670	-3.238823	2.707400
H	-3.243304	-1.805038	3.378275
C	-1.586310	-3.191158	5.204879
H	-3.758947	-3.298650	5.218480
H	-2.959064	-4.660736	4.434427
C	-0.443363	-3.711934	4.338481
H	-1.519177	-2.097275	5.278614
H	-1.503139	-3.592630	6.220134
H	-0.396576	-4.806415	4.429333
H	0.518122	-3.331133	4.700886

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M06-2X/6-31G* Energy = -8271.57578576

M06-2X/6-31G* Free Energy = -8270.693635

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.55990390

Lowest Frequency = 8.4364

M06-2X/6-31G* Geometry

C	-0.293061	3.301026	1.893549
C	1.594791	0.010054	2.765448
C	0.997309	3.421470	1.593622
H	-0.960525	2.692156	1.286272
H	-0.732851	3.841191	2.726813
C	1.677995	2.685618	0.473006
H	1.638248	4.059809	2.203189
N	1.586776	0.531979	1.584469
C	2.720769	0.192655	3.710033
C	0.440218	-0.814948	3.166126
C	2.519593	1.519916	1.037354
C	3.443706	0.886539	0.012911
H	3.129396	1.904138	1.861562
H	0.803539	0.205530	0.875381
H	0.957619	2.299375	-0.261034
H	2.356232	3.353135	-0.070576
C	-5.490229	0.603269	-1.247243
C	-5.854884	1.933145	-1.493545
C	-4.219706	0.329540	-0.700359
C	-3.284779	1.363231	-0.569373
C	-3.631474	2.697439	-0.822139
C	-4.933773	2.950749	-1.243564
C	-3.827666	-1.043190	-0.264288
C	-4.525675	-1.743102	0.744571
C	-4.103768	-3.033916	1.094233
C	-2.985253	-3.589337	0.467981
C	-2.245999	-2.897390	-0.485705
C	-2.688835	-1.616126	-0.829822
O	-2.019538	1.058144	-0.108387
O	-1.965293	-0.873843	-1.738748
P	-0.953024	0.245612	-1.098829
O	-0.035030	-0.446913	-0.111705
O	-0.421317	1.103202	-2.178109
C	-2.677158	3.820916	-0.636123
C	-1.049193	-3.498348	-1.121551
C	-3.021014	4.890095	0.237730
C	-2.164618	5.942276	0.435023
C	-0.911984	5.991722	-0.230332
C	-0.573014	4.934303	-1.118658
C	-1.476595	3.858418	-1.307305
C	-0.940647	-3.527674	-2.540886
C	0.113842	-4.151884	-3.148495
C	1.136499	-4.766988	-2.380206
C	1.060174	-4.702134	-0.961337
C	-0.057699	-4.069166	-0.358644
H	-5.220447	3.982534	-1.438851
H	-2.670190	-4.595123	0.739437
H	-3.972333	4.851348	0.762228
H	-2.430933	6.749458	1.113155
H	-0.115309	-4.014557	0.726881
H	0.184999	-4.180050	-4.232585
H	-1.713168	-3.049674	-3.134034
H	-1.199386	3.050429	-1.979468
C	-0.840803	-0.503476	2.691679
C	-1.912363	-1.320643	3.021098
C	-1.714492	-2.451152	3.810928
C	-0.444083	-2.755816	4.299104
C	0.632138	-1.933901	3.988205
H	-1.001283	0.372818	2.072314
H	-2.899095	-1.080551	2.641353

H	-2.556848	-3.094056	4.052084
H	1.626195	-2.169943	4.355975
H	-0.291486	-3.633852	4.918127
C	2.450810	0.510421	5.045749
C	3.498627	0.675302	5.944099
C	4.814095	0.492368	5.521894
C	5.085058	0.149285	4.198775
C	4.043069	0.005048	3.289649
H	4.248402	-0.273102	2.259076
H	1.421597	0.637260	5.367847
H	3.288340	0.939075	6.975299
H	5.630169	0.610959	6.227663
H	6.107945	-0.007532	3.872876
C	3.132843	-0.314355	-0.623588
C	4.051107	-0.863100	-1.514748
C	5.253918	-0.233545	-1.810552
C	5.529370	0.973625	-1.178326
Br	3.655409	-2.534707	-2.295975
H	5.958748	-0.672038	-2.506493
C	4.649048	1.535333	-0.264784
H	4.904500	2.467482	0.230499
H	2.187292	-0.820941	-0.450410
Br	7.161954	1.856016	-1.549989
C	2.111399	-5.268902	-0.192957
C	3.179559	-5.876791	-0.801386
C	3.247050	-5.955118	-2.214100
C	2.247789	-5.412880	-2.983263
H	2.053926	-5.207789	0.891045
H	3.979759	-6.300882	-0.202724
H	2.296436	-5.460872	-4.068422
H	4.096380	-6.440190	-2.685315
C	0.681982	4.965271	-1.784419
C	1.562761	5.994012	-1.565727
C	1.226291	7.045479	-0.676257
C	0.017440	7.045282	-0.028251
H	0.926959	4.146393	-2.457129
H	2.521163	6.009966	-2.076263
H	1.930954	7.855633	-0.513899
H	-0.245170	7.851147	0.652852
C	-7.232851	2.308091	-2.006778
C	-7.962912	1.147469	-2.678384
H	-7.145366	3.156914	-2.693718
H	-7.836160	2.662139	-1.158554
C	-7.868100	-0.099442	-1.803129
H	-7.504443	0.935771	-3.652938
H	-9.006577	1.420613	-2.865270
C	-6.409979	-0.531276	-1.666926
H	-8.284867	0.120338	-0.809804
H	-8.458228	-0.919848	-2.224408
H	-6.323139	-1.384657	-0.990477
H	-6.054637	-0.894996	-2.641998
C	-5.622749	-1.052972	1.540726
C	-6.506455	-2.023128	2.320772
H	-6.235409	-0.414675	0.901121
H	-5.138015	-0.363728	2.250155
C	-5.645217	-3.005042	3.109868
H	-7.172058	-1.461943	2.984521
H	-7.144454	-2.583312	1.623384
C	-4.831626	-3.858191	2.140171
H	-4.971616	-2.439347	3.770187
H	-6.260009	-3.645219	3.750898
H	-5.511244	-4.556807	1.632000
H	-4.107505	-4.481069	2.678722

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M06-2X/6-31G* Energy = -8271.57578593

M06-2X/6-31G* Free Energy = -8270.693626

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.55991031

Lowest Frequency = 8.4310

M06-2X/6-31G* Geometry

C	-0.292783	3.302029	1.892146
C	1.595270	0.011122	2.765076
C	0.997561	3.422341	1.592064
H	-0.960320	2.692998	1.285106
H	-0.732486	3.842575	2.725206
C	1.678221	2.686057	0.471701
H	1.638537	4.060943	2.201318
N	1.587245	0.532834	1.584001
C	2.721150	0.194016	3.709760
C	0.440629	-0.813737	3.165852
C	2.519972	1.520676	1.036580
C	3.444289	0.887022	0.012497
H	3.129632	1.905355	1.860666
H	0.803914	0.206357	0.874997
H	0.957844	2.299456	-0.262150
H	2.356356	3.353407	-0.072200
C	-5.490776	0.601788	-1.246956
C	-5.855954	1.931486	-1.493446
C	-4.220098	0.328628	-0.700157
C	-3.285568	1.362694	-0.569433
C	-3.632761	2.696736	-0.822381
C	-4.935193	2.949480	-1.243740
C	-3.827556	-1.043873	-0.263835
C	-4.525375	-1.743857	0.745125
C	-4.103074	-3.034476	1.094987
C	-2.984403	-3.589659	0.468800
C	-2.245347	-2.897645	-0.484991
C	-2.688534	-1.616529	-0.829264
O	-2.020178	1.058100	-0.108565
O	-1.965276	-0.874315	-1.738409
P	-0.953519	0.245980	-1.099167
O	-0.034683	-0.445596	-0.112178
O	-0.422762	1.103526	-2.178948
C	-2.678803	3.820562	-0.636658
C	-1.048513	-3.498476	-1.120885
C	-3.022975	4.889815	0.236977
C	-2.166902	5.942309	0.434039
C	-0.914251	5.991948	-0.231255
C	-0.574966	4.934443	-1.119355
C	-1.478263	3.858309	-1.307866
C	-0.939915	-3.527674	-2.540227
C	0.114550	-4.151881	-3.147861
C	1.137165	-4.767115	-2.379626
C	1.060841	-4.702348	-0.960752
C	-0.057026	-4.069396	-0.358026
H	-5.222285	3.981126	-1.439138
H	-2.669119	-4.595353	0.740332
H	-3.974291	4.850909	0.761463
H	-2.433474	6.749562	1.111987
H	-0.114652	-4.014901	0.727502
H	0.185725	-4.179948	-4.231954
H	-1.712348	-3.049519	-3.133353
H	-1.200826	3.050275	-1.979860
C	-0.840325	-0.502302	2.691194
C	-1.911916	-1.319457	3.020502
C	-1.714153	-2.449888	3.810467

C	-0.443833	-2.754479	4.298908
C	0.632437	-1.932594	3.988089
H	-1.000733	0.373915	2.071716
H	-2.898592	-1.079435	2.640570
H	-2.556537	-3.092812	4.051476
H	1.626449	-2.168603	4.355981
H	-0.291358	-3.632455	4.918044
C	4.043527	0.006577	3.289568
C	5.085361	0.151077	4.198837
C	4.814150	0.494261	5.521869
C	3.498596	0.677012	5.943882
C	2.450934	0.511849	5.045405
H	1.421648	0.638484	5.367338
H	4.249047	-0.271678	2.259067
H	6.108320	-0.005650	3.873122
H	5.630101	0.613035	6.227749
H	3.288139	0.940874	6.975024
C	4.649754	1.535636	-0.265033
C	5.530258	0.973633	-1.178225
C	5.254855	-0.233644	-1.810245
C	4.051899	-0.863016	-1.514622
Br	7.163057	1.855749	-1.549590
H	5.959835	-0.672363	-2.505891
C	3.133463	-0.313968	-0.623835
H	2.187841	-0.820442	-0.450743
H	4.905176	2.467875	0.230092
Br	3.656275	-2.534798	-2.295484
C	2.112041	-5.269195	-0.192417
C	3.180186	-5.877074	-0.800898
C	3.247665	-5.955316	-2.213604
C	2.248407	-5.413013	-2.982732
H	2.054581	-5.208175	0.891589
H	3.980389	-6.301190	-0.202261
H	2.297028	-5.460999	-4.067893
H	4.096960	-6.440408	-2.684861
C	0.680125	4.965515	-1.784923
C	1.560698	5.994435	-1.566256
C	1.223902	7.046001	-0.677029
C	0.014943	7.045715	-0.029229
H	0.925349	4.146571	-2.457460
H	2.519178	6.010462	-2.076644
H	1.928411	7.856287	-0.514661
H	-0.247908	7.851657	0.651691
C	-7.234117	2.305841	-2.006576
C	-7.963778	1.144838	-2.677954
H	-7.147039	3.154608	-2.693635
H	-7.837494	2.659765	-1.158349
C	-7.868450	-0.101874	-1.802458
H	-7.505250	0.933132	-3.652474
H	-9.007550	1.417544	-2.864871
C	-6.410165	-0.533166	-1.666291
H	-8.285190	0.117972	-0.809141
H	-8.458332	-0.922578	-2.223497
H	-6.322986	-1.386361	-0.989642
H	-6.054772	-0.897000	-2.641299
C	-5.622707	-1.053967	1.541138
C	-6.506112	-2.024309	2.321289
H	-6.235577	-0.415981	0.901432
H	-5.138219	-0.364455	2.250472
C	-5.644555	-3.005797	3.110575
H	-7.171968	-1.463274	2.984905
H	-7.143849	-2.584832	1.623939
C	-4.830692	-3.858847	2.141028

H	-4.971127	-2.439761	3.770774
H	-6.259127	-3.646043	3.751745
H	-5.510078	-4.557756	1.632957
H	-4.106391	-4.481409	2.679701

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M06-2X/6-31G* Energy = -8271.58661191

M06-2X/6-31G* Free Energy = -8270.700221

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.56396131

Lowest Frequency = 11.9787

M06-2X/6-31G* Geometry

C	1.012744	-0.712503	3.949061
C	1.770697	2.650585	1.598655
C	2.264253	-0.452487	3.578002
H	0.302036	-1.139284	3.244469
H	0.665539	-0.499813	4.956203
C	2.787998	-0.722527	2.196395
H	2.961884	-0.003495	4.287351
N	1.880747	1.381947	1.372079
C	0.444437	3.288448	1.671464
C	2.986435	3.484296	1.788492
C	3.110883	0.578083	1.432187
C	3.641767	0.261475	0.045668
H	3.861561	1.152133	1.984460
H	1.005229	0.765351	1.176340
H	2.057226	-1.294746	1.615900
H	3.714936	-1.308297	2.230847
C	-3.839934	-3.169069	1.450474
C	-3.125635	-4.099810	2.217431
C	-3.165114	-2.478821	0.422904
C	-1.786814	-2.640972	0.274405
C	-1.034361	-3.507488	1.080415
C	-1.755873	-4.257087	2.010751
C	-3.869363	-1.509679	-0.471345
C	-4.958429	-1.899947	-1.279346
C	-5.691100	-0.920181	-1.961419
C	-5.302809	0.416804	-1.862832
C	-4.164947	0.814726	-1.167433
C	-3.440327	-0.178170	-0.496748
O	-1.168391	-1.881243	-0.696105
O	-2.317872	0.182227	0.219522
P	-0.834884	-0.332036	-0.292136
O	0.000450	-0.330488	0.971897
O	-0.352399	0.375157	-1.503230
C	0.447502	-3.609542	1.021509
C	-3.774508	2.248379	-1.132635
C	1.155122	-3.912145	2.223921
C	2.516363	-4.051948	2.240571
C	3.279782	-3.879657	1.057265
C	2.592994	-3.554621	-0.144994
C	1.178451	-3.433085	-0.136765
C	-2.485632	2.667298	-1.572343
C	-2.165695	3.998411	-1.602330
C	-3.089239	4.988516	-1.175735
C	-4.368486	4.574818	-0.712211
C	-4.686637	3.192032	-0.716746
H	-1.227089	-4.989024	2.616515
H	-5.875687	1.175553	-2.392351
H	0.601647	-3.998972	3.153538
H	3.032204	-4.269586	3.172759
H	-5.668158	2.877884	-0.367371
H	-1.182844	4.313778	-1.944214
H	-1.763860	1.920480	-1.890314

H	0.678692	-3.195825	-1.069772
C	3.988178	3.505744	0.812692
C	5.117411	4.296314	0.998860
C	5.256357	5.052678	2.160611
C	4.258816	5.032246	3.133497
C	3.117377	4.261116	2.943968
H	3.873416	2.914030	-0.091391
H	5.888516	4.318923	0.235913
H	6.141946	5.663100	2.306266
H	2.327767	4.250574	3.689586
H	4.366125	5.622666	4.037508
C	0.338581	4.676561	1.475650
C	-0.901595	5.295268	1.528085
C	-2.050357	4.540087	1.762511
C	-1.955295	3.162197	1.944090
C	-0.715680	2.535232	1.914840
H	-0.658160	1.464277	2.081299
H	1.226693	5.263522	1.266412
H	-0.983047	6.364474	1.361462
H	-3.020557	5.028926	1.780157
H	-2.847324	2.564058	2.097139
C	4.997157	-0.045894	-0.086410
C	5.494210	-0.389562	-1.334940
C	4.683076	-0.431348	-2.461543
C	3.332373	-0.154945	-2.295889
Br	7.304025	-0.911799	-1.497486
H	5.081411	-0.715853	-3.428186
C	2.796388	0.198786	-1.061982
H	1.729933	0.401779	-0.996938
H	5.657863	-0.033457	0.775360
Br	2.171604	-0.360099	-3.767418
C	-5.276419	5.556238	-0.230904
C	-4.927258	6.882606	-0.202417
C	-3.654301	7.295302	-0.669705
C	-2.762765	6.369701	-1.150040
H	-6.253117	5.234273	0.121993
H	-5.626950	7.623001	0.173015
H	-1.783194	6.677982	-1.508175
H	-3.391358	8.348621	-0.649286
C	3.348840	-3.354803	-1.332269
C	4.715274	-3.469551	-1.317811
C	5.400065	-3.774415	-0.115568
C	4.696118	-3.976077	1.044419
H	2.824139	-3.071124	-2.242503
H	5.288805	-3.301173	-2.225139
H	6.484234	-3.835760	-0.120951
H	5.211233	-4.212235	1.972663
C	-3.802060	-4.960364	3.268769
C	-5.117210	-4.371367	3.772265
H	-3.110321	-5.127862	4.101743
H	-4.001994	-5.949872	2.833632
C	-5.977711	-3.946355	2.585891
H	-4.914449	-3.494413	4.400884
H	-5.639727	-5.102931	4.397295
C	-5.280746	-2.837637	1.800763
H	-6.147256	-4.812303	1.930614
H	-6.961166	-3.598987	2.919134
H	-5.265965	-1.922909	2.411617
H	-5.858305	-2.581908	0.910469
C	-5.273169	-3.372032	-1.486310
C	-6.694203	-3.615627	-1.988171
H	-5.083238	-3.948274	-0.578047
H	-4.561109	-3.756985	-2.230634

C	-6.979086	-2.730437	-3.198391
H	-6.820704	-4.674121	-2.237858
H	-7.414124	-3.384534	-1.190079
C	-6.916553	-1.260941	-2.789324
H	-6.228248	-2.931735	-3.973356
H	-7.958903	-2.956055	-3.631839
H	-7.813113	-1.019274	-2.200647
H	-6.948363	-0.613558	-3.672581

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M06-2X/6-31G* Energy = -8271.57354862

M06-2X/6-31G* Free Energy = -8270.691867

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.55873073

Lowest Frequency = 8.8171

M06-2X/6-31G* Geometry

C	-0.619439	3.304938	1.495040
C	1.653660	0.393605	2.646855
C	0.644787	3.557861	1.168516
H	-1.204415	2.563419	0.954536
H	-1.122440	3.861343	2.280715
C	1.409168	2.813354	0.108590
H	1.201126	4.324236	1.709980
N	1.589317	0.783531	1.417838
C	2.743627	0.811095	3.558510
C	0.605453	-0.518656	3.140595
C	2.393272	1.819831	0.766543
C	3.386372	1.206743	-0.204598
H	2.952995	2.354024	1.541273
H	0.858465	0.286369	0.747767
H	0.742278	2.274167	-0.576860
H	2.001034	3.504482	-0.503467
C	-4.233802	-2.192277	0.841575
C	-3.691498	-3.386471	1.338579
C	-3.594223	-1.545964	-0.238927
C	-2.396324	-2.063209	-0.730659
C	-1.830189	-3.242108	-0.235877
C	-2.511394	-3.892414	0.787664
C	-4.109486	-0.275178	-0.828930
C	-5.391565	-0.186612	-1.409762
C	-5.876628	1.066173	-1.805489
C	-5.062768	2.190877	-1.661124
C	-3.751972	2.112434	-1.200394
C	-3.281558	0.852858	-0.807873
O	-1.739404	-1.362367	-1.718892
O	-1.998032	0.728745	-0.314796
P	-0.850368	-0.081529	-1.214931
O	0.123875	-0.562206	-0.157439
O	-0.404760	0.699743	-2.385527
C	-0.560767	-3.775810	-0.785284
C	-2.918604	3.340374	-1.106040
C	-0.424868	-3.979263	-2.187568
C	0.710226	-4.539967	-2.705488
C	1.788565	-4.912186	-1.860991
C	1.679931	-4.669058	-0.463733
C	0.480786	-4.108954	0.048134
C	-1.695144	3.450327	-1.826155
C	-0.951496	4.598253	-1.749437
C	-1.364527	5.694247	-0.946602
C	-2.586753	5.590062	-0.227368
C	-3.348126	4.397269	-0.335934
H	-2.098493	-4.820652	1.178103
H	-5.442762	3.163294	-1.967994
H	-1.240670	-3.685201	-2.839760

H	0.803543	-4.702742	-3.775952
H	-4.279989	4.316900	0.220440
H	-0.020916	4.679641	-2.307021
H	-1.355962	2.612316	-2.427915
H	0.397519	-3.916207	1.116169
C	-0.700150	-0.418566	2.641886
C	-1.669155	-1.314573	3.069503
C	-1.343762	-2.316268	3.981526
C	-0.049015	-2.410980	4.491335
C	0.923776	-1.507168	4.081987
H	-0.959482	0.356045	1.927754
H	-2.675152	-1.238208	2.672328
H	-2.105868	-3.022111	4.301021
H	1.936193	-1.579701	4.467798
H	0.202981	-3.188845	5.204672
C	2.431374	1.237257	4.854083
C	3.448078	1.622210	5.720329
C	4.777866	1.552784	5.309153
C	5.093947	1.103496	4.028498
C	4.080672	0.738541	3.149276
H	4.321587	0.377624	2.152496
H	1.392887	1.274973	5.169091
H	3.203306	1.969426	6.718674
H	5.570702	1.843530	5.991083
H	6.129743	1.035639	3.712844
C	3.242912	-0.092601	-0.688852
C	4.221391	-0.611369	-1.532312
C	5.320895	0.139027	-1.929959
C	5.429157	1.439299	-1.449505
Br	4.055578	-2.403783	-2.098372
H	6.074354	-0.276702	-2.587851
C	4.486651	1.978304	-0.585679
H	4.614294	2.988551	-0.207933
H	2.379624	-0.701382	-0.435847
Br	6.918382	2.488348	-1.962779
C	-2.999888	6.676107	0.588626
C	-2.234626	7.809853	0.688038
C	-1.017047	7.913540	-0.028294
C	-0.595468	6.880511	-0.826304
H	-3.935924	6.590966	1.135238
H	-2.560034	8.634273	1.315193
H	0.337188	6.954330	-1.380346
H	-0.420193	8.816572	0.056549
C	2.780556	-4.990137	0.374383
C	3.926406	-5.534943	-0.146044
C	4.026955	-5.793852	-1.535073
C	2.981645	-5.489001	-2.370789
H	2.696949	-4.791614	1.440134
H	4.762933	-5.770741	0.504502
H	4.937696	-6.227954	-1.936101
H	3.054466	-5.676093	-3.439420
C	-4.349092	-4.152316	2.471438
C	-5.243817	-3.272890	3.340892
H	-3.575515	-4.642285	3.074545
H	-4.958757	-4.962417	2.046896
C	-6.191190	-2.476545	2.448001
H	-4.628928	-2.573596	3.926303
H	-5.798212	-3.889074	4.056188
C	-5.401821	-1.525241	1.551822
H	-6.770241	-3.173486	1.826645
H	-6.909952	-1.906828	3.045757
H	-4.993618	-0.709622	2.169357
H	-6.070038	-1.034411	0.841358

C	-6.191861	-1.444363	-1.703912
C	-7.681470	-1.172934	-1.900328
H	-6.037510	-2.202842	-0.932884
H	-5.785181	-1.880892	-2.627641
C	-7.877218	-0.046497	-2.911597
H	-8.182895	-2.088306	-2.231153
H	-8.136308	-0.884740	-0.941858
C	-7.273996	1.246853	-2.368899
H	-7.381726	-0.320256	-3.851983
H	-8.938271	0.102019	-3.137125
H	-7.924306	1.633155	-1.570985
H	-7.254373	2.018449	-3.146267

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M06-2X/6-31G* Energy = -8271.57354857

M06-2X/6-31G* Free Energy = -8270.691862

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.55873198

Lowest Frequency = 8.8151

M06-2X/6-31G* Geometry

C	-0.619573	3.304894	1.495042
C	1.653946	0.393564	2.646982
C	0.644665	3.557878	1.168611
H	-1.204486	2.563352	0.954503
H	-1.122651	3.861278	2.280686
C	1.409174	2.813473	0.108701
H	1.200912	4.324290	1.710115
N	1.589425	0.783688	1.418030
C	2.743997	0.810935	3.558575
C	0.605774	-0.518758	3.140664
C	2.393321	1.819968	0.766645
C	3.386393	1.206869	-0.204524
H	2.953068	2.354195	1.541345
H	0.858526	0.286618	0.748017
H	0.742361	2.274281	-0.576820
H	2.001037	3.504679	-0.503267
C	-5.391620	-0.186434	-1.409474
C	-5.876642	1.066349	-1.805234
C	-4.109500	-0.275028	-0.828704
C	-3.281551	0.852987	-0.807692
C	-3.751927	2.112569	-1.200263
C	-5.062725	2.191032	-1.660964
C	-3.594222	-1.545838	-0.238763
C	-4.233837	-2.192263	0.841654
C	-3.691597	-3.386553	1.338509
C	-2.511482	-3.892457	0.787574
C	-1.830232	-3.242046	-0.235876
C	-2.396333	-2.063072	-0.730535
O	-1.998024	0.728875	-0.314644
O	-1.739413	-1.362182	-1.718713
P	-0.850374	-0.081323	-1.214816
O	0.123986	-0.561933	-0.157423
O	-0.404868	0.699935	-2.385463
C	-2.918532	3.340491	-1.105949
C	-0.560870	-3.775758	-0.785409
C	-1.695056	3.450469	-1.826049
C	-0.951439	4.598411	-1.749330
C	-1.364500	5.694416	-0.946511
C	-2.586737	5.590207	-0.227303
C	-3.348076	4.397389	-0.335868
C	-0.425010	-3.978978	-2.187741
C	0.710006	-4.539729	-2.705772
C	1.788331	-4.912202	-1.861360
C	1.679752	-4.669291	-0.464061

C	0.480657	-4.109184	0.047925
H	-5.442697	3.163446	-1.967870
H	-2.098653	-4.820788	1.177871
H	-1.355833	2.612454	-2.427784
H	-0.020844	4.679806	-2.306889
H	0.397436	-3.916640	1.116001
H	0.803287	-4.702332	-3.776265
H	-1.240787	-3.684712	-2.839869
H	-4.279940	4.317017	0.220505
C	0.924209	-1.507478	4.081798
C	-0.048473	-2.411533	4.490881
C	-1.343214	-2.316865	3.981048
C	-1.668735	-1.314921	3.069338
C	-0.699854	-0.418649	2.642019
H	1.936635	-1.579997	4.467592
H	0.203617	-3.189554	5.204015
H	-2.105235	-3.022935	4.300245
H	-0.959280	0.356177	1.928150
H	-2.674731	-1.238605	2.672153
C	2.431874	1.236656	4.854324
C	3.448653	1.621458	5.720550
C	4.778392	1.552319	5.309166
C	5.094349	1.103451	4.028332
C	4.080997	0.738639	3.149139
H	4.321822	0.378026	2.152231
H	1.393427	1.274140	5.169492
H	3.203978	1.968329	6.719039
H	5.571287	1.842947	5.991078
H	6.130109	1.035804	3.712517
C	3.242810	-0.092446	-0.688832
C	4.221239	-0.611285	-1.532313
C	5.320789	0.139037	-1.929965
C	5.429162	1.439289	-1.449472
Br	4.055203	-2.403656	-2.098462
H	6.074203	-0.276712	-2.587898
C	4.486729	1.978349	-0.585598
H	4.614466	2.988572	-0.207820
H	2.379462	-0.701152	-0.435865
Br	6.918439	2.488251	-1.962786
C	2.780388	-4.990548	0.373967
C	3.926212	-5.535293	-0.146588
C	4.026709	-5.793979	-1.535661
C	2.981370	-5.488979	-2.371290
H	2.696826	-4.792206	1.439756
H	4.762750	-5.771217	0.503898
H	3.054147	-5.675893	-3.439955
H	4.937432	-6.228022	-1.936793
C	-2.999930	6.676238	0.588671
C	-2.234701	7.810010	0.688096
C	-1.017109	7.913722	-0.028203
C	-0.595476	6.880696	-0.826197
H	-3.935976	6.591075	1.135261
H	-2.560153	8.634424	1.315235
H	-0.420275	8.816767	0.056649
H	0.337196	6.954543	-1.380210
C	-7.274027	1.247091	-2.368581
C	-7.877378	-0.046245	-2.911168
H	-7.254386	2.018641	-3.145992
H	-7.924262	1.633488	-1.570652
C	-7.681616	-1.172650	-1.899869
H	-7.381993	-0.320079	-3.851588
H	-8.938443	0.102332	-3.136601
C	-6.192010	-1.444153	-1.703522

H	-8.136392	-0.884411	-0.941383
H	-8.183094	-2.088012	-2.230639
H	-6.037682	-2.202600	-0.932461
H	-5.785406	-1.880755	-2.627248
C	-5.401835	-1.525279	1.551995
C	-6.191372	-2.476724	2.447870
H	-6.069927	-1.034153	0.841621
H	-4.993551	-0.709907	2.169801
C	-5.244158	-3.273359	3.340669
H	-6.910130	-1.907074	3.045696
H	-6.770439	-3.173464	1.826300
C	-4.349387	-4.152626	2.471105
H	-4.629293	-2.574269	3.926343
H	-5.798691	-3.889701	4.055723
H	-4.959067	-4.962556	2.046258
H	-3.575937	-4.642829	3.074182

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M06-2X/6-31G* Energy = -8271.59088118

M06-2X/6-31G* Free Energy = -8270.703830

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.56399914

Lowest Frequency = 10.1234

M06-2X/6-31G* Geometry

C	-1.237658	2.401262	3.400514
C	-1.328241	3.145687	-0.538140
C	-2.459370	2.133341	2.941430
H	-0.363435	1.816838	3.113402
H	-1.071287	3.221658	4.094034
C	-2.766988	1.028934	1.969717
H	-3.304693	2.747820	3.257044
N	-1.593022	2.029906	0.059890
C	-2.350861	4.219035	-0.647173
C	-0.002425	3.368670	-1.136772
C	-2.901792	1.545039	0.521507
C	-3.404562	0.440631	-0.395645
H	-3.613615	2.372675	0.486000
H	-0.798112	1.318042	0.268512
H	-1.983130	0.261856	1.986820
H	-3.715274	0.540200	2.223354
C	2.163765	-3.653408	-0.842069
C	0.960195	-4.370527	-0.823325
C	2.409114	-2.709368	0.177169
C	1.399303	-2.415652	1.092504
C	0.174001	-3.093484	1.108228
C	0.012814	-4.104018	0.164605
C	3.690962	-1.944937	0.262136
C	4.924354	-2.600343	0.456371
C	6.109137	-1.854042	0.409755
C	6.040444	-0.475493	0.211174
C	4.833495	0.214024	0.116840
C	3.656753	-0.548748	0.168953
O	1.609935	-1.360262	1.958698
O	2.435635	0.078599	0.043183
P	1.365104	0.119689	1.301802
O	0.015832	0.111393	0.609551
O	1.690846	1.153536	2.311510
C	-0.952625	-2.690339	1.984977
C	4.832157	1.689663	-0.050528
C	-0.755150	-2.247518	3.326337
C	-1.813927	-1.838014	4.093339
C	-3.136847	-1.827178	3.575493
C	-3.345763	-2.282982	2.245209
C	-2.235087	-2.718857	1.481427

C	5.723550	2.284713	-0.989800
C	5.776819	3.644474	-1.155296
C	4.924407	4.499974	-0.407222
C	4.028205	3.911302	0.526440
C	4.013460	2.504851	0.698296
H	-0.915867	-4.670461	0.161186
H	6.965889	0.096843	0.184402
H	0.249425	-2.227346	3.732108
H	-1.647969	-1.492830	5.110487
H	3.338054	2.082548	1.436904
H	6.463201	4.084693	-1.874999
H	6.361458	1.639029	-1.587819
H	-2.402989	-3.015913	0.449290
C	0.811342	2.285683	-1.508564
C	2.044383	2.518091	-2.101139
C	2.471745	3.822886	-2.338877
C	1.677388	4.903637	-1.958349
C	0.443675	4.681145	-1.363701
H	0.488680	1.263504	-1.340918
H	2.674870	1.675242	-2.363752
H	3.437424	3.997452	-2.801957
H	-0.169846	5.521912	-1.056535
H	2.032092	5.917994	-2.107280
C	-2.893204	4.782395	0.512020
C	-3.822518	5.812136	0.407793
C	-4.219589	6.269987	-0.847021
C	-3.675009	5.711209	-2.001384
C	-2.728101	4.696925	-1.904588
H	-2.282813	4.269303	-2.798080
H	-2.569129	4.414952	1.482806
H	-4.235604	6.257590	1.306933
H	-4.950150	7.068865	-0.925422
H	-3.980696	6.071234	-2.978216
C	-2.545131	-0.501884	-0.963056
C	-3.087571	-1.529582	-1.725936
C	-4.456612	-1.671919	-1.918153
C	-5.289015	-0.738902	-1.311231
Br	-1.917513	-2.833644	-2.447082
H	-4.861929	-2.496849	-2.491652
C	-4.783029	0.321546	-0.572965
H	-5.464151	1.026097	-0.105649
H	-1.475311	-0.479812	-0.773222
Br	-7.161576	-0.979367	-1.405749
C	3.137490	4.745161	1.253939
C	3.138014	6.102652	1.058800
C	4.034932	6.691005	0.131415
C	4.906894	5.908610	-0.583718
H	2.451008	4.272842	1.952561
H	2.452206	6.735176	1.614522
H	5.596046	6.356658	-1.295878
H	4.030711	7.768118	-0.008711
C	-4.649955	-2.214114	1.689083
C	-5.695738	-1.694991	2.409629
C	-5.489388	-1.249646	3.739731
C	-4.242105	-1.324019	4.310129
H	-4.801161	-2.559400	0.669373
H	-6.679218	-1.620709	1.953574
H	-6.323966	-0.848487	4.306849
H	-4.077874	-0.977896	5.327464
C	0.630244	-5.409698	-1.876860
C	1.388385	-5.169043	-3.178841
H	-0.452704	-5.411769	-2.050853
H	0.881182	-6.409464	-1.495433

C	2.876412	-5.021025	-2.872765
H	1.017987	-4.248226	-3.650863
H	1.209242	-5.990463	-3.880094
C	3.126536	-3.785015	-2.010531
H	3.221791	-5.918728	-2.341597
H	3.463925	-4.949144	-3.793844
H	4.165462	-3.765699	-1.671354
H	3.006750	-2.884176	-2.629894
C	4.961842	-4.075791	0.817967
C	6.328019	-4.716766	0.585818
H	4.184810	-4.632131	0.288826
H	4.704762	-4.158350	1.884042
C	7.421676	-3.868842	1.229061
H	6.330675	-5.734111	0.990494
H	6.520212	-4.799041	-0.493306
C	7.474228	-2.500889	0.553736
H	7.199764	-3.746667	2.297111
H	8.397394	-4.360166	1.155710
H	7.914207	-2.617708	-0.447050
H	8.139130	-1.824851	1.102486

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M06-2X/6-31G* Energy = -8271.59088127

M06-2X/6-31G* Free Energy = -8270.703817

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.56399568

Lowest Frequency = 10.2325

M06-2X/6-31G* Geometry

C	-1.237444	2.401846	3.400110
C	-1.327819	3.146102	-0.538450
C	-2.459184	2.134020	2.941036
H	-0.363306	1.817245	3.113092
H	-1.070993	3.222297	4.093539
C	-2.766892	1.029606	1.969372
H	-3.304446	2.748621	3.256577
N	-1.592784	2.030364	0.059609
C	-2.350337	4.219528	-0.647576
C	-0.001958	3.368957	-1.137034
C	-2.901629	1.545707	0.521152
C	-3.404505	0.441250	-0.395881
H	-3.613346	2.373437	0.485565
H	-0.798086	1.318294	0.268140
H	-1.983056	0.262489	1.986435
H	-3.715189	0.540876	2.222990
C	2.163483	-3.653399	-0.842438
C	0.959830	-4.370407	-0.823911
C	2.408820	-2.709527	0.176951
C	1.398929	-2.415794	1.092216
C	0.173553	-3.093527	1.107716
C	0.012368	-4.103931	0.163949
C	3.690761	-1.945279	0.262210
C	4.924045	-2.600860	0.456564
C	6.108930	-1.854696	0.410197
C	6.040443	-0.476114	0.211774
C	4.833597	0.213574	0.117360
C	3.656752	-0.549063	0.169201
O	1.609611	-1.360553	1.958556
O	2.435717	0.078422	0.043343
P	1.365063	0.119553	1.301859
O	0.015933	0.111668	0.609352
O	1.690887	1.153166	2.311780
C	-0.953096	-2.690420	1.984457
C	4.832414	1.689214	-0.049866
C	-0.755590	-2.247663	3.325847

C	-1.814323	-1.838095	4.092862
C	-3.137266	-1.827222	3.575057
C	-3.346250	-2.283120	2.244813
C	-2.235582	-2.718958	1.480963
C	5.724024	2.284285	-0.988931
C	5.777328	3.644046	-1.154396
C	4.924747	4.499544	-0.406501
C	4.028363	3.910858	0.526978
C	4.013584	2.504400	0.698811
H	-0.916363	-4.670295	0.160367
H	6.965970	0.096103	0.185232
H	0.248987	-2.227562	3.731619
H	-1.648325	-1.492933	5.110012
H	3.338046	2.082109	1.437310
H	6.463875	4.084273	-1.873939
H	6.362058	1.638617	-1.586832
H	-2.403528	-3.016003	0.448823
C	0.811783	2.285925	-1.508760
C	2.044885	2.518266	-2.101230
C	2.472367	3.823045	-2.338898
C	1.678038	4.903839	-1.958433
C	0.444245	4.681409	-1.363915
H	0.489050	1.263760	-1.341160
H	2.675333	1.675377	-2.363811
H	3.438083	3.997551	-2.801930
H	-0.169231	5.522219	-1.056779
H	2.032791	5.918182	-2.107341
C	-2.727631	4.697191	-1.905070
C	-3.674485	5.711512	-2.002020
C	-4.218991	6.270536	-0.847736
C	-3.821892	5.812891	0.407148
C	-2.892622	4.783121	0.511528
H	-2.568539	4.415836	1.482373
H	-2.282410	4.269375	-2.798505
H	-3.980188	6.071369	-2.978909
H	-4.949521	7.069433	-0.926254
H	-4.234926	6.258517	1.306228
C	-2.545077	-0.501121	-0.963516
C	-3.087554	-1.528983	-1.726141
C	-4.456630	-1.671565	-1.917944
C	-5.289024	-0.738666	-1.310800
Br	-1.917505	-2.833031	-2.447312
H	-4.861977	-2.496658	-2.491192
C	-4.783017	0.321905	-0.572730
H	-5.464119	1.026306	-0.105155
H	-1.475214	-0.478902	-0.773925
Br	-7.161547	-0.979701	-1.404437
C	3.137463	4.744700	1.254278
C	3.137988	6.102191	1.059120
C	4.035085	6.690556	0.131915
C	4.907226	5.908178	-0.583022
H	2.450853	4.272369	1.952769
H	2.452047	6.734701	1.614696
H	5.596503	6.356237	-1.295053
H	4.030855	7.767667	-0.008239
C	-4.650517	-2.214431	1.688835
C	-5.696269	-1.695310	2.409435
C	-5.489827	-1.249816	3.739468
C	-4.242483	-1.324071	4.309757
H	-4.801828	-2.559844	0.669187
H	-6.679802	-1.621161	1.953469
H	-6.324378	-0.848664	4.306633
H	-4.078184	-0.977884	5.327061

C	0.629923	-5.409464	-1.877569
C	1.388278	-5.168819	-3.179428
H	-0.453003	-5.411413	-2.051715
H	0.880700	-6.409282	-1.496166
C	2.876275	-5.020940	-2.873120
H	1.018039	-4.247934	-3.651450
H	1.209149	-5.990180	-3.880756
C	3.126341	-3.784956	-2.010837
H	3.221490	-5.918673	-2.341889
H	3.463946	-4.949107	-3.794104
H	3.006564	-2.884104	-2.630191
H	4.165245	-3.765619	-1.671597
C	4.961323	-4.076339	0.818051
C	6.327440	-4.717462	0.585957
H	4.184254	-4.632547	0.288823
H	4.704168	-4.158950	1.884108
C	7.421127	-3.869752	1.229442
H	6.329921	-5.734868	0.990484
H	6.519742	-4.799598	-0.493162
C	7.473923	-2.501725	0.554284
H	7.199080	-3.747676	2.297478
H	8.396800	-4.361181	1.156163
H	7.914011	-2.618485	-0.446464
H	8.138843	-1.825824	1.103189

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M06-2X/6-31G* Energy = -8271.58296008

M06-2X/6-31G* Free Energy = -8270.697529

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.56223947

Lowest Frequency = 11.9660

M06-2X/6-31G* Geometry

C	-0.044021	3.416431	-2.893105
C	0.901455	3.315186	1.047889
C	1.234011	3.425231	-2.522572
H	-0.615456	2.489435	-2.906927
H	-0.535228	4.332415	-3.210777
C	1.988714	2.205695	-2.070390
H	1.797046	4.360943	-2.520370
N	1.266878	2.383986	0.228127
C	1.828363	4.392434	1.465889
C	-0.468492	3.296262	1.581911
C	2.467771	2.374882	-0.611513
C	3.466943	1.317538	-0.178087
H	2.947305	3.354777	-0.523669
H	0.623638	1.515303	0.069091
H	1.358377	1.311379	-2.152622
H	2.882018	2.051919	-2.689525
C	-4.495905	-3.120374	-0.721708
C	-5.654261	-2.538001	-1.252467
C	-3.435039	-2.287527	-0.307137
C	-3.496423	-0.917066	-0.562692
C	-4.655448	-0.315582	-1.071254
C	-5.724290	-1.150358	-1.382594
C	-2.234361	-2.841380	0.388785
C	-2.337807	-3.490949	1.635656
C	-1.189199	-4.065520	2.192166
C	0.015890	-4.000946	1.493471
C	0.163822	-3.325704	0.280996
C	-0.984117	-2.684395	-0.210485
O	-2.416391	-0.131585	-0.220870
O	-0.914003	-1.879035	-1.330279
P	-1.006578	-0.263568	-1.065769
O	0.060486	0.135652	-0.066964

O	-1.073462	0.422197	-2.381125
C	-4.781151	1.156665	-1.211797
C	1.477121	-3.357004	-0.413003
C	-3.810209	1.916938	-1.926088
C	-3.926125	3.279708	-2.011870
C	-5.007145	3.970443	-1.400937
C	-5.991012	3.215088	-0.704593
C	-5.849724	1.804622	-0.631263
C	2.284809	-4.527365	-0.266282
C	3.563631	-4.580643	-0.746160
C	4.118924	-3.482797	-1.456258
C	3.286694	-2.360163	-1.707199
C	1.982446	-2.310361	-1.150968
H	-6.629360	-0.701547	-1.787399
H	0.895666	-4.456627	1.942593
H	-2.978176	1.401493	-2.397996
H	-3.182285	3.854902	-2.558543
H	1.418586	-1.394126	-1.266451
H	4.169696	-5.470788	-0.597118
H	1.870142	-5.389887	0.246122
H	-6.589061	1.232358	-0.074619
C	-0.714618	3.775145	2.878230
C	-2.001580	3.739774	3.394603
C	-3.048103	3.244603	2.616425
C	-2.812119	2.782540	1.324236
C	-1.524996	2.805179	0.801832
H	0.107173	4.151135	3.479781
H	-2.189268	4.096933	4.401850
H	-4.057513	3.225878	3.015751
H	-1.354052	2.486115	-0.223896
H	-3.625587	2.399875	0.718555
C	3.125820	4.083433	1.892525
C	3.976139	5.099444	2.313071
C	3.541793	6.423651	2.296108
C	2.250544	6.733706	1.873686
C	1.387245	5.720133	1.473562
H	0.374431	5.949384	1.156261
H	3.455758	3.047549	1.909193
H	4.976865	4.856454	2.654455
H	4.210065	7.215694	2.618909
H	1.912929	7.764728	1.863103
C	4.779020	1.449032	-0.642615
C	5.716007	0.479133	-0.321810
C	5.398377	-0.607506	0.483596
C	4.094922	-0.704494	0.949790
Br	7.453068	0.593423	-1.054425
H	6.133022	-1.370009	0.711832
C	3.116774	0.232983	0.624738
H	2.093749	0.076465	0.954038
H	5.062968	2.286642	-1.273284
Br	3.623521	-2.187364	2.012101
C	3.802923	-1.280449	-2.471218
C	5.096815	-1.295446	-2.924352
C	5.941568	-2.394414	-2.631897
C	5.457326	-3.468998	-1.927905
H	3.148541	-0.437569	-2.680344
H	5.491114	-0.453904	-3.487311
H	6.093434	-4.325897	-1.719701
H	6.971374	-2.383671	-2.975938
C	-7.074098	3.897368	-0.088829
C	-7.175668	5.262658	-0.163467
C	-6.197078	6.014558	-0.859152
C	-5.140128	5.382184	-1.462160

H	-7.822988	3.314793	0.441887
H	-8.008715	5.773895	0.309122
H	-6.289802	7.094880	-0.913345
H	-4.387064	5.952965	-1.999662
C	-6.852408	-3.368120	-1.674087
C	-6.506428	-4.832957	-1.927611
H	-7.308008	-2.919489	-2.563735
H	-7.612437	-3.316226	-0.881316
C	-5.677597	-5.371894	-0.765242
H	-5.925544	-4.921519	-2.854753
H	-7.423247	-5.415895	-2.063388
C	-4.344726	-4.631724	-0.681578
H	-6.235954	-5.236163	0.171836
H	-5.495379	-6.445663	-0.877035
H	-3.789191	-4.947663	0.204559
H	-3.718242	-4.921591	-1.537533
C	-3.643167	-3.465170	2.411768
C	-3.692928	-4.498853	3.534487
H	-4.499492	-3.589376	1.744354
H	-3.752209	-2.459347	2.842938
C	-2.425921	-4.417534	4.381379
H	-4.586256	-4.335528	4.146195
H	-3.777066	-5.506949	3.104902
C	-1.215436	-4.785566	3.527440
H	-2.313455	-3.394103	4.762396
H	-2.487538	-5.081362	5.249954
H	-0.284647	-4.578675	4.067372
H	-1.228615	-5.869376	3.343742

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M06-2X/6-31G* Energy = -8271.58934615

M06-2X/6-31G* Free Energy = -8270.702726

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.56328711

Lowest Frequency = 12.8638

M06-2X/6-31G* Geometry

C	1.297213	2.207062	-3.657621
C	1.206976	3.312172	0.205838
C	2.512780	2.062772	-3.131767
H	0.452162	1.586763	-3.358714
H	1.106562	2.956110	-4.421840
C	2.849348	1.064925	-2.059342
H	3.328005	2.708556	-3.463627
N	1.536198	2.168217	-0.299432
C	2.198684	4.418405	0.283643
C	-0.151615	3.544327	0.720745
C	2.887514	1.711179	-0.659496
C	3.402091	0.725919	0.377645
H	3.554198	2.575923	-0.670938
H	0.786336	1.408297	-0.492423
H	2.118721	0.247526	-2.039907
H	3.838676	0.624236	-2.231615
C	-1.853557	-3.700832	0.960806
C	-0.604988	-4.328392	1.060062
C	-2.111772	-2.871986	-0.151394
C	-1.078657	-2.583382	-1.041954
C	0.189710	-3.168892	-0.940963
C	0.370815	-4.080537	0.095155
C	-3.439512	-2.220876	-0.366335
C	-4.614137	-2.982454	-0.543749
C	-5.851336	-2.328377	-0.610551
C	-5.893454	-0.935526	-0.538201
C	-4.743076	-0.155903	-0.466183
C	-3.513222	-0.824678	-0.407123

O	-1.320978	-1.636586	-2.016130
O	-2.355918	-0.084640	-0.296778
P	-1.239273	-0.077842	-1.518200
O	0.070419	0.117608	-0.778942
O	-1.615921	0.798368	-2.649474
C	1.328629	-2.764802	-1.801243
C	-4.840467	1.325284	-0.414446
C	1.168241	-2.456919	-3.184732
C	2.233988	-2.043165	-3.939572
C	3.526291	-1.893995	-3.368636
C	3.699733	-2.215449	-1.994635
C	2.583918	-2.658527	-1.242464
C	-4.117523	2.140701	-1.331911
C	-4.232166	3.504249	-1.283457
C	-5.047433	4.141252	-0.311983
C	-5.769441	3.333066	0.609699
C	-5.654906	1.921596	0.522647
H	1.334230	-4.576673	0.190260
H	-6.856395	-0.431261	-0.591368
H	0.185816	-2.543297	-3.633547
H	2.095703	-1.801492	-4.990169
H	-6.199698	1.306052	1.235807
H	-3.675261	4.120636	-1.984752
H	-3.470723	1.672688	-2.068005
H	2.719720	-2.850622	-0.181044
C	-0.608577	4.862595	0.889038
C	-1.872713	5.100080	1.408894
C	-2.692222	4.031354	1.770005
C	-2.254270	2.720448	1.586529
C	-0.989065	2.472205	1.071662
H	0.024768	5.695607	0.602456
H	-2.228427	6.118418	1.527670
H	-3.679489	4.224599	2.180343
H	-0.661386	1.444642	0.950051
H	-2.899891	1.883960	1.832899
C	2.547900	4.961218	1.522027
C	3.464512	6.006059	1.582599
C	4.006992	6.527650	0.410107
C	3.639329	6.001519	-0.826825
C	2.740154	4.942341	-0.894102
H	2.443028	4.517880	-1.850300
H	2.104702	4.561214	2.429298
H	3.748361	6.418184	2.545329
H	4.713906	7.349712	0.460035
H	4.052432	6.415901	-1.740679
C	2.567044	-0.209320	0.991696
C	3.125965	-1.126426	1.874350
C	4.489423	-1.168227	2.141090
C	5.299430	-0.248494	1.486062
Br	1.998212	-2.426590	2.665181
H	4.909569	-1.910807	2.808726
C	4.774121	0.707055	0.628151
H	5.438027	1.404669	0.126910
H	1.508833	-0.267486	0.749747
Br	7.175321	-0.371661	1.683890
C	-6.543501	3.965672	1.619565
C	-6.585240	5.333441	1.719083
C	-5.865378	6.138250	0.800739
C	-5.122436	5.553882	-0.193669
H	-7.094303	3.343625	2.320833
H	-7.173560	5.805648	2.499883
H	-4.565396	6.164085	-0.900525
H	-5.909287	7.219727	0.886852

C	4.968725	-2.008845	-1.392837
C	6.011853	-1.483892	-2.112905
C	5.841162	-1.171387	-3.485206
C	4.630402	-1.381618	-4.098589
H	5.093605	-2.252397	-0.340711
H	6.965735	-1.303322	-1.624927
H	6.674220	-0.764614	-4.050554
H	4.493119	-1.138480	-5.149197
C	-0.258792	-5.245141	2.216986
C	-1.093736	-4.944139	3.457937
H	0.812040	-5.155725	2.436870
H	-0.424476	-6.289738	1.918118
C	-2.571773	-4.929683	3.076907
H	-0.809358	-3.960825	3.858338
H	-0.894350	-5.684883	4.239037
C	-2.861477	-3.796467	2.094094
H	-2.830475	-5.893454	2.616982
H	-3.206795	-4.817316	3.961684
H	-2.832075	-2.837732	2.632141
H	-3.881719	-3.881105	1.711209
C	-4.528908	-4.483569	-0.764452
C	-5.853111	-5.203054	-0.519745
H	-3.735770	-4.927311	-0.158456
H	-4.222572	-4.644054	-1.808361
C	-6.977329	-4.505297	-1.280030
H	-5.764300	-6.250987	-0.824230
H	-6.084429	-5.198526	0.554848
C	-7.158269	-3.088259	-0.742227
H	-6.719611	-4.467023	-2.346356
H	-7.916945	-5.060834	-1.194338
H	-7.632679	-3.143817	0.248025
H	-7.845162	-2.518985	-1.378108

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M06-2X/6-31G* Energy = -8271.58934598

M06-2X/6-31G* Free Energy = -8270.702722

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.56326562

Lowest Frequency = 13.0320

M06-2X/6-31G* Geometry

C	-1.296703	2.208454	3.656871
C	-1.204696	3.312808	-0.206849
C	-2.511975	2.065020	3.130113
H	-0.451968	1.587325	3.358814
H	-1.105987	2.957666	4.420910
C	-2.848717	1.066958	2.057952
H	-3.326883	2.711715	3.460990
N	-1.534545	2.168889	0.298029
C	-2.195844	4.419586	-0.284726
C	0.154126	3.544617	-0.721375
C	-2.886207	1.712796	0.657864
C	-3.401241	0.727443	-0.378993
H	-3.552459	2.577882	0.668942
H	-0.784970	1.408090	0.491496
H	-2.118490	0.249202	2.038983
H	-3.838291	0.626811	2.230200
C	4.611999	-2.984845	0.544796
C	5.849693	-2.331722	0.611704
C	3.438000	-2.222400	0.366925
C	3.512802	-0.826258	0.407491
C	4.743148	-0.158426	0.466773
C	5.892909	-0.938918	0.539123
C	2.109853	-2.872650	0.151796
C	1.851397	-3.701684	-0.960223

C	0.602510	-4.328564	-1.059522
C	-0.373350	-4.079917	-0.094858
C	-0.191986	-3.168062	0.941013
C	1.076691	-2.583187	1.041990
O	2.356145	-0.085298	0.296616
O	1.319269	-1.636075	2.015798
P	1.238735	-0.077568	1.517222
O	-0.070320	0.118156	0.776722
O	1.614724	0.798958	2.648450
C	4.841593	1.322693	0.414930
C	-1.330739	-2.763203	1.801151
C	4.119018	2.138647	1.332203
C	4.234555	3.502115	1.283686
C	5.050375	4.138505	0.312284
C	5.771982	3.329785	-0.609245
C	5.656564	1.918395	-0.522082
C	-1.170157	-2.454942	3.184529
C	-2.235653	-2.040401	3.939295
C	-3.527909	-1.890796	3.368396
C	-3.701600	-2.212731	1.994534
C	-2.586027	-2.656532	1.242421
H	6.856223	-0.435383	0.592409
H	-1.336981	-4.575614	-0.190015
H	3.471795	1.671130	2.068232
H	3.677940	4.118909	1.984849
H	-2.721965	-2.848839	0.181055
H	-2.097143	-1.798415	4.989790
H	-0.187774	-2.541652	3.633364
H	6.201075	1.302440	-1.235100
C	0.611643	4.862755	-0.889033
C	1.876022	5.099956	-1.408454
C	2.695203	4.031068	-1.769788
C	2.256642	2.720265	-1.587035
C	0.991206	2.472321	-1.072598
H	-0.021466	5.695905	-0.602326
H	2.232141	6.118212	-1.526729
H	3.682670	4.224083	-2.179753
H	0.663006	1.444865	-0.951601
H	2.901974	1.883620	-1.833625
C	-2.545029	4.962253	-1.523167
C	-3.461084	6.007582	-1.583819
C	-4.003017	6.529787	-0.411353
C	-3.635352	6.003799	0.825636
C	-2.736728	4.944157	0.892997
H	-2.439632	4.519776	1.849232
H	-2.102238	4.561773	-2.430426
H	-3.744918	6.419602	-2.546597
H	-4.709500	7.352213	-0.461343
H	-4.048024	6.418657	1.739469
C	-2.566647	-0.207879	-0.993538
C	-3.126263	-1.125394	-1.875326
C	-4.489951	-1.167526	-2.140771
C	-5.299454	-0.247655	-1.485340
Br	-1.999180	-2.425945	-2.666464
H	-4.910642	-1.910543	-2.807574
C	-4.773494	0.708295	-0.628299
H	-5.437056	1.405900	-0.126590
H	-1.508255	-0.265933	-0.752493
Br	-7.175538	-0.371684	-1.680794
C	-4.970570	-2.005799	1.392798
C	-6.013329	-1.479853	2.112672
C	-5.842340	-1.166765	3.484800
C	-4.631678	-1.377474	4.098201

H	-5.095743	-2.249907	0.340848
H	-6.967109	-1.298929	1.624626
H	-4.494167	-1.133960	5.148691
H	-6.675103	-0.759201	4.050014
C	6.546551	3.961824	-1.619068
C	6.589180	5.329559	-1.718681
C	5.869735	6.134896	-0.800479
C	5.126300	5.551074	0.193878
H	7.097036	3.339379	-2.320231
H	7.177884	5.801320	-2.499461
H	5.914347	7.216337	-0.886659
H	4.569558	6.161683	0.900618
C	7.156013	-3.092600	0.743736
C	6.973907	-4.509387	1.281803
H	7.843263	-2.523733	1.379591
H	7.630517	-3.148728	-0.246439
C	5.849229	-5.206427	0.521539
H	6.716102	-4.470703	2.348091
H	7.913098	-5.065668	1.196323
C	4.525579	-4.485835	0.765958
H	6.080673	-5.202326	-0.553025
H	5.759565	-6.254217	0.826259
H	3.732090	-4.929146	0.160119
H	4.219117	-4.645718	1.809922
C	2.859568	-3.797981	-2.093240
C	2.568646	-4.929940	-3.077182
H	3.879540	-3.884592	-1.710045
H	2.831929	-2.838696	-2.630377
C	1.090447	-4.943285	-3.457610
H	3.203374	-4.816985	-3.962091
H	2.826971	-5.894373	-2.618454
C	0.256029	-5.245119	-2.216503
H	0.806274	-3.959457	-3.856903
H	0.890424	-5.683198	-4.239331
H	0.422230	-6.289785	-1.918173
H	-0.814915	-5.155946	-2.435882

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M06-2X/6-31G* Energy = -8271.58934622

M06-2X/6-31G* Free Energy = -8270.702711

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.56327257

Lowest Frequency = 12.9620

M06-2X/6-31G* Geometry

C	-1.297343	2.208191	3.656487
C	-1.206562	3.312587	-0.206726
C	-2.512816	2.063668	3.130473
H	-0.452116	1.588091	3.357654
H	-1.106953	2.957280	4.420729
C	-2.849134	1.065700	2.058093
H	-3.328229	2.709269	3.462223
N	-1.536201	2.168464	0.297914
C	-2.198018	4.419073	-0.284210
C	0.152148	3.544689	-0.721342
C	-2.887569	1.711754	0.658147
C	-3.402531	0.726223	-0.378576
H	-3.554111	2.576619	0.669561
H	-0.786695	1.408221	0.490481
H	-2.118275	0.248485	2.038613
H	-3.838316	0.624738	2.230495
C	1.853382	-3.701510	-0.960347
C	0.604761	-4.329002	-1.059267
C	2.111713	-2.872179	0.151478
C	1.078615	-2.583068	1.041885

C	-0.189770	-3.168651	0.941326
C	-0.370968	-4.080738	-0.094372
C	3.439577	-2.221244	0.366253
C	4.613987	-2.983073	0.544106
C	5.851372	-2.329332	0.610806
C	5.893894	-0.936505	0.538103
C	4.743725	-0.156623	0.465777
C	3.513682	-0.825054	0.406618
O	1.320902	-1.635515	2.015347
O	2.356782	-0.084578	0.295691
P	1.238891	-0.077256	1.515931
O	-0.070038	0.116952	0.775016
O	1.613940	0.800211	2.646785
C	-1.328518	-2.764147	1.801621
C	4.841370	1.324552	0.414092
C	-1.167807	-2.455662	3.184938
C	-2.233326	-2.041429	3.939841
C	-3.525722	-1.892288	3.369117
C	-3.699509	-2.214394	1.995307
C	-2.583935	-2.658015	1.243089
C	4.118469	2.139911	1.331657
C	4.233240	3.503448	1.283434
C	5.048578	4.140514	0.312051
C	5.770456	3.332400	-0.609799
C	5.655827	1.920912	-0.522936
H	-1.334395	-4.576903	-0.189209
H	6.856962	-0.432483	0.591284
H	-0.185298	-2.541956	3.633593
H	-2.094734	-1.799278	4.990288
H	6.200542	1.305426	-1.236206
H	3.676348	4.119776	1.984789
H	3.471505	1.671892	2.067599
H	-2.720008	-2.850531	0.181776
C	0.989513	2.472604	-1.072595
C	2.254900	2.720899	-1.586976
C	2.693132	4.031826	-1.769676
C	1.873693	5.100503	-1.408285
C	0.609369	4.862963	-0.888885
H	0.661605	1.445039	-0.951627
H	2.900470	1.884431	-1.833553
H	3.680545	4.225093	-2.179656
H	-0.023903	5.695952	-0.602076
H	2.229561	6.118854	-1.526500
C	-2.547171	4.962155	-1.522494
C	-3.463566	6.007202	-1.582865
C	-4.005891	6.528719	-0.410269
C	-3.638282	6.002312	0.826563
C	-2.739320	4.942940	0.893641
H	-2.442228	4.518278	1.849758
H	-2.104095	4.562210	-2.429852
H	-3.747351	6.419546	-2.545521
H	-4.712639	7.350934	-0.460032
H	-4.051265	6.416631	1.740501
C	-4.774665	0.707340	-0.628563
C	-5.300412	-0.248762	-1.485599
C	-4.490778	-1.169042	-2.140321
C	-3.127207	-1.127134	-1.874205
Br	-7.176417	-0.372113	-1.682321
H	-4.911294	-1.912127	-2.807165
C	-2.567840	-0.209473	-0.992417
H	-1.509534	-0.267626	-0.750927
H	-5.438319	1.405309	-0.127479
Br	-1.999843	-2.427987	-2.664458

C	6.544518	3.965095	-1.619600
C	6.586436	5.332883	-1.718865
C	5.866741	6.137615	-0.800331
C	5.123759	5.553155	0.193998
H	7.095207	3.343114	-2.321016
H	7.174776	5.805149	-2.499615
H	4.566821	6.163298	0.900987
H	5.910793	7.219103	-0.886235
C	-4.968557	-2.007697	1.393655
C	-6.011366	-1.481948	2.113611
C	-5.840328	-1.168817	3.485728
C	-4.629544	-1.379200	4.099013
H	-5.093727	-2.251791	0.341695
H	-6.965237	-1.301223	1.625664
H	-6.673133	-0.761431	4.051009
H	-4.491975	-1.135570	5.149470
C	0.258408	-5.246019	-2.215926
C	1.092910	-4.944870	-3.457138
H	-0.812517	-5.156900	-2.435472
H	0.424478	-6.290549	-1.917030
C	2.571069	-4.930567	-3.076590
H	0.808402	-3.961487	-3.857285
H	0.893256	-5.685502	-4.238278
C	2.861284	-3.797606	-2.093611
H	2.829841	-5.894473	-2.616988
H	3.205807	-4.818063	-3.961556
H	3.881464	-3.882901	-1.710677
H	2.832503	-2.838767	-2.631499
C	4.528331	-4.484075	0.765474
C	5.852322	-5.204055	0.521085
H	3.735048	-4.927877	0.159716
H	4.221974	-4.643979	1.809470
C	6.976730	-4.506334	1.281120
H	5.763193	-6.251836	0.826008
H	6.083669	-5.200046	-0.553505
C	7.158079	-3.089541	0.742808
H	6.719019	-4.467607	2.347433
H	7.916190	-5.062168	1.195629
H	7.632513	-3.145588	-0.247408
H	7.845116	-2.520236	1.378510

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M06-2X/6-31G* Energy = -8271.58934625

M06-2X/6-31G* Free Energy = -8270.702702

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.56326984

Lowest Frequency = 12.9969

M06-2X/6-31G* Geometry

C	-1.296974	2.208105	3.656353
C	-1.206732	3.312685	-0.206721
C	-2.512481	2.063576	3.130427
H	-0.451761	1.588000	3.357481
H	-1.106529	2.957211	4.420566
C	-2.848916	1.065593	2.058102
H	-3.327863	2.709206	3.462201
N	-1.536199	2.168475	0.297825
C	-2.198400	4.419005	-0.284146
C	0.151958	3.545108	-0.721252
C	-2.887490	1.711639	0.658147
C	-3.402417	0.726064	-0.378550
H	-3.554096	2.576449	0.669604
H	-0.786528	1.408337	0.490433
H	-2.118068	0.248377	2.038560
H	-3.838078	0.624636	2.230628

C	1.853467	-3.701444	-0.960360
C	0.604832	-4.328899	-1.059358
C	2.111752	-2.872111	0.151473
C	1.078600	-2.582946	1.041801
C	-0.189780	-3.168520	0.941184
C	-0.370943	-4.080608	-0.094521
C	3.439635	-2.221245	0.366334
C	4.614000	-2.983114	0.544284
C	5.851405	-2.329410	0.611072
C	5.893986	-0.936589	0.538354
C	4.743846	-0.156668	0.465919
C	3.513798	-0.825053	0.406678
O	1.320827	-1.635404	2.015279
O	2.356900	-0.084569	0.295630
P	1.239069	-0.077112	1.515926
O	-0.069802	0.117349	0.774962
O	1.614236	0.800204	2.646853
C	-1.328553	-2.764029	1.801445
C	4.841489	1.324503	0.414171
C	-1.167884	-2.455581	3.184779
C	-2.233434	-2.041398	3.939663
C	-3.525821	-1.892279	3.368907
C	-3.699561	-2.214337	1.995080
C	-2.583951	-2.657901	1.242880
C	4.118655	2.139876	1.331766
C	4.233364	3.503416	1.283460
C	5.048557	4.140457	0.311946
C	5.770376	3.332323	-0.609934
C	5.655844	1.920835	-0.522965
H	-1.334377	-4.576752	-0.189407
H	6.857067	-0.432597	0.591579
H	-0.185383	-2.541850	3.633453
H	-2.094880	-1.799276	4.990120
H	6.200527	1.305324	-1.236236
H	3.676519	4.119760	1.984837
H	3.471774	1.671865	2.067783
H	-2.719984	-2.850406	0.181562
C	0.989654	2.473242	-1.072387
C	2.255021	2.721867	-1.586665
C	2.692911	4.032905	-1.769384
C	1.873142	5.101367	-1.408106
C	0.608842	4.863500	-0.888804
H	0.662038	1.445586	-0.951420
H	2.900839	1.885558	-1.833135
H	3.680311	4.226432	-2.179280
H	-0.024679	5.696326	-0.602077
H	2.228750	6.119808	-1.526331
C	-2.547889	4.961857	-1.522435
C	-3.464494	6.006719	-1.582766
C	-4.006708	6.528274	-0.410133
C	-3.638773	6.002087	0.826691
C	-2.739586	4.942898	0.893736
H	-2.442261	4.518391	1.849847
H	-2.104894	4.561890	-2.429822
H	-3.748542	6.418889	-2.545419
H	-4.713627	7.350342	-0.459868
H	-4.051676	6.416431	1.740654
C	-2.567650	-0.209468	-0.992524
C	-3.126966	-1.127166	-1.874310
C	-4.490556	-1.169270	-2.140279
C	-5.300267	-0.249161	-1.485405
Br	-1.999493	-2.427809	-2.664754
H	-4.911039	-1.912389	-2.807104

C	-4.774583	0.706966	-0.628369
H	-5.438288	1.404793	-0.127158
H	-1.509303	-0.267454	-0.751162
Br	-7.176269	-0.372798	-1.681959
C	6.544261	3.965001	-1.619882
C	6.586041	5.332784	-1.719274
C	5.866391	6.137533	-0.800718
C	5.123599	5.553093	0.193763
H	7.094908	3.343009	-2.321321
H	7.174228	5.805033	-2.500149
H	4.566691	6.163246	0.900766
H	5.910329	7.219017	-0.886728
C	-4.968600	-2.007674	1.393410
C	-6.011450	-1.482015	2.113374
C	-5.840461	-1.168933	3.485504
C	-4.629676	-1.379274	4.098804
H	-5.093743	-2.251714	0.341435
H	-6.965324	-1.301328	1.625420
H	-6.673299	-0.761614	4.050783
H	-4.492136	-1.135678	5.149272
C	0.258530	-5.245876	-2.216061
C	1.093026	-4.944578	-3.457240
H	-0.812398	-5.156806	-2.435609
H	0.424663	-6.290419	-1.917248
C	2.571185	-4.930371	-3.076687
H	0.808530	-3.961135	-3.857245
H	0.893359	-5.685097	-4.238483
C	2.861460	-3.797569	-2.093538
H	2.829911	-5.894355	-2.617228
H	3.205932	-4.817771	-3.961634
H	2.832885	-2.838657	-2.631301
H	3.881591	-3.883074	-1.710515
C	4.528283	-4.484108	0.765658
C	5.852261	-5.204137	0.521351
H	3.735018	-4.927887	0.159860
H	4.221861	-4.643999	1.809637
C	6.976644	-4.506456	1.281458
H	5.763080	-6.251918	0.826258
H	6.083675	-5.200127	-0.553223
C	7.158075	-3.089668	0.743164
H	6.718867	-4.467723	2.347754
H	7.916090	-5.062323	1.196030
H	7.632578	-3.145726	-0.247018
H	7.845090	-2.520392	1.378916

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M06-2X/6-31G* Energy = -8271.58624139

M06-2X/6-31G* Free Energy = -8270.700460

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.56226939

Lowest Frequency = 8.6837

M06-2X/6-31G* Geometry

C	-1.652434	1.652388	3.562638
C	-2.093971	2.728838	-0.336899
C	-2.813705	1.175920	3.116996
H	-0.693415	1.311116	3.173819
H	-1.620968	2.406886	4.344144
C	-2.928958	0.141347	2.032489
H	-3.750521	1.548832	3.534176
N	-2.082023	1.556867	0.208994
C	-3.320888	3.566107	-0.310970
C	-0.890566	3.240760	-1.010453
C	-3.239538	0.762833	0.659293
C	-3.526260	-0.294747	-0.395617

H	-4.106807	1.421695	0.734207
H	-1.147280	1.014974	0.324564
H	-2.001034	-0.437578	1.953676
H	-3.736769	-0.563357	2.255532
C	5.239727	-1.679806	0.057695
C	6.249531	-0.720197	-0.091720
C	3.889714	-1.279186	-0.033968
C	3.578476	0.082679	-0.127339
C	4.578067	1.057057	-0.271018
C	5.898975	0.616002	-0.281025
C	2.782449	-2.283506	-0.000319
C	2.659629	-3.298484	-0.972285
C	1.652139	-4.258893	-0.819398
C	0.753393	-4.154051	0.241985
C	0.759536	-3.086153	1.135985
C	1.812152	-2.169767	0.994394
O	2.254739	0.465879	-0.159379
O	1.881919	-1.066482	1.820603
P	1.285032	0.312695	1.168914
O	-0.075277	0.002327	0.575056
O	1.448764	1.412538	2.147596
C	4.281462	2.505226	-0.412091
C	-0.353009	-2.904694	2.102551
C	4.951892	3.261652	-1.416366
C	4.740125	4.609596	-1.549184
C	3.826995	5.287558	-0.697872
C	3.148992	4.535865	0.300410
C	3.405480	3.148689	0.432726
C	-1.655156	-3.363911	1.738375
C	-2.722221	-3.227583	2.585116
C	-2.574659	-2.598610	3.848962
C	-1.287126	-2.121361	4.218147
C	-0.192830	-2.301158	3.333401
H	6.690240	1.356535	-0.382337
H	-0.020237	-4.912404	0.336739
H	5.635229	2.749384	-2.088798
H	5.260052	5.174932	-2.319225
H	0.781845	-1.938712	3.640538
H	-3.707824	-3.573217	2.281566
H	-1.806563	-3.789725	0.749986
H	2.892581	2.602689	1.219428
C	0.081817	2.355275	-1.504867
C	1.189071	2.850792	-2.178549
C	1.330663	4.222781	-2.377481
C	0.379020	5.109132	-1.874818
C	-0.730019	4.623392	-1.196862
H	-0.025268	1.283268	-1.374024
H	1.945331	2.161535	-2.538820
H	2.197260	4.603422	-2.907933
H	-1.466831	5.312220	-0.796226
H	0.515522	6.178572	-1.996113
C	-3.876236	4.034995	-1.504025
C	-5.022327	4.822754	-1.468262
C	-5.594031	5.167811	-0.245451
C	-5.025087	4.720960	0.945868
C	-3.892622	3.914219	0.917233
H	-3.435025	3.555340	1.836538
H	-3.412532	3.775706	-2.451231
H	-5.463814	5.173791	-2.395145
H	-6.481934	5.791599	-0.220399
H	-5.462964	5.001177	1.898353
C	-2.551201	-1.234131	-0.748387
C	-2.864592	-2.193769	-1.701491

C	-4.114647	-2.257840	-2.309355
C	-5.061706	-1.311983	-1.941361
Br	-1.543489	-3.464606	-2.181679
H	-4.341035	-3.017564	-3.047586
C	-4.782406	-0.329005	-0.997768
H	-5.542703	0.400858	-0.737615
H	-1.560802	-1.210802	-0.297211
Br	-6.771907	-1.361085	-2.748329
C	-1.132157	-1.458721	5.465664
C	-2.205643	-1.270020	6.296739
C	-3.489569	-1.737879	5.923234
C	-3.668288	-2.388265	4.728664
H	-0.146293	-1.092375	5.739394
H	-2.077456	-0.755657	7.244098
H	-4.650809	-2.751900	4.436845
H	-4.332376	-1.580728	6.589553
C	2.201006	5.185799	1.135161
C	1.939443	6.523250	0.981623
C	2.618080	7.274806	-0.011139
C	3.538887	6.671501	-0.830856
H	1.682851	4.588012	1.881051
H	1.210969	7.014676	1.619634
H	2.406901	8.334859	-0.118466
H	4.060850	7.244937	-1.593476
C	7.721554	-1.087588	-0.065428
C	7.994456	-2.424474	0.618581
H	8.286551	-0.283645	0.419012
H	8.088520	-1.139152	-1.100555
C	7.035983	-3.481362	0.077517
H	7.844666	-2.324402	1.701386
H	9.037320	-2.719113	0.462238
C	5.595476	-3.111595	0.423323
H	7.149270	-3.549178	-1.013739
H	7.269720	-4.469903	0.486090
H	4.901808	-3.821462	-0.032250
H	5.449911	-3.217602	1.508256
C	3.517949	-3.266624	-2.225641
C	3.473524	-4.563951	-3.031349
H	4.552380	-3.002774	-1.991046
H	3.142328	-2.442926	-2.850005
C	2.035193	-5.052060	-3.183617
H	3.941561	-4.403743	-4.008051
H	4.060214	-5.338510	-2.518169
C	1.474966	-5.395861	-1.806723
H	1.423762	-4.259020	-3.636340
H	1.982045	-5.923728	-3.843886
H	1.983416	-6.292991	-1.426354
H	0.410734	-5.654748	-1.872136

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M06-2X/6-31G* Energy = -8271.58559184

M06-2X/6-31G* Free Energy = -8270.700080

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.56199716

Lowest Frequency = 11.5688

M06-2X/6-31G* Geometry

C	-1.546250	3.007013	-2.770634
C	-2.200738	2.659308	0.966017
C	-2.657306	2.274828	-2.706613
H	-0.590915	2.617459	-2.417609
H	-1.547607	4.013765	-3.180868
C	-2.702743	0.897802	-2.101467
H	-3.600525	2.687439	-3.067568
N	-2.034843	1.707801	0.113723

C	-1.048349	3.135171	1.760749
C	-3.523058	3.301590	1.181821
C	-3.070581	0.950245	-0.602293
C	-3.168002	-0.439346	0.010361
H	-4.030295	1.457028	-0.472310
H	-1.007315	1.385561	-0.156731
H	-1.737815	0.390376	-2.220895
H	-3.459613	0.274642	-2.590779
C	4.880662	-2.167851	-0.501251
C	4.776615	-3.532909	-0.798334
C	3.705733	-1.428955	-0.260318
C	2.453768	-2.027244	-0.451423
C	2.330531	-3.397250	-0.734453
C	3.514367	-4.119336	-0.877027
C	3.757124	0.005495	0.157307
C	4.326214	0.425994	1.377913
C	4.343399	1.794524	1.683860
C	3.758612	2.710339	0.804541
C	3.121451	2.313609	-0.366110
C	3.143898	0.946900	-0.665374
O	1.325275	-1.249003	-0.292188
O	2.450509	0.483544	-1.766271
P	0.954945	-0.075968	-1.395654
O	0.282836	0.987260	-0.549328
O	0.303025	-0.602830	-2.614604
C	1.018659	-4.085930	-0.817031
C	2.397519	3.278582	-1.227652
C	0.854853	-5.338449	-0.158391
C	-0.359780	-5.971062	-0.132399
C	-1.492828	-5.391457	-0.761998
C	-1.322889	-4.166970	-1.463809
C	-0.054304	-3.537110	-1.482026
C	2.570189	3.255731	-2.641452
C	1.921782	4.156726	-3.442050
C	1.042652	5.124429	-2.888221
C	0.846705	5.140748	-1.479306
C	1.549266	4.209613	-0.671552
H	3.445483	-5.180247	-1.109859
H	3.770321	3.769218	1.058078
H	1.702150	-5.770392	0.367523
H	-0.477683	-6.914232	0.395507
H	1.386393	4.219618	0.404709
H	2.064515	4.134607	-4.519196
H	3.225321	2.508822	-3.076434
H	0.051367	-2.607876	-2.033619
C	-4.155740	3.950957	0.117333
C	-5.372599	4.591373	0.328575
C	-5.960991	4.574275	1.591542
C	-5.325167	3.933035	2.652945
C	-4.097282	3.310491	2.455462
H	-3.676018	3.961345	-0.858421
H	-5.860427	5.104660	-0.493656
H	-6.914334	5.067976	1.751141
H	-3.585368	2.823914	3.280640
H	-5.781580	3.924477	3.637265
C	-1.032861	4.457108	2.228676
C	0.046662	4.921631	2.970444
C	1.102870	4.063028	3.274622
C	1.081403	2.741416	2.833090
C	0.013796	2.274831	2.075164
H	0.014452	1.247788	1.728915
H	-1.859063	5.121197	1.993275
H	0.061478	5.950443	3.315399

H	1.941098	4.424388	3.863194
H	1.901235	2.069167	3.065916
C	-2.060122	-1.066990	0.580597
C	-2.211682	-2.323796	1.154515
C	-3.425490	-2.998760	1.135334
C	-4.500562	-2.372072	0.519645
Br	-0.725148	-3.129167	1.977245
H	-3.519992	-3.992685	1.555306
C	-4.396823	-1.098919	-0.025253
H	-5.266916	-0.630397	-0.475006
H	-1.078591	-0.604584	0.583110
Br	-6.147531	-3.291680	0.403552
C	-0.067786	6.076425	-0.925944
C	-0.755046	6.949051	-1.730770
C	-0.552743	6.937366	-3.133120
C	0.329235	6.048859	-3.695105
H	-0.205953	6.086855	0.152217
H	-1.452322	7.658949	-1.295881
H	0.487642	6.031865	-4.770493
H	-1.097004	7.636804	-3.760258
C	-2.444068	-3.572770	-2.105709
C	-3.678833	-4.164463	-2.041586
C	-3.852157	-5.380907	-1.332776
C	-2.784994	-5.979775	-0.711873
H	-2.293791	-2.631232	-2.629839
H	-4.538889	-3.696125	-2.512398
H	-4.839410	-5.829567	-1.277444
H	-2.913388	-6.914600	-0.171170
C	5.999825	-4.403143	-1.019239
C	7.250246	-3.602404	-1.374461
H	5.781986	-5.143048	-1.797221
H	6.194834	-4.973754	-0.099943
C	7.406149	-2.433995	-0.404844
H	7.161807	-3.211042	-2.396214
H	8.130199	-4.253601	-1.353027
C	6.230042	-1.471499	-0.551307
H	7.444181	-2.818769	0.624086
H	8.344823	-1.899007	-0.582472
H	6.292709	-0.675999	0.195343
H	6.302841	-0.964172	-1.524350
C	4.798592	-0.598240	2.395742
C	5.716187	-0.006564	3.463170
H	5.283326	-1.445058	1.904168
H	3.904794	-1.017753	2.880567
C	5.097066	1.259536	4.048747
H	5.900579	-0.750654	4.244667
H	6.689733	0.240806	3.017783
C	4.976525	2.321321	2.958428
H	4.102090	1.019786	4.449008
H	5.694601	1.643391	4.882063
H	5.979712	2.704856	2.724915
H	4.400543	3.183278	3.318275

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M06-2X/6-31G* Energy = -8271.58624145

M06-2X/6-31G* Free Energy = -8270.700390

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.56226686

Lowest Frequency = 8.7598

M06-2X/6-31G* Geometry

C	-1.651159	1.657001	3.560191
C	-2.089774	2.731333	-0.339260
C	-2.813088	1.181780	3.114934
H	-0.692592	1.314431	3.171420

H	-1.618721	2.411886	4.341287
C	-2.929845	0.146808	2.031000
H	-3.749374	1.556074	3.532065
N	-2.080409	1.559218	0.206398
C	-3.314848	3.571314	-0.313381
C	-0.885198	3.240712	-1.012671
C	-3.239423	0.767783	0.657263
C	-3.527693	-0.290634	-0.396390
H	-4.105632	1.428135	0.731401
H	-1.147019	1.015247	0.322567
H	-2.002705	-0.433458	1.952412
H	-3.738609	-0.556666	2.254439
C	2.655800	-3.301579	-0.971375
C	1.646844	-4.260480	-0.818608
C	2.779764	-2.286562	0.000404
C	1.809259	-2.171174	0.994750
C	0.755181	-3.085911	1.136125
C	0.747824	-4.154040	0.242394
C	3.888478	-1.283799	-0.033107
C	5.237923	-1.686183	0.059216
C	6.249022	-0.727862	-0.089980
C	5.900286	0.608739	-0.279715
C	4.579941	1.051551	-0.270407
C	3.579099	0.078471	-0.126961
O	1.880307	-1.067718	1.820628
O	2.255870	0.463311	-0.159783
P	1.285279	0.311934	1.168015
O	-0.074888	0.002943	0.573257
O	1.449730	1.411916	2.146431
C	-0.357407	-2.902517	2.102297
C	4.285291	2.500061	-0.411941
C	-1.660117	-3.360129	1.738082
C	-2.727164	-3.222050	2.584574
C	-2.579008	-2.592815	3.848222
C	-1.290922	-2.117036	4.217393
C	-0.196709	-2.298615	3.332908
C	4.957165	3.255303	-1.416181
C	4.747362	4.603486	-1.549473
C	3.834884	5.283007	-0.698677
C	3.155544	4.532570	0.299654
C	3.409935	3.145018	0.432375
H	-0.026888	-4.911293	0.337064
H	6.692589	1.348197	-0.380788
H	-1.812007	-3.786077	0.749833
H	-3.713170	-3.566446	2.280924
H	2.895973	2.600019	1.219083
H	5.268351	5.167860	-2.319501
H	5.640003	2.741902	-2.088253
H	0.778369	-1.937258	3.640064
C	0.085236	2.353176	-1.507191
C	1.193824	2.846398	-2.180419
C	1.338656	4.218108	-2.378817
C	0.388798	5.106458	-1.876267
C	-0.721493	4.623045	-1.198699
H	-0.024358	1.281394	-1.376644
H	1.948583	2.155510	-2.540723
H	2.206349	4.596949	-2.908799
H	-1.456780	5.313450	-0.797973
H	0.527699	6.175628	-1.997222
C	-3.886140	3.920584	0.914683
C	-5.016846	4.729832	0.943070
C	-5.584487	5.178041	-0.248350
C	-5.013187	4.831848	-1.471046

C	-3.868828	4.041578	-1.506558
H	-3.405418	3.781377	-2.453657
H	-3.429562	3.560698	1.834098
H	-5.454340	5.010929	1.895474
H	-6.471030	5.803772	-0.223483
H	-5.453620	5.183966	-2.398022
C	-2.553481	-1.230950	-0.749083
C	-2.868507	-2.191722	-1.700516
C	-4.119341	-2.256019	-2.306776
C	-5.065519	-1.309231	-1.938889
Br	-1.548727	-3.464002	-2.180594
H	-4.346953	-3.016640	-3.043710
C	-4.784591	-0.325119	-0.996946
H	-5.544270	0.405377	-0.736766
H	-1.562551	-1.207667	-0.299007
Br	-6.776736	-1.358631	-2.743646
C	2.208358	5.184134	1.134026
C	1.948801	6.521945	0.980067
C	2.628745	7.272227	-0.012749
C	3.548827	6.667318	-0.832129
H	1.689149	4.587334	1.879978
H	1.220932	7.014599	1.617824
H	4.071775	7.239786	-1.594799
H	2.419163	8.332558	-0.120440
C	-1.135309	-1.454064	5.464656
C	-2.208666	-1.263704	6.295523
C	-3.493130	-1.730109	5.922032
C	-3.672498	-2.380737	4.727686
H	-0.149032	-1.088806	5.738364
H	-2.079958	-0.749107	7.242685
H	-4.335828	-1.571664	6.588184
H	-4.655436	-2.743243	4.435861
C	1.468538	-5.397630	-1.805519
C	2.030039	-5.055369	-3.182271
H	0.403963	-5.655002	-1.871372
H	1.975442	-6.295315	-1.424384
C	3.468923	-4.569061	-3.029456
H	1.419916	-4.261776	-3.635796
H	1.976106	-5.927340	-3.842078
C	3.514547	-3.271324	-2.224482
H	4.054321	-5.344074	-2.515469
H	3.937735	-4.410031	-4.005981
H	3.139962	-2.447600	-2.849445
H	4.549178	-3.008410	-1.989720
C	5.591707	-3.118366	0.425242
C	7.031883	-3.489977	0.080041
H	4.897297	-3.827404	-0.030493
H	5.445595	-3.224025	1.510138
C	7.991459	-2.434229	0.621364
H	7.264230	-4.478763	0.488822
H	7.145513	-3.558063	-1.011168
C	7.720569	-1.097104	-0.062967
H	7.841299	-2.333792	1.704090
H	9.034021	-2.730217	0.465544
H	8.087927	-1.149284	-1.097924
H	8.286360	-0.293801	0.421617

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M06-2X/6-31G* Energy = -8271.58468891

M06-2X/6-31G* Free Energy = -8270.699324

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.56174409

Lowest Frequency = 7.7702

M06-2X/6-31G* Geometry

C	-1.706639	1.331529	3.820530
C	-1.909424	2.967114	0.079717
C	-2.884925	1.035417	3.274763
H	-0.766497	0.946169	3.427004
H	-1.641515	1.974575	4.694115
C	-3.046295	0.165486	2.059154
H	-3.800844	1.446514	3.702392
N	-1.997219	1.743846	0.488258
C	-3.097966	3.859627	0.131318
C	-0.644601	3.491846	-0.456456
C	-3.234792	0.993169	0.776933
C	-3.557017	0.129996	-0.432253
H	-4.048000	1.707485	0.916134
H	-1.115048	1.120837	0.584748
H	-2.175557	-0.488559	1.934550
H	-3.928310	-0.475756	2.157343
C	2.284026	-3.416979	-1.199371
C	1.178672	-4.276279	-1.220843
C	2.457559	-2.563316	-0.089327
C	1.450944	-2.479998	0.871986
C	0.303659	-3.286692	0.840550
C	0.238842	-4.218543	-0.192082
C	3.663466	-1.693355	0.065714
C	4.960620	-2.246276	0.140372
C	6.070961	-1.392041	0.160125
C	5.871720	-0.011083	0.153818
C	4.603663	0.560042	0.189169
C	3.502847	-0.306756	0.164144
O	1.594374	-1.525471	1.856034
O	2.234913	0.232852	0.149282
P	1.198263	0.002510	1.416962
O	-0.160554	-0.032798	0.745043
O	1.458505	0.900676	2.563617
C	-0.836794	-3.120874	1.776852
C	4.446247	2.036485	0.228908
C	-2.155606	-3.382533	1.295475
C	-3.249886	-3.255216	2.108047
C	-3.111845	-2.831017	3.455495
C	-1.806516	-2.547545	3.942847
C	-0.687001	-2.715897	3.087715
C	3.672583	2.658961	1.250196
C	3.558140	4.022354	1.297545
C	4.180192	4.847572	0.325029
C	4.948155	4.232300	-0.702581
C	5.075203	2.818947	-0.713784
H	-0.611269	-4.895309	-0.234882
H	6.736430	0.649316	0.176622
H	-2.291584	-3.645562	0.249731
H	-4.246219	-3.448010	1.716710
H	5.657530	2.350427	-1.504805
H	2.963399	4.489891	2.078247
H	3.168357	2.043998	1.989273
H	0.300025	-2.505787	3.484425
C	0.349997	2.624885	-0.939899
C	1.516020	3.144635	-1.485375
C	1.696908	4.524708	-1.568900
C	0.721880	5.390185	-1.074420
C	-0.444768	4.880914	-0.522370
H	0.216362	1.548106	-0.903134
H	2.286569	2.466167	-1.836510
H	2.605033	4.930071	-2.006544
H	-1.201124	5.555055	-0.133833
H	0.879285	6.463111	-1.116957

C	-3.597982	4.434602	-1.038859
C	-4.711091	5.267307	-0.975918
C	-5.303659	5.548769	0.253133
C	-4.789681	4.992754	1.423423
C	-3.691270	4.141584	1.365959
H	-3.281240	3.691787	2.267642
H	-3.118484	4.222838	-1.990097
H	-5.110660	5.701859	-1.886290
H	-6.165663	6.206641	0.299864
H	-5.244950	5.220806	2.381652
C	-2.652729	-0.838349	-0.881469
C	-2.999122	-1.611830	-1.981310
C	-4.213468	-1.461588	-2.644450
C	-5.089005	-0.490643	-2.178764
Br	-1.777003	-2.922920	-2.595517
H	-4.465288	-2.078098	-3.498801
C	-4.774551	0.309899	-1.085772
H	-5.477120	1.066738	-0.751222
H	-1.690659	-0.976568	-0.390554
Br	-6.745983	-0.245594	-3.057955
C	5.524682	5.049160	-1.712217
C	5.335279	6.408131	-1.709693
C	4.570660	7.020552	-0.685194
C	4.014630	6.257348	0.310110
H	6.110844	4.574590	-2.495345
H	5.773839	7.021135	-2.491128
H	3.423683	6.718648	1.097673
H	4.431132	8.097333	-0.691394
C	-1.657643	-2.085392	5.278285
C	-2.752329	-1.904357	6.083078
C	-4.052820	-2.179744	5.593376
C	-4.227096	-2.634140	4.310744
H	-0.657723	-1.864816	5.642328
H	-2.627683	-1.543309	7.099229
H	-4.912131	-2.030971	6.240255
H	-5.222493	-2.848955	3.928942
C	0.940485	-5.245496	-2.362317
C	1.607356	-4.784998	-3.655063
H	-0.139498	-5.375556	-2.505863
H	1.332775	-6.235211	-2.089195
C	3.076711	-4.476412	-3.378991
H	1.104584	-3.878412	-4.020041
H	1.503510	-5.551257	-4.430077
C	3.205045	-3.308278	-2.402825
H	3.554841	-5.369274	-2.952641
H	3.610934	-4.239372	-4.304791
H	4.246614	-3.184912	-2.095517
H	2.942767	-2.375467	-2.922949
C	5.149320	-3.745325	0.307353
C	6.555964	-4.218985	-0.050648
H	4.403725	-4.304823	-0.261463
H	4.949944	-3.983734	1.362285
C	7.596459	-3.361044	0.663310
H	6.667282	-5.274962	0.216388
H	6.706944	-4.143976	-1.136882
C	7.494051	-1.918706	0.174611
H	7.412844	-3.400048	1.744834
H	8.608399	-3.742982	0.493192
H	7.898635	-1.862058	-0.846122
H	8.117917	-1.258534	0.787148

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M06-2X/6-31G* Energy = -8271.58468913

M06-2X/6-31G* Free Energy = -8270.699317

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.56173928

Lowest Frequency = 7.7783

M06-2X/6-31G* Geometry

C	-1.706574	1.332227	3.820210
C	-1.908900	2.967451	0.079367
C	-2.884894	1.036210	3.274451
H	-0.766497	0.946742	3.426648
H	-1.641380	1.975247	4.693800
C	-3.046339	0.166240	2.058888
H	-3.800774	1.447405	3.702073
N	-1.996954	1.744174	0.487827
C	-3.097236	3.860226	0.130923
C	-0.643927	3.491981	-0.456669
C	-3.234683	0.993802	0.776575
C	-3.557027	0.130440	-0.432459
H	-4.047774	1.708280	0.915646
H	-1.114948	1.120933	0.584463
H	-2.175667	-0.487922	1.934382
H	-3.928413	-0.474923	2.157132
C	4.960114	-2.247042	0.140274
C	6.070641	-1.393057	0.159936
C	3.663059	-1.693851	0.065690
C	3.502728	-0.307216	0.164088
C	4.603759	0.559324	0.189038
C	5.871693	-0.012045	0.153627
C	2.457004	-2.563630	-0.089180
C	2.283253	-3.417470	-1.199059
C	1.177805	-4.276639	-1.220286
C	0.238051	-4.218596	-0.191461
C	0.303077	-3.286576	0.840989
C	1.450480	-2.480012	0.872209
O	2.234946	0.232699	0.149228
O	1.594129	-1.525368	1.856086
P	1.198144	0.002580	1.416865
O	-0.160592	-0.032749	0.744761
O	1.458303	0.900870	2.563433
C	4.446673	2.035809	0.228711
C	-0.837315	-3.120395	1.777296
C	3.673177	2.658516	1.249982
C	3.559156	4.021946	1.297314
C	4.181450	4.846962	0.324783
C	4.949192	4.231450	-0.702855
C	5.075828	2.818059	-0.714028
C	-2.156167	-3.381980	1.296002
C	-3.250414	-3.254314	2.108566
C	-3.112285	-2.829810	3.455909
C	-1.806897	-2.546486	3.943197
C	-0.687424	-2.715201	3.088082
H	6.736543	0.648170	0.176381
H	-0.612166	-4.895245	-0.234086
H	3.168762	2.043704	1.989065
H	2.964566	4.489678	2.078016
H	0.299649	-2.505205	3.484743
H	-4.246781	-3.447072	1.717296
H	-2.292194	-3.645269	0.250327
H	5.658008	2.349343	-1.505040
C	0.350557	2.624833	-0.940009
C	1.516714	3.144353	-1.485421
C	1.697836	4.524389	-1.569006
C	0.722932	5.390053	-1.074612
C	-0.443836	4.881010	-0.522607
H	0.216758	1.548071	-0.903199
H	2.287184	2.465739	-1.836458

H	2.606040	4.929578	-2.006640
H	-1.200063	5.555321	-0.134117
H	0.880518	6.462952	-1.117164
C	-3.596845	4.435538	-1.039277
C	-4.709744	5.268530	-0.976448
C	-5.302503	5.549943	0.252524
C	-4.788937	4.993588	1.422832
C	-3.690744	4.142129	1.365469
H	-3.281028	3.692059	2.267162
H	-3.117187	4.223812	-1.990444
H	-5.108997	5.703339	-1.886837
H	-6.164334	6.208050	0.299191
H	-5.244367	5.221593	2.380995
C	-2.652945	-0.838211	-0.881420
C	-2.999524	-1.611919	-1.981042
C	-4.213837	-1.461576	-2.644221
C	-5.089160	-0.490295	-2.178816
Br	-1.777761	-2.923524	-2.594877
H	-4.465808	-2.078285	-3.498385
C	-4.774523	0.310448	-1.086023
H	-5.476926	1.067525	-0.751656
H	-1.690893	-0.976495	-0.390480
Br	-6.746040	-0.245095	-3.058134
C	-1.657925	-2.084139	5.278559
C	-2.752571	-1.902734	6.083325
C	-4.053119	-2.177924	5.593669
C	-4.227491	-2.632527	4.311122
H	-0.657956	-1.863719	5.642564
H	-2.627839	-1.541550	7.099418
H	-5.222937	-2.847213	3.929373
H	-4.912408	-2.028832	6.240506
C	5.525940	5.048125	-1.712512
C	5.336988	6.407160	-1.709973
C	4.572609	7.019822	-0.685442
C	4.016351	6.256794	0.309870
H	6.111906	4.573363	-2.495671
H	5.775726	7.020022	-2.491419
H	4.433439	8.096650	-0.691612
H	3.425577	6.718295	1.097446
C	7.493617	-1.920017	0.174327
C	7.595769	-3.362327	0.663160
H	8.117693	-1.259899	0.786710
H	7.898100	-1.863580	-0.846463
C	6.555056	-4.220106	-0.050687
H	7.412205	-3.401209	1.744696
H	8.607620	-3.744492	0.493003
C	5.148517	-3.746123	0.307312
H	6.706022	-4.145225	-1.136930
H	6.666145	-5.276085	0.216445
H	4.402812	-4.305523	-0.261459
H	4.949107	-3.984427	1.362266
C	3.204168	-3.309022	-2.402617
C	3.075635	-4.477282	-3.378610
H	4.245775	-3.185697	-2.095418
H	2.941912	-2.376263	-2.922847
C	1.606216	-4.785791	-3.654461
H	3.609747	-4.240405	-4.304519
H	3.553746	-5.370125	-2.952204
C	0.939446	-5.246030	-2.361570
H	1.103472	-3.879224	-4.019520
H	1.502231	-5.552173	-4.429338
H	1.331691	-6.235728	-2.088313
H	-0.140561	-5.376063	-2.505002

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M06-2X/6-31G* Energy = -8271.57807576

M06-2X/6-31G* Free Energy = -8270.693022

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.56140849

Lowest Frequency = 9.2538

M06-2X/6-31G* Geometry

C	-0.389705	-0.202361	2.897717
C	0.814347	3.177032	1.338270
C	0.914246	0.000936	3.071493
H	-0.787291	-0.511625	1.931636
H	-1.099400	-0.077294	3.711417
C	1.917470	-0.128484	1.958795
H	1.295322	0.314805	4.044269
N	1.190892	1.985952	0.993678
C	-0.527526	3.652510	0.981704
C	1.727733	4.064281	2.097813
C	2.381125	1.261778	1.471916
C	3.441886	1.174974	0.392632
H	2.784667	1.820227	2.321183
H	0.567086	1.388961	0.374924
H	1.482309	-0.669754	1.113420
H	2.812944	-0.671708	2.282714
C	-4.494627	-3.135562	-0.092804
C	-5.687257	-2.672491	-0.663296
C	-3.413989	-2.241217	0.058971
C	-3.498308	-0.959899	-0.485919
C	-4.689242	-0.474980	-1.042810
C	-5.772262	-1.346492	-1.092071
C	-2.168837	-2.630274	0.786775
C	-2.196919	-2.988489	2.151575
C	-1.016936	-3.431221	2.759279
C	0.146605	-3.533320	1.996628
C	0.222372	-3.131539	0.663688
C	-0.952127	-2.603795	0.099165
O	-2.398846	-0.134339	-0.387346
O	-0.941224	-2.086501	-1.173970
P	-1.067787	-0.447975	-1.334906
O	0.052017	0.192033	-0.540744
O	-1.296903	-0.149446	-2.761053
C	-4.821945	0.931392	-1.500466
C	1.484023	-3.350997	-0.093786
C	-3.926444	1.475757	-2.464845
C	-4.035110	2.787302	-2.843917
C	-5.021075	3.639233	-2.280258
C	-5.923691	3.099318	-1.321592
C	-5.808561	1.729896	-0.964409
C	2.014688	-2.399749	-1.012401
C	3.192495	-2.642024	-1.668378
C	3.919311	-3.842356	-1.462013
C	3.397020	-4.803577	-0.554758
C	2.176278	-4.527421	0.109646
H	-6.704091	-0.988410	-1.525608
H	1.053629	-3.894771	2.476884
H	-3.149576	0.843881	-2.885869
H	-3.346234	3.198020	-3.577543
H	1.770297	-5.283815	0.777263
H	3.580636	-1.911330	-2.372431
H	1.481263	-1.472162	-1.180065
H	-6.486371	1.323583	-0.216288
C	3.022516	4.310250	1.627089
C	3.868641	5.153953	2.337959
C	3.431190	5.742182	3.523178

C	2.141219	5.500678	3.991945
C	1.282604	4.674677	3.274918
H	3.355742	3.851692	0.700181
H	4.868560	5.350543	1.965355
H	4.095618	6.395055	4.080232
H	0.271557	4.490078	3.625481
H	1.800866	5.960979	4.913585
C	-1.563825	2.737298	0.736628
C	-2.829685	3.200877	0.408409
C	-3.076212	4.571323	0.323710
C	-2.047925	5.483989	0.558496
C	-0.778436	5.031530	0.891166
H	0.024654	5.740976	1.062873
H	-1.396846	1.667149	0.812753
H	-3.623380	2.485674	0.220511
H	-4.072674	4.924908	0.070880
H	-2.235963	6.549685	0.479308
C	3.096924	0.950765	-0.941077
C	4.111235	0.861524	-1.886787
C	5.454541	0.974756	-1.545665
C	5.769217	1.194445	-0.210620
Br	3.648775	0.561739	-3.691108
H	6.229564	0.899695	-2.298683
C	4.781418	1.300514	0.760920
H	5.057202	1.485721	1.794932
H	2.057152	0.835613	-1.240031
Br	7.582870	1.374525	0.291529
C	4.111901	-6.013873	-0.348377
C	5.290085	-6.251875	-1.007443
C	5.811997	-5.291088	-1.909001
C	5.141002	-4.116057	-2.130422
H	3.705881	-6.748487	0.342560
H	5.828773	-7.180020	-0.842732
H	5.531963	-3.374855	-2.823015
H	6.745405	-5.492538	-2.425561
C	-6.882057	3.958521	-0.720091
C	-6.940146	5.288416	-1.052872
C	-6.046833	5.823701	-2.014265
C	-5.113909	5.016119	-2.614380
H	-7.566465	3.542478	0.015049
H	-7.674560	5.935942	-0.583719
H	-6.106304	6.876213	-2.274124
H	-4.423035	5.419683	-3.350227
C	-6.906631	-3.563186	-0.812844
C	-6.572098	-5.051394	-0.755707
H	-7.614637	-3.328230	-0.005152
H	-7.419858	-3.318865	-1.749378
C	-5.666698	-5.327846	0.441147
H	-6.052756	-5.349954	-1.675457
H	-7.493507	-5.640095	-0.698831
C	-4.334206	-4.601998	0.270723
H	-6.162775	-4.981132	1.358829
H	-5.488268	-6.401583	0.559285
H	-3.719402	-4.720034	1.166361
H	-3.765283	-5.080875	-0.539211
C	-3.455353	-2.774942	2.975038
C	-3.430605	-3.515020	4.310151
H	-4.347978	-3.047335	2.406791
H	-3.549431	-1.694575	3.163627
C	-2.117639	-3.241781	5.038051
H	-4.288803	-3.208876	4.917257
H	-3.529419	-4.595345	4.134870
C	-0.953411	-3.805265	4.227700

H	-1.992845	-2.157046	5.157323
H	-2.122586	-3.678044	6.042293
H	-0.954508	-4.900796	4.317251
H	0.002625	-3.463396	4.640485

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M06-2X/6-31G* Energy = -8271.58751627

M06-2X/6-31G* Free Energy = -8270.701943

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.56157414

Lowest Frequency = 10.8204

M06-2X/6-31G* Geometry

C	-2.267895	1.181734	-3.814132
C	-2.652389	2.903480	-0.385623
C	-3.182423	0.733732	-2.956659
H	-1.219302	0.901170	-3.718366
H	-2.543816	1.840217	-4.633424
C	-2.865910	-0.181646	-1.810001
H	-4.227466	1.032494	-3.060896
N	-2.275408	1.665406	-0.345835
C	-1.646788	3.934040	-0.680216
C	-4.055747	3.303058	-0.131137
C	-3.142252	0.483265	-0.441787
C	-2.910728	-0.500819	0.686750
H	-4.181881	0.817764	-0.426092
H	-1.198823	1.481645	-0.353925
H	-1.818320	-0.512121	-1.855760
H	-3.494658	-1.080313	-1.845044
C	4.207519	-2.624639	-1.329122
C	3.852752	-3.523892	-2.345223
C	3.203604	-1.857174	-0.712880
C	1.896363	-1.922630	-1.194801
C	1.514095	-2.849488	-2.167190
C	2.513137	-3.640739	-2.724838
C	3.438934	-0.961814	0.456445
C	3.763679	-1.481389	1.724735
C	3.847449	-0.600407	2.811934
C	3.621222	0.762176	2.612821
C	3.256448	1.294624	1.377440
C	3.149276	0.394224	0.312511
O	0.965851	-1.041001	-0.693945
O	2.672702	0.821230	-0.913106
P	1.074514	0.542913	-1.167131
O	0.273684	1.265015	-0.105163
O	0.761657	0.728692	-2.604327
C	0.082697	-3.004631	-2.519625
C	2.990141	2.746401	1.233075
C	-0.366262	-2.878563	-3.861217
C	-1.695518	-3.011953	-4.170446
C	-2.652800	-3.289682	-3.159542
C	-2.204282	-3.439822	-1.817359
C	-0.828700	-3.280178	-1.524965
C	2.280780	3.431914	2.259880
C	2.117961	4.790240	2.223850
C	2.659166	5.558215	1.160086
C	3.330387	4.878976	0.105583
C	3.475310	3.469283	0.165811
H	2.238161	-4.373475	-3.481656
H	3.714197	1.435587	3.462615
H	0.359060	-2.638631	-4.633075
H	-2.037301	-2.885487	-5.194408
H	4.003814	2.961386	-0.635910
H	1.573985	5.300948	3.014518
H	1.854539	2.851695	3.072889

H	-0.495189	-3.351727	-0.490510
C	-4.674513	4.233322	-0.971684
C	-5.987356	4.621538	-0.727049
C	-6.673651	4.107350	0.370916
C	-6.051620	3.197527	1.224845
C	-4.747253	2.789350	0.973016
H	-4.124644	4.636526	-1.816774
H	-6.472115	5.331067	-1.389462
H	-7.694399	4.420544	0.566167
H	-4.251538	2.084176	1.636292
H	-6.581602	2.808133	2.087846
C	-0.603636	3.647338	-1.573246
C	0.370181	4.605598	-1.817995
C	0.308314	5.843937	-1.184468
C	-0.738652	6.138616	-0.310301
C	-1.723349	5.192500	-0.064790
H	-2.535321	5.408670	0.623513
H	-0.557186	2.689416	-2.083587
H	1.184338	4.375838	-2.497871
H	1.085457	6.580510	-1.364029
H	-0.775439	7.103451	0.185522
C	-1.613891	-0.854586	1.056828
C	-1.419452	-1.873674	1.976750
C	-2.485161	-2.552826	2.558847
C	-3.768489	-2.178539	2.175149
Br	0.367672	-2.367067	2.364883
H	-2.325091	-3.361039	3.262600
C	-3.998509	-1.161269	1.255626
H	-5.015237	-0.922423	0.957813
H	-0.750341	-0.358159	0.631907
Br	-5.247484	-3.154166	2.840672
C	3.864777	5.642163	-0.968095
C	3.757749	7.010319	-0.981755
C	3.099022	7.686078	0.076486
C	2.556186	6.973391	1.116056
H	4.373633	5.119182	-1.773965
H	4.181184	7.581890	-1.802094
H	2.046023	7.483681	1.929705
H	3.025880	8.769318	0.058909
C	-3.156714	-3.686121	-0.794491
C	-4.496884	-3.746843	-1.078385
C	-4.945933	-3.588720	-2.414374
C	-4.045017	-3.375975	-3.428478
H	-2.801538	-3.804096	0.225735
H	-5.210224	-3.905328	-0.273415
H	-6.008284	-3.640973	-2.632974
H	-4.386069	-3.255218	-4.453633
C	4.880836	-4.418462	-3.012715
C	6.314910	-3.922626	-2.838302
H	4.636608	-4.521619	-4.075910
H	4.799875	-5.426449	-2.581583
C	6.565866	-3.558480	-1.376714
H	6.477635	-3.033336	-3.460998
H	7.018382	-4.688838	-3.180227
C	5.664217	-2.395359	-0.970544
H	6.354493	-4.431304	-0.743163
H	7.614714	-3.289520	-1.214503
H	5.771299	-2.170494	0.094277
H	5.995226	-1.487527	-1.495276
C	3.873692	-2.985064	1.920380
C	4.405733	-3.392151	3.294281
H	4.487313	-3.437116	1.136171
H	2.870981	-3.413021	1.772262

C	3.753465	-2.560250	4.394584
H	4.231243	-4.461721	3.449688
H	5.492485	-3.237042	3.330372
C	4.146922	-1.096897	4.212561
H	2.660730	-2.655979	4.329307
H	4.053343	-2.914392	5.386194
H	5.221061	-0.988826	4.420035
H	3.626457	-0.461475	4.937350

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M06-2X/6-31G* Energy = -8271.58751601

M06-2X/6-31G* Free Energy = -8270.701928

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.56157193

Lowest Frequency = 10.8464

M06-2X/6-31G* Geometry

C	-2.266912	1.178918	-3.815766
C	-2.653936	2.901618	-0.387002
C	-3.181501	0.730753	-2.958441
H	-1.218190	0.899013	-3.719561
H	-2.542970	1.836926	-4.635391
C	-2.865042	-0.184112	-1.811352
H	-4.226658	1.028936	-3.063200
N	-2.276195	1.663774	-0.347583
C	-1.649054	3.932967	-0.681289
C	-4.057551	3.300193	-0.132240
C	-3.142302	0.481117	-0.443471
C	-2.910552	-0.502313	0.685582
H	-4.182154	0.814976	-0.428320
H	-1.199435	1.480662	-0.355578
H	-1.817290	-0.514176	-1.856535
H	-3.493393	-1.083057	-1.846394
C	3.764366	-1.479259	1.724926
C	3.847323	-0.598338	2.812235
C	3.439513	-0.959757	0.456614
C	3.149051	0.396110	0.312788
C	3.255322	1.296481	1.377851
C	3.620145	0.764116	2.613248
C	3.204845	-1.855173	-0.712795
C	4.209255	-2.622171	-1.328868
C	3.855084	-3.521726	-2.344875
C	2.515529	-3.639463	-2.724520
C	1.516005	-2.848728	-2.167059
C	1.897710	-1.921372	-1.194858
O	2.672643	0.822945	-0.912958
O	0.966656	-1.040126	-0.694370
P	1.074771	0.543816	-1.167745
O	0.273021	1.265689	-0.106284
O	0.762507	0.729239	-2.605103
C	2.988097	2.748092	1.233530
C	0.084658	-3.005106	-2.519160
C	2.278288	3.433137	2.260345
C	2.114443	4.791340	2.224268
C	2.655062	5.559691	1.160477
C	3.326807	4.880906	0.106014
C	3.472747	3.471320	0.166260
C	-0.364698	-2.879762	-3.860685
C	-1.693894	-3.014422	-4.169643
C	-2.650740	-3.292730	-3.158487
C	-2.201824	-3.441990	-1.816319
C	-0.826318	-3.281134	-1.524236
H	3.712510	1.437472	3.463152
H	2.241042	-4.372533	-3.481193
H	1.852489	2.852664	3.073405

H	1.570137	5.301664	3.014956
H	-0.492585	-3.352100	-0.489809
H	-2.035961	-2.888514	-5.193579
H	0.360260	-2.639393	-4.632754
H	4.001657	2.963830	-0.635447
C	-4.748498	2.785620	0.971859
C	-6.053109	3.192803	1.224064
C	-6.675924	4.102483	0.370560
C	-5.990184	4.617520	-0.727362
C	-4.677111	4.230309	-0.972364
H	-4.252202	2.080513	1.634772
H	-6.582666	2.802739	2.087026
H	-7.696854	4.414901	0.566104
H	-4.127674	4.634188	-1.817416
H	-6.475563	5.326929	-1.389452
C	-0.605561	3.647295	-1.574282
C	0.367552	4.606369	-1.818650
C	0.304611	5.844507	-1.184827
C	-0.742668	6.138144	-0.310682
C	-1.726627	5.191186	-0.065506
H	-2.538824	5.406526	0.622792
H	-0.558349	2.689560	-2.084909
H	1.182006	4.377443	-2.498466
H	1.081181	6.581732	-1.364137
H	-0.780247	7.102820	0.185394
C	-3.998012	-1.162881	1.254902
C	-3.767456	-2.179417	2.175116
C	-2.483942	-2.552792	2.559081
C	-1.418545	-1.873523	1.976519
Br	-5.245912	-3.155359	2.841372
H	-2.323497	-3.360443	3.263395
C	-1.613530	-0.855200	1.055878
H	-0.750251	-0.358615	0.630587
H	-5.014866	-0.924703	0.956986
Br	0.368799	-2.365690	2.365110
C	-3.153869	-3.688585	-0.793181
C	-4.494055	-3.750481	-1.076793
C	-4.943482	-3.593384	-2.412759
C	-4.042921	-3.380352	-3.427134
H	-2.798444	-3.805775	0.227052
H	-5.207098	-3.909082	-0.271582
H	-4.384278	-3.260336	-4.452275
H	-6.005824	-3.646620	-2.631164
C	3.860741	5.644461	-0.967632
C	3.752843	7.012550	-0.981265
C	3.093585	7.687855	0.076933
C	2.551106	6.974794	1.116433
H	4.370009	5.121828	-1.773469
H	4.175982	7.584406	-1.801560
H	3.019715	8.771048	0.059369
H	2.040549	7.484744	1.930048
C	4.147027	-1.094723	4.212853
C	3.754845	-2.558438	4.394755
H	3.625921	-0.459822	4.937639
H	5.221048	-0.985736	4.420461
C	4.407671	-3.389703	3.294305
H	2.662186	-2.655140	4.329654
H	4.055190	-2.912404	5.386289
C	3.875217	-2.982880	1.920490
H	5.494311	-3.233785	3.330334
H	4.233991	-4.459423	3.449620
H	4.488944	-3.434611	1.136186
H	2.872681	-3.411314	1.772553

C	5.665792	-2.392056	-0.970196
C	6.568093	-3.554765	-1.376094
H	5.772681	-2.166956	0.094597
H	5.996369	-1.484137	-1.495060
C	6.317517	-3.919239	-2.837670
H	7.616780	-3.285233	-1.213778
H	6.357088	-4.427616	-0.742457
C	4.883707	-4.415813	-3.012185
H	6.479902	-3.029961	-3.460470
H	7.021410	-4.685165	-3.179373
H	4.803229	-5.423798	-2.580951
H	4.639631	-4.519216	-4.075393

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M06-2X/6-31G* Energy = -8271.58557565

M06-2X/6-31G* Free Energy = -8270.699533

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.56193039

Lowest Frequency = 16.4136

M06-2X/6-31G* Geometry

C	-1.432258	3.067507	-2.761703
C	-2.091128	2.735497	0.964316
C	-2.569867	2.376513	-2.705141
H	-0.493679	2.642869	-2.404204
H	-1.394603	4.074284	-3.170156
C	-2.669716	1.001110	-2.102537
H	-3.495044	2.824306	-3.070712
N	-1.965771	1.777804	0.112251
C	-0.918765	3.166745	1.755630
C	-3.387012	3.428207	1.186394
C	-3.033413	1.065447	-0.602610
C	-3.186993	-0.319849	0.008132
H	-3.971626	1.610431	-0.470597
H	-0.950809	1.411982	-0.164533
H	-1.725742	0.455961	-2.223840
H	-3.451134	0.409585	-2.592449
C	4.346327	0.259857	1.374902
C	4.421510	1.626810	1.679206
C	3.757864	-0.137774	0.155870
C	3.182153	0.827510	-0.666276
C	3.216270	2.194128	-0.367978
C	3.872745	2.565174	0.800491
C	3.647427	-1.569212	-0.260804
C	4.791028	-2.355509	-0.502589
C	4.630885	-3.715366	-0.798961
C	3.345693	-4.249651	-0.876046
C	2.192397	-3.479947	-0.732325
C	2.371880	-2.116065	-0.450075
O	2.468903	0.392208	-1.766194
O	1.276066	-1.292367	-0.290111
P	0.952836	-0.106544	-1.394381
O	0.325127	0.984790	-0.548616
O	0.278741	-0.608083	-2.611873
C	2.529545	3.187289	-1.227914
C	0.854123	-4.115936	-0.813986
C	2.696050	3.156288	-2.642304
C	2.081012	4.081536	-3.441572
C	1.244029	5.084676	-2.885545
C	1.054818	5.110691	-1.475854
C	1.721547	4.152214	-0.669640
C	0.642917	-5.362438	-0.157239
C	-0.594584	-5.948912	-0.132393
C	-1.704670	-5.326599	-0.762102
C	-1.488606	-4.108181	-1.461846

C	-0.197374	-3.525832	-1.477956
H	3.929029	3.622914	1.052794
H	3.233456	-5.306918	-1.108510
H	3.319322	2.383452	-3.078800
H	2.218571	4.052484	-4.519225
H	-0.056869	-2.600321	-2.028047
H	-0.748017	-6.887683	0.394205
H	1.473173	-5.826748	0.368244
H	1.562260	4.169474	0.407128
C	-3.951739	3.460038	2.463970
C	-5.154756	4.127041	2.669090
C	-5.774441	4.789382	1.611127
C	-5.194763	4.783031	0.344051
C	-4.003544	4.098409	0.125392
H	-3.452031	2.956446	3.286417
H	-5.604137	4.136432	3.656637
H	-6.708093	5.317608	1.776474
H	-3.531595	4.089293	-0.854107
H	-5.669467	5.312268	-0.475748
C	-0.849090	4.488587	2.218696
C	0.248929	4.911564	2.958152
C	1.269860	4.011996	3.264369
C	1.194297	2.690742	2.827596
C	0.107629	2.265078	2.072733
H	0.064965	1.237399	1.731248
H	-1.647772	5.184865	1.981383
H	0.305720	5.940173	3.299429
H	2.122809	4.341128	3.850686
H	1.986445	1.986707	3.062284
C	-2.106810	-0.991771	0.580934
C	-2.311018	-2.240885	1.155634
C	-3.551205	-2.865985	1.134286
C	-4.598284	-2.196662	0.515253
Br	-0.860111	-3.105134	1.982648
H	-3.687124	-3.854699	1.555199
C	-4.441414	-0.929183	-0.030029
H	-5.290705	-0.425834	-0.481928
H	-1.107038	-0.570040	0.586060
Br	-6.281348	-3.048117	0.394098
C	-2.586139	-3.472394	-2.104723
C	-3.841979	-4.018252	-2.043154
C	-4.061204	-5.228055	-1.335764
C	-3.017747	-5.866700	-0.714176
H	-2.400528	-2.536538	-2.627714
H	-4.683418	-3.518144	-2.514909
H	-3.181324	-6.796784	-0.174821
H	-5.064369	-5.640130	-1.282549
C	0.182877	6.084589	-0.919890
C	-0.470571	6.984405	-1.722937
C	-0.275412	6.962259	-3.126163
C	0.565990	6.036799	-3.690735
H	0.049929	6.101951	0.158819
H	-1.135394	7.723599	-1.286081
H	-0.792704	7.683048	-3.751959
H	0.718873	6.011850	-4.766771
C	5.080240	2.128004	2.951206
C	5.159911	1.063518	4.042693
H	4.542125	3.013789	3.311704
H	6.097824	2.468786	2.713730
C	5.722522	-0.228646	3.456871
H	4.157227	0.866749	4.447144
H	5.776335	1.422967	4.873130
C	4.776928	-0.781931	2.393363

H	6.704285	-0.023678	3.007961
H	5.877521	-0.978904	4.238860
H	5.222945	-1.650077	1.902395
H	3.867215	-1.161083	2.881813
C	6.167887	-1.715292	-0.553637
C	7.303244	-2.725573	-0.407219
H	6.263514	-0.922705	0.192596
H	6.261188	-1.211824	-1.526938
C	7.099059	-3.886537	-1.376708
H	8.263200	-2.229862	-0.585027
H	7.325474	-3.111493	0.621750
C	5.817051	-4.635223	-1.020804
H	7.026295	-3.491842	-2.398414
H	7.951546	-4.573310	-1.355718
H	5.988950	-5.213420	-0.101639
H	5.568376	-5.365515	-1.798624

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M06-2X/6-31G* Energy = -8271.58510984

M06-2X/6-31G* Free Energy = -8270.699275

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.56124679

Lowest Frequency = 11.1689

M06-2X/6-31G* Geometry

C	-1.829824	0.094121	-4.038960
C	-2.638603	2.360081	-1.258487
C	-2.827612	-0.311026	-3.255397
H	-0.794792	-0.026149	-3.725641
H	-2.026721	0.538821	-5.011056
C	-2.629045	-0.928212	-1.900454
H	-3.863403	-0.182997	-3.577543
N	-2.324686	1.204185	-0.760427
C	-1.588761	3.354316	-1.519825
C	-4.047998	2.715844	-1.551667
C	-3.172677	0.000261	-0.790118
C	-3.254476	-0.710710	0.544918
H	-4.178863	0.310472	-1.076531
H	-1.315697	1.053275	-0.426936
H	-1.567082	-1.145217	-1.725129
H	-3.186520	-1.869076	-1.812338
C	5.139490	-0.333441	1.385069
C	5.465463	0.806591	2.131709
C	4.165289	-0.239032	0.369002
C	3.426096	0.943247	0.231851
C	3.708166	2.076053	1.004959
C	4.761559	1.990097	1.910893
C	3.882438	-1.385744	-0.546698
C	4.867897	-1.941460	-1.389303
C	4.533809	-3.042442	-2.190659
C	3.221549	-3.517881	-2.199360
C	2.207479	-2.930694	-1.447718
C	2.577363	-1.873625	-0.611909
O	2.448363	1.028578	-0.734951
O	1.603438	-1.204652	0.108444
P	1.069904	0.136426	-0.666553
O	0.082036	0.779301	0.282143
O	0.643812	-0.144811	-2.063430
C	2.898296	3.321971	0.947877
C	0.794934	-3.354854	-1.613388
C	3.526693	4.574330	0.701203
C	2.820105	5.746820	0.781853
C	1.444106	5.742384	1.134476
C	0.805913	4.491028	1.359018
C	1.555938	3.293335	1.248971

C	0.298777	-3.531035	-2.936537
C	-0.989519	-3.932905	-3.164864
C	-1.869860	-4.190010	-2.082409
C	-1.386352	-4.014876	-0.756004
C	-0.048697	-3.585318	-0.548220
H	4.996651	2.865174	2.514133
H	2.972587	-4.360055	-2.842369
H	4.584040	4.587655	0.450019
H	3.311420	6.699237	0.597385
H	0.293812	-3.423284	0.471754
H	-1.361451	-4.037443	-4.180880
H	0.955915	-3.301118	-3.769784
H	1.058400	2.345458	1.430197
C	-5.034070	2.565822	-0.569854
C	-6.344675	2.940748	-0.842661
C	-6.675790	3.451379	-2.096789
C	-5.694928	3.600864	-3.075110
C	-4.377801	3.248584	-2.800691
H	-4.764953	2.165488	0.404977
H	-7.106439	2.835215	-0.077202
H	-7.700814	3.737545	-2.310088
H	-3.600984	3.367320	-3.550248
H	-5.954376	3.998705	-4.050613
C	-0.318066	2.936191	-1.939692
C	0.687687	3.874441	-2.133209
C	0.424008	5.228079	-1.935915
C	-0.851598	5.652478	-1.562070
C	-1.859475	4.721560	-1.356564
H	-2.844533	5.045035	-1.033188
H	-0.132742	1.888248	-2.157699
H	1.675594	3.537903	-2.429760
H	1.215926	5.958572	-2.071404
H	-1.049658	6.706527	-1.400496
C	-2.110678	-1.030014	1.278711
C	-2.243378	-1.794020	2.428490
C	-3.474149	-2.257017	2.878890
C	-4.592567	-1.942135	2.120003
Br	-0.674844	-2.335430	3.329836
H	-3.552528	-2.871025	3.768078
C	-4.501723	-1.172470	0.966243
H	-5.396697	-0.960303	0.388900
H	-1.124454	-0.699155	0.966975
Br	-6.271965	-2.644261	2.634698
C	-2.273290	-4.242828	0.330928
C	-3.587559	-4.569017	0.112321
C	-4.070478	-4.729043	-1.211141
C	-3.226554	-4.561146	-2.279911
H	-1.887652	-4.131034	1.340010
H	-4.268057	-4.694151	0.950589
H	-3.588008	-4.690307	-3.297257
H	-5.110652	-4.995230	-1.373279
C	-0.565009	4.472338	1.730191
C	-1.264633	5.641797	1.885825
C	-0.630009	6.888060	1.658035
C	0.689757	6.935776	1.284156
H	-1.039100	3.506793	1.892333
H	-2.309660	5.618982	2.181288
H	-1.193165	7.808051	1.785323
H	1.181551	7.890523	1.112721
C	6.567837	0.799251	3.174680
C	6.907988	-0.599509	3.682811
H	6.284964	1.453736	4.006494
H	7.470558	1.242315	2.730198

C	7.073163	-1.550740	2.500767
H	6.098856	-0.966730	4.327356
H	7.816551	-0.565032	4.292908
C	5.754475	-1.676875	1.742080
H	7.852236	-1.164362	1.828298
H	7.401044	-2.540001	2.836497
H	5.029161	-2.208498	2.375283
H	5.881126	-2.304324	0.857596
C	6.230806	-1.283858	-1.527745
C	7.292006	-2.217914	-2.104191
H	6.568334	-0.864485	-0.577862
H	6.109825	-0.422320	-2.200626
C	6.774392	-2.875588	-3.380293
H	8.211392	-1.655658	-2.297930
H	7.539298	-2.995832	-1.368103
C	5.563104	-3.746100	-3.055784
H	6.488050	-2.093822	-4.095758
H	7.552746	-3.480557	-3.856867
H	5.906543	-4.646141	-2.526145
H	5.083437	-4.098414	-3.975671

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M06-2X/6-31G* Energy = -8271.58510984

M06-2X/6-31G* Free Energy = -8270.699274

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.56124762

Lowest Frequency = 11.1785

M06-2X/6-31G* Geometry

C	-1.829823	0.094434	-4.038915
C	-2.638869	2.360124	-1.258382
C	-2.827576	-0.310870	-3.255391
H	-0.794778	-0.025858	-3.725633
H	-2.026746	0.539237	-5.010957
C	-2.628965	-0.928156	-1.900500
H	-3.863382	-0.182878	-3.577504
N	-2.324895	1.204222	-0.760334
C	-1.589004	3.354271	-1.519880
C	-4.048290	2.715818	-1.551431
C	-3.172728	0.000201	-0.790121
C	-3.254463	-0.710813	0.544892
H	-4.178946	0.310262	-1.076578
H	-1.315869	1.053335	-0.426935
H	-1.566991	-1.145129	-1.725190
H	-3.186392	-1.869055	-1.812452
C	4.867948	-1.941314	-1.389277
C	4.533908	-3.042260	-2.190697
C	3.882449	-1.385647	-0.546685
C	2.577384	-1.873541	-0.611955
C	2.207555	-2.930604	-1.447797
C	3.221662	-3.517740	-2.199430
C	4.165258	-0.238947	0.369046
C	5.139423	-0.333373	1.385139
C	5.465400	0.806657	2.131786
C	4.761536	1.990175	1.910935
C	3.708162	2.076142	1.004982
C	3.426083	0.943344	0.231865
O	1.603417	-1.204582	0.108375
O	2.448371	1.028698	-0.734934
P	1.069938	0.136491	-0.666735
O	0.081975	0.779375	0.281836
O	0.644074	-0.144837	-2.063654
C	0.795032	-3.354807	-1.613497
C	2.898247	3.322033	0.947896
C	0.298837	-3.530884	-2.936646

C	-0.989468	-3.932729	-3.164972
C	-1.869787	-4.189912	-2.082516
C	-1.386237	-4.014904	-0.756111
C	-0.048576	-3.585361	-0.548331
C	3.526585	4.574421	0.701201
C	2.819926	5.746871	0.781786
C	1.443922	5.742366	1.134407
C	0.805803	4.490985	1.359010
C	1.555891	3.293329	1.248972
H	2.972742	-4.359909	-2.842462
H	4.996625	2.865255	2.514173
H	0.955942	-3.300870	-3.769892
H	-1.361427	-4.037182	-4.180986
H	1.058401	2.345430	1.430216
H	3.311183	6.699312	0.597290
H	4.583937	4.587789	0.450041
H	0.293968	-3.423419	0.471644
C	-4.378224	3.248761	-2.800338
C	-5.695400	3.600953	-3.074625
C	-6.676196	3.451157	-2.096285
C	-6.344964	2.940324	-0.842268
C	-5.034306	2.565496	-0.569598
H	-3.601457	3.367720	-3.549911
H	-5.954949	3.998952	-4.050035
H	-7.701263	3.737246	-2.309482
H	-4.765089	2.165054	0.405161
H	-7.106677	2.834571	-0.076789
C	-0.318391	2.936016	-1.939896
C	0.687472	3.874133	-2.133430
C	0.423984	5.227802	-1.936035
C	-0.851534	5.652342	-1.562072
C	-1.859513	4.721540	-1.356510
H	-2.844485	5.045133	-1.032988
H	-0.133220	1.888054	-2.157953
H	1.675307	3.537474	-2.430078
H	1.215991	5.958198	-2.071526
H	-1.049448	6.706408	-1.400435
C	-2.110595	-1.030079	1.278603
C	-2.243184	-1.794077	2.428397
C	-3.473911	-2.257162	2.878846
C	-4.592388	-1.942347	2.120027
Br	-0.674587	-2.335375	3.329687
H	-3.552200	-2.871209	3.768014
C	-4.501659	-1.172622	0.966290
H	-5.396675	-0.960496	0.388997
H	-1.124410	-0.699202	0.966782
Br	-6.271718	-2.644608	2.634754
C	-0.565090	4.472238	1.730284
C	-1.264759	5.641666	1.885946
C	-0.630219	6.887954	1.658067
C	0.689517	6.935723	1.284085
H	-1.039120	3.506673	1.892492
H	-2.309760	5.618804	2.181501
H	1.181256	7.890488	1.112586
H	-1.193410	7.807921	1.785372
C	-2.273145	-4.242922	0.330835
C	-3.587442	-4.569011	0.112248
C	-4.070405	-4.728897	-1.211216
C	-3.226506	-4.560967	-2.280002
H	-1.887461	-4.131239	1.339908
H	-4.267915	-4.694177	0.950531
H	-5.110599	-4.995016	-1.373348
H	-3.588006	-4.690040	-3.297342

C	5.563213	-3.745803	-3.055905
C	6.774500	-2.875235	-3.380269
H	5.083550	-4.097955	-3.975856
H	5.906637	-4.645935	-2.526416
C	7.292076	-2.217717	-2.104071
H	6.488150	-2.093377	-4.095631
H	7.552865	-3.480123	-3.856923
C	6.230871	-1.283703	-1.527570
H	7.539292	-2.995730	-1.368056
H	8.211497	-1.655479	-2.297688
H	6.568348	-0.864470	-0.577607
H	6.109950	-0.422068	-2.200335
C	5.754393	-1.676813	1.742152
C	7.073082	-1.550673	2.500838
H	5.881033	-2.304260	0.857666
H	5.029086	-2.208443	2.375357
C	6.907873	-0.599479	3.682907
H	7.400999	-2.539932	2.836530
H	7.852137	-1.164244	1.828375
C	6.567724	0.799296	3.174815
H	6.098716	-0.966721	4.327408
H	7.816407	-0.565014	4.293046
H	7.470457	1.242408	2.730408
H	6.284783	1.453734	4.006643

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M06-2X/6-31G* Energy = -8271.58451769

M06-2X/6-31G* Free Energy = -8270.698261

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.56146881

Lowest Frequency = 17.5442

M06-2X/6-31G* Geometry

C	1.209056	3.129634	2.746953
C	2.005471	2.876727	-1.083252
C	2.405391	2.551869	2.651062
H	0.313073	2.625265	2.386754
H	1.075506	4.111751	3.194207
C	2.610921	1.197638	2.028096
H	3.292393	3.069556	3.019265
N	1.911056	1.933446	-0.210090
C	0.840999	3.197780	-1.938328
C	3.257760	3.652080	-1.273499
C	2.998860	1.284848	0.536625
C	3.235657	-0.097710	-0.054420
H	3.910715	1.875495	0.419800
H	0.905365	1.519322	0.038073
H	1.701532	0.592870	2.129659
H	3.419162	0.653052	2.529754
C	-4.653074	-2.540482	0.536982
C	-4.417702	-3.868227	0.917211
C	-3.555379	-1.709496	0.238769
C	-2.252193	-2.173663	0.457186
C	-1.996639	-3.505407	0.820901
C	-3.104981	-4.327149	1.018135
C	-3.741029	-0.321201	-0.285452
C	-4.343644	-0.057194	-1.532493
C	-4.479161	1.274856	-1.950465
C	-3.969617	2.305135	-1.157457
C	-3.296748	2.069338	0.038892
C	-3.211575	0.734900	0.454208
O	-1.202637	-1.303723	0.243408
O	-2.493143	0.415145	1.589605
P	-0.951879	-0.038246	1.273041
O	-0.353507	1.019646	0.366386

O	-0.282078	-0.427188	2.533954
C	-0.623058	-4.056936	0.929344
C	-2.628220	3.171164	0.773727
C	-0.338882	-5.319350	0.333570
C	0.931413	-5.831844	0.332626
C	2.003133	-5.114734	0.926986
C	1.715791	-3.878279	1.566905
C	0.392302	-3.373269	1.559206
C	-1.957306	4.182236	0.028356
C	-1.319483	5.220568	0.651188
C	-1.303189	5.319309	2.066533
C	-1.960364	4.309119	2.822870
C	-2.619916	3.248791	2.149336
H	-2.934213	-5.360941	1.312544
H	-4.073440	3.331746	-1.504912
H	-1.141142	-5.857431	-0.164388
H	1.139944	-6.784640	-0.147810
H	-3.111002	2.482297	2.740643
H	-0.805373	5.978156	0.063551
H	-1.935542	4.107111	-1.054114
H	0.196901	-2.431353	2.063074
C	3.834109	3.752506	-2.542633
C	4.997614	4.494503	-2.715158
C	5.565752	5.163070	-1.632516
C	4.974398	5.087726	-0.372946
C	3.824042	4.328164	-0.187868
H	3.374515	3.242407	-3.384161
H	5.456400	4.557108	-3.696390
H	6.468008	5.749967	-1.772386
H	3.343995	4.263822	0.785848
H	5.408253	5.621367	0.466379
C	-0.080174	2.202343	-2.295101
C	-1.146714	2.511475	-3.131684
C	-1.302685	3.808707	-3.616125
C	-0.392134	4.804645	-3.261260
C	0.681647	4.500138	-2.433645
H	1.394467	5.271750	-2.159179
H	0.031915	1.190418	-1.923712
H	-1.859337	1.735871	-3.394729
H	-2.136161	4.046175	-4.270794
H	-0.516790	5.816460	-3.632977
C	2.193869	-0.847510	-0.601637
C	2.466517	-2.101943	-1.134710
C	3.739853	-2.655567	-1.097108
C	4.749134	-1.907509	-0.506373
Br	1.062379	-3.078215	-1.917228
H	3.929501	-3.649819	-1.482643
C	4.522851	-0.632975	-0.003060
H	5.342824	-0.069335	0.431540
H	1.171565	-0.483795	-0.613645
Br	6.474980	-2.663599	-0.355264
C	-1.913477	4.376282	4.241389
C	-1.250604	5.396024	4.874689
C	-0.605952	6.407578	4.119777
C	-0.633656	6.368685	2.748631
H	-2.404469	3.594637	4.814699
H	-1.216078	5.432239	5.959030
H	-0.138396	7.139245	2.162638
H	-0.089491	7.213029	4.633051
C	2.774672	-3.148293	2.173689
C	4.060579	-3.621346	2.134347
C	4.350366	-4.849561	1.486596
C	3.345867	-5.578078	0.900781

H	2.534561	-2.201066	2.652181
H	4.871273	-3.049876	2.578173
H	5.376109	-5.203709	1.449559
H	3.563647	-6.522280	0.407057
C	-5.551463	-4.835351	1.202857
C	-6.872023	-4.136667	1.516863
H	-5.262173	-5.499967	2.024306
H	-5.692854	-5.479463	0.323156
C	-7.141373	-3.052782	0.476570
H	-6.819528	-3.674089	2.510950
H	-7.685593	-4.868919	1.543826
C	-6.062864	-1.974559	0.552866
H	-7.144059	-3.504145	-0.525692
H	-8.126814	-2.600030	0.627509
H	-6.182705	-1.415513	1.492301
H	-6.201444	-1.237753	-0.242341
C	-4.722307	-1.198618	-2.460911
C	-5.687043	-0.779620	-3.567862
H	-5.131376	-2.042290	-1.900296
H	-3.793927	-1.575311	-2.914889
C	-5.183763	0.485429	-4.257555
H	-5.802363	-1.598273	-4.285483
H	-6.679811	-0.585481	-3.138748
C	-5.160743	1.637908	-3.256680
H	-4.170590	0.305191	-4.642637
H	-5.812825	0.745114	-5.115254
H	-6.195120	1.943303	-3.044866
H	-4.668176	2.517637	-3.689212

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M06-2X/6-31G* Energy = -8271.58451767

M06-2X/6-31G* Free Energy = -8270.698263

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.56146633

Lowest Frequency = 17.5447

M06-2X/6-31G* Geometry

C	1.208832	3.130058	2.746211
C	2.005433	2.877043	-1.083110
C	2.405187	2.552267	2.650737
H	0.312954	2.625630	2.385824
H	1.075156	4.112183	3.193408
C	2.610933	1.197966	2.027979
H	3.292070	3.069972	3.019214
N	1.911003	1.933487	-0.210281
C	0.840960	3.198511	-1.938072
C	3.257862	3.652230	-1.273292
C	2.998809	1.284973	0.536474
C	3.235642	-0.097674	-0.054369
H	3.910648	1.875637	0.419525
H	0.905214	1.519299	0.037762
H	1.701647	0.593063	2.129652
H	3.419275	0.653582	2.529685
C	-4.344284	-0.057411	-1.532030
C	-4.479919	1.274635	-1.949977
C	-3.741305	-0.321397	-0.285151
C	-3.211675	0.734741	0.454331
C	-3.296988	2.069176	0.039056
C	-3.970153	2.304928	-1.157139
C	-3.555459	-1.709721	0.238938
C	-4.653005	-2.540850	0.537302
C	-4.417423	-3.868648	0.917222
C	-3.104638	-4.327466	1.017830
C	-1.996426	-3.505573	0.820525
C	-2.252195	-2.173824	0.456988

O	-2.492840	0.415006	1.589524
O	-1.202757	-1.303845	0.242924
P	-0.951702	-0.038290	1.272304
O	-0.353793	1.019531	0.365222
O	-0.281225	-0.426984	2.532946
C	-2.628417	3.171047	0.773768
C	-0.622765	-4.056955	0.928853
C	-1.957938	4.182382	0.028346
C	-1.320241	5.220805	0.651156
C	-1.303581	5.319364	2.066512
C	-1.960290	4.308902	2.822882
C	-2.619761	3.248505	2.149381
C	-0.338455	-5.319237	0.332872
C	0.931864	-5.831667	0.331966
C	2.003483	-5.114632	0.926604
C	1.716022	-3.878264	1.566647
C	0.392499	-3.373313	1.558890
H	-4.074076	3.331528	-1.504590
H	-2.933693	-5.361286	1.312037
H	-1.936431	4.107435	-1.054143
H	-0.806533	5.978635	0.063479
H	0.197027	-2.431473	2.062866
H	1.140485	-6.784381	-0.148592
H	-1.140652	-5.857280	-0.165235
H	-3.110467	2.481799	2.740730
C	3.834063	3.752701	-2.542494
C	4.997716	4.494451	-2.715121
C	5.566209	5.162684	-1.632467
C	4.975038	5.087264	-0.372811
C	3.824518	4.327984	-0.187650
H	3.374196	3.242883	-3.384048
H	5.456304	4.557125	-3.696440
H	6.468596	5.749371	-1.772375
H	3.344626	4.263657	0.786135
H	5.409187	5.620626	0.466541
C	-0.080185	2.203171	-2.295176
C	-1.146742	2.512496	-3.131681
C	-1.302766	3.809858	-3.615750
C	-0.392226	4.805702	-3.260564
C	0.681562	4.500988	-2.433033
H	1.394325	5.272585	-2.158386
H	0.031879	1.191116	-1.924122
H	-1.859297	1.736906	-3.394949
H	-2.136241	4.047503	-4.270355
H	-0.516887	5.817632	-3.631966
C	4.522769	-0.633049	-0.002655
C	4.749107	-1.907553	-0.506027
C	3.739936	-2.655560	-1.096998
C	2.466639	-2.101877	-1.134862
Br	6.474943	-2.663621	-0.354875
H	3.929644	-3.649789	-1.482559
C	2.193956	-0.847402	-0.601908
H	1.171715	-0.483544	-0.614329
H	5.342687	-0.069468	0.432126
Br	1.062671	-3.078057	-1.917809
C	2.774799	-3.148348	2.173696
C	4.060710	-3.621434	2.134583
C	4.350601	-4.849576	1.486760
C	3.346214	-5.577984	0.900611
H	2.534599	-2.201166	2.652233
H	4.871330	-3.050039	2.578627
H	3.564088	-6.522125	0.406811
H	5.376345	-5.203737	1.449891

C	-1.913033	4.375864	4.241395
C	-1.250254	5.395688	4.874665
C	-0.606079	6.407519	4.119724
C	-0.634142	6.368815	2.748577
H	-2.403663	3.594008	4.814725
H	-1.215446	5.431759	5.959001
H	-0.089676	7.213025	4.632969
H	-0.139235	7.139588	2.162568
C	-5.161878	1.637636	-3.256009
C	-5.184694	0.485229	-4.256958
H	-4.669690	2.517573	-3.688540
H	-6.196323	1.942649	-3.043973
C	-5.687821	-0.779922	-3.567352
H	-4.171483	0.305170	-4.642021
H	-5.813771	0.744865	-5.114662
C	-4.723131	-1.198873	-2.460334
H	-6.680669	-0.585979	-3.138343
H	-5.802933	-1.598560	-4.285023
H	-5.132340	-2.042411	-1.899621
H	-3.794801	-1.575778	-2.914235
C	-6.062837	-1.975034	0.553711
C	-7.141318	-3.053298	0.477552
H	-6.201719	-1.238083	-0.241307
H	-6.182415	-1.416173	1.493288
C	-6.871546	-4.137439	1.517470
H	-8.126719	-2.600616	0.628970
H	-7.144371	-3.504413	-0.524819
C	-5.551054	-4.835941	1.202796
H	-6.818744	-3.675133	2.511666
H	-7.685056	-4.869752	1.544503
H	-5.692687	-5.479662	0.322846
H	-5.261496	-5.500919	2.023855

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M06-2X/6-31G* Energy = -8271.57916914

M06-2X/6-31G* Free Energy = -8270.697616

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.55673165

Lowest Frequency = 6.9755

M06-2X/6-31G* Geometry

C	1.796205	2.982970	-2.274578
C	3.753874	-0.017803	-1.148051
C	2.241544	3.136360	-1.028730
H	0.956771	2.328206	-2.514636
H	2.236581	3.547074	-3.093516
C	1.673796	2.397665	0.150640
H	3.062836	3.823540	-0.817920
N	2.696187	0.267614	-0.464903
C	3.739893	-0.978205	-2.262751
C	5.044500	0.637890	-0.780888
C	2.615696	1.271764	0.615366
C	2.175433	0.585627	1.894235
H	3.615190	1.684738	0.763941
H	1.728186	-0.140642	-0.707474
H	0.689070	1.983445	-0.091833
H	1.541313	3.074662	1.002687
C	-4.098807	-1.327170	1.374304
C	-3.745809	-2.623039	1.779193
C	-3.590516	-0.824730	0.161360
C	-2.650695	-1.570302	-0.554391
C	-2.223395	-2.826719	-0.118313
C	-2.819973	-3.346617	1.026078
C	-3.936004	0.529242	-0.359882
C	-5.245791	0.884095	-0.735989

C	-5.490404	2.178089	-1.217826
C	-4.428611	3.073698	-1.348243
C	-3.116472	2.727175	-1.038142
C	-2.890538	1.437392	-0.553540
O	-2.112174	-1.025849	-1.699446
O	-1.598194	1.014043	-0.308777
P	-0.921033	0.091035	-1.512992
O	0.248290	-0.574345	-0.817128
O	-0.755508	0.845355	-2.773438
C	-1.110383	-3.541408	-0.787840
C	-2.016488	3.705695	-1.232872
C	0.033410	-3.881861	-0.012977
C	1.084716	-4.555172	-0.575189
C	1.056129	-4.932232	-1.944465
C	-0.079056	-4.579678	-2.728306
C	-1.147809	-3.872059	-2.121181
C	-1.787216	4.254374	-2.524452
C	-0.832978	5.217648	-2.717949
C	-0.047961	5.691160	-1.634882
C	-0.267894	5.144399	-0.340499
C	-1.257968	4.143264	-0.172121
H	-2.507443	-4.329408	1.374809
H	-4.625432	4.076977	-1.721958
H	0.060275	-3.560474	1.025650
H	1.960967	-4.804847	0.017781
H	-1.423967	3.725150	0.818696
H	-0.653366	5.622154	-3.710907
H	-2.368893	3.874001	-3.358537
H	-2.007634	-3.592502	-2.724087
C	5.484304	1.748659	-1.501815
C	6.680847	2.365716	-1.147145
C	7.435183	1.873100	-0.084390
C	6.994539	0.760926	0.629725
C	5.797478	0.139685	0.283623
H	4.879380	2.129302	-2.319763
H	7.022571	3.233514	-1.701851
H	8.367586	2.356851	0.188374
H	5.442921	-0.725649	0.837618
H	7.581291	0.375312	1.457198
C	2.556041	-1.606621	-2.689429
C	2.599467	-2.504098	-3.746685
C	3.806613	-2.794883	-4.379964
C	4.983476	-2.181201	-3.959487
C	4.952543	-1.276274	-2.906868
H	5.872134	-0.802719	-2.581646
H	1.602817	-1.409272	-2.205456
H	1.685038	-2.988528	-4.072971
H	3.823765	-3.508357	-5.198562
H	5.926087	-2.406746	-4.447305
C	0.881055	0.080493	2.009467
C	0.523659	-0.607048	3.159784
C	1.402995	-0.771431	4.224373
C	2.677559	-0.232013	4.097568
Br	-1.202761	-1.375334	3.197579
H	1.110193	-1.306361	5.119878
C	3.080592	0.432881	2.944355
H	4.090772	0.824733	2.869648
H	0.168052	0.171284	1.197564
Br	3.903386	-0.427301	5.527359
C	0.523991	5.608444	0.743778
C	1.507251	6.544028	0.546694
C	1.736684	7.075623	-0.746828
C	0.971212	6.663425	-1.807447

H	0.336842	5.202876	1.735726
H	2.108772	6.887981	1.382765
H	1.138338	7.071385	-2.801368
H	2.516222	7.817498	-0.891338
C	-0.107700	-4.948514	-4.100945
C	0.941225	-5.627641	-4.668433
C	2.072295	-5.974343	-3.887996
C	2.125479	-5.633947	-2.559922
H	-0.977890	-4.678052	-4.693411
H	0.906621	-5.905119	-5.717624
H	2.896349	-6.513096	-4.346232
H	2.992535	-5.893701	-1.957691
C	-4.283965	-3.238200	3.058077
C	-4.758880	-2.194888	4.067885
H	-3.510560	-3.876318	3.501810
H	-5.124322	-3.901157	2.808681
C	-5.660716	-1.176866	3.374702
H	-3.890224	-1.674178	4.493948
H	-5.278878	-2.685588	4.897062
C	-4.871966	-0.417046	2.311555
H	-6.506327	-1.699805	2.906444
H	-6.080753	-0.470048	4.097682
H	-4.126831	0.223225	2.808704
H	-5.523689	0.263809	1.758565
C	-6.350195	-0.159358	-0.744662
C	-7.750273	0.448928	-0.778943
H	-6.253047	-0.843653	0.101497
H	-6.207575	-0.781132	-1.640453
C	-7.842225	1.492900	-1.888421
H	-8.492531	-0.343092	-0.922488
H	-7.970278	0.925498	0.186578
C	-6.885157	2.644342	-1.590746
H	-7.573575	1.025411	-2.844610
H	-8.864294	1.872409	-1.989756
H	-7.291821	3.235913	-0.758112
H	-6.822217	3.325527	-2.446575

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M06-2X/6-31G* Energy = -8271.57556321

M06-2X/6-31G* Free Energy = -8270.693419

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.55685200

Lowest Frequency = 7.8563

M06-2X/6-31G* Geometry

C	-0.682657	-3.839648	0.689380
C	-2.025486	-1.277818	2.574247
C	-1.895355	-3.638557	0.176305
H	0.124598	-3.127808	0.524206
H	-0.444572	-4.742048	1.245651
C	-2.278368	-2.403042	-0.590637
H	-2.682219	-4.376950	0.332452
N	-2.054957	-0.932088	1.330717
C	-3.171490	-2.004600	3.184686
C	-0.880496	-0.923567	3.429838
C	-3.021687	-1.402788	0.319358
C	-3.606313	-0.197339	-0.391850
H	-3.822720	-1.930256	0.841579
H	-1.256090	-0.345249	0.900614
H	-1.391336	-1.927405	-1.027053
H	-2.948780	-2.652031	-1.420306
C	5.067870	-1.154466	-1.023213
C	5.243642	-2.355544	-1.722771
C	3.793822	-0.845268	-0.500624
C	2.703392	-1.655842	-0.823375

C	2.858667	-2.856589	-1.527801
C	4.147624	-3.194354	-1.929550
C	3.578818	0.343108	0.379558
C	4.268145	0.488015	1.603884
C	4.115932	1.676005	2.329845
C	3.300543	2.690175	1.823107
C	2.557724	2.553130	0.652361
C	2.676522	1.329876	-0.024797
O	1.456243	-1.287242	-0.361737
O	1.923679	1.094829	-1.157159
P	0.686464	0.034734	-1.006684
O	-0.216171	0.475789	0.123323
O	0.123777	-0.250523	-2.348581
C	1.720265	-3.758961	-1.838977
C	1.775322	3.707060	0.132383
C	1.778264	-5.121711	-1.432019
C	0.754670	-5.987369	-1.718295
C	-0.388556	-5.546284	-2.434073
C	-0.442587	-4.189972	-2.857910
C	0.626693	-3.313117	-2.545005
C	0.447313	3.581951	-0.369230
C	-0.226387	4.681146	-0.832090
C	0.368195	5.969697	-0.828459
C	1.692140	6.105322	-0.329603
C	2.368499	4.952070	0.140710
H	4.290232	-4.124281	-2.477046
H	3.204214	3.615663	2.386942
H	2.646604	-5.463983	-0.874860
H	0.803708	-7.024298	-1.394753
H	3.392461	5.059977	0.491712
H	-1.232321	4.567950	-1.227243
H	-0.041507	2.614527	-0.354333
H	0.568595	-2.276620	-2.868213
C	-1.079547	-0.803423	4.814174
C	-0.029405	-0.420595	5.637365
C	1.226442	-0.168435	5.087587
C	1.433959	-0.308480	3.717084
C	0.390361	-0.689150	2.883739
H	-2.060958	-0.990588	5.237989
H	-0.191826	-0.314731	6.704864
H	2.047474	0.136245	5.730457
H	0.571409	-0.800012	1.819739
H	2.408472	-0.110298	3.283191
C	-4.405118	-1.362175	3.319381
C	-5.468593	-2.028580	3.920897
C	-5.302345	-3.334394	4.377282
C	-4.070038	-3.971612	4.244864
C	-2.997715	-3.305443	3.660054
H	-2.031620	-3.789276	3.551468
H	-4.520384	-0.341241	2.963979
H	-6.424480	-1.527315	4.032728
H	-6.134005	-3.855238	4.840834
H	-3.941805	-4.988256	4.601769
C	-4.866450	0.265386	-0.011857
C	-5.371429	1.423660	-0.589575
C	-4.641938	2.147231	-1.524433
C	-3.393196	1.658294	-1.893059
Br	-7.084511	2.042718	-0.074751
H	-5.031989	3.062873	-1.952232
C	-2.873850	0.484166	-1.363522
H	-1.902212	0.137830	-1.703218
H	-5.456305	-0.271071	0.725216
Br	-2.339904	2.627166	-3.121131

C	2.299021	7.389563	-0.326200
C	1.620551	8.485952	-0.792062
C	0.299840	8.350973	-1.287142
C	-0.309171	7.122413	-1.304805
H	3.313462	7.486298	0.052713
H	2.093220	9.463372	-0.785092
H	-1.321248	7.010744	-1.685485
H	-0.226778	9.226410	-1.654649
C	-1.580277	-3.735334	-3.578152
C	-2.620797	-4.586770	-3.850554
C	-2.570139	-5.936699	-3.420122
C	-1.479521	-6.404296	-2.732101
H	-1.606353	-2.694751	-3.894328
H	-3.487104	-4.231825	-4.400698
H	-3.399143	-6.601458	-3.643645
H	-1.434676	-7.440172	-2.404655
C	6.597989	-2.787636	-2.253940
C	7.583929	-1.631360	-2.399801
H	6.463504	-3.302883	-3.211252
H	7.023237	-3.530206	-1.563612
C	7.582364	-0.791028	-1.126176
H	7.290508	-0.998662	-3.247320
H	8.584734	-2.018689	-2.616815
C	6.209319	-0.156637	-0.918016
H	7.828806	-1.431762	-0.267446
H	8.346166	-0.007938	-1.171653
H	6.179312	0.382130	0.031628
H	6.047068	0.607450	-1.691958
C	5.068333	-0.669187	2.180280
C	6.038041	-0.237030	3.277200
H	5.600188	-1.209608	1.394477
H	4.355843	-1.396937	2.599226
C	5.310637	0.618899	4.309765
H	6.485538	-1.120662	3.743571
H	6.858761	0.345824	2.836431
C	4.818018	1.907744	3.655687
H	4.458249	0.048108	4.705685
H	5.959304	0.854043	5.159816
H	5.679065	2.569986	3.488497
H	4.144009	2.449497	4.329420

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M06-2X/6-31G* Energy = -8271.57556350

M06-2X/6-31G* Free Energy = -8270.693392

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.55684315

Lowest Frequency = 7.8991

M06-2X/6-31G* Geometry

C	0.682956	3.840002	0.688352
C	2.025803	1.278997	2.573751
C	1.895633	3.638737	0.175291
H	-0.124339	3.128151	0.523413
H	0.444909	4.742569	1.244371
C	2.278552	2.403042	-0.591401
H	2.682503	4.377173	0.331197
N	2.055348	0.932614	1.330403
C	3.171601	2.006391	3.183819
C	0.880907	0.924855	3.429511
C	3.021910	1.402931	0.318701
C	3.606159	0.197123	-0.392244
H	3.823146	1.930402	0.840613
H	1.256587	0.345519	0.900657
H	1.391459	1.927371	-1.027652
H	2.948916	2.651833	-1.421172

C	-5.067723	1.154013	-1.022835
C	-5.243698	2.354982	-1.722527
C	-3.793570	0.844987	-0.500406
C	-2.703241	1.655594	-0.823433
C	-2.858728	2.856232	-1.528001
C	-4.147775	3.193842	-1.929595
C	-3.578329	-0.343260	0.379893
C	-4.267393	-0.488023	1.604385
C	-4.114926	-1.675884	2.330499
C	-3.299574	-2.690078	1.823741
C	-2.557041	-2.553185	0.652800
C	-2.676064	-1.330030	-0.024515
O	-1.456000	1.287153	-0.361957
O	-1.923455	-1.095047	-1.157041
P	-0.686227	-0.034903	-1.006774
O	0.216495	-0.475808	0.123197
O	-0.123705	0.250243	-2.348768
C	-1.720450	3.758659	-1.839445
C	-1.774729	-3.707163	0.132792
C	-1.778549	5.121469	-1.432697
C	-0.755057	5.987180	-1.719177
C	0.388163	5.546091	-2.434961
C	0.442284	4.189722	-2.858601
C	-0.626892	3.312814	-2.545492
C	-0.446937	-3.582157	-0.369427
C	0.226568	-4.681455	-0.832336
C	-0.367992	-5.970009	-0.828197
C	-1.691721	-6.105540	-0.328746
C	-2.367878	-4.952192	0.141611
H	-4.290539	4.123678	-2.477206
H	-3.203063	-3.615466	2.387709
H	-2.646878	5.463748	-0.875524
H	-0.804173	7.024154	-1.395788
H	-3.391698	-5.060040	0.493049
H	1.232332	-4.568329	-1.227940
H	0.041901	-2.614734	-0.354974
H	-0.568718	2.276272	-2.868546
C	1.079996	0.805386	4.813902
C	0.029959	0.422659	5.637270
C	-1.225828	0.169934	5.087614
C	-1.433385	0.309305	3.717052
C	-0.389890	0.689863	2.883525
H	2.061361	0.992992	5.237632
H	0.192416	0.317303	6.704813
H	-2.046777	-0.134671	5.730626
H	-0.570980	0.800175	1.819471
H	-2.407843	0.110682	3.283245
C	4.405421	1.364428	3.318887
C	5.468654	2.031457	3.920152
C	5.301968	3.337426	4.375917
C	4.069458	3.974185	4.243135
C	2.997387	3.307403	3.658585
H	2.031147	3.790880	3.549706
H	4.521026	0.343342	2.964035
H	6.424689	1.530539	4.032269
H	6.133433	3.858751	4.839276
H	3.940874	4.990950	4.599572
C	2.873611	-0.484239	-1.363929
C	3.392516	-1.658750	-1.893067
C	4.640906	-2.148228	-1.524005
C	5.370531	-1.424797	-0.589128
Br	2.339019	-2.627395	-3.121132
H	5.030604	-3.064171	-1.951484

C	4.865988	-0.266129	-0.011840
H	5.455937	0.270230	0.725226
H	1.902199	-0.137560	-1.703918
Br	7.083118	-2.044666	-0.073649
C	-2.298597	-7.389783	-0.324830
C	-1.620320	-8.486258	-0.790769
C	-0.299823	-8.351368	-1.286445
C	0.309177	-7.122811	-1.304613
H	-3.312876	-7.486447	0.054535
H	-2.092977	-9.463680	-0.783406
H	1.321087	-7.011211	-1.685755
H	0.226636	-9.226877	-1.654010
C	1.579978	3.735071	-3.578824
C	2.620422	4.586550	-3.851390
C	2.569669	5.936540	-3.421164
C	1.479039	6.404152	-2.733170
H	1.606121	2.694446	-3.894857
H	3.486740	4.231593	-4.401510
H	3.398606	6.601334	-3.644828
H	1.434120	7.440076	-2.405887
C	-6.598171	2.786886	-2.253524
C	-7.583982	1.630476	-2.399184
H	-6.463891	3.302111	-3.210877
H	-7.023420	3.529428	-1.563165
C	-7.582202	0.790280	-1.125470
H	-7.290561	0.997729	-3.246666
H	-8.584855	2.017662	-2.616142
C	-6.209062	0.156085	-0.917339
H	-7.828670	1.431074	-0.266792
H	-8.345907	0.007085	-1.170807
H	-6.178902	-0.382508	0.032398
H	-6.046800	-0.608124	-1.691159
C	-5.067542	0.669202	2.180787
C	-6.036980	0.237137	3.277984
H	-5.599610	1.209471	1.395023
H	-4.355020	1.397072	2.599474
C	-5.309287	-0.618569	4.310528
H	-6.484442	1.120811	3.744313
H	-6.857752	-0.345848	2.837487
C	-4.816676	-1.907468	3.656547
H	-4.456879	-0.047639	4.706206
H	-5.957768	-0.853653	5.160738
H	-5.677686	-2.569842	3.489681
H	-4.142441	-2.449024	4.330214

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M06-2X/6-31G* Energy = -8271.58696660

M06-2X/6-31G* Free Energy = -8270.700747

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.56075210

Lowest Frequency = 11.7007

M06-2X/6-31G* Geometry

C	0.407078	-2.644690	-3.786696
C	-0.661045	-3.878863	0.027020
C	1.268796	-3.127273	-2.893229
H	0.103291	-1.597928	-3.762372
H	-0.005522	-3.280612	-4.565503
C	1.878836	-2.293247	-1.804538
H	1.566749	-4.177454	-2.925355
N	0.064091	-2.856038	-0.292049
C	-2.106174	-3.833265	-0.240591
C	-0.069940	-5.088099	0.646636
C	1.526307	-2.812552	-0.396109
C	2.153619	-1.924114	0.658764

H	1.904390	-3.833393	-0.289116
H	-0.441661	-1.928114	-0.576180
H	1.560737	-1.247305	-1.902595
H	2.974200	-2.306836	-1.872637
C	-0.034680	4.966543	-1.009493
C	1.181909	5.286640	-1.628242
C	-0.250531	3.650624	-0.561990
C	0.684049	2.662411	-0.867923
C	1.906784	2.965323	-1.464947
C	2.144399	4.289609	-1.812339
C	-1.422686	3.236027	0.259228
C	-1.595490	3.720015	1.571796
C	-2.659174	3.221779	2.335564
C	-3.543401	2.306027	1.766195
C	-3.372545	1.779623	0.485983
C	-2.260925	2.235657	-0.235385
O	0.391613	1.354939	-0.553338
O	-1.952673	1.683756	-1.462618
P	-0.723381	0.587590	-1.501581
O	-1.125818	-0.608821	-0.665198
O	-0.256049	0.435610	-2.898586
C	2.920938	1.889807	-1.628713
C	-4.362563	0.818961	-0.061139
C	3.814771	1.644299	-0.550735
C	4.731645	0.630141	-0.619021
C	4.787479	-0.214695	-1.757830
C	3.911891	0.041415	-2.850028
C	2.977952	1.107659	-2.756289
C	-4.765431	0.891759	-1.427940
C	-5.793564	0.121392	-1.900525
C	-6.492269	-0.774604	-1.047594
C	-6.075726	-0.882408	0.307946
C	-4.999416	-0.081032	0.765560
H	3.097790	4.547836	-2.268882
H	-4.400457	1.981139	2.351775
H	3.729066	2.258514	0.342771
H	5.405974	0.432055	0.210330
H	-4.686345	-0.179705	1.801976
H	-6.103521	0.203046	-2.939554
H	-4.254419	1.583438	-2.087684
H	2.260406	1.262281	-3.557702
C	0.824416	-4.966240	1.717350
C	1.353787	-6.105809	2.311498
C	1.004707	-7.367482	1.833028
C	0.113676	-7.492446	0.769110
C	-0.435856	-6.356895	0.184479
H	1.088404	-3.979204	2.088761
H	2.037812	-6.008269	3.148000
H	1.424470	-8.255788	2.294438
H	-1.140837	-6.444369	-0.636680
H	-0.158742	-8.475073	0.398438
C	-2.588575	-3.101703	-1.336344
C	-3.952878	-3.056676	-1.584460
C	-4.838717	-3.732969	-0.748804
C	-4.363461	-4.462701	0.340348
C	-3.000187	-4.523651	0.591625
H	-2.623367	-5.083010	1.442574
H	-1.895385	-2.585746	-1.992284
H	-4.328511	-2.481066	-2.423915
H	-5.906029	-3.682243	-0.942073
H	-5.060681	-4.974728	0.995708
C	3.478324	-2.167109	1.025352
C	4.109675	-1.288624	1.893374

C	3.464929	-0.169787	2.408201
C	2.152397	0.055170	2.012215
Br	5.939708	-1.559507	2.296642
H	3.982492	0.521685	3.062603
C	1.479287	-0.812635	1.161103
H	0.459711	-0.586491	0.865639
H	4.024059	-3.010966	0.613162
Br	1.268011	1.632248	2.564807
C	-6.767275	-1.776532	1.168642
C	-7.830061	-2.514157	0.711039
C	-8.248408	-2.401565	-0.638483
C	-7.588668	-1.556471	-1.496850
H	-6.441294	-1.859464	2.202512
H	-8.357711	-3.185298	1.382033
H	-7.904747	-1.464521	-2.533144
H	-9.093357	-2.985893	-0.989897
C	3.949065	-0.824669	-3.975222
C	4.797867	-1.902451	-4.002729
C	5.652943	-2.169530	-2.903653
C	5.650049	-1.342029	-1.808202
H	3.268697	-0.633490	-4.800783
H	4.807534	-2.565112	-4.862689
H	6.310156	-3.033577	-2.933042
H	6.285634	-1.545566	-0.948067
C	1.505569	6.702966	-2.066950
C	0.268633	7.585083	-2.224366
H	2.076516	6.672690	-3.001606
H	2.170380	7.156383	-1.317853
C	-0.643079	7.429368	-1.009021
H	-0.284727	7.289167	-3.125033
H	0.570247	8.628941	-2.359909
C	-1.150693	5.992021	-0.925537
H	-0.081354	7.679715	-0.097956
H	-1.490560	8.120403	-1.064698
H	-1.755736	5.839423	-0.027876
H	-1.830312	5.806948	-1.769889
C	-0.576130	4.678884	2.167580
C	-0.940443	5.191376	3.562216
H	-0.406816	5.528557	1.500308
H	0.392122	4.160939	2.204563
C	-1.535179	4.074131	4.413478
H	-0.050902	5.621328	4.033821
H	-1.678702	6.000064	3.478743
C	-2.851356	3.627984	3.782842
H	-0.837689	3.225132	4.444602
H	-1.696957	4.406576	5.443903
H	-3.576114	4.451743	3.850208
H	-3.284556	2.787478	4.335855

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M06-2X/6-31G* Energy = -8271.58991225

M06-2X/6-31G* Free Energy = -8270.703587

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.55988888

Lowest Frequency = 14.2177

M06-2X/6-31G* Geometry

C	-1.160727	4.053143	-0.497445
C	-3.394190	1.537348	1.039046
C	-1.905832	3.357319	-1.354586
H	-0.245594	3.644890	-0.064117
H	-1.424862	5.069072	-0.216849
C	-1.574232	1.954016	-1.776239
H	-2.808088	3.798420	-1.780719
N	-2.511649	1.019560	0.253955

C	-3.006778	1.908869	2.410849
C	-4.786299	1.775306	0.587924
C	-2.574279	0.917221	-1.215082
C	-2.272593	-0.508583	-1.647395
H	-3.585888	1.182850	-1.533144
H	-1.513139	0.772097	0.621514
H	-0.563089	1.704544	-1.435426
H	-1.592527	1.858234	-2.868622
C	3.888793	-2.557983	0.243981
C	3.166742	-3.708222	0.596952
C	3.518686	-1.320785	0.806106
C	2.369057	-1.241278	1.597671
C	1.549962	-2.352723	1.829456
C	2.019066	-3.583994	1.379461
C	4.205901	-0.041641	0.451330
C	5.555847	0.223127	0.749109
C	6.119392	1.442477	0.342740
C	5.324028	2.392753	-0.300761
C	3.969935	2.184444	-0.546842
C	3.435849	0.952528	-0.160103
O	1.999911	-0.002999	2.080691
O	2.082081	0.731274	-0.317431
P	1.187770	0.979913	1.046808
O	-0.130058	0.329986	0.707626
O	1.253345	2.372842	1.550947
C	0.147620	-2.190816	2.290983
C	3.101101	3.232077	-1.137533
C	-0.224832	-1.345088	3.374242
C	-1.544484	-1.100363	3.649610
C	-2.576409	-1.681613	2.864199
C	-2.213758	-2.542467	1.792184
C	-0.841377	-2.781354	1.535380
C	3.116472	4.546518	-0.596528
C	2.297502	5.523745	-1.097733
C	1.411818	5.250694	-2.172420
C	1.402804	3.942825	-2.732766
C	2.256947	2.952106	-2.189094
H	1.414231	-4.468727	1.568344
H	5.771474	3.337893	-0.603493
H	0.553155	-0.871283	3.963032
H	-1.822560	-0.436801	4.466217
H	2.230561	1.949256	-2.607876
H	2.300974	6.519932	-0.662658
H	3.763647	4.752071	0.250942
H	-0.568468	-3.377971	0.667580
C	-5.556462	0.705521	0.121617
C	-6.869681	0.926903	-0.280869
C	-7.407236	2.211815	-0.229051
C	-6.639375	3.276004	0.240614
C	-5.332245	3.058672	0.664214
H	-5.125710	-0.293082	0.109700
H	-7.473251	0.095997	-0.631994
H	-8.430031	2.383338	-0.549403
H	-4.724400	3.876708	1.040438
H	-7.061013	4.274924	0.282937
C	-1.689610	2.299641	2.680835
C	-1.314408	2.619484	3.980182
C	-2.251264	2.562200	5.009551
C	-3.572889	2.198981	4.739773
C	-3.955694	1.883184	3.442515
H	-4.978893	1.589242	3.226321
H	-0.951765	2.386884	1.890806
H	-0.286452	2.913829	4.164949

H	-1.958751	2.811803	6.025114
H	-4.303354	2.164074	5.541741
C	-0.962308	-0.989663	-1.666349
C	-0.730892	-2.321765	-1.977706
C	-1.764951	-3.194827	-2.297561
C	-3.059008	-2.689606	-2.280367
Br	1.039886	-2.969237	-1.824405
H	-1.574607	-4.239144	-2.515870
C	-3.326436	-1.362886	-1.969447
H	-4.353252	-1.010950	-1.954073
H	-0.128736	-0.366422	-1.369967
Br	-4.508896	-3.875382	-2.546273
C	0.520236	3.662912	-3.809989
C	-0.333766	4.624071	-4.286249
C	-0.336541	5.921521	-3.716199
C	0.520615	6.227039	-2.690632
H	0.531886	2.665833	-4.244614
H	-1.007490	4.397498	-5.107404
H	0.528295	7.222935	-2.254199
H	-1.016189	6.675305	-4.102014
C	-3.237863	-3.104981	0.984266
C	-4.559468	-2.820441	1.218159
C	-4.922303	-1.976621	2.298918
C	-3.953457	-1.429906	3.104367
H	-2.957260	-3.765711	0.168649
H	-5.323957	-3.248753	0.574926
H	-5.971642	-1.770971	2.492271
H	-4.224026	-0.797666	3.945865
C	3.527607	-5.076162	0.050937
C	4.276700	-4.995743	-1.277028
H	2.612411	-5.668666	-0.060633
H	4.154307	-5.606055	0.781967
C	5.443141	-4.020021	-1.148184
H	3.592744	-4.642809	-2.062234
H	4.623537	-5.990234	-1.576090
C	4.926131	-2.611634	-0.865012
H	6.096511	-4.347045	-0.327547
H	6.051418	-4.011570	-2.058494
H	4.436194	-2.221094	-1.770473
H	5.758391	-1.931120	-0.669144
C	6.351370	-0.741447	1.611038
C	7.860885	-0.549577	1.486517
H	6.075085	-1.777307	1.398882
H	6.054593	-0.568711	2.655736
C	8.217538	0.921935	1.680795
H	8.375152	-1.177777	2.221158
H	8.195530	-0.876418	0.492027
C	7.586301	1.757959	0.569885
H	7.840508	1.256303	2.656047
H	9.302781	1.067431	1.686848
H	8.132521	1.571890	-0.365864
H	7.698800	2.827248	0.780774

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M06-2X/6-31G* Energy = -8271.58173157

M06-2X/6-31G* Free Energy = -8270.697299

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.55752827

Lowest Frequency = 12.8042

M06-2X/6-31G* Geometry

C	-2.915610	-2.158996	-2.821228
C	-2.323829	-2.616740	0.932067
C	-1.985916	-3.110355	-2.737929
H	-2.697744	-1.131477	-2.531002

H	-3.919373	-2.367126	-3.183899
C	-0.601791	-2.863037	-2.196606
H	-2.225073	-4.132121	-3.036655
N	-1.478253	-2.286054	0.019863
C	-2.982026	-1.556314	1.726265
C	-2.653206	-4.033232	1.232790
C	-0.521546	-3.152404	-0.680618
C	0.864188	-2.879469	-0.106742
H	-0.779010	-4.197134	-0.487044
H	-1.408648	-1.217049	-0.316215
H	-0.296992	-1.827689	-2.387177
H	0.135706	-3.511319	-2.682669
C	-1.002474	4.020228	1.405078
C	-2.354596	3.915776	1.763320
C	-0.595558	3.566572	0.132441
C	-1.525707	2.932767	-0.687966
C	-2.867562	2.761353	-0.327022
C	-3.260204	3.301807	0.892448
C	0.820731	3.648392	-0.341422
C	1.476795	4.884676	-0.508081
C	2.836030	4.895204	-0.848245
C	3.500042	3.685291	-1.051637
C	2.855957	2.451954	-0.989634
C	1.495177	2.461134	-0.652003
O	-1.063624	2.362207	-1.857008
O	0.814126	1.266595	-0.558067
P	-0.381501	0.891414	-1.637903
O	-1.346383	0.073693	-0.799224
O	0.128583	0.385039	-2.929134
C	-3.780311	1.944236	-1.163766
C	3.616676	1.194588	-1.207169
C	-3.828798	2.121210	-2.576160
C	-4.622768	1.325348	-3.356617
C	-5.410798	0.293112	-2.782437
C	-5.372684	0.111574	-1.372051
C	-4.551500	0.960594	-0.586360
C	3.144389	0.172842	-2.079694
C	3.844491	-0.996682	-2.220005
C	5.039283	-1.232274	-1.491169
C	5.521550	-0.211188	-0.625526
C	4.794773	1.000774	-0.522067
H	-4.300835	3.200509	1.196626
H	4.555046	3.701433	-1.318091
H	-3.214757	2.891552	-3.029291
H	-4.649353	1.466855	-4.433785
H	5.145058	1.759868	0.174520
H	3.475659	-1.773791	-2.885448
H	2.226003	0.326818	-2.637436
H	-4.501610	0.791037	0.487730
C	-2.536310	-4.518760	2.538078
C	-2.865346	-5.841463	2.813771
C	-3.342988	-6.667868	1.798328
C	-3.488633	-6.175005	0.503130
C	-3.138848	-4.860035	0.214768
H	-2.179908	-3.862340	3.326586
H	-2.756490	-6.224825	3.822935
H	-3.608977	-7.696797	2.018925
H	-3.255489	-4.454166	-0.787084
H	-3.876255	-6.814027	-0.283571
C	-4.264398	-1.775768	2.248428
C	-4.878739	-0.798944	3.022833
C	-4.203267	0.386752	3.311226
C	-2.920183	0.601451	2.811967

C	-2.311506	-0.358284	2.011617
H	-1.316441	-0.173603	1.621981
H	-4.780727	-2.706225	2.031742
H	-5.878761	-0.966686	3.409625
H	-4.676514	1.141932	3.931990
H	-2.388793	1.521109	3.033888
C	1.832165	-3.882643	-0.162143
C	3.088912	-3.649357	0.383181
C	3.415323	-2.446364	1.002351
C	2.433346	-1.464346	1.046725
Br	4.374187	-5.036442	0.328913
H	4.400537	-2.281984	1.425608
C	1.177303	-1.657275	0.485075
H	0.467711	-0.840905	0.516309
H	1.609313	-4.847298	-0.607936
Br	2.755368	0.156819	1.959417
C	6.683436	-0.458990	0.152351
C	7.332820	-1.665640	0.078003
C	6.854058	-2.680380	-0.786307
C	5.739093	-2.464176	-1.556348
H	7.041720	0.322903	0.817405
H	8.215181	-1.848691	0.683635
H	5.354138	-3.250443	-2.201428
H	7.364860	-3.637705	-0.826647
C	-6.138522	-0.937040	-0.795761
C	-6.899516	-1.765717	-1.580282
C	-6.939577	-1.581410	-2.984543
C	-6.214732	-0.573148	-3.568551
H	-6.108788	-1.064581	0.283417
H	-7.480602	-2.563933	-1.128087
H	-7.549279	-2.239877	-3.595723
H	-6.239753	-0.425761	-4.645342
C	-2.868736	4.430893	3.095040
C	-1.774671	4.544001	4.154102
H	-3.681611	3.781714	3.444669
H	-3.318534	5.422150	2.943293
C	-0.572626	5.282463	3.571865
H	-1.458464	3.541460	4.474797
H	-2.162070	5.056798	5.040536
C	0.030613	4.486475	2.417032
H	-0.896079	6.268535	3.210766
H	0.189625	5.455784	4.338270
H	0.526278	3.588068	2.814808
H	0.823694	5.061584	1.933650
C	0.695561	6.185465	-0.429724
C	1.585691	7.405626	-0.205821
H	-0.082686	6.133718	0.335641
H	0.159588	6.304927	-1.382553
C	2.732196	7.408060	-1.213160
H	0.987582	8.318906	-0.289733
H	1.997401	7.382382	0.813121
C	3.620089	6.187024	-0.986508
H	2.316734	7.380971	-2.228834
H	3.327283	8.323534	-1.131950
H	4.205472	6.341062	-0.068707
H	4.348030	6.083602	-1.798617

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M06-2X/6-31G* Energy = -8271.58303048

M06-2X/6-31G* Free Energy = -8270.697594

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.55806897

Lowest Frequency = 17.5389

M06-2X/6-31G* Geometry

C	1.892150	0.246363	2.991464
C	0.663004	-2.851235	1.785822
C	0.645851	0.099212	3.438379
H	2.092642	0.453370	1.942188
H	2.746446	0.170027	3.659334
C	-0.569846	0.187874	2.560506
H	0.468182	-0.126150	4.491018
N	-0.105080	-1.884826	1.413446
C	1.687191	-3.365754	0.863775
C	0.482109	-3.489673	3.124030
C	-1.128328	-1.209648	2.216351
C	-2.424681	-1.184048	1.413015
H	-1.283809	-1.782714	3.136877
H	0.009986	-1.369699	0.437812
H	-0.343116	0.705250	1.619936
H	-1.348497	0.757267	3.078633
C	2.911182	4.058539	-0.212944
C	4.290719	3.966808	-0.437921
C	2.153603	2.872770	-0.105909
C	2.752234	1.642642	-0.396194
C	4.126328	1.535463	-0.645425
C	4.871520	2.711369	-0.617082
C	0.709850	2.908723	0.277208
C	0.283372	3.453099	1.510047
C	-1.090802	3.562058	1.762132
C	-2.002578	3.155625	0.785321
C	-1.610704	2.548570	-0.406280
C	-0.233507	2.384653	-0.612995
O	1.974372	0.504194	-0.346713
O	0.219564	1.728252	-1.735708
P	0.827111	0.219574	-1.508935
O	-0.211368	-0.590447	-0.746910
O	1.403851	-0.272309	-2.775928
C	4.807330	0.254903	-0.971015
C	-2.653029	2.150793	-1.388711
C	5.943308	-0.147745	-0.214175
C	6.655297	-1.269466	-0.550238
C	6.289902	-2.046438	-1.680839
C	5.159704	-1.643417	-2.443986
C	4.421714	-0.495923	-2.057727
C	-3.614940	3.125113	-1.783109
C	-4.672525	2.790101	-2.585075
C	-4.841868	1.454772	-3.037900
C	-3.858331	0.490237	-2.687465
C	-2.767707	0.864962	-1.862479
H	5.941128	2.647814	-0.808568
H	-3.070135	3.257846	0.980063
H	6.235817	0.449310	0.645727
H	7.517498	-1.572288	0.038801
H	-2.051288	0.105219	-1.559478
H	-5.406755	3.539098	-2.871203
H	-3.499056	4.145266	-1.426846
H	3.552601	-0.207670	-2.643824
C	-0.510412	-4.461300	3.271759
C	-0.698359	-5.078537	4.504796
C	0.107099	-4.734201	5.587321
C	1.101796	-3.770934	5.436904
C	1.292774	-3.145863	4.207710
H	-1.132513	-4.732949	2.423113
H	-1.473123	-5.829906	4.616841
H	-0.039469	-5.217536	6.547840
H	2.058435	-2.386733	4.083695
H	1.731908	-3.502366	6.278682

C	2.788070	-4.073894	1.365523
C	3.800307	-4.481214	0.504741
C	3.711659	-4.210207	-0.858666
C	2.595546	-3.545591	-1.366811
C	1.586270	-3.125246	-0.516843
H	0.723492	-2.616860	-0.933982
H	2.860850	-4.288314	2.426536
H	4.663115	-5.006950	0.900476
H	4.511454	-4.511162	-1.529818
H	2.515473	-3.334268	-2.427379
C	-3.266955	-0.074758	1.424539
C	-4.447589	-0.102135	0.690610
C	-4.830053	-1.209797	-0.051464
C	-3.971800	-2.302201	-0.057111
Br	-5.522442	1.444135	0.633011
H	-5.735685	-1.202405	-0.646531
C	-2.782607	-2.304538	0.657864
H	-2.130398	-3.169493	0.599746
H	-3.008300	0.830923	1.958128
Br	-4.417139	-3.802199	-1.117509
C	-4.020516	-0.852100	-3.123096
C	-5.122029	-1.224897	-3.849650
C	-6.102353	-0.262696	-4.199830
C	-5.960893	1.045018	-3.809463
H	-3.266189	-1.583667	-2.843315
H	-5.244728	-2.258957	-4.157787
H	-6.709896	1.785888	-4.077986
H	-6.968308	-0.566378	-4.780260
C	4.796901	-2.399425	-3.591960
C	5.516703	-3.508580	-3.957252
C	6.639904	-3.914761	-3.191229
C	7.014918	-3.200928	-2.080719
H	3.933850	-2.074277	-4.168439
H	5.233866	-4.078132	-4.837274
H	7.205388	-4.791578	-3.492228
H	7.879113	-3.504403	-1.494620
C	5.182583	5.193535	-0.486058
C	4.418230	6.481545	-0.780721
H	5.687463	5.296446	0.485201
H	5.974484	5.036929	-1.226576
C	3.186737	6.565356	0.116482
H	4.098296	6.490561	-1.830592
H	5.073251	7.346697	-0.634924
C	2.230087	5.417445	-0.197369
H	3.499034	6.510745	1.169148
H	2.669653	7.521383	-0.015337
H	1.380709	5.430179	0.488799
H	1.799948	5.575292	-1.197098
C	1.296700	3.824514	2.581040
C	0.708272	4.686185	3.695924
H	2.168012	4.316971	2.143784
H	1.674541	2.889311	3.016451
C	-0.599279	4.076648	4.192951
H	1.435083	4.778640	4.509476
H	0.513913	5.700999	3.321415
C	-1.629922	4.114066	3.068552
H	-0.415207	3.035693	4.495083
H	-0.979315	4.608407	5.071269
H	-1.949271	5.154323	2.913991
H	-2.533534	3.559002	3.349047

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M06-2X/6-31G* Energy = -8271.58057082

M06-2X/6-31G* Free Energy = -8270.696720

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.55636228

Lowest Frequency = 12.5731

M06-2X/6-31G* Geometry

C	-2.223984	-2.830894	-2.822193
C	-1.471196	-3.212304	1.053728
C	-1.096161	-3.527041	-2.684219
H	-2.265629	-1.775929	-2.556828
H	-3.135951	-3.278509	-3.209868
C	0.171992	-2.929471	-2.133892
H	-1.068073	-4.582768	-2.959056
N	-0.791297	-2.657126	0.111566
C	-2.333076	-2.369388	1.913166
C	-1.403712	-4.669164	1.328488
C	0.351125	-3.213530	-0.626937
C	1.617001	-2.569423	-0.072550
H	0.401462	-4.291403	-0.451796
H	-1.046894	-1.604593	-0.203759
H	0.180048	-1.846808	-2.304266
H	1.053554	-3.341700	-2.638293
C	-1.985219	3.597566	1.571363
C	-3.216959	3.123695	2.047352
C	-1.577920	3.243184	0.268960
C	-2.353968	2.348497	-0.466281
C	-3.550063	1.800737	0.015416
C	-3.974419	2.249952	1.263773
C	-0.280233	3.701160	-0.318497
C	-0.000603	5.065128	-0.537220
C	1.279077	5.438840	-0.968844
C	2.237509	4.452934	-1.206618
C	1.961534	3.092707	-1.094161
C	0.673579	2.738213	-0.669289
O	-1.842337	1.917347	-1.673676
O	0.354414	1.405064	-0.527865
P	-0.760380	0.701400	-1.525157
O	-1.388754	-0.351748	-0.631716
O	-0.226568	0.352131	-2.858802
C	-4.243732	0.693290	-0.689733
C	3.020191	2.080654	-1.343047
C	-4.751520	-0.388717	0.085050
C	-5.327938	-1.479962	-0.505809
C	-5.432234	-1.571781	-1.917764
C	-4.933875	-0.495268	-2.703003
C	-4.353477	0.629348	-2.061715
C	2.792509	0.946627	-2.173888
C	3.767595	-0.002876	-2.333340
C	5.016153	0.104364	-1.666894
C	5.254423	1.241904	-0.846071
C	4.239872	2.223265	-0.721210
H	-4.910807	1.867479	1.666561
H	3.229603	4.751168	-1.540009
H	-4.644737	-0.356922	1.164542
H	-5.696497	-2.301188	0.105121
H	4.410761	3.067049	-0.055626
H	3.584409	-0.868876	-2.965360
H	1.839621	0.839092	-2.682726
H	-3.966348	1.433776	-2.678509
C	-1.153360	-5.131910	2.623461
C	-1.108901	-6.499585	2.870960
C	-1.347920	-7.403826	1.837874
C	-1.627951	-6.943041	0.552827
C	-1.650492	-5.577090	0.293131
H	-0.984692	-4.419578	3.425723
H	-0.895456	-6.859661	3.871967

H	-1.322928	-8.470606	2.036550
H	-1.877856	-5.198114	-0.700484
H	-1.830692	-7.647302	-0.247403
C	-1.947902	-1.058899	2.230253
C	-2.716990	-0.303292	3.108029
C	-3.878312	-0.839870	3.660052
C	-4.276142	-2.137032	3.334259
C	-3.499770	-2.905468	2.475521
H	-3.796487	-3.921184	2.231651
H	-1.042613	-0.633163	1.811926
H	-2.407682	0.708546	3.350760
H	-4.476431	-0.246753	4.345765
H	-5.184657	-2.552434	3.757998
C	2.820383	-3.273000	-0.121655
C	3.972563	-2.690058	0.392711
C	3.965621	-1.426832	0.976461
C	2.753284	-0.748926	1.018017
Br	5.588716	-3.671713	0.340270
H	4.874255	-0.987196	1.373569
C	1.591774	-1.291525	0.483428
H	0.687408	-0.697460	0.503209
H	2.863868	-4.273550	-0.541102
Br	2.633258	0.924818	1.883855
C	6.477685	1.331326	-0.130223
C	7.418030	0.336172	-0.221626
C	7.181606	-0.794195	-1.041618
C	6.011853	-0.902360	-1.750513
H	6.649473	2.199595	0.501182
H	8.346631	0.409911	0.336151
H	5.816778	-1.781246	-2.360695
H	7.923980	-1.584708	-1.094811
C	-5.002871	-0.591558	-4.119194
C	-5.541837	-1.698667	-4.722431
C	-6.048323	-2.765120	-3.938278
C	-5.993885	-2.701086	-2.568927
H	-4.606677	0.226204	-4.715054
H	-5.582150	-1.763299	-5.805254
H	-6.478911	-3.633533	-4.427704
H	-6.377943	-3.516488	-1.960542
C	-3.742872	3.508395	3.417729
C	-2.637494	3.939854	4.378532
H	-4.314017	2.669483	3.834682
H	-4.457661	4.335870	3.306498
C	-1.744234	4.973690	3.698562
H	-2.028328	3.070265	4.662333
H	-3.074745	4.340087	5.299092
C	-1.043650	4.358803	2.489221
H	-2.360447	5.823769	3.374561
H	-0.997820	5.366605	4.396383
H	-0.279530	3.645883	2.834314
H	-0.492947	5.126401	1.940786
C	-1.102482	6.103357	-0.410763
C	-0.570134	7.526140	-0.257258
H	-1.783135	5.858480	0.408494
H	-1.713147	6.047311	-1.323568
C	0.464294	7.816904	-1.341328
H	-1.400580	8.238038	-0.306004
H	-0.103054	7.642898	0.730922
C	1.666687	6.892378	-1.167946
H	0.007988	7.650704	-2.325760
H	0.788272	8.862230	-1.307735
H	2.244335	7.223762	-0.293162
H	2.341530	6.972660	-2.027180

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M06-2X/6-31G* Energy = -8271.57835944

M06-2X/6-31G* Free Energy = -8270.694733

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.55489056

Lowest Frequency = 10.8140

M06-2X/6-31G* Geometry

C	-1.740942	3.800911	-0.237698
C	0.807932	2.789875	1.937460
C	-0.543996	4.149825	-0.705998
H	-2.102562	2.775502	-0.315265
H	-2.417658	4.530907	0.199107
C	0.409963	3.173470	-1.332619
H	-0.208313	5.184500	-0.625422
N	1.082976	2.239439	0.805284
C	1.203184	4.192181	2.244131
C	0.116658	2.005368	2.980319
C	1.613586	2.880147	-0.412642
C	2.641293	1.910879	-0.981195
H	2.093507	3.821799	-0.132514
H	0.822011	1.196164	0.584183
H	-0.112837	2.238440	-1.569071
H	0.812902	3.567735	-2.274079
C	-4.215519	-3.020316	-0.489856
C	-5.262897	-2.442245	-1.219209
C	-3.111366	-2.225475	-0.122731
C	-3.000852	-0.926447	-0.631233
C	-4.037153	-0.334985	-1.362190
C	-5.169321	-1.104772	-1.609669
C	-2.047442	-2.707775	0.808447
C	-2.326898	-3.057357	2.147039
C	-1.265640	-3.441109	2.979415
C	0.040301	-3.431780	2.484776
C	0.353303	-3.033795	1.186955
C	-0.725531	-2.690349	0.363413
O	-1.876822	-0.183935	-0.340921
O	-0.494373	-2.231179	-0.918008
P	-0.414096	-0.600313	-1.022833
O	0.585358	-0.116839	-0.000646
O	-0.345295	-0.200945	-2.446957
C	-3.950041	1.071884	-1.834703
C	1.767553	-2.943796	0.744374
C	-2.931496	1.463964	-2.750568
C	-2.867341	2.756421	-3.199016
C	-3.792441	3.738145	-2.753974
C	-4.808434	3.352850	-1.836653
C	-4.866900	2.002115	-1.402482
C	2.739687	-2.435586	1.654076
C	4.071307	-2.419890	1.337757
C	4.523108	-2.917603	0.087133
C	3.555324	-3.365437	-0.854536
C	2.181425	-3.366021	-0.499537
H	-5.985773	-0.657440	-2.173213
H	0.850736	-3.728870	3.147400
H	-2.200578	0.729749	-3.075216
H	-2.088003	3.051976	-3.897821
H	1.456241	-3.725285	-1.223550
H	4.801901	-2.016808	2.034703
H	2.400954	-2.037103	2.606285
H	-5.641873	1.709854	-0.696803
C	0.300954	2.347120	4.328116
C	-0.283292	1.578563	5.326696
C	-1.062587	0.473949	4.987515

C	-1.265762	0.143861	3.649091
C	-0.685004	0.904631	2.642669
H	0.917186	3.201157	4.590682
H	-0.126927	1.839127	6.368321
H	-1.516598	-0.127669	5.769764
H	-0.865082	0.638733	1.606294
H	-1.871053	-0.714674	3.375561
C	0.213295	5.131755	2.545037
C	0.572006	6.439622	2.851102
C	1.916269	6.807341	2.884360
C	2.904595	5.866065	2.609630
C	2.549932	4.559279	2.286708
H	3.317644	3.817902	2.084120
H	-0.830338	4.833102	2.518506
H	-0.198641	7.171620	3.069452
H	2.193179	7.827476	3.130388
H	3.952320	6.145535	2.647372
C	2.353777	1.106576	-2.078908
C	3.226898	0.078256	-2.413665
C	4.407473	-0.147219	-1.717052
C	4.687485	0.693304	-0.645819
Br	2.734832	-1.089543	-3.807452
H	5.071249	-0.962639	-1.984751
C	3.823092	1.709569	-0.267424
H	4.061365	2.314318	0.601948
H	1.421298	1.189015	-2.623465
Br	6.267550	0.423206	0.362469
C	3.996386	-3.821456	-2.125943
C	5.330972	-3.840186	-2.441134
C	6.295175	-3.415921	-1.492795
C	5.899566	-2.967287	-0.257860
H	3.251218	-4.141078	-2.848972
H	5.654629	-4.183633	-3.418784
H	6.632234	-2.631404	0.470166
H	7.349898	-3.448546	-1.748685
C	-5.719693	4.335674	-1.366980
C	-5.623116	5.638562	-1.784378
C	-4.610010	6.022173	-2.697222
C	-3.718906	5.092827	-3.169711
H	-6.495261	4.035140	-0.666809
H	-6.324748	6.381838	-1.418103
H	-4.543424	7.056395	-3.020960
H	-2.936871	5.380419	-3.867968
C	-6.515110	-3.220573	-1.578610
C	-6.321157	-4.734196	-1.523481
H	-6.861182	-2.913049	-2.571495
H	-7.313359	-2.940429	-0.876391
C	-5.618845	-5.120685	-0.224300
H	-5.706327	-5.059884	-2.372437
H	-7.288992	-5.238046	-1.614152
C	-4.220476	-4.509000	-0.187726
H	-6.207065	-4.756025	0.629886
H	-5.549335	-6.208820	-0.125109
H	-3.729614	-4.719617	0.765823
H	-3.598081	-4.999047	-0.950299
C	-3.727063	-2.890979	2.716404
C	-3.940915	-3.662585	4.016421
H	-4.487496	-3.168044	1.983873
H	-3.891261	-1.818464	2.905453
C	-2.810336	-3.364068	4.996168
H	-4.913192	-3.399698	4.445623
H	-3.962031	-4.740691	3.805941
C	-1.485989	-3.860436	4.421247

H	-2.762570	-2.278424	5.163497
H	-2.995080	-3.829479	5.969830
H	-1.466799	-4.957916	4.477154
H	-0.645408	-3.509037	5.030572

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M06-2X/6-31G* Energy = -8271.59163984

M06-2X/6-31G* Free Energy = -8270.706854

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.55596438

Lowest Frequency = 11.6820

M06-2X/6-31G* Geometry

C	2.432929	3.684732	-1.924361
C	3.739726	1.369741	0.271438
C	2.114846	3.971763	-0.663223
H	1.898901	2.907246	-2.470086
H	3.220002	4.217216	-2.451488
C	1.043339	3.241805	0.094115
H	2.657548	4.749596	-0.125060
N	2.463433	1.296265	0.331198
C	4.441568	0.485900	-0.694233
C	4.575003	2.276472	1.115818
C	1.618861	2.209988	1.093609
C	0.528693	1.365793	1.751286
H	2.191635	2.745727	1.860109
H	1.646878	0.155727	-0.348021
H	0.380832	2.717532	-0.606957
H	0.433289	3.962942	0.651845
C	-2.874612	-2.773611	0.606522
C	-2.066136	-3.785387	1.141286
C	-2.428428	-2.082450	-0.546148
C	-1.185037	-2.398577	-1.087192
C	-0.354598	-3.388280	-0.555820
C	-0.835779	-4.077787	0.549022
C	-3.181309	-0.921981	-1.108548
C	-4.505532	-1.023463	-1.580380
C	-5.216989	0.144368	-1.886925
C	-4.575587	1.383169	-1.806116
C	-3.227254	1.494770	-1.489263
C	-2.547650	0.323372	-1.148782
O	-0.712323	-1.632518	-2.152024
O	-1.215671	0.421750	-0.783292
P	-0.050011	-0.223866	-1.721705
O	1.040685	-0.620329	-0.682842
O	0.346620	0.606964	-2.872009
C	1.008441	-3.646584	-1.079279
C	-2.513062	2.799833	-1.513938
C	1.229644	-3.896564	-2.461578
C	2.484137	-4.193144	-2.923410
C	3.594956	-4.241980	-2.039779
C	3.387991	-3.943374	-0.663807
C	2.075603	-3.655082	-0.210749
C	-1.562650	3.059302	-2.541675
C	-0.869797	4.240459	-2.563741
C	-1.054033	5.214670	-1.547315
C	-2.012853	4.966720	-0.526234
C	-2.746915	3.750849	-0.549225
H	-0.209966	-4.852344	0.987511
H	-5.128143	2.287181	-2.053359
H	0.385631	-3.860823	-3.143125
H	2.645101	-4.404617	-3.977574
H	-3.461225	3.552177	0.245466
H	-0.138421	4.432208	-3.344206
H	-1.371840	2.296802	-3.289492

H	1.909910	-3.408003	0.836636
C	4.554204	2.176760	2.509264
C	5.355534	3.012560	3.282054
C	6.175484	3.954973	2.666498
C	6.202767	4.053779	1.276505
C	5.414579	3.209384	0.501657
H	3.913310	1.438117	2.985171
H	5.339514	2.926215	4.363825
H	6.797243	4.609138	3.269609
H	5.434266	3.270477	-0.582903
H	6.844724	4.784877	0.795413
C	5.711433	-0.018857	-0.392595
C	6.332831	-0.906321	-1.263568
C	5.702705	-1.274028	-2.450248
C	4.448283	-0.755942	-2.765512
C	3.817219	0.123527	-1.894739
H	2.846890	0.537879	-2.152748
H	6.199106	0.269537	0.534374
H	7.306590	-1.316698	-1.014829
H	6.188648	-1.969062	-3.127075
H	3.954843	-1.037378	-3.690242
C	0.866078	0.101762	2.244834
C	-0.124072	-0.740976	2.724044
C	-1.459892	-0.362242	2.736928
C	-1.772729	0.899380	2.252982
Br	0.346136	-2.461752	3.361664
H	-2.229159	-1.031282	3.100153
C	-0.803781	1.773256	1.777249
H	-1.111085	2.728378	1.367252
H	1.891306	-0.250753	2.198755
Br	-3.595315	1.402824	2.156706
C	-2.171057	5.918628	0.516299
C	-1.404289	7.055644	0.547789
C	-0.445684	7.299482	-0.466763
C	-0.278447	6.401806	-1.490334
H	-2.904563	5.722160	1.294511
H	-1.527613	7.773718	1.352700
H	0.463819	6.573917	-2.265366
H	0.157916	8.201046	-0.427633
C	4.502603	-3.958369	0.216013
C	5.753882	-4.284926	-0.240428
C	5.953716	-4.610807	-1.604256
C	4.899749	-4.582745	-2.481985
H	4.341227	-3.713766	1.262849
H	6.597012	-4.299452	0.443771
H	6.947059	-4.878552	-1.952491
H	5.047338	-4.824238	-3.532115
C	-2.463351	-4.566645	2.377265
C	-3.436520	-3.798174	3.262988
H	-1.557886	-4.827094	2.936371
H	-2.926922	-5.515125	2.071760
C	-4.605673	-3.304254	2.416622
H	-2.909630	-2.951523	3.723120
H	-3.789573	-4.434934	4.080667
C	-4.145650	-2.341154	1.320359
H	-5.092292	-4.174715	1.956028
H	-5.361141	-2.810304	3.036227
H	-4.964160	-2.194653	0.612195
H	-3.973870	-1.342003	1.741779
C	-5.112303	-2.384719	-1.872645
C	-6.638628	-2.365276	-1.884751
H	-4.731293	-3.144473	-1.186498
H	-4.757123	-2.687144	-2.868531

C	-7.132440	-1.255980	-2.810866
H	-7.019405	-3.340154	-2.205992
H	-7.018239	-2.189209	-0.868290
C	-6.680530	0.105695	-2.286558
H	-6.721225	-1.421049	-3.815092
H	-8.223218	-1.275417	-2.902803
H	-7.284417	0.363267	-1.404839
H	-6.876453	0.887403	-3.028561

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M06-2X/6-31G* Energy = -8271.58907092

M06-2X/6-31G* Free Energy = -8270.703869

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.55605112

Lowest Frequency = 12.5504

M06-2X/6-31G* Geometry

C	2.991760	2.583460	-2.559006
C	3.888679	0.993899	0.461391
C	2.768078	3.268749	-1.438950
H	2.295152	1.812000	-2.886259
H	3.863731	2.772966	-3.179371
C	1.574073	3.032318	-0.562257
H	3.472291	4.036187	-1.114079
N	2.612797	1.110499	0.460435
C	4.492676	-0.201203	-0.182504
C	4.827270	1.989467	1.062645
C	1.927866	2.355966	0.788993
C	0.654590	2.060002	1.572172
H	2.571306	3.035348	1.360463
H	1.708194	-0.131074	0.056443
H	0.840927	2.403876	-1.085346
H	1.093263	3.992162	-0.343518
C	-3.281208	-2.645069	0.921135
C	-2.735705	-3.706085	1.657659
C	-2.587305	-2.167446	-0.207533
C	-1.315180	-2.669142	-0.487429
C	-0.712867	-3.662896	0.285378
C	-1.474118	-4.196361	1.323828
C	-3.126097	-1.072187	-1.066760
C	-4.345976	-1.190664	-1.763905
C	-4.825389	-0.094520	-2.495097
C	-4.060700	1.071525	-2.570186
C	-2.813684	1.180766	-1.965545
C	-2.368463	0.092233	-1.216717
O	-0.608999	-2.115386	-1.550159
O	-1.125800	0.162969	-0.600037
P	0.082801	-0.679636	-1.292226
O	1.063449	-0.928383	-0.104950
O	0.626065	-0.082993	-2.525338
C	0.694035	-4.089370	0.092434
C	-1.962463	2.387907	-2.161926
C	1.534212	-4.155366	1.240194
C	2.823823	-4.602221	1.143589
C	3.358600	-5.008963	-0.106854
C	2.542107	-4.897626	-1.266561
C	1.208519	-4.431398	-1.136613
C	-1.060318	2.422086	-3.261170
C	-0.271387	3.520233	-3.478761
C	-0.325515	4.637666	-2.606076
C	-1.230109	4.610830	-1.508147
C	-2.045814	3.464508	-1.312144
H	-1.041294	-4.992945	1.925882
H	-4.430011	1.912887	-3.152647
H	1.134825	-3.812038	2.190900

H	3.458816	-4.647833	2.024558
H	-2.717624	3.433228	-0.456986
H	0.432016	3.537225	-4.307023
H	-0.982671	1.549736	-3.901159
H	0.586060	-4.365509	-2.024620
C	4.733785	2.324054	2.416154
C	5.631337	3.228835	2.975698
C	6.620007	3.808319	2.184032
C	6.718347	3.474245	0.834465
C	5.833300	2.557439	0.276795
H	3.958749	1.866766	3.026846
H	5.558629	3.480005	4.029077
H	7.317367	4.516868	2.619888
H	5.905442	2.280820	-0.771570
H	7.490606	3.922854	0.217679
C	3.893066	-0.760028	-1.318294
C	4.453597	-1.882575	-1.916851
C	5.614422	-2.448476	-1.394584
C	6.219360	-1.890190	-0.269765
C	5.668450	-0.763103	0.328503
H	6.141265	-0.320307	1.200755
H	3.004370	-0.302011	-1.743600
H	3.984786	-2.315174	-2.794930
H	6.044473	-3.326037	-1.865637
H	7.123820	-2.330826	0.138179
C	-0.358855	3.020592	1.665613
C	-1.563840	2.684884	2.264894
C	-1.820255	1.410771	2.758035
C	-0.791456	0.485100	2.678933
Br	-2.941709	3.984934	2.368886
H	-2.785935	1.153942	3.176259
C	0.446613	0.804268	2.137531
H	1.213709	0.042499	2.099608
H	-0.229679	4.017148	1.257153
Br	-1.101902	-1.302107	3.208026
C	-1.244296	5.706741	-0.602885
C	-0.384690	6.763633	-0.769393
C	0.520392	6.786018	-1.859676
C	0.543317	5.750056	-2.758039
H	-1.926499	5.674318	0.242819
H	-0.395338	7.589063	-0.064056
H	1.243272	5.751570	-3.589582
H	1.197097	7.626696	-1.977968
C	3.081713	-5.282655	-2.523561
C	4.357410	-5.778152	-2.618872
C	5.159766	-5.912756	-1.458365
C	4.674072	-5.525631	-0.235392
H	2.457926	-5.186344	-3.408657
H	4.754563	-6.078260	-3.583818
H	6.164415	-6.316308	-1.544359
H	5.288743	-5.612279	0.657208
C	-3.451006	-4.291709	2.860539
C	-4.418249	-3.303859	3.508433
H	-2.707664	-4.637175	3.588045
H	-4.009383	-5.184036	2.544238
C	-5.325293	-2.701968	2.439037
H	-3.846847	-2.499483	3.989994
H	-5.002037	-3.804671	4.287403
C	-4.496532	-1.898544	1.440228
H	-5.857972	-3.508645	1.916295
H	-6.085711	-2.054810	2.888021
H	-5.124340	-1.533267	0.624326
H	-4.107911	-0.998193	1.942070

C	-5.074403	-2.523328	-1.818565
C	-6.541560	-2.389140	-2.219073
H	-4.984754	-3.061938	-0.872770
H	-4.557370	-3.148419	-2.561059
C	-6.664208	-1.544518	-3.484134
H	-6.974402	-3.383677	-2.367655
H	-7.105185	-1.910581	-1.405950
C	-6.164441	-0.128894	-3.207959
H	-6.062884	-2.001515	-4.280691
H	-7.699354	-1.512392	-3.839018
H	-6.903659	0.392379	-2.583370
H	-6.093371	0.444496	-4.138683

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M06-2X/6-31G* Energy = -8271.59495411

M06-2X/6-31G* Free Energy = -8270.706421

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.55898760

Lowest Frequency = 11.4585

M06-2X/6-31G* Geometry

C	-0.981788	3.998156	2.820934
C	0.871517	3.788060	-0.314286
C	-1.740473	4.168035	1.740194
H	-0.694301	2.997465	3.139797
H	-0.635946	4.836246	3.418841
C	-2.216180	3.015417	0.903597
H	-2.023013	5.171632	1.419581
N	-0.018238	2.876075	-0.112651
C	0.565228	4.977441	-1.149870
C	2.218985	3.622929	0.254150
C	-1.445009	2.897695	-0.437908
C	-1.796544	1.606087	-1.169869
H	-1.659989	3.767111	-1.065031
H	0.176395	1.987308	0.505417
H	-2.082356	2.074390	1.445567
H	-3.282067	3.129274	0.675445
C	-1.351493	-3.824226	-0.370992
C	-2.716720	-3.507163	-0.414017
C	-0.538085	-3.145312	0.558120
C	-1.079901	-2.152034	1.380975
C	-2.437574	-1.799606	1.330266
C	-3.227135	-2.535355	0.443078
C	0.939579	-3.351390	0.597497
C	1.542161	-4.576897	0.933123
C	2.933360	-4.708729	0.814108
C	3.696294	-3.609175	0.420603
C	3.135685	-2.353679	0.192675
C	1.747022	-2.248061	0.301597
O	-0.217272	-1.524780	2.255554
O	1.149990	-1.005093	0.202509
P	0.762473	-0.342508	1.671848
O	-0.127928	0.834207	1.327151
O	1.938226	-0.179243	2.551167
C	-3.025705	-0.644863	2.061285
C	3.986728	-1.189290	-0.150345
C	-2.510490	-0.145252	3.295767
C	-3.044851	0.974469	3.879514
C	-4.124930	1.679211	3.283699
C	-4.678109	1.161836	2.082659
C	-4.108260	0.004589	1.504643
C	3.646620	-0.345486	-1.247767
C	4.485489	0.661545	-1.642456
C	5.711342	0.899732	-0.965611
C	6.033290	0.096343	0.162603

C	5.150332	-0.946914	0.542487
H	-4.292912	-2.326999	0.390326
H	4.772818	-3.725034	0.310183
H	-1.679585	-0.653693	3.767316
H	-2.629365	1.348865	4.811859
H	5.399547	-1.559453	1.405647
H	4.230284	1.287516	-2.494230
H	2.724205	-0.541148	-1.786432
H	-4.518620	-0.328114	0.558269
C	2.444651	2.725607	1.309491
C	3.737347	2.466275	1.742588
C	4.811575	3.134276	1.158678
C	4.592025	4.062778	0.140498
C	3.305459	4.302326	-0.321214
H	1.623918	2.219289	1.804123
H	3.881618	1.721670	2.518496
H	5.827769	2.916607	1.477073
H	3.142284	4.992253	-1.143068
H	5.434767	4.571589	-0.316392
C	0.132632	4.821685	-2.469986
C	-0.134561	5.943783	-3.247152
C	0.017157	7.218616	-2.705262
C	0.446713	7.374223	-1.388927
C	0.733653	6.256071	-0.612723
H	1.080139	6.363798	0.411171
H	0.015578	3.822192	-2.882646
H	-0.461320	5.822470	-4.274674
H	-0.196633	8.092850	-3.311867
H	0.564983	8.367269	-0.967950
C	-0.802116	0.733350	-1.613268
C	-1.154295	-0.472265	-2.205506
C	-2.479577	-0.842828	-2.379095
C	-3.452490	0.041734	-1.934743
Br	0.207331	-1.642025	-2.783502
H	-2.747025	-1.793310	-2.824761
C	-3.137790	1.258044	-1.344833
H	-3.936718	1.901851	-0.990716
H	0.249281	0.949533	-1.462707
Br	-5.269341	-0.476611	-2.067570
C	7.235740	0.360602	0.872290
C	8.084710	1.360903	0.470108
C	7.773785	2.145831	-0.668510
C	6.614870	1.917603	-1.366770
H	7.472778	-0.250249	1.739671
H	9.002759	1.550101	1.018054
H	6.364852	2.521002	-2.236473
H	8.458573	2.926766	-0.985390
C	-5.736384	1.861681	1.442381
C	-6.213356	3.034464	1.971128
C	-5.658516	3.554797	3.167641
C	-4.642552	2.890999	3.808977
H	-6.143291	1.451024	0.519540
H	-7.018191	3.569714	1.476412
H	-6.042279	4.485376	3.574331
H	-4.208875	3.292284	4.721380
C	-3.665714	-4.149152	-1.408977
C	-2.932597	-4.781239	-2.589444
H	-4.380458	-3.388890	-1.749542
H	-4.258499	-4.924113	-0.903152
C	-1.808376	-5.668722	-2.064408
H	-2.493245	-3.999425	-3.226227
H	-3.633556	-5.348041	-3.210577
C	-0.756390	-4.819590	-1.352814

H	-2.228541	-6.405946	-1.366617
H	-1.335550	-6.229473	-2.877170
H	-0.026538	-5.467492	-0.863153
H	-0.186908	-4.251354	-2.097935
C	0.717918	-5.692263	1.550803
C	1.379366	-7.061944	1.420237
H	-0.297374	-5.704602	1.147187
H	0.603795	-5.454715	2.618416
C	2.817296	-6.992175	1.929916
H	0.803277	-7.807251	1.978317
H	1.380164	-7.376702	0.367029
C	3.632963	-6.031570	1.066673
H	2.810037	-6.639771	2.969416
H	3.284628	-7.982436	1.928365
H	3.831774	-6.509971	0.096979
H	4.612562	-5.844689	1.520437

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M06-2X/6-31G* Energy = -8271.58482868

M06-2X/6-31G* Free Energy = -8270.695490

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.55950538

Lowest Frequency = 15.7364

M06-2X/6-31G* Geometry

C	-0.587607	3.216832	3.058263
C	-0.940200	3.257859	-0.898975
C	-1.793136	3.099193	2.505128
H	0.113140	2.382598	3.065400
H	-0.280651	4.146859	3.531544
C	-2.304154	1.835040	1.877083
H	-2.483743	3.944914	2.507122
N	-1.375926	2.169813	-0.348809
C	-1.819359	4.463884	-0.917753
C	0.390458	3.337904	-1.518243
C	-2.642517	2.017363	0.378281
C	-3.484207	0.865946	-0.151164
H	-3.214596	2.941107	0.259908
H	-0.739384	1.307674	-0.226676
H	-1.570434	1.026615	1.983138
H	-3.230910	1.520103	2.373586
C	2.987189	-3.550143	-1.220396
C	1.967125	-4.349803	-1.748219
C	2.708054	-2.761761	-0.085239
C	1.412505	-2.720224	0.437182
C	0.391233	-3.566461	-0.029103
C	0.716629	-4.356415	-1.134497
C	3.766709	-1.890608	0.512984
C	4.951725	-2.413715	1.066373
C	5.977432	-1.531905	1.432748
C	5.801081	-0.159285	1.249716
C	4.604278	0.391239	0.795859
C	3.579516	-0.508570	0.476018
O	1.171557	-1.809966	1.449778
O	2.360224	-0.037474	0.038753
P	1.056186	-0.230748	1.029709
O	-0.114058	-0.060996	0.079774
O	1.139995	0.596278	2.257670
C	-0.973592	-3.683405	0.553766
C	4.474821	1.856938	0.589891
C	-1.657092	-4.932731	0.417412
C	-2.971515	-5.076725	0.764368
C	-3.697447	-3.993770	1.326988
C	-2.996219	-2.786712	1.582860
C	-1.647557	-2.648160	1.163226

C	5.519189	2.537885	-0.099041
C	5.461567	3.888377	-0.325649
C	4.347902	4.648723	0.116157
C	3.296426	3.975010	0.797121
C	3.386788	2.578780	1.030798
H	-0.061636	-4.972243	-1.577559
H	6.612861	0.514561	1.517916
H	-1.117690	-5.788994	0.025888
H	-3.474394	-6.030118	0.622750
H	2.588172	2.083024	1.578307
H	6.267695	4.393311	-0.852742
H	6.367701	1.961749	-0.458540
H	-1.185174	-1.677860	1.276162
C	1.188477	2.195296	-1.690508
C	2.459289	2.310601	-2.236231
C	2.940287	3.554379	-2.636830
C	2.145957	4.691719	-2.492600
C	0.879700	4.588427	-1.937699
H	0.837092	1.212218	-1.399146
H	3.074652	1.421588	-2.327262
H	3.940038	3.640576	-3.051182
H	0.277185	5.481058	-1.813596
H	2.522180	5.663712	-2.792809
C	-1.618338	5.479529	0.018736
C	-2.442983	6.600566	0.002860
C	-3.458378	6.708763	-0.945376
C	-3.652739	5.694918	-1.880359
C	-2.833891	4.568984	-1.869772
H	-2.982249	3.770912	-2.592043
H	-0.823232	5.377581	0.752286
H	-2.291359	7.389972	0.732035
H	-4.099108	7.584630	-0.955340
H	-4.443185	5.777719	-2.619078
C	-2.959469	-0.217462	-0.853154
C	-3.803371	-1.271042	-1.197340
C	-5.148161	-1.286017	-0.858082
C	-5.644739	-0.194668	-0.156822
Br	-3.077475	-2.769084	-2.081542
H	-5.777147	-2.135685	-1.093748
C	-4.841582	0.881768	0.185492
H	-5.264584	1.712501	0.743203
H	-1.902799	-0.294927	-1.080844
Br	-7.442421	-0.230020	0.424773
C	2.170726	4.725378	1.232325
C	2.096060	6.076076	1.004289
C	3.142020	6.744577	0.320603
C	4.240564	6.045833	-0.112109
H	1.370583	4.196948	1.746000
H	1.237528	6.644703	1.352130
H	5.048502	6.553706	-0.633667
H	3.073316	7.814478	0.147890
C	-3.683982	-1.715608	2.211738
C	-5.014053	-1.821007	2.526707
C	-5.725533	-3.008150	2.223832
C	-5.076435	-4.074489	1.652152
H	-3.129486	-0.806962	2.429919
H	-5.538518	-0.985962	2.983388
H	-6.784775	-3.070322	2.454541
H	-5.610423	-4.997181	1.438349
C	2.178057	-5.223135	-2.970447
C	3.364765	-4.778848	-3.820793
H	1.258560	-5.237899	-3.566081
H	2.347123	-6.258279	-2.641274

C	4.580732	-4.568598	-2.923626
H	3.124185	-3.836422	-4.329987
H	3.570574	-5.523117	-4.596976
C	4.322888	-3.432804	-1.935660
H	4.786796	-5.496483	-2.372265
H	5.473593	-4.343250	-3.515982
H	4.325265	-2.475397	-2.477557
H	5.147934	-3.363311	-1.223067
C	5.076516	-3.902523	1.336163
C	6.521451	-4.355402	1.531797
H	4.594390	-4.483029	0.545091
H	4.504923	-4.121122	2.249527
C	7.220751	-3.449757	2.542138
H	6.539616	-5.399183	1.861478
H	7.057405	-4.311162	0.573062
C	7.297995	-2.027282	1.992855
H	6.652253	-3.453834	3.481062
H	8.226507	-3.816442	2.771702
H	8.051836	-1.996831	1.193148
H	7.645559	-1.333956	2.766694

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M06-2X/6-31G* Energy = -8271.58482869

M06-2X/6-31G* Free Energy = -8270.695490

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.55950465

Lowest Frequency = 15.7428

M06-2X/6-31G* Geometry

C	-0.586824	3.216728	3.058192
C	-0.939100	3.257542	-0.898870
C	-1.792321	3.099520	2.504890
H	0.113490	2.382141	3.065645
H	-0.279490	4.146784	3.531174
C	-2.303861	1.835476	1.877083
H	-2.482461	3.945624	2.506471
N	-1.375272	2.169592	-0.348877
C	-1.817781	4.463927	-0.917538
C	0.391580	3.337190	-1.518135
C	-2.641952	2.017679	0.378180
C	-3.484007	0.866518	-0.151233
H	-3.213723	2.941601	0.259658
H	-0.738985	1.307101	-0.226329
H	-1.570561	1.026727	1.983422
H	-3.230871	1.521155	2.373495
C	4.951232	-2.414534	1.066494
C	5.977104	-1.532888	1.432792
C	3.766295	-1.891246	0.513089
C	3.579341	-0.509182	0.476132
C	4.604273	0.390464	0.795877
C	5.800997	-0.160241	1.249697
C	2.707470	-2.762193	-0.085150
C	2.986423	-3.550511	-1.220412
C	1.966174	-4.349934	-1.748236
C	0.715712	-4.356374	-1.134431
C	0.390485	-3.566448	-0.028963
C	1.411965	-2.720459	0.437311
O	2.360049	-0.037831	0.039079
O	1.171343	-1.810251	1.450069
P	1.056206	-0.230986	1.030246
O	-0.114274	-0.060960	0.080601
O	1.140307	0.595866	2.258299
C	4.475025	1.856172	0.589811
C	-0.974364	-3.683173	0.553869
C	5.519429	2.536845	-0.099319

C	5.462021	3.887324	-0.326080
C	4.348542	4.647912	0.115760
C	3.297019	3.974466	0.796936
C	3.387167	2.578248	1.030772
C	-1.658090	-4.932393	0.417447
C	-2.972532	-5.076205	0.764373
C	-3.698363	-3.993133	1.326939
C	-2.996936	-2.786195	1.582863
C	-1.648193	-2.647879	1.163376
H	6.612918	0.513474	1.517799
H	-0.062689	-4.971994	-1.577545
H	6.367810	1.960518	-0.458827
H	6.268194	4.392054	-0.853300
H	-1.185667	-1.677676	1.276508
H	-3.475513	-6.029547	0.622770
H	-1.118817	-5.788752	0.025950
H	2.588524	2.082672	1.578414
C	1.189227	2.194344	-1.690483
C	2.460051	2.309271	-2.236265
C	2.941384	3.552901	-2.636919
C	2.147419	4.690488	-2.492605
C	0.881189	4.587574	-1.937577
H	0.837529	1.211376	-1.399147
H	3.075153	1.420079	-2.327319
H	3.941123	3.638792	-3.051365
H	0.278966	5.480386	-1.813371
H	2.523911	5.662368	-2.792844
C	-2.832382	4.569298	-1.869460
C	-3.650750	5.695584	-1.880160
C	-3.455810	6.709532	-0.945411
C	-2.440323	6.601073	0.002704
C	-1.616175	5.479672	0.018709
H	-0.821006	5.377538	0.752163
H	-2.981157	3.771161	-2.591576
H	-4.441260	5.778579	-2.618789
H	-4.096140	7.585690	-0.955457
H	-2.288225	7.390576	0.731677
C	-4.841409	0.882881	0.185316
C	-5.644937	-0.193298	-0.156916
C	-5.148756	-1.284861	-0.858130
C	-3.803944	-1.270426	-1.197290
Br	-7.442611	-0.228050	0.424749
H	-5.778075	-2.134265	-1.093856
C	-2.959625	-0.217189	-0.853042
H	-1.902971	-0.295070	-1.080651
H	-5.264136	1.713839	0.742903
Br	-3.078662	-2.768700	-2.081624
C	-3.684555	-1.714955	2.211634
C	-5.014694	-1.820090	2.526464
C	-5.726358	-3.007089	2.223542
C	-5.077384	-4.073582	1.651962
H	-3.129914	-0.806421	2.429906
H	-5.539037	-0.984896	2.983017
H	-5.611537	-4.996180	1.438161
H	-6.785636	-3.069083	2.454137
C	2.171550	4.725115	1.232270
C	2.097117	6.075806	1.004109
C	3.143119	6.744032	0.320219
C	4.241463	6.045030	-0.112582
H	1.371423	4.196906	1.746198
H	1.238745	6.644646	1.352000
H	3.074622	7.813934	0.147432
H	5.049445	6.552706	-0.634265

C	7.297601	-2.028468	1.992878
C	7.220176	-3.450933	2.542162
H	7.645272	-1.335198	2.766719
H	8.051434	-1.998109	1.193163
C	6.520625	-4.356486	1.531912
H	6.651779	-3.454920	3.481147
H	8.225899	-3.817774	2.771620
C	5.075754	-3.903349	1.336413
H	7.056493	-4.312370	0.573124
H	6.538643	-5.400255	1.861634
H	4.593401	-4.483828	0.545467
H	4.504244	-4.121751	2.249874
C	4.322112	-3.433347	-1.935728
C	4.579586	-4.568912	-2.924054
H	4.324767	-2.475755	-2.477294
H	5.147226	-3.364353	-1.223168
C	3.363447	-4.778766	-3.821074
H	5.472385	-4.343546	-3.516496
H	4.785597	-5.496977	-2.372978
C	2.176823	-5.223096	-2.970633
H	3.122907	-3.836192	-4.330009
H	3.569037	-5.522885	-4.597459
H	2.345828	-6.258319	-2.641683
H	1.257230	-5.237642	-3.566121

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M06-2X/6-31G* Energy = -8271.57659338

M06-2X/6-31G* Free Energy = -8270.692741

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.55255051

Lowest Frequency = 12.2878

M06-2X/6-31G* Geometry

C	1.161011	2.249856	2.968262
C	1.079875	-1.300925	3.097652
C	2.313906	1.612257	2.774393
H	0.452681	2.375161	2.150516
H	0.897182	2.680516	3.929911
C	2.708011	1.017216	1.455428
H	3.020342	1.499082	3.598343
N	1.447456	-0.995829	1.894925
C	2.066164	-1.621455	4.157249
C	-0.353515	-1.341099	3.423492
C	2.780078	-0.530021	1.489817
C	3.167420	-1.086420	0.129623
H	3.504178	-0.833900	2.249728
H	0.664603	-0.934491	1.138601
H	2.000806	1.316284	0.672085
H	3.696665	1.386851	1.162606
C	-3.021015	3.624236	-1.475950
C	-2.177779	4.656709	-1.907516
C	-2.462465	2.512942	-0.804658
C	-1.073834	2.397149	-0.722540
C	-0.217886	3.412112	-1.160937
C	-0.798542	4.545545	-1.715573
C	-3.322678	1.441886	-0.214230
C	-4.311998	1.739632	0.750056
C	-5.220373	0.741131	1.124468
C	-5.102694	-0.533844	0.567315
C	-4.070879	-0.888443	-0.298263
C	-3.160026	0.122508	-0.651309
O	-0.537714	1.267956	-0.140257
O	-2.138648	-0.157337	-1.526075
P	-0.582908	-0.156486	-1.005401
O	-0.431247	-1.175372	0.108891

O	0.304009	-0.141267	-2.184954
C	1.260647	3.291735	-1.035806
C	-4.015204	-2.263401	-0.857785
C	1.981510	2.403844	-1.885110
C	3.345813	2.311592	-1.790056
C	4.064102	3.062667	-0.821279
C	3.346291	3.938706	0.040113
C	1.938834	4.047884	-0.108482
C	-5.221168	-2.854309	-1.333828
C	-5.234791	-4.124558	-1.845252
C	-4.041362	-4.889340	-1.919349
C	-2.834274	-4.306443	-1.445981
C	-2.849004	-2.992530	-0.913584
H	-0.147928	5.349026	-2.054733
H	-5.816779	-1.301346	0.860267
H	1.432324	1.781740	-2.584103
H	3.898190	1.634580	-2.437468
H	-1.922382	-2.573932	-0.532847
H	-6.160507	-4.558533	-2.214845
H	-6.136375	-2.269012	-1.309104
H	1.390782	4.719029	0.549633
C	-0.828378	-2.249329	4.381298
C	-2.184925	-2.302254	4.670919
C	-3.066267	-1.433822	4.026807
C	-2.594053	-0.510298	3.097002
C	-1.241865	-0.461185	2.788882
H	-0.136246	-2.924848	4.874960
H	-2.554998	-3.020337	5.395121
H	-4.127827	-1.474069	4.253388
H	-0.879175	0.263025	2.066411
H	-3.277205	0.170829	2.601078
C	3.044789	-2.596628	3.937229
C	3.939623	-2.919259	4.951340
C	3.868266	-2.261639	6.178110
C	2.893047	-1.290824	6.398729
C	1.981132	-0.979801	5.396093
H	1.209329	-0.232418	5.556238
H	3.089204	-3.105718	2.977379
H	4.690925	-3.683938	4.784303
H	4.571639	-2.510772	6.966253
H	2.837815	-0.781351	7.355093
C	4.335064	-0.617289	-0.482497
C	4.623301	-1.015149	-1.778650
C	3.785616	-1.856741	-2.503165
C	2.650082	-2.328972	-1.865032
Br	6.165474	-0.321374	-2.633357
H	4.004571	-2.116040	-3.531625
C	2.350104	-1.981288	-0.552636
H	1.430119	-2.353774	-0.122732
H	4.998368	0.079035	0.021752
Br	1.422352	-3.407699	-2.799076
C	-1.630198	-5.057219	-1.519867
C	-1.626263	-6.321916	-2.048723
C	-2.830502	-6.903495	-2.518563
C	-4.008138	-6.203707	-2.454985
H	-0.710087	-4.594342	-1.174721
H	-0.698571	-6.882968	-2.111771
H	-4.933846	-6.643812	-2.817534
H	-2.815164	-7.906616	-2.934021
C	4.051511	4.639076	1.054106
C	5.403680	4.471347	1.211989
C	6.118885	3.598471	0.355211
C	5.465989	2.916459	-0.641113

H	3.494505	5.300701	1.712766
H	5.931921	5.005922	1.995584
H	7.189093	3.473167	0.489389
H	6.004760	2.234991	-1.294969
C	-2.713416	5.912284	-2.571138
C	-4.108316	5.732682	-3.163609
H	-2.007249	6.243093	-3.340479
H	-2.747948	6.715917	-1.821602
C	-5.016208	5.057662	-2.140042
H	-4.051629	5.104787	-4.062052
H	-4.511707	6.702760	-3.471813
C	-4.500643	3.655699	-1.824204
H	-5.038735	5.659960	-1.220567
H	-6.045502	4.995904	-2.508184
H	-5.104968	3.199534	-1.037650
H	-4.640398	3.015561	-2.707307
C	-4.323246	3.089954	1.448899
C	-5.645508	3.395557	2.148001
H	-4.062769	3.894462	0.757790
H	-3.517761	3.078369	2.199291
C	-6.070546	2.210882	3.011084
H	-5.542551	4.304178	2.750057
H	-6.423288	3.593694	1.397164
C	-6.335775	0.999730	2.120869
H	-5.267017	1.979402	3.724168
H	-6.963505	2.448587	3.598257
H	-7.271947	1.164265	1.568859
H	-6.495695	0.100782	2.727637

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M06-2X/6-31G* Energy = -8271.59160527

M06-2X/6-31G* Free Energy = -8270.704871

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.55523713

Lowest Frequency = 17.0055

M06-2X/6-31G* Geometry

C	3.259175	3.135767	-1.246789
C	3.880149	0.584087	0.926411
C	2.823062	3.444957	-0.027689
H	2.696197	2.455079	-1.884493
H	4.167108	3.568543	-1.658053
C	1.568276	2.863756	0.555755
H	3.392966	4.129329	0.601045
N	2.606692	0.695981	0.852961
C	4.571115	-0.360581	0.009494
C	4.730328	1.335372	1.901926
C	1.845980	1.720154	1.563121
C	0.562343	1.075977	2.081539
H	2.415970	2.131223	2.404862
H	1.650448	-0.216407	0.007793
H	0.924631	2.480050	-0.246270
H	1.008726	3.650172	1.073854
C	-3.451616	-2.170284	0.441809
C	-2.912631	-3.364004	0.940455
C	-2.780129	-1.509317	-0.615240
C	-1.587380	-2.040537	-1.100764
C	-1.013696	-3.208837	-0.591050
C	-1.716469	-3.857195	0.416766
C	-3.229900	-0.177542	-1.119201
C	-4.510024	0.041335	-1.665227
C	-4.940296	1.354259	-1.902545
C	-4.056817	2.415442	-1.694890
C	-2.735397	2.211792	-1.312759
C	-2.345684	0.902989	-1.024300

O	-0.895897	-1.321920	-2.075450
O	-1.053006	0.685929	-0.578066
P	0.017320	-0.120687	-1.501891
O	0.930514	-0.812731	-0.444466
O	0.655648	0.685023	-2.557314
C	0.328923	-3.681241	-1.004798
C	-1.762594	3.336498	-1.249160
C	1.265311	-4.017576	0.013974
C	2.518252	-4.464483	-0.306287
C	2.917739	-4.597011	-1.662617
C	1.999830	-4.227978	-2.684525
C	0.704380	-3.777020	-2.323947
C	-1.854928	4.316751	-0.223607
C	-0.951650	5.348185	-0.159403
C	0.081631	5.473059	-1.125980
C	0.156957	4.512524	-2.172042
C	-0.774247	3.443414	-2.200489
H	-1.294920	-4.766736	0.840088
H	-4.387886	3.431542	-1.899920
H	0.973888	-3.863638	1.050249
H	3.233816	-4.707073	0.475245
H	-0.682920	2.689534	-2.977257
H	-1.018948	6.088654	0.634293
H	-2.635662	4.217858	0.525489
H	0.007051	-3.501225	-3.109984
C	5.730182	2.193473	1.437373
C	6.533793	2.880472	2.341138
C	6.358627	2.698413	3.711919
C	5.375139	1.830229	4.178804
C	4.560745	1.151511	3.276318
H	5.861438	2.322680	0.366767
H	7.302138	3.554355	1.975554
H	6.991565	3.229977	4.415528
H	3.791343	0.471694	3.635211
H	5.241364	1.679275	5.245245
C	5.781118	-0.948432	0.395928
C	6.412478	-1.865430	-0.437682
C	5.842970	-2.197035	-1.663685
C	4.642325	-1.608755	-2.059969
C	4.012271	-0.685156	-1.235265
H	3.096296	-0.204246	-1.564359
H	6.221083	-0.694719	1.355694
H	7.347791	-2.320937	-0.127583
H	6.328188	-2.917493	-2.314649
H	4.195013	-1.876572	-3.013157
C	-0.655234	1.754511	2.057942
C	-1.815935	1.087595	2.423484
C	-1.807315	-0.231585	2.852830
C	-0.582819	-0.885248	2.888800
Br	-3.478977	1.975360	2.241519
H	-2.721629	-0.735450	3.138185
C	0.593138	-0.253442	2.512712
H	1.522557	-0.813421	2.503759
H	-0.729605	2.769139	1.685321
Br	-0.529769	-2.692192	3.458248
C	1.165864	4.646238	-3.162493
C	2.062743	5.681856	-3.110226
C	2.002657	6.625697	-2.055677
C	1.037981	6.522312	-1.086538
H	1.215353	3.901918	-3.953075
H	2.830939	5.777040	-3.871676
H	0.983164	7.249407	-0.279988
H	2.724507	7.436056	-2.020095

C	2.409001	-4.320682	-4.042180
C	3.664560	-4.766553	-4.368268
C	4.572145	-5.150150	-3.349850
C	4.205635	-5.065086	-2.030528
H	1.705972	-4.028974	-4.818020
H	3.966185	-4.833098	-5.409090
H	5.560459	-5.510763	-3.619923
H	4.902025	-5.343918	-1.243305
C	-3.562988	-4.129825	2.074608
C	-4.416258	-3.234025	2.964149
H	-2.780634	-4.622724	2.662075
H	-4.192728	-4.928430	1.658068
C	-5.390037	-2.444762	2.095312
H	-3.757929	-2.555238	3.522351
H	-4.954746	-3.835218	3.703970
C	-4.662054	-1.532240	1.105783
H	-6.014779	-3.157934	1.540662
H	-6.067544	-1.841784	2.708629
H	-5.379191	-1.179139	0.361989
H	-4.327272	-0.616320	1.609517
C	-5.365491	-1.131058	-2.113011
C	-6.851190	-0.788499	-2.187795
H	-5.191220	-2.011223	-1.490262
H	-5.020117	-1.412655	-3.118419
C	-7.047150	0.471019	-3.028909
H	-7.405497	-1.631442	-2.612943
H	-7.247427	-0.618583	-1.176599
C	-6.352914	1.659365	-2.366057
H	-6.621187	0.302722	-4.026410
H	-8.110663	0.691588	-3.166455
H	-6.941187	1.968944	-1.490518
H	-6.336980	2.521073	-3.042224

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M06-2X/6-31G* Energy = -8271.57551943

M06-2X/6-31G* Free Energy = -8270.691592

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.55145034

Lowest Frequency = 11.4108

M06-2X/6-31G* Geometry

C	2.086494	2.353414	2.523582
C	1.354587	-0.963162	3.262885
C	3.085589	1.499588	2.307030
H	1.289213	2.470869	1.790892
H	2.042140	2.971421	3.415916
C	3.175796	0.640548	1.080703
H	3.883960	1.395338	3.043223
N	1.603685	-0.952046	1.994337
C	2.407590	-1.288973	4.257060
C	-0.005999	-0.668525	3.739969
C	2.933075	-0.862124	1.375340
C	2.975155	-1.686372	0.097721
H	3.681520	-1.209847	2.091544
H	0.758527	-0.861876	1.300522
H	2.450359	0.968824	0.325569
H	4.174345	0.735640	0.641666
C	-2.330858	3.900258	-1.659764
C	-1.388517	4.744089	-2.263444
C	-1.882554	2.787141	-0.913292
C	-0.523359	2.469363	-0.920963
C	0.426734	3.285273	-1.543207
C	-0.028698	4.435477	-2.174039
C	-2.832904	1.915488	-0.156144
C	-3.686542	2.440561	0.840012

C	-4.682770	1.620200	1.384292
C	-4.790562	0.295566	0.954669
C	-3.902612	-0.279143	0.048813
C	-2.894472	0.552467	-0.465179
O	-0.101478	1.345560	-0.244064
O	-1.988270	0.040212	-1.362961
P	-0.431797	-0.157945	-0.882837
O	-0.411797	-1.009211	0.373353
O	0.388796	-0.473638	-2.067897
C	1.865788	2.905650	-1.556609
C	-4.103247	-1.684056	-0.396820
C	2.290084	1.829038	-2.385769
C	3.605076	1.448083	-2.411802
C	4.566626	2.094545	-1.590865
C	4.148581	3.170865	-0.758681
C	2.785369	3.569155	-0.779151
C	-3.033196	-2.622262	-0.470668
C	-3.268373	-3.911849	-0.866574
C	-4.571228	-4.354255	-1.215163
C	-5.644472	-3.424548	-1.145948
C	-5.375184	-2.095269	-0.732798
H	0.697407	5.086060	-2.657141
H	-5.571013	-0.332655	1.379210
H	1.551163	1.289094	-2.966771
H	3.921445	0.617028	-3.036965
H	-6.197738	-1.383715	-0.706496
H	-2.444146	-4.619479	-0.915423
H	-2.032576	-2.315809	-0.186688
H	2.465559	4.384950	-0.134179
C	-0.837999	0.200886	3.019354
C	-2.121395	0.460382	3.480690
C	-2.581313	-0.139423	4.650933
C	-1.754086	-0.995591	5.376882
C	-0.465349	-1.253013	4.929949
H	-0.487395	0.676061	2.108427
H	-2.763371	1.126202	2.914085
H	-3.589351	0.064276	5.000588
H	0.182132	-1.922577	5.487682
H	-2.113339	-1.462917	6.287740
C	2.646919	-0.421825	5.326485
C	3.620340	-0.739148	6.267578
C	4.333128	-1.932066	6.160030
C	4.079583	-2.808289	5.106592
C	3.122186	-2.486436	4.150714
H	2.915219	-3.163753	3.325504
H	2.078204	0.500692	5.401132
H	3.817938	-0.058707	7.089330
H	5.084898	-2.181921	6.901892
H	4.626237	-3.742240	5.028865
C	4.016120	-1.488772	-0.814247
C	3.971471	-2.133416	-2.041066
C	2.906916	-2.944435	-2.416867
C	1.901651	-3.143981	-1.484183
Br	5.374459	-1.833932	-3.280902
H	2.855797	-3.382465	-3.405874
C	1.948000	-2.569057	-0.221161
H	1.119850	-2.743046	0.451826
H	4.842369	-0.819637	-0.596820
Br	0.358255	-4.118449	-1.954354
C	-6.951565	-3.854534	-1.497807
C	-7.181228	-5.146640	-1.894599
C	-6.111979	-6.073725	-1.960531
C	-4.839267	-5.684924	-1.629280

H	-7.767564	-3.137883	-1.447261
H	-8.184240	-5.464989	-2.161813
H	-4.013845	-6.390521	-1.680227
H	-6.305791	-7.093899	-2.277448
C	5.093404	3.770428	0.115197
C	6.387258	3.317113	0.168558
C	6.802782	2.243962	-0.658287
C	5.915288	1.652121	-1.522283
H	4.765300	4.585471	0.755507
H	7.098672	3.777564	0.847345
H	7.828755	1.892391	-0.605704
H	6.217923	0.816596	-2.149830
C	-1.794487	5.998985	-3.014420
C	-3.247297	5.978631	-3.481456
H	-1.118419	6.146460	-3.863662
H	-1.647714	6.864687	-2.352709
C	-4.149989	5.549835	-2.328610
H	-3.360592	5.267192	-4.309525
H	-3.532178	6.965211	-3.861279
C	-3.815327	4.122592	-1.902175
H	-4.005826	6.233611	-1.479882
H	-5.205579	5.610046	-2.613055
H	-4.408496	3.839659	-1.030386
H	-4.121139	3.429899	-2.699601
C	-3.453294	3.836879	1.394284
C	-4.657174	4.392063	2.151020
H	-3.145687	4.527952	0.606447
H	-2.595441	3.779675	2.082225
C	-5.157088	3.367632	3.165914
H	-4.383034	5.331108	2.642634
H	-5.464621	4.623332	1.442232
C	-5.655871	2.123504	2.435022
H	-4.331427	3.098952	3.840040
H	-5.956518	3.783186	3.787950
H	-6.612063	2.359589	1.947116
H	-5.869734	1.316546	3.145767

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M06-2X/6-31G* Energy = -8271.57502465

M06-2X/6-31G* Free Energy = -8270.689650

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.55276055

Lowest Frequency = 10.0081

M06-2X/6-31G* Geometry

C	2.528897	-0.259097	1.876562
C	1.238666	-2.663576	-0.706674
C	1.348552	-0.158705	2.484013
H	2.614890	-0.449989	0.810152
H	3.458280	-0.122898	2.422782
C	0.008683	-0.383183	1.823878
H	1.323941	0.059016	3.551323
N	0.438247	-1.779629	-0.202979
C	1.561564	-2.701349	-2.144347
C	1.842614	-3.699186	0.182181
C	-0.093671	-1.781277	1.176871
C	-1.522739	-2.290759	1.115624
H	0.504760	-2.481812	1.761407
H	0.037605	-0.970893	-0.789614
H	-0.210749	0.384495	1.071675
H	-0.783873	-0.320494	2.575546
C	2.497393	4.521184	0.697061
C	3.876374	4.459509	0.456401
C	1.704191	3.383902	0.445693
C	2.270398	2.282066	-0.196116

C	3.651456	2.187730	-0.407226
C	4.432138	3.280585	-0.045620
C	0.277935	3.286665	0.877534
C	-0.076337	3.320424	2.243430
C	-1.429575	3.203205	2.588890
C	-2.391451	3.085433	1.584285
C	-2.069187	2.995149	0.231029
C	-0.704101	3.058074	-0.086423
O	1.459289	1.225320	-0.537607
O	-0.287266	2.871313	-1.389481
P	0.328805	1.395605	-1.745781
O	-0.667428	0.316509	-1.362082
O	0.947107	1.438391	-3.087876
C	4.254635	0.923021	-0.894323
C	-3.135980	2.886992	-0.796465
C	3.818054	0.316531	-2.106523
C	4.335635	-0.889895	-2.498532
C	5.273939	-1.587246	-1.691334
C	5.712734	-0.985394	-0.478351
C	5.203393	0.289830	-0.122588
C	-3.000233	3.550333	-2.052473
C	-4.016324	3.536084	-2.967880
C	-5.244453	2.879554	-2.692441
C	-5.396676	2.224288	-1.440757
C	-4.315118	2.227536	-0.522553
H	5.507664	3.225099	-0.203357
H	-3.440279	3.062966	1.871233
H	3.062769	0.816057	-2.709360
H	4.004635	-1.346352	-3.428011
H	-4.434149	1.684155	0.412363
H	-3.897741	4.044573	-3.921162
H	-2.077617	4.071793	-2.276254
H	5.522988	0.741014	0.814789
C	1.101422	-4.814749	0.575586
C	1.689258	-5.775293	1.394158
C	3.010801	-5.624125	1.810071
C	3.749528	-4.514351	1.405876
C	3.170669	-3.548173	0.587966
H	0.072690	-4.927365	0.243171
H	1.114301	-6.642504	1.702738
H	3.466076	-6.376008	2.446856
H	3.749217	-2.686751	0.261813
H	4.782264	-4.392788	1.716694
C	2.430184	-3.697932	-2.620642
C	2.723489	-3.780332	-3.976056
C	2.176739	-2.858696	-4.867607
C	1.318291	-1.863762	-4.402121
C	0.991629	-1.796409	-3.054944
H	0.283099	-1.040796	-2.737907
H	2.878871	-4.406372	-1.933229
H	3.386085	-4.561875	-4.334628
H	2.418499	-2.917502	-5.924536
H	0.893233	-1.130485	-5.078668
C	-1.868684	-3.413852	1.865295
C	-3.177085	-3.882208	1.825362
C	-4.147313	-3.259412	1.053250
C	-3.775604	-2.139104	0.314618
Br	-3.641366	-5.412009	2.836724
H	-5.163202	-3.634384	1.023438
C	-2.479657	-1.638493	0.333265
H	-2.217255	-0.764144	-0.261459
H	-1.127720	-3.924052	2.473387
Br	-5.074751	-1.268768	-0.741666

C	-6.635946	1.593451	-1.145394
C	-7.660765	1.596634	-2.056945
C	-7.501058	2.237583	-3.309980
C	-6.321566	2.866493	-3.616165
H	-6.756363	1.107304	-0.180784
H	-8.602785	1.112427	-1.818214
H	-6.193164	3.367370	-4.572348
H	-8.318994	2.232577	-4.023765
C	6.597126	-1.707913	0.367959
C	7.021038	-2.968155	0.028315
C	6.594268	-3.562264	-1.185781
C	5.749437	-2.882968	-2.026698
H	6.925932	-1.244699	1.295030
H	7.693536	-3.512400	0.684802
H	6.943783	-4.556099	-1.448120
H	5.419357	-3.328924	-2.961395
C	4.797138	5.625727	0.764947
C	4.061181	6.958017	0.887908
H	5.316773	5.419700	1.711703
H	5.575946	5.686418	-0.003241
C	2.834211	6.792555	1.781176
H	3.737446	7.295138	-0.105236
H	4.737543	7.722705	1.283509
C	1.848343	5.822150	1.135349
H	3.147593	6.407123	2.761831
H	2.344153	7.755719	1.956482
H	0.999188	5.632405	1.797101
H	1.420438	6.293457	0.238813
C	1.001703	3.376812	3.313553
C	0.461425	3.660494	4.714413
H	1.766901	4.114008	3.059023
H	1.523992	2.410100	3.304754
C	-0.775109	2.813642	4.998085
H	1.247440	3.473841	5.453499
H	0.190402	4.721839	4.797790
C	-1.887883	3.215004	4.034557
H	-0.529846	1.751398	4.857865
H	-1.108763	2.935259	6.033697
H	-2.236541	4.223906	4.296637
H	-2.754229	2.553173	4.143112

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M06-2X/6-31G* Energy = -8271.57835516

M06-2X/6-31G* Free Energy = -8270.692354

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.55337115

Lowest Frequency = 9.2023

M06-2X/6-31G* Geometry

C	-2.746893	-0.368330	-1.744715
C	-1.347129	-2.760692	0.544153
C	-1.621392	-0.457155	-2.450079
H	-2.733217	-0.221097	-0.668102
H	-3.722418	-0.438697	-2.219384
C	-0.240010	-0.447226	-1.847115
H	-1.676242	-0.611159	-3.527821
N	-0.449541	-1.927628	0.124790
C	-1.755970	-2.817657	1.963720
C	-1.982539	-3.722149	-0.403464
C	0.102239	-1.828695	-1.243415
C	1.597167	-2.103423	-1.205209
H	-0.372074	-2.606777	-1.844286
H	-0.053986	-1.155318	0.765236
H	-0.143053	0.319003	-1.070614
H	0.510401	-0.226787	-2.613163

C	-2.161072	4.616192	-0.579121
C	-3.537942	4.702178	-0.331644
C	-1.492813	3.403222	-0.321607
C	-2.179008	2.367458	0.308170
C	-3.564033	2.411081	0.509775
C	-4.220265	3.586554	0.161623
C	-0.083946	3.142731	-0.746911
C	0.262046	3.095925	-2.114449
C	1.587672	2.808694	-2.465507
C	2.538825	2.623632	-1.460886
C	2.220165	2.630885	-0.101637
C	0.868737	2.820948	0.221695
O	-1.483731	1.225299	0.632664
O	0.434043	2.668460	1.523797
P	-0.339321	1.255621	1.831973
O	0.565183	0.109727	1.404365
O	-0.940325	1.296229	3.181571
C	-4.284298	1.181183	0.924405
C	3.314333	2.468512	0.891370
C	-3.897485	0.450250	2.084259
C	-4.465206	-0.767351	2.353432
C	-5.415173	-1.348741	1.471199
C	-5.816441	-0.615381	0.319495
C	-5.253066	0.666564	0.091910
C	4.532091	3.166885	0.641539
C	5.635999	2.979111	1.428896
C	5.594228	2.091755	2.536888
C	4.374467	1.417279	2.814140
C	3.248576	1.622431	1.975456
H	-5.296907	3.645257	0.310473
H	3.565753	2.397249	-1.743582
H	-3.130873	0.857605	2.739532
H	-4.166832	-1.322880	3.238806
H	2.354031	1.042232	2.166735
H	6.557378	3.517717	1.221417
H	4.574500	3.860155	-0.193711
H	-5.527051	1.207262	-0.811973
C	-1.287772	-4.852852	-0.835704
C	-1.908287	-5.756992	-1.693921
C	-3.219007	-5.534806	-2.110461
C	-3.914937	-4.412971	-1.664204
C	-3.302936	-3.504726	-0.806047
H	-0.271386	-5.026480	-0.491196
H	-1.368733	-6.636238	-2.030662
H	-3.700881	-6.241779	-2.778347
H	-3.848960	-2.635920	-0.444553
H	-4.940627	-4.238769	-1.973483
C	-1.199837	-1.965657	2.932245
C	-1.602666	-2.053203	4.257571
C	-2.530436	-3.017620	4.647686
C	-3.069029	-3.885704	3.699864
C	-2.696339	-3.781895	2.365087
H	-3.136576	-4.453909	1.637303
H	-0.443431	-1.234386	2.676953
H	-1.183736	-1.356801	4.975838
H	-2.833474	-3.093001	5.687604
H	-3.786635	-4.643981	3.997436
C	2.053162	-3.332025	-1.680944
C	3.418484	-3.586061	-1.724168
C	4.343776	-2.633571	-1.323321
C	3.869008	-1.409562	-0.858188
Br	4.028446	-5.256180	-2.369208
H	5.407499	-2.830934	-1.378325

C	2.508057	-1.133355	-0.774360
H	2.163283	-0.178052	-0.384257
H	1.353486	-4.081706	-2.037545
Br	5.124595	-0.087680	-0.366761
C	4.319916	0.524329	3.917242
C	5.421954	0.316796	4.705905
C	6.635765	0.993271	4.429879
C	6.718629	1.860484	3.370841
H	3.383676	0.011867	4.121778
H	5.369457	-0.366847	5.547662
H	7.646750	2.383490	3.154082
H	7.501281	0.821336	5.062510
C	-6.711737	-1.220367	-0.603754
C	-7.184373	-2.491657	-0.393959
C	-6.798414	-3.215069	0.762130
C	-5.941888	-2.652116	1.674511
H	-7.010042	-0.657878	-1.485207
H	-7.864927	-2.944942	-1.108608
H	-7.187787	-4.215708	0.923380
H	-5.641299	-3.198283	2.564857
C	-4.327102	5.963748	-0.630076
C	-3.447720	7.204498	-0.768443
H	-4.882096	5.816323	-1.567618
H	-5.081247	6.112141	0.150703
C	-2.263455	6.899993	-1.682335
H	-3.071167	7.503556	0.218244
H	-4.040284	8.040178	-1.154655
C	-1.378842	5.829079	-1.048668
H	-2.636310	6.546670	-2.654133
H	-1.672962	7.801779	-1.873540
H	-0.579329	5.532051	-1.733219
H	-0.870916	6.255992	-0.172103
C	-0.818705	3.205850	-3.176997
C	-0.266486	3.382676	-4.590021
H	-1.513895	4.017109	-2.945768
H	-1.421669	2.286150	-3.128684
C	0.858485	2.386406	-4.852487
H	-1.076654	3.264233	-5.316893
H	0.124624	4.402334	-4.709389
C	2.024077	2.681680	-3.912465
H	0.485784	1.367473	-4.675747
H	1.192996	2.431638	-5.893971
H	2.504125	3.618664	-4.228272
H	2.792204	1.903697	-3.987923

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M06-2X/6-31G* Energy = -8271.58516195

M06-2X/6-31G* Free Energy = -8270.696971

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.55446134

Lowest Frequency = 14.4986

M06-2X/6-31G* Geometry

C	1.534690	3.252939	-3.513530
C	2.941946	-0.234816	-2.035890
C	2.414784	3.490481	-2.542849
H	0.565275	2.813847	-3.284814
H	1.742637	3.499034	-4.550843
C	2.158556	3.135191	-1.106367
H	3.382470	3.935049	-2.779820
N	2.323703	0.712236	-1.410571
C	2.218427	-1.411155	-2.549616
C	4.415449	-0.127660	-2.242225
C	2.915288	1.864701	-0.691973
C	2.802065	1.516686	0.784263

H	3.969624	1.937982	-0.969599
H	1.262881	0.681502	-1.222267
H	1.085623	2.968905	-0.959467
H	2.466489	3.947936	-0.436088
C	-4.769169	-1.851036	1.060986
C	-4.533891	-3.188371	1.406830
C	-3.805175	-1.156361	0.301951
C	-2.563709	-1.757313	0.061785
C	-2.307670	-3.094203	0.401303
C	-3.330251	-3.792377	1.037377
C	-4.069971	0.188332	-0.300671
C	-5.117845	0.388272	-1.223359
C	-5.306185	1.667205	-1.769607
C	-4.390333	2.677955	-1.485274
C	-3.280624	2.483345	-0.662634
C	-3.179754	1.234458	-0.038517
O	-1.592354	-1.023594	-0.584028
O	-2.148130	0.992084	0.839796
P	-0.846258	0.190936	0.258534
O	-0.193131	1.018997	-0.829419
O	-0.068506	-0.312889	1.413754
C	-1.008304	-3.752962	0.099730
C	-2.217466	3.519186	-0.584278
C	-0.976055	-4.996084	-0.590703
C	0.215117	-5.622931	-0.864080
C	1.450314	-5.047213	-0.464508
C	1.420924	-3.809912	0.234544
C	0.179445	-3.188776	0.508589
C	-1.894289	4.213077	-1.787633
C	-0.913375	5.165918	-1.826483
C	-0.178234	5.493892	-0.659710
C	-0.486015	4.809922	0.550149
C	-1.508778	3.821782	0.560413
H	-3.156148	-4.831531	1.311364
H	-4.533682	3.653131	-1.946003
H	-1.913919	-5.443258	-0.911265
H	0.226399	-6.572708	-1.394227
H	-1.703831	3.287463	1.486123
H	-0.666440	5.664963	-2.760189
H	-2.419744	3.945180	-2.699239
H	0.176221	-2.259953	1.070922
C	5.290108	-0.959654	-1.539626
C	6.663175	-0.831866	-1.729406
C	7.160347	0.110048	-2.627500
C	6.284995	0.930591	-3.335493
C	4.911191	0.817634	-3.142538
H	4.887918	-1.700731	-0.852103
H	7.343291	-1.471359	-1.176157
H	8.231279	0.204434	-2.776018
H	4.216956	1.461088	-3.677189
H	6.671267	1.662652	-4.037313
C	2.939594	-2.512303	-3.041911
C	2.270347	-3.646349	-3.478984
C	0.878479	-3.697683	-3.436393
C	0.155173	-2.606345	-2.961526
C	0.815021	-1.465617	-2.528981
H	0.221189	-0.627420	-2.183082
H	4.022183	-2.488369	-3.079059
H	2.839013	-4.496565	-3.840806
H	0.357615	-4.592048	-3.763882
H	-0.927944	-2.638806	-2.905196
C	1.748163	1.980252	1.559504
C	1.580511	1.480571	2.845536

C	2.440725	0.537145	3.386052
C	3.498449	0.101921	2.593437
Br	0.036649	1.980661	3.802641
H	2.271911	0.123293	4.372504
C	3.696180	0.582354	1.310041
H	4.520920	0.205857	0.712772
H	1.010475	2.660315	1.150613
Br	4.655628	-1.253961	3.234745
C	0.274701	5.114343	1.713838
C	1.289998	6.035990	1.668813
C	1.592884	6.713931	0.461602
C	0.873407	6.446855	-0.675325
H	0.062380	4.574538	2.632877
H	1.867730	6.248828	2.563007
H	1.100621	6.954693	-1.609434
H	2.397263	7.443010	0.441552
C	2.640714	-3.228190	0.677219
C	3.838381	-3.847863	0.424873
C	3.872311	-5.066455	-0.301572
C	2.707779	-5.651865	-0.731319
H	2.596038	-2.298853	1.242377
H	4.758530	-3.416301	0.812075
H	4.826510	-5.546163	-0.499005
H	2.731744	-6.594144	-1.274202
C	-5.563856	-4.017224	2.152678
C	-6.603486	-3.172893	2.886221
H	-5.052496	-4.689054	2.850871
H	-6.080653	-4.664036	1.429198
C	-7.133849	-2.082292	1.959249
H	-6.144702	-2.702287	3.765367
H	-7.414733	-3.812475	3.249142
C	-6.003050	-1.130817	1.576896
H	-7.552957	-2.544779	1.054141
H	-7.943548	-1.521346	2.437284
H	-6.351272	-0.383878	0.859440
H	-5.700309	-0.562047	2.467883
C	-5.953015	-0.777585	-1.727689
C	-7.286101	-0.346814	-2.334808
H	-6.117590	-1.521032	-0.946480
H	-5.359929	-1.291984	-2.498471
C	-7.064749	0.757860	-3.363636
H	-7.779506	-1.212550	-2.788790
H	-7.950549	0.022703	-1.541170
C	-6.480385	1.988626	-2.675726
H	-6.369753	0.397765	-4.133449
H	-7.999796	1.020137	-3.869482
H	-7.267633	2.461156	-2.071204
H	-6.174436	2.736387	-3.415782

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M06-2X/6-31G* Energy = -8271.57596113

M06-2X/6-31G* Free Energy = -8270.689571

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8277.55155300

Lowest Frequency = 15.2088

M06-2X/6-31G* Geometry

C	-2.996794	0.806690	-2.066195
C	-1.521794	-2.692504	-0.524885
C	-2.018162	0.066643	-2.577368
H	-2.818566	1.516157	-1.263160
H	-4.013684	0.727845	-2.441754
C	-0.579472	0.118726	-2.149623
H	-2.244165	-0.629558	-3.387641
N	-0.557288	-1.840649	-0.643271

C	-1.886635	-3.269952	0.789074
C	-2.289873	-3.149766	-1.720390
C	-0.014723	-1.290543	-1.896950
C	1.511019	-1.369248	-1.829384
H	-0.339579	-1.935613	-2.719932
H	-0.053368	-1.343793	0.238047
H	-0.436043	0.739825	-1.259054
H	-0.003535	0.570484	-2.964913
C	-1.783730	4.492206	0.886866
C	-3.144234	4.566216	1.215503
C	-1.187492	3.227862	0.704509
C	-1.924073	2.078793	0.999399
C	-3.296653	2.130840	1.274146
C	-3.883934	3.388661	1.356210
C	0.197033	3.054200	0.166560
C	0.541014	3.461502	-1.139423
C	1.850542	3.241060	-1.589354
C	2.771383	2.601238	-0.757914
C	2.438109	2.106673	0.503564
C	1.125441	2.347871	0.932633
O	-1.316184	0.850683	0.885322
O	0.676575	1.812789	2.125116
P	-0.146010	0.407487	1.980841
O	0.678541	-0.567856	1.152322
O	-0.713551	0.027429	3.290197
C	-4.089795	0.876368	1.302772
C	3.394411	1.282922	1.285134
C	-3.739500	-0.207506	2.157445
C	-4.422041	-1.392700	2.082922
C	-5.459164	-1.587813	1.131308
C	-5.817319	-0.505828	0.279410
C	-5.127596	0.726733	0.410575
C	4.327517	0.474640	0.577159
C	5.180747	-0.372566	1.228487
C	5.179922	-0.454498	2.644465
C	4.286737	0.382611	3.367753
C	3.404566	1.241190	2.663229
H	-4.949540	3.452633	1.568510
H	3.781656	2.452937	-1.134248
H	-2.915076	-0.089677	2.856719
H	-4.150307	-2.217665	2.736859
H	2.718223	1.854679	3.236272
H	5.865363	-1.005085	0.667085
H	4.339995	0.518502	-0.504579
H	-5.385215	1.545366	-0.258879
C	-1.731478	-4.029339	-2.647973
C	-2.482283	-4.440897	-3.746687
C	-3.786755	-3.981352	-3.911232
C	-4.347333	-3.113414	-2.974940
C	-3.603989	-2.697755	-1.875465
H	-0.715342	-4.391003	-2.508849
H	-2.047828	-5.123365	-4.469893
H	-4.369463	-4.305197	-4.767828
H	-4.032294	-2.015318	-1.144556
H	-5.366472	-2.757567	-3.088998
C	-1.193281	-2.932761	1.963355
C	-1.548414	-3.506200	3.176703
C	-2.565315	-4.457391	3.234276
C	-3.238668	-4.822686	2.070477
C	-2.912986	-4.227134	0.857767
H	-3.459491	-4.510756	-0.034273
H	-0.365951	-2.234432	1.952444
H	-1.018615	-3.201111	4.072527

H	-2.830386	-4.915265	4.182471
H	-4.025004	-5.570424	2.104722
C	2.305638	-0.508473	-2.589197
C	3.683129	-0.678926	-2.600001
C	4.312697	-1.682337	-1.879036
C	3.513004	-2.492861	-1.085062
Br	4.752184	0.576464	-3.523762
H	5.390968	-1.788861	-1.887178
C	2.131117	-2.356773	-1.058210
H	1.551830	-3.007299	-0.412495
H	1.884149	0.306287	-3.163993
Br	4.346128	-3.767026	0.029446
C	4.288659	0.320554	4.787215
C	5.129857	-0.535015	5.450318
C	6.011375	-1.375674	4.726402
C	6.033498	-1.336233	3.355851
H	3.601084	0.958649	5.335896
H	5.120164	-0.576338	6.535147
H	6.703771	-1.980165	2.791607
H	6.668479	-2.052949	5.263465
C	-6.806702	-0.713010	-0.719348
C	-7.409101	-1.937314	-0.867596
C	-7.061078	-3.011871	-0.011619
C	-6.115958	-2.836293	0.967587
H	-7.073581	0.117428	-1.368819
H	-8.161828	-2.085291	-1.636337
H	-7.550605	-3.973391	-0.132380
H	-5.844651	-3.653895	1.630371
C	-3.857818	5.895779	1.378344
C	-2.904665	7.066249	1.608755
H	-4.445882	6.090950	0.470171
H	-4.579898	5.820568	2.198845
C	-1.766951	7.014387	0.592473
H	-2.483864	7.007605	2.620823
H	-3.452251	8.011864	1.541211
C	-0.937750	5.750031	0.803242
H	-2.186681	7.018166	-0.423415
H	-1.124038	7.896356	0.677512
H	-0.175055	5.654023	0.025746
H	-0.382737	5.838861	1.748188
C	-0.522036	3.989286	-2.088200
C	0.057227	4.693115	-3.313571
H	-1.222557	4.648840	-1.570026
H	-1.125513	3.129115	-2.420773
C	1.147713	3.836668	-3.950591
H	-0.744825	4.905898	-4.027758
H	0.487875	5.658909	-3.015381
C	2.306320	3.672130	-2.971010
H	0.729010	2.851396	-4.202060
H	1.504659	4.280790	-4.885439
H	2.839524	4.629756	-2.888397
H	3.035598	2.946421	-3.347900

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M06-2X/6-31G* Energy = -8277.56244573

M06-2X/6-31G* Free Energy = -8276.677787

M06-2X/def2-TZVPP-SMD(dibutylether) Energy = -8276.56003994

Lowest Frequency = 8.8607

M06-2X/6-31G* Geometry

C	-0.349799	3.180632	1.256883
C	1.830103	0.233628	2.403882
C	0.963436	3.313315	1.083926
H	-0.961093	2.593612	0.571923

H	-0.868135	3.679173	2.071341
C	1.729570	2.659733	-0.032355
H	1.545537	3.915969	1.783082
N	1.851785	0.548678	1.150628
C	2.918795	0.631105	3.323987
C	0.690297	-0.540389	2.918038
C	2.687871	1.571734	0.503128
C	3.566142	0.971887	-0.578607
H	3.327351	2.012254	1.271951
H	1.087136	0.178621	0.504086
H	1.040502	2.211284	-0.756287
H	2.349101	3.391462	-0.564691
C	-5.559553	-0.761143	-1.359690
C	-6.232999	0.433336	-1.645007
C	-4.261035	-0.708149	-0.812557
C	-3.603606	0.526320	-0.740468
C	-4.264567	1.728640	-1.013668
C	-5.589774	1.654836	-1.425915
C	-3.559249	-1.904203	-0.256857
C	-4.090916	-2.655009	0.815155
C	-3.333603	-3.709287	1.351307
C	-2.030474	-3.921349	0.898725
C	-1.454460	-3.143612	-0.100747
C	-2.264878	-2.177133	-0.708754
O	-2.282073	0.569358	-0.343442
O	-1.776434	-1.441126	-1.759933
P	-1.153869	0.050975	-1.457589
O	0.104729	-0.088579	-0.643682
O	-1.173839	0.828054	-2.712468
C	-3.575025	3.033923	-0.820514
C	-0.004403	-3.199281	-0.403633
C	-2.490893	3.408681	-1.664766
C	-1.841210	4.597760	-1.464549
C	-2.219807	5.476713	-0.415044
C	-3.309062	5.111271	0.423615
C	-3.974067	3.878777	0.188495
C	0.476271	-3.225544	-1.741803
C	1.816046	-3.139285	-2.003555
C	2.755578	-2.984921	-0.949729
C	2.286792	-2.986215	0.393410
C	0.895068	-3.115584	0.635553
H	-6.121666	2.581223	-1.633351
H	-1.426214	-4.695839	1.367752
H	-2.175687	2.726590	-2.448451
H	-1.009038	4.878276	-2.105757
H	0.531770	-3.085810	1.661672
H	2.176879	-3.152738	-3.027106
H	-0.237593	-3.300698	-2.554573
H	-4.797993	3.593271	0.839294
C	0.868820	-1.429708	3.987016
C	-0.196753	-2.210184	4.419523
C	-1.443381	-2.086656	3.805318
C	-1.631765	-1.174094	2.768727
C	-0.570622	-0.401573	2.320228
H	1.844372	-1.525251	4.454963
H	-0.054436	-2.915918	5.231384
H	-2.274350	-2.702631	4.138323
H	-0.726986	0.302571	1.510450
H	-2.598857	-1.071752	2.286560
C	4.250180	0.362953	2.987508
C	5.269337	0.716094	3.864982
C	4.963172	1.345958	5.070320
C	3.636884	1.609828	5.407770

C	2.611119	1.240557	4.544174
H	1.573540	1.432722	4.801205
H	4.468630	-0.145997	2.052304
H	6.300991	0.497019	3.608245
H	5.760093	1.626407	5.751777
H	3.400567	2.098447	6.347218
C	3.008942	0.443817	-1.747349
C	3.864613	-0.014700	-2.740095
C	5.249002	0.007485	-2.599525
C	5.771255	0.499087	-1.413876
Br	3.140531	-0.746344	-4.320844
H	5.894707	-0.373407	-3.381837
C	4.949943	0.997359	-0.410150
H	5.391852	1.401739	0.495603
H	1.930298	0.372285	-1.871380
Br	7.640277	0.435800	-1.131978
C	3.227705	-2.817444	1.445295
C	4.560751	-2.630397	1.172728
C	5.023625	-2.605252	-0.166630
C	4.140078	-2.797730	-1.198702
H	2.869712	-2.841248	2.472858
H	5.269575	-2.504732	1.987242
H	4.479683	-2.783620	-2.231909
H	6.074392	-2.417411	-0.371527
C	-3.682327	5.979583	1.483665
C	-3.004714	7.151706	1.702470
C	-1.919205	7.514836	0.867844
C	-1.538860	6.696565	-0.164811
H	-4.516418	5.695642	2.120693
H	-3.298698	7.807713	2.516207
H	-1.390469	8.445435	1.050317
H	-0.706139	6.968215	-0.808674
C	-7.662497	0.445043	-2.154952
C	-8.095983	-0.882452	-2.773106
H	-7.784386	1.261456	-2.875181
H	-8.330083	0.678367	-1.313058
C	-7.696166	-2.038831	-1.859758
H	-7.608321	-1.013247	-3.747657
H	-9.176265	-0.875458	-2.951431
C	-6.175759	-2.097613	-1.736060
H	-8.146051	-1.892360	-0.867249
H	-8.073748	-2.991164	-2.246209
H	-5.870378	-2.883358	-1.040394
H	-5.752315	-2.387880	-2.708298
C	-5.387792	-2.239286	1.493338
C	-6.027513	-3.359974	2.308874
H	-6.105624	-1.838363	0.777007
H	-5.154643	-1.398857	2.166258
C	-5.000398	-3.976764	3.253393
H	-6.885091	-2.967287	2.864756
H	-6.409948	-4.136039	1.631635
C	-3.876184	-4.615175	2.441257
H	-4.596384	-3.185632	3.901305
H	-5.461180	-4.722974	3.908833
H	-4.259715	-5.533670	1.975077
H	-3.053191	-4.929738	3.094272