Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Molecular design Principles towards Exo-Exclusive Diels-Alder Reactions

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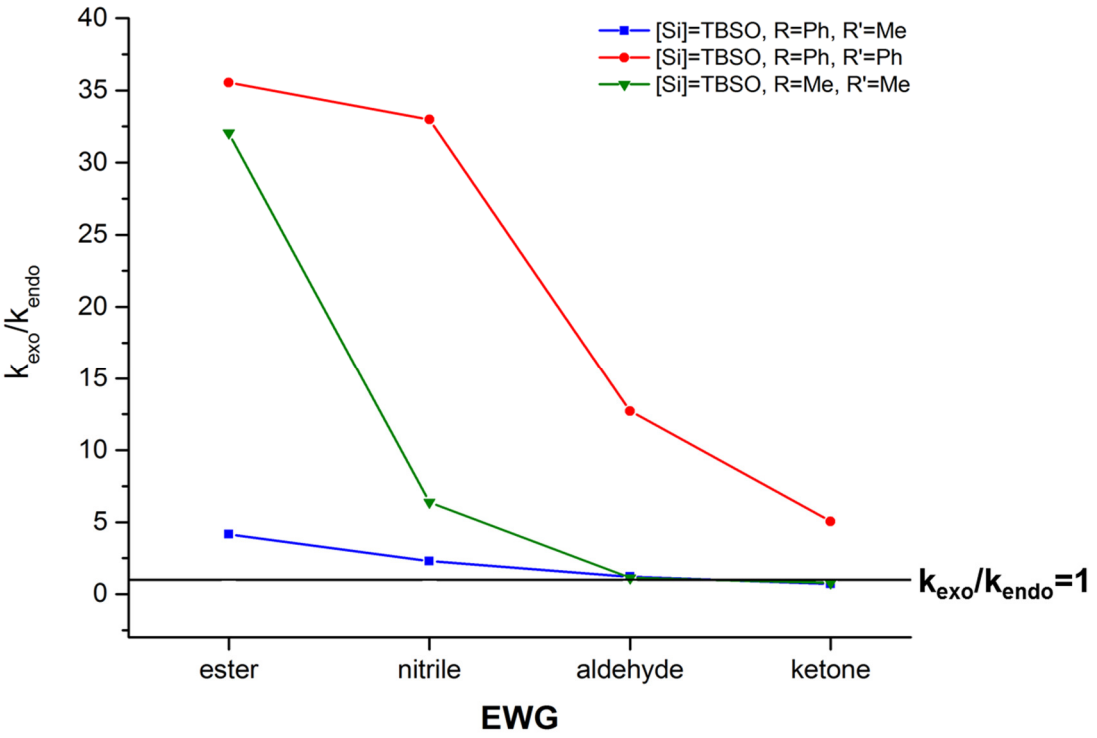


Figure S1 The calculated product ratio k_{exo}/k_{endo} of the Diels-Alder reaction pathways with different EWG, substituent at C_4 of diene(R) and C_β of dienophile(R').

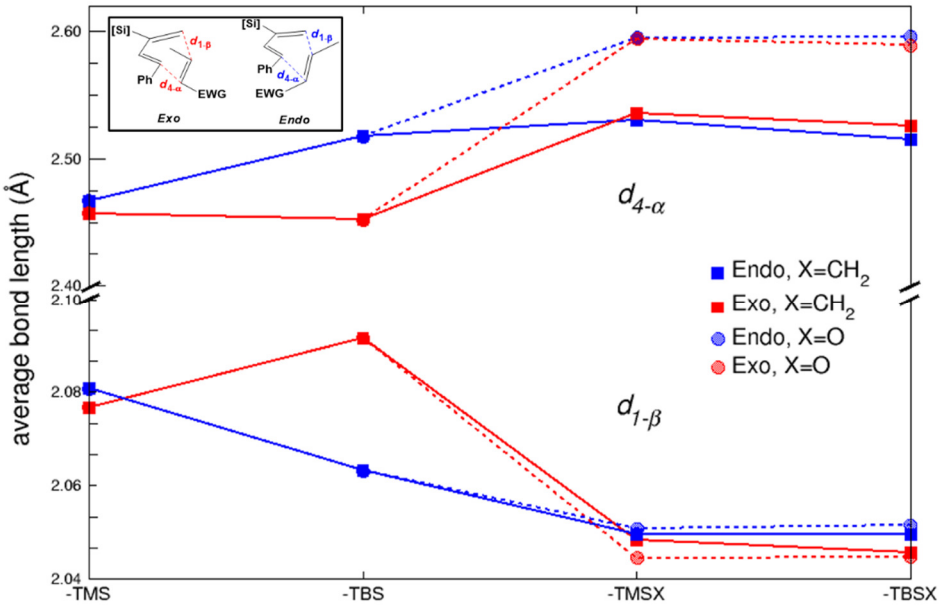


Figure S2. The average bond lengths of the two newly formed C-C bonds in the exo or endo transition states for dienes with different [Si] substituent at C_2 calculated at the M06-2X/6-311++G(d,p) level.

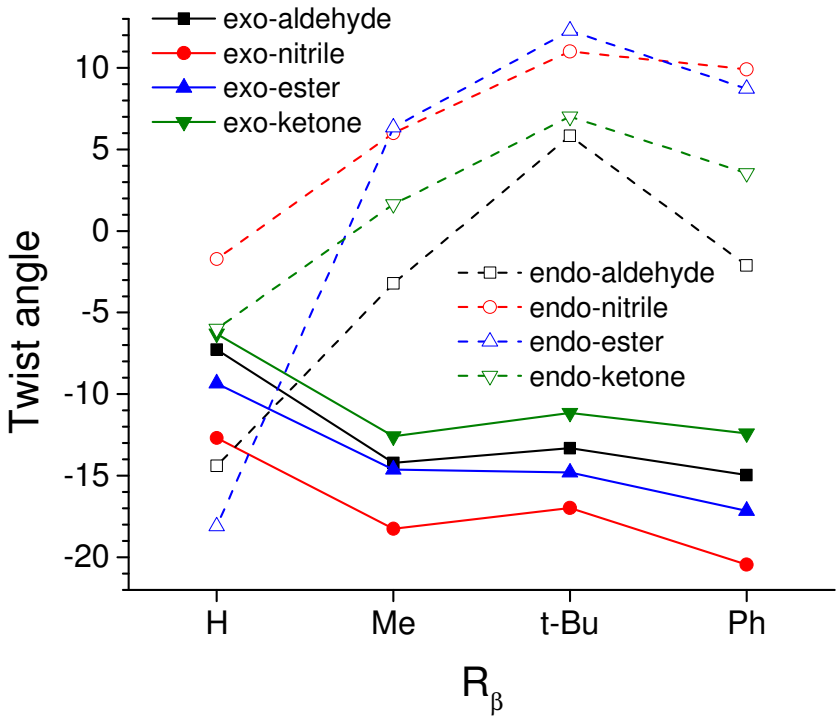


Figure S3. The twist angle in the exo or endo transition states for dienes with different R_β substituent at C_β calculated at the M06-2X/6-311++G(d,p) level.

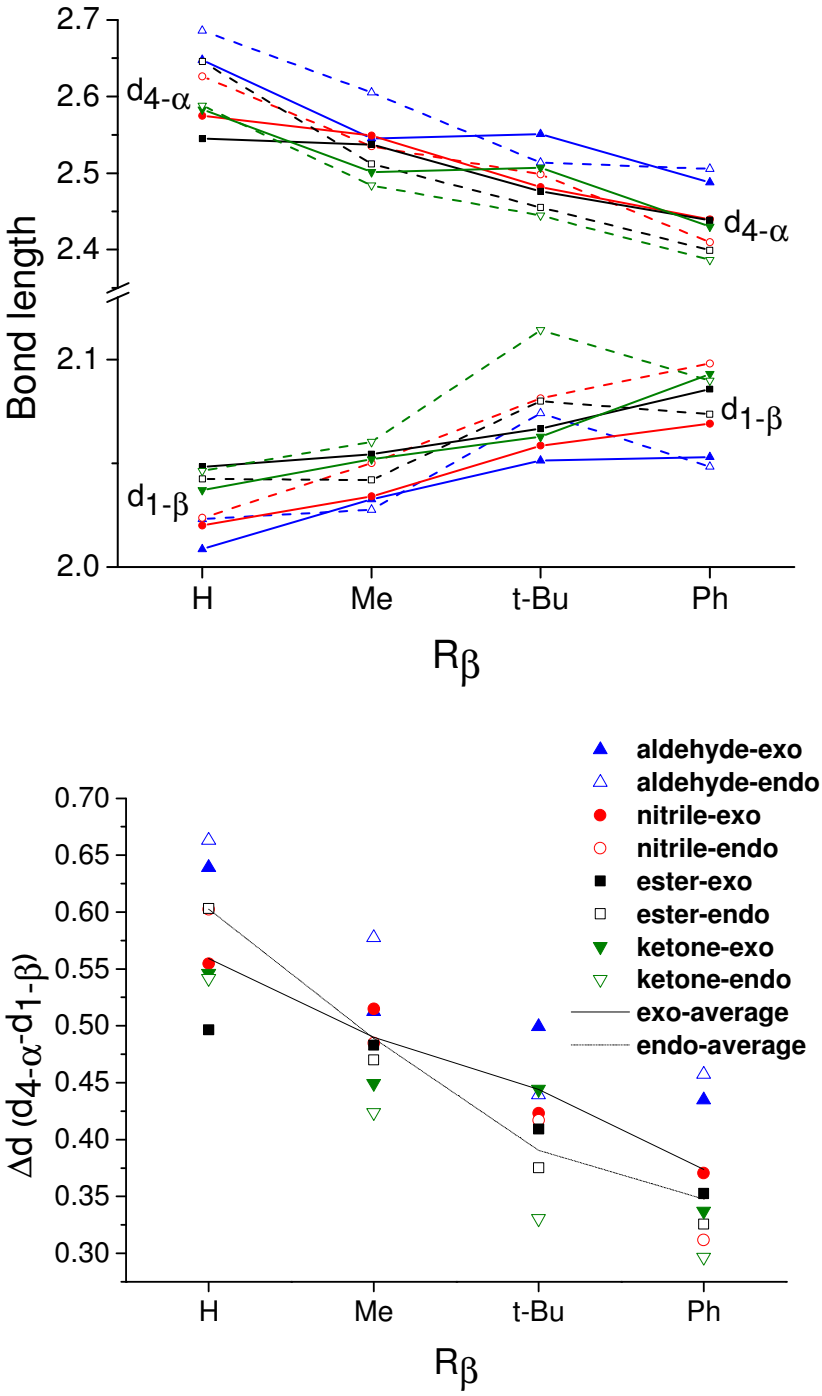
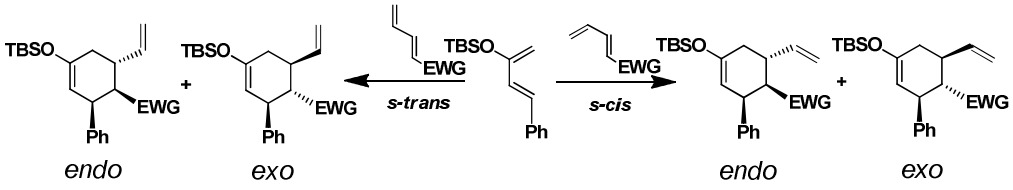


Figure S4. (Top) The bond lengths and (Bottom) the bond length differences of the two newly formed C-C bonds in the exo or endo transition states for dienes with different R_β substituent at C_β calculated at the M06-2X/6-311++G(d,p) level.

Table S1. Computed activation energy (kcal/mol) and product distribution ratio at the M06-2X/6-311++G(d,p) level for Diels-Alder reactions between a [Si]=TBSO and R=phenyl substituted diene and a trans-ethenyl substituted dienophile with different EWG's.



EWG	Isomer	$\Delta E_a^{\ddagger}$ (kcal/mol)		k_{exo}/k_{endo}
		Exo	Endo	
-$COOCH_3$	s-cis	13.20	15.45	15.5789
	s-trans	17.08	17.43	1.5228
-CN	s-cis	12.93	14.71	5.7527
	s-trans	17.58	17.28	0.6949
-CHO	s-cis	14.79	15.65	2.8486
	s-trans	18.28	17.63	0.4511
-$COCH_3$	s-cis	14.34	14.90	2.0008
	s-trans	18.96	16.57	0.0539

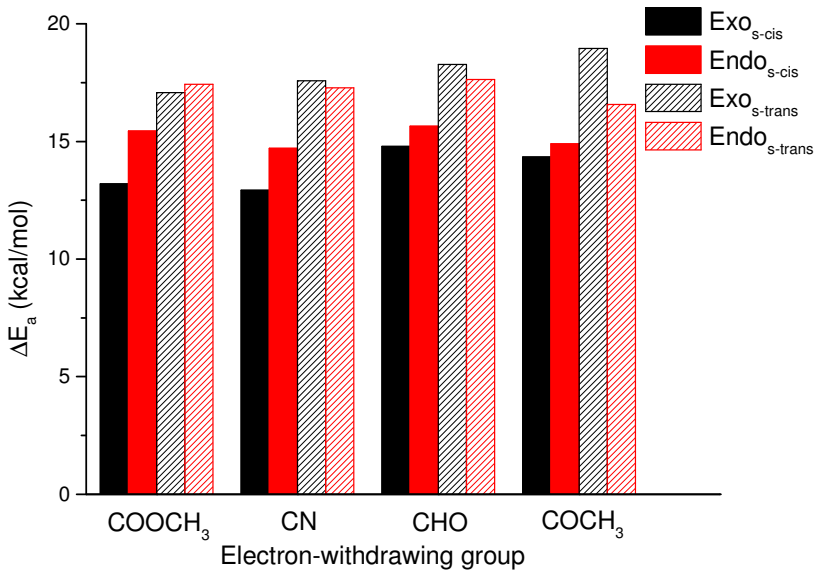


Figure S5. Computed activation energy (kcal/mol) at the M06-2X/6-311++G(d,p) level for Diels-Alder reactions involving dienophiles with a trans-ethenyl substitution of R_β and different EWG's and dienes with [Si]=TBSO and R=Ph substituent.

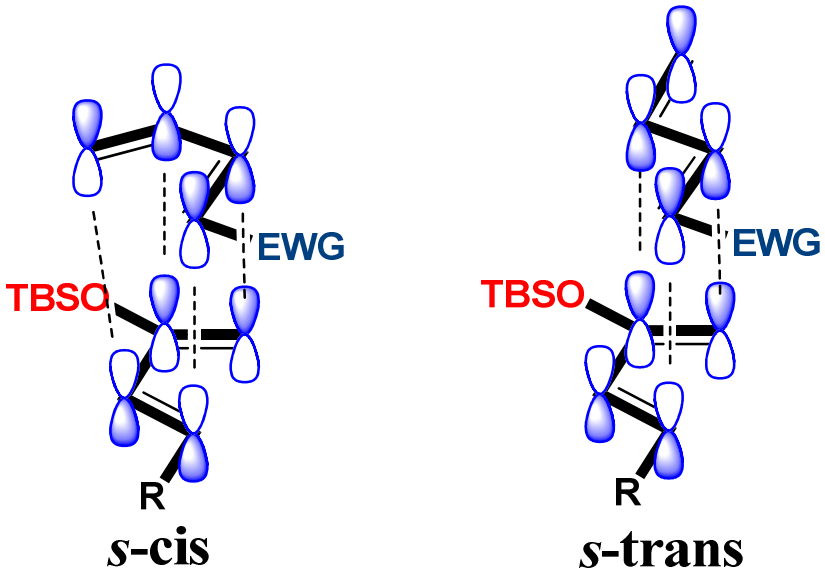
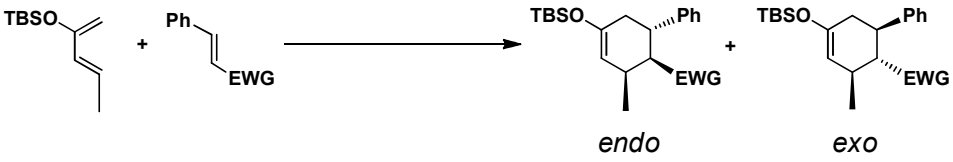
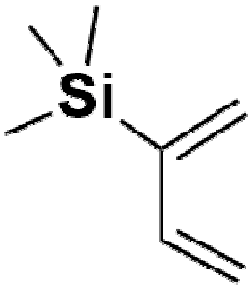


Figure S6. The exo transition state geometry for a dienophile with a trans- C_β ethenyl substitution at the *s*-cis or *s*-trans conformation. Only the *s*-cis conformation forms secondary orbital interaction between the ethenyl group and the diene fragment.

Table S2. Computed activation energy (kcal/mol) and product distribution ratio at the M06-2X/6-311++G(d,p) level for Diels-Alder reactions between a [Si]-TBSO and R-methyl substituted diene and a trans- R_β phenyl substituted dienophile with different EWG's.



EWG	$\Delta E_a^{\ddagger}$		k_{exo}/k_{endo}
	Exo	Endo	
-$COOCH_3$	12.14	15.29	203.2994
-CN	13.50	15.83	50.8855
-CHO	13.53	15.66	36.4818



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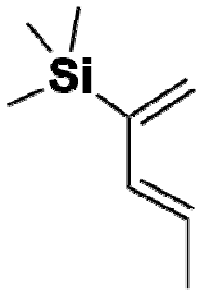
C	-0.95043	-0.85143	-0.10732
C	3.05428	1.89938	-0.82693
C	2.62764	0.7129	1.98928
C	4.58582	-0.64342	0.021
Si	2.95758	0.29827	0.17567
H	0.92996	-2.58825	-1.40873
H	2.7184	-2.45272	-0.98323
H	0.09413	0.88316	-0.66353
H	-0.84681	-1.89308	0.1886
H	-1.94894	-0.46906	-0.06628
H	3.87154	2.52964	-0.46164
H	3.23822	1.69309	-1.88542
H	2.13239	2.48413	-0.75445
H	1.67647	1.23933	2.11142
H	2.58512	-0.19463	2.59888
H	3.41824	1.35298	2.39382
H	4.81527	-0.8917	-1.01929
H	5.40807	-0.03038	0.40361
H	4.57324	-1.57346	0.59664



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C	2.62764	0.7129	1.98928
C	4.58582	-0.64342	0.021
C	-2.38753	-0.30111	-0.04825
Si	2.95758	0.29827	0.17567
H	0.92996	-2.58825	-1.40873
H	2.7184	-2.45272	-0.98323
H	0.09413	0.88316	-0.66353
H	-0.84681	-1.89308	0.1886
H	3.87154	2.52964	-0.46164
H	3.23822	1.69309	-1.88542
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H	1.67647	1.23933	2.11142
H	2.58512	-0.19463	2.59888
H	3.41824	1.35298	2.39382
H	4.81527	-0.8917	-1.01929
H	5.40807	-0.03038	0.40361
H	4.57324	-1.57346	0.59664
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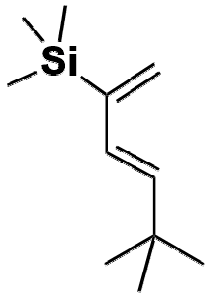

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C	-0.95043	-0.85143	-0.10732
C	3.05428	1.89938	-0.82693
C	2.62764	0.7129	1.98928
C	4.58582	-0.64342	0.021
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H	2.58512	-0.19463	2.59888
H	3.41824	1.35298	2.39382
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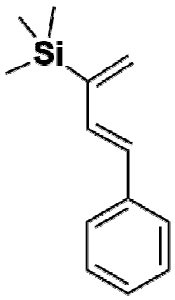

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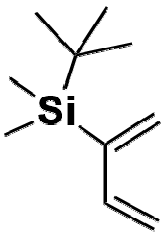

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C	1.94584	2.10881	-0.90804
C	1.49188	0.93948	1.90039
C	4.73298	0.79722	0.72476
C	3.84072	-1.52836	0.93344
C	4.24358	-0.51716	-1.34451
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H	1.82503	-2.29475	-1.16161
H	-0.873	0.96389	-0.69995
H	-1.68523	-1.8552	0.14049
H	-2.8476	-0.47332	-0.0768
H	2.67386	2.83701	-0.53912
H	2.16616	1.91482	-1.96127
H	0.96099	2.58253	-0.85844
H	0.47939	1.35289	1.92674
H	1.49967	0.05411	2.54244
H	2.16406	1.68198	2.33984
H	5.75422	0.39576	0.71979
H	4.75302	1.73943	0.16941
H	4.47835	1.02272	1.76413
H	3.19871	-2.32045	0.54188
H	4.86937	-1.91112	0.93936
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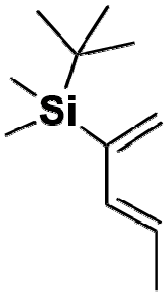

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C	3.765	-0.23342	0.09608
C	1.94584	2.10881	-0.90804
C	1.49188	0.93948	1.90039
C	4.73298	0.79722	0.72476
C	3.84072	-1.52836	0.93344
C	4.24358	-0.51716	-1.34451
C	-3.29201	-0.32302	-0.04835
Si	1.98588	0.51781	0.12159
H	0.03207	-2.42534	-1.54851
H	1.82503	-2.29475	-1.16161
H	-0.873	0.96389	-0.69995
H	-1.68523	-1.8552	0.14049
H	2.67386	2.83701	-0.53912
H	2.16616	1.91482	-1.96127
H	0.96099	2.58253	-0.85844
H	0.47939	1.35289	1.92674
H	1.49967	0.05411	2.54244
H	2.16406	1.68198	2.33984
H	5.75422	0.39576	0.71979
H	4.75302	1.73943	0.16941
H	4.47835	1.02272	1.76413
H	3.19871	-2.32045	0.54188
H	4.86937	-1.91112	0.93936
H	3.55313	-1.3554	1.97474
H	4.25904	0.39132	-1.95404
H	5.26689	-0.91374	-1.32673
H	3.61849	-1.24923	-1.86061

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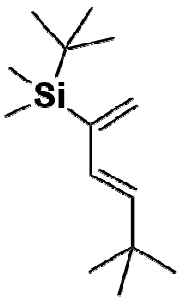

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C	1.94584	2.10881	-0.90804
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C	3.84072	-1.52836	0.93344
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C	-3.61319	0.45343	-1.3078
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H	-1.68523	-1.8552	0.14049
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H	2.16616	1.91482	-1.96127
H	0.96099	2.58253	-0.85844
H	0.47939	1.35289	1.92674
H	1.49967	0.05411	2.54244
H	2.16406	1.68198	2.33984
H	5.75422	0.39576	0.71979
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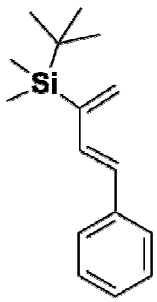

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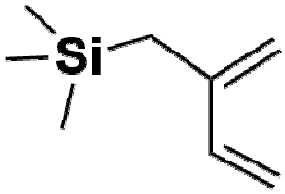
Optimized potential energies (E)	-913.153418
Gibbs's free energies (G)	-913.200929

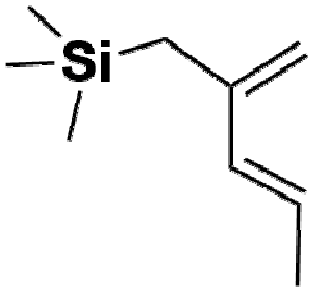
C	0.84207	-1.84315	-1.11471
C	0.62198	-0.63142	-0.57513
C	-0.75351	-0.09799	-0.49561
C	-1.83586	-0.8155	-0.14157
C	3.765	-0.23342	0.09608
C	1.94584	2.10881	-0.90804
C	1.49188	0.93948	1.90039
C	4.73298	0.79722	0.72476
C	3.84072	-1.52836	0.93344
C	4.24358	-0.51716	-1.34451
C	-3.22426	-0.34593	-0.05268
C	-4.19036	-1.19302	0.51685
C	-3.64751	0.9141	-0.51402
C	-5.52081	-0.79802	0.63411
C	-4.97456	1.3102	-0.39543
C	-5.91972	0.45773	0.18055
Si	1.98588	0.51781	0.12159
H	0.03207	-2.42534	-1.54851
H	1.82503	-2.29475	-1.16161
H	-0.873	0.96389	-0.69995
H	-1.68523	-1.8552	0.14049
H	2.67386	2.83701	-0.53912
H	2.16616	1.91482	-1.96127
H	0.96099	2.58253	-0.85844
H	0.47939	1.35289	1.92674
H	1.49967	0.05411	2.54244
H	2.16406	1.68198	2.33984
H	5.75422	0.39576	0.71979
H	4.75302	1.73943	0.16941
H	4.47835	1.02272	1.76413
H	3.19871	-2.32045	0.54188

H	4.86937	-1.91112	0.93936
H	3.55313	-1.3554	1.97474
H	4.25904	0.39132	-1.95404
H	5.26689	-0.91374	-1.32673
H	3.61849	-1.24923	-1.86061
H	-3.88829	-2.17225	0.87404
H	-2.93651	1.58673	-0.97947
H	-6.24499	-1.47139	1.07923
H	-5.27698	2.28592	-0.75973
H	-6.95446	0.76885	0.26823



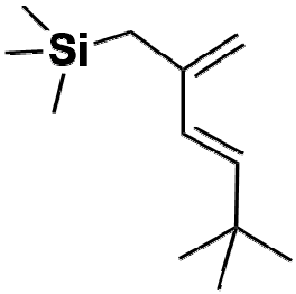
Charge	0
Number of imaginary frequencies	0
Optimized potential energies (E)	-603.675935
Gibbs's free energies (G)	-603.715804

C	-1.24149	2.69868	-0.37432
C	-1.12714	1.40796	-0.73302
C	0.17665	0.71964	-0.76516
C	1.21578	0.96453	0.05288
C	-2.32574	0.58398	-1.14236
C	-4.59209	-1.38915	-0.55063
C	-1.81213	-1.92965	0.66719
C	-3.52618	0.41668	1.71971
Si	-3.05004	-0.58446	0.19183
H	-0.37621	3.29832	-0.1173
H	-2.2067	3.19237	-0.34743
H	0.26361	-0.0697	-1.50879
H	1.0825	1.69868	0.8441
H	2.17707	0.49499	0.03416
H	-3.1422	1.242	-1.45832
H	-2.07213	-0.03612	-2.01157
H	-4.34565	-1.97407	-1.44242
H	-5.06579	-2.06538	0.1681
H	-5.33492	-0.63885	-0.83899
H	-1.53167	-2.53678	-0.19929
H	-0.89605	-1.50741	1.08866
H	-2.24699	-2.60116	1.41471
H	-2.65747	0.92392	2.14864
H	-4.27293	1.18026	1.48056
H	-3.95032	-0.23319	2.49169



Charge	0
Number of imaginary frequencies	0
Optimized potential energies (E)	-642.956032
Gibbs's free energies (G)	-642.99813

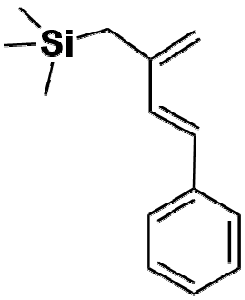
C	-1.24149	2.69868	-0.37432
C	-1.12714	1.40796	-0.73302
C	0.17665	0.71964	-0.76516
C	1.21578	0.96453	0.05288
C	-2.32574	0.58398	-1.14236
C	-4.59209	-1.38915	-0.55063
C	-1.81213	-1.92965	0.66719
C	-3.52618	0.41668	1.71971
C	2.59932	0.28875	0.02594
Si	-3.05004	-0.58446	0.19183
H	-0.37621	3.29832	-0.1173
H	-2.2067	3.19237	-0.34743
H	0.26361	-0.0697	-1.50879
H	1.0825	1.69868	0.8441
H	-3.1422	1.242	-1.45832
H	-2.07213	-0.03612	-2.01157
H	-4.34565	-1.97407	-1.44242
H	-5.06579	-2.06538	0.1681
H	-5.33492	-0.63885	-0.83899
H	-1.53167	-2.53678	-0.19929
H	-0.89605	-1.50741	1.08866
H	-2.24699	-2.60116	1.41471
H	-2.65747	0.92392	2.14864
H	-4.27293	1.18026	1.48056
H	-3.95032	-0.23319	2.49169
H	3.3626	1.0363	0.08487
H	2.68726	-0.3772	0.85881
H	2.7094	-0.26238	-0.88457



Charge	0
Number of imaginary frequencies	0
Optimized potential energies (E)	-760.787209
Gibbs's free energies (G)	-760.834296

C	-1.24149	2.69868	-0.37432
C	-1.12714	1.40796	-0.73302
C	0.17665	0.71964	-0.76516
C	1.21578	0.96453	0.05288
C	-2.32574	0.58398	-1.14236
C	-4.59209	-1.38915	-0.55063
C	-1.81213	-1.92965	0.66719
C	-3.52618	0.41668	1.71971
C	2.59932	0.28875	0.02594
C	2.76191	-0.51303	1.29996
C	2.66296	-0.61686	-1.18571
C	3.65522	1.37032	-0.0613
Si	-3.05004	-0.58446	0.19183
H	-0.37621	3.29832	-0.1173
H	-2.2067	3.19237	-0.34743
H	0.26361	-0.0697	-1.50879
H	1.0825	1.69868	0.8441
H	-3.1422	1.242	-1.45832
H	-2.07213	-0.03612	-2.01157
H	-4.34565	-1.97407	-1.44242
H	-5.06579	-2.06538	0.1681
H	-5.33492	-0.63885	-0.83899
H	-1.53167	-2.53678	-0.19929
H	-0.89605	-1.50741	1.08866
H	-2.24699	-2.60116	1.41471
H	-2.65747	0.92392	2.14864
H	-4.27293	1.18026	1.48056
H	-3.95032	-0.23319	2.49169
H	2.6891	0.15508	2.19147
H	1.96581	-1.29235	1.37289
H	3.75624	-1.0208	1.31924

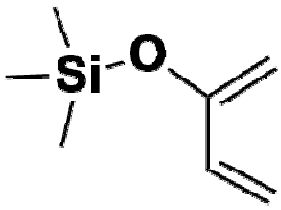
H	2.51684	-0.02525	-2.12119
H	3.65454	-1.12732	-1.24172
H	1.86655	-1.39729	-1.12992
H	4.67677	0.91982	-0.08265
H	3.51626	1.97506	-0.98944
H	3.5878	2.05123	0.82091



Charge	0
Number of imaginary frequencies	0
Optimized potential energies (E)	-834.614761
Gibbs's free energies (G)	-834.662314

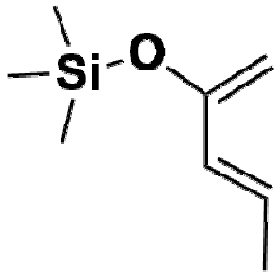
C	-1.24149	2.69868	-0.37432
C	-1.12714	1.40796	-0.73302
C	0.17665	0.71964	-0.76516
C	1.21578	0.96453	0.05288
C	-2.32574	0.58398	-1.14236
C	-4.59209	-1.38915	-0.55063
C	-1.81213	-1.92965	0.66719
C	-3.52618	0.41668	1.71971
C	2.5341	0.32061	0.02721
C	3.42909	0.56801	1.08248
C	2.95762	-0.53673	-1.00514
C	4.68915	-0.02412	1.11646
C	4.21424	-1.12949	-0.97106
C	5.08748	-0.87864	0.09031
Si	-3.05004	-0.58446	0.19183
H	-0.37621	3.29832	-0.1173
H	-2.2067	3.19237	-0.34743
H	0.26361	-0.0697	-1.50879
H	1.0825	1.69868	0.8441
H	-3.1422	1.242	-1.45832
H	-2.07213	-0.03612	-2.01157
H	-4.34565	-1.97407	-1.44242
H	-5.06579	-2.06538	0.1681
H	-5.33492	-0.63885	-0.83899
H	-1.53167	-2.53678	-0.19929
H	-0.89605	-1.50741	1.08866
H	-2.24699	-2.60116	1.41471
H	-2.65747	0.92392	2.14864
H	-4.27293	1.18026	1.48056
H	-3.95032	-0.23319	2.49169
H	3.12658	1.23213	1.88576

H	2.3042	-0.73353	-1.84698
H	5.3593	0.18296	1.94345
H	4.5193	-1.7856	-1.7789
H	6.0681	-1.34026	0.11143



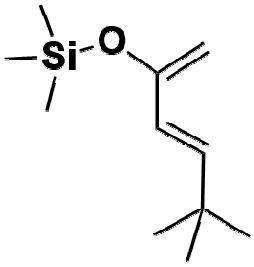
Charge	0
Number of imaginary frequencies	0
Optimized potential energies (E)	-639.653178
Gibbs's free energies (G)	-639.692829

C	-1.20994	-1.89517	0.65963
C	-0.9164	-0.63063	0.31045
C	0.44217	-0.06926	0.26024
C	1.56844	-0.76625	0.03631
C	-3.94015	2.06086	-0.64315
C	-4.08865	-0.91848	-1.45385
C	-4.30323	-0.10004	1.53551
O	-1.84514	0.31478	-0.01925
Si	-3.54056	0.30291	-0.13479
H	-0.4237	-2.57367	0.95868
H	-2.22261	-2.27396	0.6673
H	0.47609	1.00843	0.3882
H	1.4832	-1.83156	-0.16377
H	2.56741	-0.38367	0.01207
H	-3.46	2.31248	-1.59283
H	-5.01947	2.19574	-0.7651
H	-3.59505	2.77545	0.10929
H	-3.61438	-0.69356	-2.41354
H	-3.84716	-1.95216	-1.19453
H	-5.1728	-0.85618	-1.59476
H	-4.10545	-1.12617	1.85442
H	-3.9215	0.57179	2.30983
H	-5.38973	0.02874	1.48897



Charge	0
Number of imaginary frequencies	0
Optimized potential energies (E)	-678.933595
Gibbs's free energies (G)	-678.975968

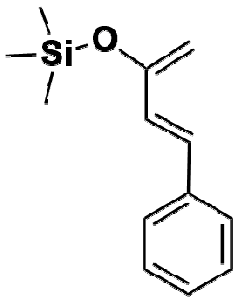
C	-1.20994	-1.89517	0.65963
C	-0.9164	-0.63063	0.31045
C	0.44217	-0.06926	0.26024
C	1.56844	-0.76625	0.03631
C	-3.94015	2.06086	-0.64315
C	-4.08865	-0.91848	-1.45385
C	-4.30323	-0.10004	1.53551
C	3.00622	-0.21562	0.00142
O	-1.84514	0.31478	-0.01925
Si	-3.54056	0.30291	-0.13479
H	-0.4237	-2.57367	0.95868
H	-2.22261	-2.27396	0.6673
H	0.47609	1.00843	0.3882
H	1.4832	-1.83156	-0.16377
H	-3.46	2.31248	-1.59283
H	-5.01947	2.19574	-0.7651
H	-3.59505	2.77545	0.10929
H	-3.61438	-0.69356	-2.41354
H	-3.84716	-1.95216	-1.19453
H	-5.1728	-0.85618	-1.59476
H	-4.10545	-1.12617	1.85442
H	-3.9215	0.57179	2.30983
H	-5.38973	0.02874	1.48897
H	3.69543	-1.0253	-0.11819
H	3.10817	0.46369	-0.81897
H	3.21402	0.29733	0.91717



Charge	0
Number of imaginary frequencies	0
Optimized potential energies (E)	-796.763487
Gibbs's free energies (G)	-796.81113

C	-1.20994	-1.89517	0.65963
C	-0.9164	-0.63063	0.31045
C	0.44217	-0.06926	0.26024
C	1.56844	-0.76625	0.03631
C	-3.94015	2.06086	-0.64315
C	-4.08865	-0.91848	-1.45385
C	-4.30323	-0.10004	1.53551
C	3.00622	-0.21562	0.00142
C	3.12747	0.7231	-1.18031
C	3.26443	0.52289	1.29764
C	3.95908	-1.383	-0.14554
O	-1.84514	0.31478	-0.01925
Si	-3.54056	0.30291	-0.13479
H	-0.4237	-2.57367	0.95868
H	-2.22261	-2.27396	0.6673
H	0.47609	1.00843	0.3882
H	1.4832	-1.83156	-0.16377
H	-3.46	2.31248	-1.59283
H	-5.01947	2.19574	-0.7651
H	-3.59505	2.77545	0.10929
H	-3.61438	-0.69356	-2.41354
H	-3.84716	-1.95216	-1.19453
H	-5.1728	-0.85618	-1.59476
H	-4.10545	-1.12617	1.85442
H	-3.9215	0.57179	2.30983
H	-5.38973	0.02874	1.48897
H	2.91154	0.18011	-2.13162
H	2.40499	1.56842	-1.08079
H	4.15934	1.14553	-1.24099
H	3.14862	-0.16703	2.16774
H	4.30066	0.93877	1.31195
H	2.5433	1.36719	1.41426

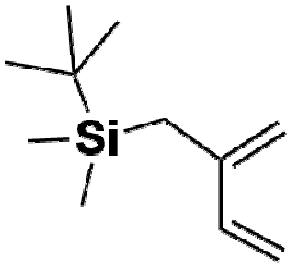
H	5.01623	-1.02453	-0.17551
H	3.84847	-2.08558	0.71505
H	3.74814	-1.94027	-1.0897



Charge	0
Number of imaginary frequencies	0
Optimized potential energies (E)	-870.591256
Gibbs's free energies (G)	-870.637904

C	-1.20994	-1.89517	0.65963
C	-0.9164	-0.63063	0.31045
C	0.44217	-0.06926	0.26024
C	1.56844	-0.76625	0.03631
C	-3.94015	2.06086	-0.64315
C	-4.08865	-0.91848	-1.45385
C	-4.30323	-0.10004	1.53551
C	2.93804	-0.24173	0.00308
C	3.97858	-1.09365	-0.40514
C	3.27066	1.07746	0.36181
C	5.29659	-0.6477	-0.46474
C	4.58543	1.52339	0.30134
C	5.60655	0.66451	-0.11324
O	-1.84514	0.31478	-0.01925
Si	-3.54056	0.30291	-0.13479
H	-0.4237	-2.57367	0.95868
H	-2.22261	-2.27396	0.6673
H	0.47609	1.00843	0.3882
H	1.4832	-1.83156	-0.16377
H	-3.46	2.31248	-1.59283
H	-5.01947	2.19574	-0.7651
H	-3.59505	2.77545	0.10929
H	-3.61438	-0.69356	-2.41354
H	-3.84716	-1.95216	-1.19453
H	-5.1728	-0.85618	-1.59476
H	-4.10545	-1.12617	1.85442
H	-3.9215	0.57179	2.30983
H	-5.38973	0.02874	1.48897
H	3.74538	-2.1168	-0.68166
H	2.49773	1.75808	0.69875
H	6.08032	-1.32526	-0.78485

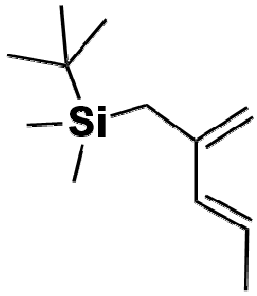
H	4.81827	2.54421	0.58374
H	6.63126	1.01558	-0.15642



Charge	0
Number of imaginary frequencies	0
Optimized potential energies (E)	-721.498890
Gibbs's free energies (G)	-721.541549

C	-0.49659	2.42112	-1.57429
C	-0.37698	1.08476	-1.48909
C	0.90877	0.43798	-1.16829
C	1.86515	0.94293	-0.36889
C	-3.09623	0.31984	1.03451
C	-3.68325	-1.87791	-1.1233
C	-1.0581	-1.99573	0.45925
C	-3.95246	-0.52517	2.00401
C	-1.98866	1.02517	1.84669
C	-3.99934	1.38682	0.38107
C	-1.53927	0.15844	-1.76126
Si	-2.3297	-0.82812	-0.31372
H	0.3514	3.07996	-1.42781
H	-1.44584	2.88909	-1.8104
H	1.05371	-0.54571	-1.6094
H	1.66829	1.88869	0.1304
H	2.81286	0.50267	-0.13884
H	-4.1471	-2.55976	-0.40515
H	-4.47605	-1.26374	-1.56031
H	-3.25923	-2.48812	-1.9274
H	-0.65709	-2.67663	-0.29844
H	-0.2154	-1.46044	0.90289
H	-1.51475	-2.61105	1.24064
H	-4.36862	0.11694	2.79104
H	-4.79433	-1.00792	1.49914
H	-3.36573	-1.30517	2.49943
H	-1.35558	1.65516	1.2168
H	-2.4387	1.66869	2.61409
H	-1.34286	0.30816	2.36194
H	-4.80354	0.93852	-0.2113
H	-4.47239	2.00696	1.15351
H	-3.43338	2.05628	-0.27208

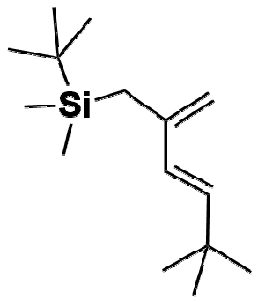
H	-1.2193	-0.61182	-2.47693
H	-2.34669	0.70932	-2.25425



Charge	0
Number of imaginary frequencies	0
Optimized potential energies (E)	-760.779512
Gibbs's free energies (G)	-760.824699

C	-0.49659	2.42112	-1.57429
C	-0.37698	1.08476	-1.48909
C	0.90877	0.43798	-1.16829
C	1.86515	0.94293	-0.36889
C	-3.09623	0.31984	1.03451
C	-3.68325	-1.87791	-1.1233
C	-1.0581	-1.99573	0.45925
C	-3.95246	-0.52517	2.00401
C	-1.98866	1.02517	1.84669
C	-3.99934	1.38682	0.38107
C	-1.53927	0.15844	-1.76126
C	3.22915	0.30929	-0.03779
Si	-2.3297	-0.82812	-0.31372
H	0.3514	3.07996	-1.42781
H	-1.44584	2.88909	-1.8104
H	1.05371	-0.54571	-1.6094
H	1.66829	1.88869	0.1304
H	-4.1471	-2.55976	-0.40515
H	-4.47605	-1.26374	-1.56031
H	-3.25923	-2.48812	-1.9274
H	-0.65709	-2.67663	-0.29844
H	-0.2154	-1.46044	0.90289
H	-1.51475	-2.61105	1.24064
H	-4.36862	0.11694	2.79104
H	-4.79433	-1.00792	1.49914
H	-3.36573	-1.30517	2.49943
H	-1.35558	1.65516	1.2168
H	-2.4387	1.66869	2.61409
H	-1.34286	0.30816	2.36194
H	-4.80354	0.93852	-0.2113
H	-4.47239	2.00696	1.15351

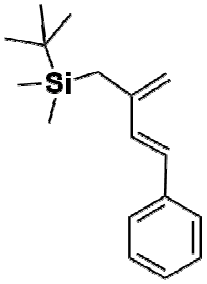
H	-3.43338	2.05628	-0.27208
H	-1.2193	-0.61182	-2.47693
H	-2.34669	0.70932	-2.25425
H	3.99357	1.05539	-0.10012
H	3.20408	-0.09375	0.95308
H	3.4375	-0.47403	-0.73628



Charge	0
Number of imaginary frequencies	0
Optimized potential energies (E)	-878.610226
Gibbs's free energies (G)	-878.659793

C	-0.49659	2.42112	-1.57429
C	-0.37698	1.08476	-1.48909
C	0.90877	0.43798	-1.16829
C	1.86515	0.94293	-0.36889
C	-3.09623	0.31984	1.03451
C	-3.68325	-1.87791	-1.1233
C	-1.0581	-1.99573	0.45925
C	-3.95246	-0.52517	2.00401
C	-1.98866	1.02517	1.84669
C	-3.99934	1.38682	0.38107
C	-1.53927	0.15844	-1.76126
C	3.22915	0.30929	-0.03779
C	3.21214	-0.12547	1.41242
C	3.43404	-0.88219	-0.94921
C	4.30525	1.34876	-0.26978
Si	-2.3297	-0.82812	-0.31372
H	0.3514	3.07996	-1.42781
H	-1.44584	2.88909	-1.8104
H	1.05371	-0.54571	-1.6094
H	1.66829	1.88869	0.1304
H	-4.1471	-2.55976	-0.40515
H	-4.47605	-1.26374	-1.56031
H	-3.25923	-2.48812	-1.9274
H	-0.65709	-2.67663	-0.29844
H	-0.2154	-1.46044	0.90289
H	-1.51475	-2.61105	1.24064
H	-4.36862	0.11694	2.79104
H	-4.79433	-1.00792	1.49914
H	-3.36573	-1.30517	2.49943
H	-1.35558	1.65516	1.2168
H	-2.4387	1.66869	2.61409

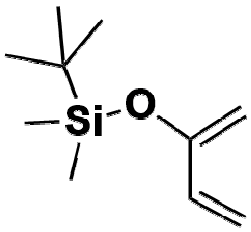
H	-1.34286	0.30816	2.36194
H	-4.80354	0.93852	-0.2113
H	-4.47239	2.00696	1.15351
H	-3.43338	2.05628	-0.27208
H	-1.2193	-0.61182	-2.47693
H	-2.34669	0.70932	-2.25425
H	3.03564	0.75243	2.07919
H	2.40047	-0.87245	1.58464
H	4.18705	-0.592	1.69314
H	3.42006	-0.56067	-2.01827
H	4.41592	-1.37119	-0.74011
H	2.62427	-1.63476	-0.79311
H	5.31335	0.92726	-0.03947
H	4.29764	1.68501	-1.33436
H	4.13552	2.23666	0.38543



Charge	0
Number of imaginary frequencies	0
Optimized potential energies (E)	-952.438139
Gibbs's free energies (G)	-952.489699

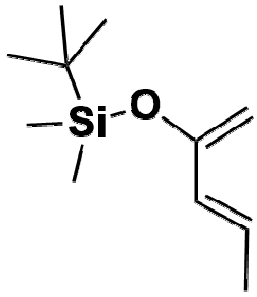
C	-0.49659	2.42112	-1.57429
C	-0.37698	1.08476	-1.48909
C	0.90877	0.43798	-1.16829
C	1.86515	0.94293	-0.36889
C	-3.09623	0.31984	1.03451
C	-3.68325	-1.87791	-1.1233
C	-1.0581	-1.99573	0.45925
C	-3.95246	-0.52517	2.00401
C	-1.98866	1.02517	1.84669
C	-3.99934	1.38682	0.38107
C	3.16489	0.33914	-0.05339
C	3.95092	0.91455	0.95997
C	3.67405	-0.7933	-0.7156
C	5.18721	0.37717	1.30968
C	4.90683	-1.3314	-0.3658
C	5.67065	-0.75107	0.64994
C	-1.53927	0.15844	-1.76126
Si	-2.3297	-0.82812	-0.31372
H	0.3514	3.07996	-1.42781
H	-1.44584	2.88909	-1.8104
H	1.05371	-0.54571	-1.6094
H	1.66829	1.88869	0.1304
H	-4.1471	-2.55976	-0.40515
H	-4.47605	-1.26374	-1.56031
H	-3.25923	-2.48812	-1.9274
H	-0.65709	-2.67663	-0.29844
H	-0.2154	-1.46044	0.90289
H	-1.51475	-2.61105	1.24064
H	-4.36862	0.11694	2.79104
H	-4.79433	-1.00792	1.49914
H	-3.36573	-1.30517	2.49943
H	-1.35558	1.65516	1.2168

H	-2.4387	1.66869	2.61409
H	-1.34286	0.30816	2.36194
H	-4.80354	0.93852	-0.2113
H	-4.47239	2.00696	1.15351
H	-3.43338	2.05628	-0.27208
H	3.58105	1.79233	1.48005
H	3.10748	-1.25071	-1.51819
H	5.77235	0.83998	2.09662
H	5.2794	-2.20365	-0.89165
H	6.6332	-1.17183	0.91753
H	-1.2193	-0.61182	-2.47693
H	-2.34669	0.70932	-2.25425



Charge	0
Number of imaginary frequencies	0
Optimized potential energies (E)	-757.476136
Gibbs's free energies (G)	-757.518035

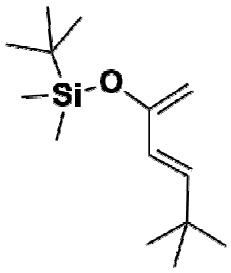
C	-0.51241	2.38049	-1.57591
C	-0.38323	1.0731	-1.3029
C	0.8925	0.40682	-1.00056
C	1.9137	0.96306	-0.32655
C	-3.25115	0.25813	0.96121
C	-3.41317	-1.76699	-1.44335
C	-1.06259	-1.94951	0.53708
C	-4.10997	-0.6748	1.84336
C	-2.27996	1.0492	1.86429
C	-4.17925	1.25214	0.23084
O	-1.4701	0.24191	-1.39479
Si	-2.27707	-0.78878	-0.31484
H	0.35539	3.02387	-1.61594
H	-1.48246	2.80768	-1.79431
H	0.96336	-0.61809	-1.35318
H	1.77475	1.96202	0.0797
H	2.86467	0.51834	-0.11968
H	-3.98683	-2.51112	-0.88353
H	-4.11866	-1.1195	-1.97001
H	-2.82407	-2.29825	-2.19657
H	-0.52511	-2.55126	-0.20175
H	-0.32137	-1.41883	1.13924
H	-1.5963	-2.64199	1.19573
H	-4.67445	-0.08299	2.57488
H	-4.8375	-1.24282	1.25553
H	-3.50012	-1.38852	2.40577
H	-1.65053	1.73276	1.28768
H	-2.84625	1.65318	2.58489
H	-1.62287	0.38959	2.43866
H	-4.91414	0.74154	-0.39872
H	-4.73584	1.85259	0.96167
H	-3.61731	1.94158	-0.40451



Charge	0
Number of imaginary frequencies	0
Optimized potential energies (E)	-796.756114
Gibbs's free energies (G)	-796.800882

C	-0.51241	2.38049	-1.57591
C	-0.38323	1.0731	-1.3029
C	0.8925	0.40682	-1.00056
C	1.9137	0.96306	-0.32655
C	-3.25115	0.25813	0.96121
C	-3.41317	-1.76699	-1.44335
C	-1.06259	-1.94951	0.53708
C	-4.10997	-0.6748	1.84336
C	-2.27996	1.0492	1.86429
C	-4.17925	1.25214	0.23084
C	3.28238	0.323	-0.02882
O	-1.4701	0.24191	-1.39479
Si	-2.27707	-0.78878	-0.31484
H	0.35539	3.02387	-1.61594
H	-1.48246	2.80768	-1.79431
H	0.96336	-0.61809	-1.35318
H	1.77475	1.96202	0.0797
H	-3.98683	-2.51112	-0.88353
H	-4.11866	-1.1195	-1.97001
H	-2.82407	-2.29825	-2.19657
H	-0.52511	-2.55126	-0.20175
H	-0.32137	-1.41883	1.13924
H	-1.5963	-2.64199	1.19573
H	-4.67445	-0.08299	2.57488
H	-4.8375	-1.24282	1.25553
H	-3.50012	-1.38852	2.40577
H	-1.65053	1.73276	1.28768
H	-2.84625	1.65318	2.58489
H	-1.62287	0.38959	2.43866
H	-4.91414	0.74154	-0.39872
H	-4.73584	1.85259	0.96167

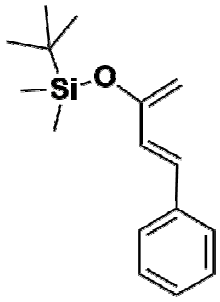
H	-3.61731	1.94158	-0.40451
H	4.03572	1.08271	-0.01391
H	3.24863	-0.16455	0.92305
H	3.51376	-0.39387	-0.78873



Charge	0
Number of imaginary frequencies	0
Optimized potential energies (E)	-914.587457
Gibbs's free energies (G)	-914.636765

C	-0.51241	2.38049	-1.57591
C	-0.38323	1.0731	-1.3029
C	0.8925	0.40682	-1.00056
C	1.9137	0.96306	-0.32655
C	-3.25115	0.25813	0.96121
C	-3.41317	-1.76699	-1.44335
C	-1.06259	-1.94951	0.53708
C	-4.10997	-0.6748	1.84336
C	-2.27996	1.0492	1.86429
C	-4.17925	1.25214	0.23084
C	3.28238	0.323	-0.02882
C	3.24963	-0.23728	1.37739
C	3.52078	-0.78094	-1.03716
C	4.34506	1.39452	-0.15078
O	-1.4701	0.24191	-1.39479
Si	-2.27707	-0.78878	-0.31484
H	0.35539	3.02387	-1.61594
H	-1.48246	2.80768	-1.79431
H	0.96336	-0.61809	-1.35318
H	1.77475	1.96202	0.0797
H	-3.98683	-2.51112	-0.88353
H	-4.11866	-1.1195	-1.97001
H	-2.82407	-2.29825	-2.19657
H	-0.52511	-2.55126	-0.20175
H	-0.32137	-1.41883	1.13924
H	-1.5963	-2.64199	1.19573
H	-4.67445	-0.08299	2.57488
H	-4.8375	-1.24282	1.25553
H	-3.50012	-1.38852	2.40577
H	-1.65053	1.73276	1.28768
H	-2.84625	1.65318	2.58489
H	-1.62287	0.38959	2.43866

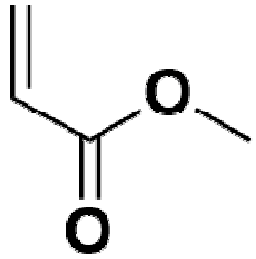
H	-4.91414	0.74154	-0.39872
H	-4.73584	1.85259	0.96167
H	-3.61731	1.94158	-0.40451
H	3.04853	0.57617	2.11516
H	2.44753	-1.00834	1.46986
H	4.22742	-0.7122	1.63289
H	3.5184	-0.36728	-2.07415
H	4.50703	-1.27187	-0.85484
H	2.72092	-1.55613	-0.96121
H	5.3561	0.96936	0.05901
H	4.34874	1.82256	-1.18191
H	4.15074	2.21904	0.57646



Charge	0
Number of imaginary frequencies	0
Optimized potential energies (E)	-988.415255
Gibbs's free energies (G)	-988.466939

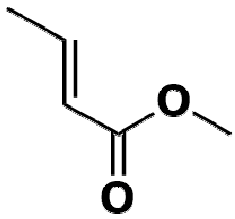
C	-0.51241	2.38049	-1.57591
C	-0.38323	1.0731	-1.3029
C	0.8925	0.40682	-1.00056
C	1.9137	0.96306	-0.32655
C	-3.25115	0.25813	0.96121
C	-3.41317	-1.76699	-1.44335
C	-1.06259	-1.94951	0.53708
C	-4.10997	-0.6748	1.84336
C	-2.27996	1.0492	1.86429
C	-4.17925	1.25214	0.23084
C	3.21755	0.35332	-0.04292
C	4.07679	0.98558	0.87199
C	3.65865	-0.83977	-0.64407
C	5.31936	0.44275	1.18913
C	4.8982	-1.3826	-0.32699
C	5.73521	-0.74623	0.59283
O	-1.4701	0.24191	-1.39479
Si	-2.27707	-0.78878	-0.31484
H	0.35539	3.02387	-1.61594
H	-1.48246	2.80768	-1.79431
H	0.96336	-0.61809	-1.35318
H	1.77475	1.96202	0.0797
H	-3.98683	-2.51112	-0.88353
H	-4.11866	-1.1195	-1.97001
H	-2.82407	-2.29825	-2.19657
H	-0.52511	-2.55126	-0.20175
H	-0.32137	-1.41883	1.13924
H	-1.5963	-2.64199	1.19573
H	-4.67445	-0.08299	2.57488
H	-4.8375	-1.24282	1.25553
H	-3.50012	-1.38852	2.40577

H	-1.65053	1.73276	1.28768
H	-2.84625	1.65318	2.58489
H	-1.62287	0.38959	2.43866
H	-4.91414	0.74154	-0.39872
H	-4.73584	1.85259	0.96167
H	-3.61731	1.94158	-0.40451
H	3.75992	1.91151	1.34099
H	3.03461	-1.33989	-1.37545
H	5.96254	0.94895	1.90033
H	5.21881	-2.30177	-0.80481
H	6.70294	-1.17064	0.83467



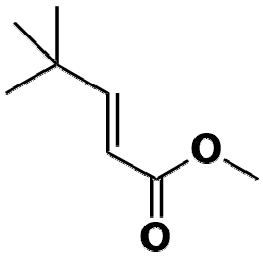
Charge	0
Number of imaginary frequencies	0
Optimized potential energies (E)	-306.333606
Gibbs's free energies (G)	-306.364152

C	2.17048	-0.77424	-0.00022
C	1.49338	0.37386	-0.00018
C	0.01538	0.48518	-0.00003
C	-2.05229	-0.67035	0.00026
O	-0.57237	1.54704	0.00001
O	-0.61167	-0.70691	0.0001
H	3.25437	-0.78094	-0.00034
H	1.66392	-1.73168	-0.00013
H	1.99944	1.33246	-0.00028
H	-2.36774	-1.71097	0.00033
H	-2.41959	-0.15827	0.89027
H	-2.41979	-0.15833	-0.8897



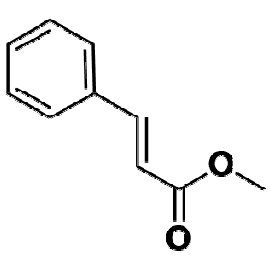
Charge	0
Number of imaginary frequencies	0
Optimized potential energies (E)	-345.612956
Gibbs's free energies (G)	-345.6453

C	-1.67514	-0.41578	0.00017
C	-0.83873	0.62807	0.00009
C	0.63329	0.53188	-0.00007
C	2.52666	-0.89382	-0.00028
C	-3.17429	-0.30117	0.00034
O	1.36761	1.50018	-0.00012
O	1.09538	-0.7377	-0.00014
H	-1.24766	-1.41386	0.00012
H	-1.20527	1.64968	0.00013
H	2.70053	-1.96749	-0.00032
H	2.96103	-0.43632	-0.89002
H	2.9612	-0.43635	0.88939
H	-3.5268	0.24582	-0.87942
H	-3.65106	-1.2818	0.00014
H	-3.52663	0.24536	0.88047



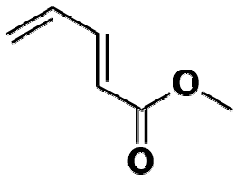
Charge	0
Number of imaginary frequencies	0
Optimized potential energies (E)	-463.445861
Gibbs's free energies (G)	-463.484904

C	2.17048	-0.77424	-0.00022
C	1.49328	0.36112	-0.17035
C	0.01527	0.47131	-0.1854
C	-2.05229	-0.67121	-0.01132
C	3.71045	-0.78375	-0.00039
C	4.19041	-0.05957	-1.24039
C	4.19073	-0.07682	1.24935
C	4.17711	-2.22405	-0.0104
O	-0.57257	1.52139	-0.34278
O	-0.61167	-0.70747	-0.00736
H	1.66401	-1.72099	0.14277
H	1.99926	1.30902	-0.31351
H	-2.36766	-1.70023	0.14384
H	-2.41882	-0.03242	0.79295
H	-2.42066	-0.29727	-0.9672
H	3.81296	-0.5698	-2.1589
H	3.82239	0.99447	-1.24171
H	5.30632	-0.04423	-1.27802
H	3.81308	-0.59932	2.16087
H	5.30666	-0.06253	1.28711
H	3.82322	0.97729	1.26521
H	5.29264	-2.27451	-0.0114
H	3.79991	-2.76101	0.89285
H	3.79896	-2.7487	-0.92047



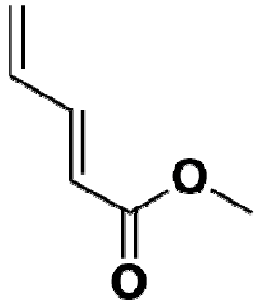
Charge	0
Number of imaginary frequencies	0
Optimized potential energies (E)	-537.272791
Gibbs's free energies (G)	-537.312487

C	0.1637	-0.25731	0.
C	1.06788	0.73731	0.
C	2.52611	0.53457	-0.00001
C	4.31023	-1.02607	0.00001
C	-1.29464	-0.12829	0.
C	-2.07047	-1.29982	0.
C	-1.96061	1.11089	0.
C	-3.46135	-1.241	0.
C	-3.34819	1.16955	0.
C	-4.10505	-0.00529	0.
O	3.3297	1.44702	0.
O	2.89437	-0.76603	0.
H	0.53858	-1.27646	-0.00001
H	0.78255	1.7823	0.
H	4.40543	-2.10954	0.00002
H	4.77669	-0.60162	-0.88982
H	4.77668	-0.60159	0.88983
H	-1.57214	-2.26354	0.
H	-1.39274	2.03355	0.
H	-4.04047	-2.15735	0.
H	-3.84487	2.13318	0.00001
H	-5.18787	0.04581	0.



Charge	0
Number of imaginary frequencies	0
Optimized potential energies (E)	-383.684604
Gibbs's free energies (G)	-383.718707

C	-1.20423	-0.6134	-0.0004
C	-0.47417	0.50681	-0.00054
C	1.0028	0.51634	-0.00026
C	2.97708	-0.74913	0.00057
O	1.66201	1.5284	-0.00039
O	1.54819	-0.70869	0.00025
H	-0.67433	-1.56066	-0.00017
H	-0.91505	1.49669	-0.00092
H	3.24142	-1.80308	0.00098
H	3.36988	-0.2557	-0.88851
H	3.36949	-0.25509	0.88948
C	-2.67141	-0.68932	-0.0006
C	-3.50577	0.35097	0.00104
H	-3.08664	-1.69204	-0.00213
H	-4.57831	0.20175	0.00076
H	-3.15381	1.37681	0.00277

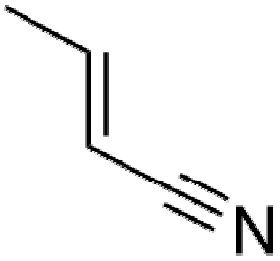


Charge	0
Number of imaginary frequencies	0
Optimized potential energies (E)	-383.689175
Gibbs's free energies (G)	-383.723414

C	2.15281	-0.76856	-0.00022
C	1.49204	0.38387	-0.00019
C	0.01113	0.48333	0.00002
C	-2.02974	-0.66889	0.00025
O	-0.58475	1.53198	0.
O	-0.60008	-0.70727	0.0001
H	1.62687	-1.71582	-0.00011
H	1.99721	1.34228	-0.0003
H	-2.35219	-1.70634	0.00031
H	-2.39322	-0.15346	0.88933
H	-2.3934	-0.15352	-0.8888
C	3.69253	-0.79796	-0.00043
C	4.38773	-1.927	-0.00047
H	4.1681	0.192	-0.00051
H	5.48579	-1.94796	-0.0006
H	3.91215	-2.91696	-0.00039

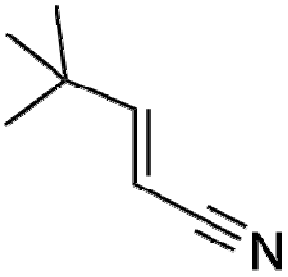
Charge	0
Number of imaginary frequencies	0
Optimized potential energies (E)	-170.755969
Gibbs's free energies (G)	-170.781849

C	1.31917	0.98022	0.
C	0.	0.77211	0.
C	-0.57757	-0.53371	0.
N	-1.06979	-1.57976	0.
H	1.71519	1.98809	0.
H	2.02794	0.16116	0.
H	-0.70415	1.59732	0.



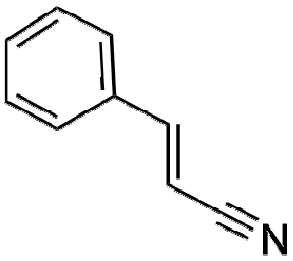
Charge	0
Number of imaginary frequencies	0
Optimized potential energies (E)	-210.038400
Gibbs's free energies (G)	-210.066651

C	0.88303	-0.38425	0.
C	-0.13152	0.49158	0.
C	-1.49799	0.08809	0.
C	2.32616	-0.00466	0.
N	-2.61505	-0.21285	0.
H	0.6544	-1.44699	0.
H	0.04713	1.56241	0.
H	2.46532	1.07771	-0.00006
H	2.83016	-0.42384	0.8774
H	2.83019	-0.42395	-0.87734



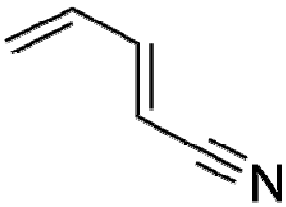
Charge	0
Number of imaginary frequencies	0
Optimized potential energies (E)	-327.868460
Gibbs's free energies (G)	-327.901783

C	1.31917	0.98022	0.
C	0.01193	0.76742	-0.17132
C	-0.56502	-0.53864	-0.18025
C	1.88237	2.41354	0.
C	1.39187	3.1173	-1.24761
C	1.38331	3.12081	1.24217
C	3.39412	2.33046	0.00535
N	-1.05646	-1.585	-0.19149
H	2.01801	0.16506	0.14269
H	-0.68231	1.58874	-0.31371
H	1.74114	2.57802	-2.16066
H	0.27607	3.15333	-1.26017
H	1.77961	4.16378	-1.28535
H	1.72574	2.58386	2.15918
H	1.77129	4.16722	1.27982
H	0.26746	3.15741	1.24679
H	3.84275	3.35305	0.00494
H	3.75029	1.7887	0.91424
H	3.7565	1.78538	-0.89911



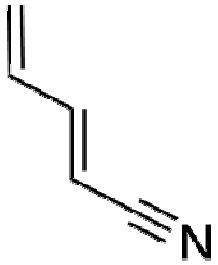
Charge	0
Number of imaginary frequencies	0
Optimized potential energies (E)	-401.694654
Gibbs's free energies (G)	-401.728525

C	1.07701	-0.4458	0.
C	2.06708	0.46901	0.00001
C	3.43776	0.09727	0.
C	-0.36107	-0.18543	-0.00001
C	-1.23759	-1.28378	0.00001
C	-0.91155	1.10918	-0.00001
C	-2.61709	-1.09911	0.
C	-2.28785	1.29231	0.
C	-3.1465	0.18964	0.
N	4.56173	-0.18072	-0.00001
H	1.35942	-1.49487	-0.00003
H	1.87321	1.5356	0.00003
H	-0.8289	-2.28865	0.
H	-0.26448	1.97827	-0.00001
H	-3.27643	-1.95936	0.
H	-2.69591	2.29651	0.
H	-4.22028	0.33769	0.



Charge	0
Number of imaginary frequencies	0
Optimized potential energies (E)	-248.106466
Gibbs's free energies (G)	-248.13551

C	1.31797	0.96342	0.
C	0.	0.78308	0.
C	-0.58359	-0.52793	0.
N	-1.06405	-1.5733	0.
H	2.00513	0.12623	0.
H	-0.69671	1.61262	0.
C	1.90923	2.38539	0.
C	1.1543	3.4754	-0.00002
H	3.00684	2.4235	0.
H	1.57596	4.48949	-0.00004
H	0.05669	3.43729	-0.00002

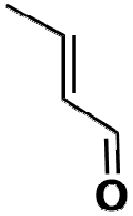


Charge	0
Number of imaginary frequencies	0
Optimized potential energies (E)	-248.111696
Gibbs's free energies (G)	-248.141293

C	1.31797	0.96342	0.
C	0.	0.78308	0.
C	-0.58359	-0.52793	0.
N	-1.06405	-1.5733	0.
H	2.00513	0.12623	0.
H	-0.69671	1.61262	0.
C	1.90923	2.38539	0.
C	3.21445	2.61878	0.
H	1.16224	3.19048	0.00002
H	3.63611	3.63288	0.00002
H	3.96144	1.81369	-0.00003

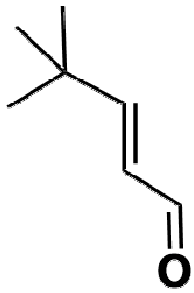
Charge	0
Number of imaginary frequencies	0
Optimized potential energies (E)	-191.822255
Gibbs's free energies (G)	-191.848554

C	1.75987	0.14232	0.00005
C	0.56163	-0.44923	0.00004
C	-0.67353	0.34877	0.00001
O	-1.79336	-0.12112	-0.00008
H	2.68222	-0.42616	0.00006
H	1.85033	1.22475	0.00003
H	0.44812	-1.52878	0.00005
H	-0.52161	1.44793	-0.00008



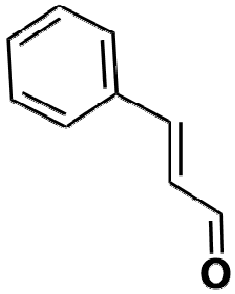
Charge	0
Number of imaginary frequencies	0
Optimized potential energies (E)	-231.102533
Gibbs's free energies (G)	-231.130753

C	1.03814	0.39997	0.00009
C	-0.091	-0.32484	-0.00001
C	-1.39861	0.32965	-0.00006
C	2.42978	-0.16048	0.00015
O	-2.46725	-0.25315	-0.00019
H	0.93995	1.48467	0.00012
H	-0.08215	-1.41161	-0.00005
H	-1.36523	1.43928	-0.00008
H	2.59632	-0.79043	-0.87914
H	3.18295	0.62763	0.00001
H	2.59636	-0.79015	0.87963



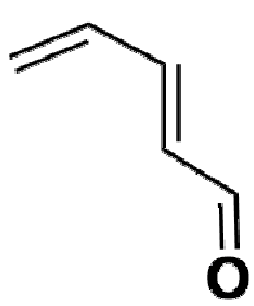
Charge	0
Number of imaginary frequencies	0
Optimized potential energies (E)	-348.935061
Gibbs's free energies (G)	-348.968967

C	1.75987	0.14232	0.00005
C	0.56823	-0.4385	0.16848
C	-0.6671	0.3592	0.1638
C	3.07086	-0.6657	0.00007
C	3.10217	-1.52134	1.24878
C	3.09546	-1.53256	-1.24098
C	4.22987	0.30844	-0.00748
O	-1.78117	-0.10134	0.31062
H	1.84467	1.21557	-0.14411
H	0.46044	-1.50879	0.31406
H	-0.52112	1.44873	0.01266
H	3.0584	-0.87919	2.16102
H	2.23155	-2.2201	1.26295
H	4.04062	-2.12532	1.28657
H	3.04616	-0.89877	-2.15878
H	4.03399	-2.13644	-1.27859
H	2.22513	-2.23183	-1.24399
H	5.20263	-0.23992	-0.00712
H	4.18868	0.95434	-0.91719
H	4.19309	0.96311	0.89615



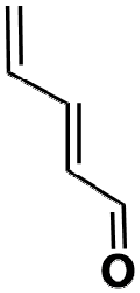
Charge	0
Number of imaginary frequencies	0
Optimized potential energies (E)	-422.762177
Gibbs's free energies (G)	-422.796758

C	0.93325	-0.58489	-0.00001
C	1.99482	0.24722	-0.00002
C	3.35148	-0.28882	-0.00002
C	-0.48497	-0.23739	-0.00001
C	-1.43384	-1.27451	0.
C	-0.94712	1.09173	-0.00001
C	-2.7977	-0.9978	0.00001
C	-2.30806	1.36692	0.
C	-3.23867	0.32422	0.00001
O	4.36489	0.38821	0.00003
H	1.14237	-1.65381	-0.00001
H	1.89994	1.32792	-0.00002
H	3.41858	-1.39669	0.00003
H	-1.09254	-2.30447	0.
H	-0.24007	1.91249	-0.00001
H	-3.51406	-1.8112	0.00001
H	-2.64833	2.39609	0.
H	-4.30013	0.54404	0.00001



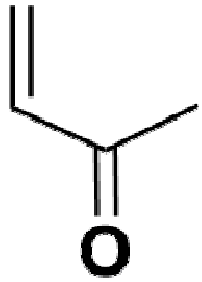
Charge	0
Number of imaginary frequencies	0
Optimized potential energies (E)	-269.173196
Gibbs's free energies (G)	-269.202559

C	1.75095	0.14572	0.00005
C	0.563	-0.45516	0.00003
C	-0.67348	0.34882	-0.00003
O	-1.78448	-0.12051	-0.00005
H	1.82569	1.22942	0.00002
H	0.44921	-1.53399	0.00005
H	-0.5204	1.4458	-0.00005
C	3.06986	-0.64931	0.00011
C	3.10768	-1.97468	0.00017
H	3.97656	-0.02957	0.00012
H	4.04828	-2.54166	0.00023
H	2.20098	-2.59442	0.00015



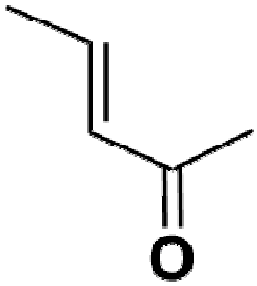
Charge	0
Number of imaginary frequencies	0
Optimized potential energies (E)	-269.178368
Gibbs's free energies (G)	-269.208465

C	1.75095	0.14572	0.00005
C	0.563	-0.45516	0.00003
C	-0.67348	0.34882	-0.00003
O	-1.78448	-0.12051	-0.00005
H	1.82569	1.22942	0.00002
H	0.44921	-1.53399	0.00005
H	-0.5204	1.4458	-0.00005
C	3.06986	-0.64931	0.00011
C	4.25952	-0.06385	0.00012
H	2.94524	-1.74048	0.00011
H	5.20011	-0.63083	0.00015
H	4.38413	1.02732	0.00012



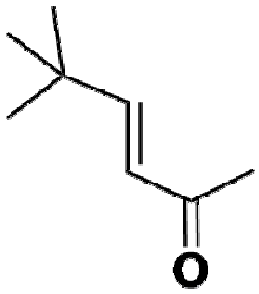
Charge	0
Number of imaginary frequencies	0
Optimized potential energies (E)	-231.107405
Gibbs's free energies (G)	-231.136238

C	1.93825	0.17525	-0.00002
C	0.87605	-0.63357	0.00001
C	-0.54218	-0.18731	0.00016
C	-0.86039	1.29353	0.
O	-1.43112	-1.02436	-0.00008
H	2.94646	-0.22331	-0.0001
H	1.84572	1.2556	0.00005
H	0.99795	-1.71264	-0.00006
H	-0.43529	1.78106	0.88184
H	-0.43511	1.78093	-0.88184
H	-1.94107	1.42584	-0.00012



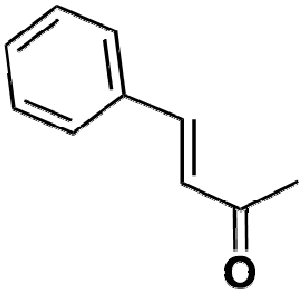
Charge	0
Number of imaginary frequencies	0
Optimized potential energies (E)	-270.389262
Gibbs's free energies (G)	-270.4204

C	-1.30596	0.31763	0.00003
C	-0.29234	-0.55831	-0.00009
C	1.14417	-0.2057	-0.00008
C	1.56292	1.25241	0.00008
C	-2.75512	-0.04858	0.00007
O	1.98396	-1.09545	-0.0001
H	-1.08685	1.3831	0.00012
H	-0.48731	-1.62766	-0.00016
H	1.17399	1.76946	-0.88164
H	1.17476	1.76893	0.88246
H	2.65029	1.30856	-0.00035
H	-3.25811	0.37325	-0.87713
H	-2.90233	-1.12991	0.00005
H	-3.25806	0.3732	0.87732



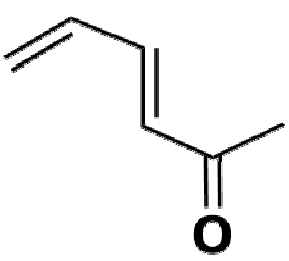
Charge	0
Number of imaginary frequencies	0
Optimized potential energies (E)	-388.219278
Gibbs's free energies (G)	-388.255635

C	1.93825	0.17525	-0.00002
C	0.88073	-0.62175	0.16999
C	-0.53706	-0.17439	0.18597
C	-0.86045	1.29338	-0.00165
C	3.37041	-0.3909	-0.00014
C	3.54232	-1.25002	1.23468
C	3.55499	-1.21783	-1.25488
C	4.34104	0.77091	0.01979
O	-1.42148	-1.00004	0.35015
H	1.84174	1.24557	-0.14435
H	1.00656	-1.69091	0.31254
H	-0.38962	1.89661	0.77969
H	-0.48589	1.65249	-0.96436
H	-1.94002	1.42851	0.03903
H	3.38048	-0.64179	2.1568
H	2.80737	-2.09041	1.22874
H	4.57171	-1.68113	1.27194
H	3.4019	-0.58616	-2.16265
H	4.58498	-1.64749	-1.293
H	2.82054	-2.05837	-1.27799
H	5.39474	0.40121	0.02088
H	4.19375	1.41577	-0.87961
H	4.18395	1.39283	0.93358



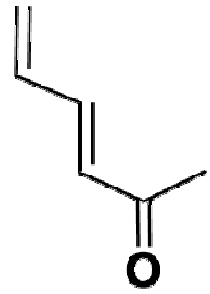
Charge	0
Number of imaginary frequencies	0
Optimized potential energies (E)	-462.046349
Gibbs's free energies (G)	-462.083047

C	0.58352	0.39722	-0.00022
C	1.56446	-0.52519	-0.00026
C	3.00794	-0.21903	-0.00045
C	3.47618	1.22448	0.00023
C	-0.86141	0.15998	-0.0001
C	-1.7255	1.26837	-0.00006
C	-1.43013	-1.12698	-0.00002
C	-3.10738	1.10217	0.00008
C	-2.80893	-1.29258	0.00008
C	-3.65397	-0.17962	0.00013
O	3.81887	-1.13689	0.00031
H	0.86569	1.44691	-0.0003
H	1.346	-1.58818	-0.00018
H	3.10787	1.75515	-0.88224
H	3.10704	1.75466	0.88265
H	4.56479	1.24195	0.00075
H	-1.30437	2.26853	-0.00009
H	-0.79184	-2.00236	-0.00005
H	-3.75558	1.97115	0.00013
H	-3.2296	-2.29181	0.00014
H	-4.72975	-0.31383	0.00023



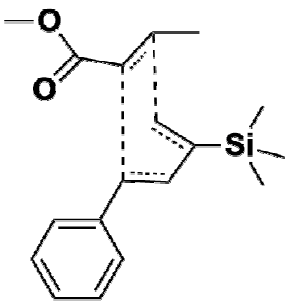
Charge	0
Number of imaginary frequencies	0
Optimized potential energies (E)	-308.458388
Gibbs's free energies (G)	-308.490743

C	1.92159	0.16754	0.
C	0.87066	-0.6483	0.00001
C	-0.54554	-0.18708	0.00004
C	-0.8334	1.29561	0.
O	-1.43926	-1.00604	-0.00004
H	1.81091	1.24654	0.
H	0.99102	-1.72697	0.
H	-0.3954	1.76753	0.88232
H	-0.3953	1.76752	-0.88227
H	-1.91031	1.44729	-0.00006
C	3.3596	-0.38356	-0.00004
C	3.62956	-1.6817	-0.00003
H	4.14341	0.38575	-0.00004
H	4.65509	-2.07472	-0.00003
H	2.84576	-2.45101	-0.00002



Charge	0
Number of imaginary frequencies	0
Optimized potential energies (E)	-308.462909
Gibbs's free energies (G)	-308.495168

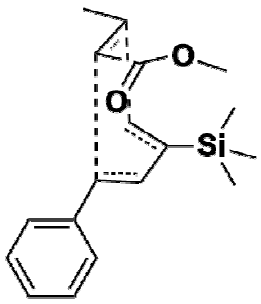
C	1.92159	0.16754	0.
C	0.87066	-0.6483	0.00001
C	-0.54554	-0.18708	0.00004
C	-0.8334	1.29561	0.
O	-1.43926	-1.00604	-0.00004
H	1.81091	1.24654	0.
H	0.99102	-1.72697	0.
H	-0.3954	1.76753	0.88232
H	-0.3953	1.76752	-0.88227
H	-1.91031	1.44729	-0.00006
C	3.3596	-0.38356	-0.00004
C	4.42799	0.40169	-0.00005
H	3.42852	-1.47966	-0.00007
H	5.45352	0.00867	-0.00009
H	4.35907	1.49779	-0.00001



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1140.926746
Gibbs's free energies (G)	-1140.982052

C	0.60523	1.23344	0.63599
C	-0.57152	0.6097	1.03882
C	-0.65322	-0.79895	0.99376
C	0.41248	-1.6071	0.65276
C	-3.54487	1.1577	0.27524
C	-2.63586	1.16934	3.19213
C	-1.76227	3.44137	1.30794
C	0.30187	-3.04676	0.39046
C	1.40618	-3.87913	0.60315
C	-0.87968	-3.61707	-0.10298
C	1.3244	-5.24593	0.3662
C	-0.96192	-4.98179	-0.34072
C	0.13892	-5.80265	-0.1022
Si	-2.12921	1.6032	1.4342
H	1.57418	0.76507	0.77614
H	0.64289	2.31984	0.6118
H	-1.63067	-1.26541	1.10597
H	1.41542	-1.24994	0.86696
H	-4.48298	1.56692	0.66121
H	-3.38966	1.56391	-0.72666
H	-3.66769	0.07463	0.18696
H	-2.8485	0.10078	3.28386
H	-1.83864	1.41306	3.89844
H	-3.53462	1.71831	3.48614
H	-1.46079	3.73159	0.29798
H	-2.65719	4.01553	1.5631
H	-0.96804	3.7378	1.9979
H	2.33507	-3.44734	0.96083
H	-1.73136	-2.98236	-0.32317
H	2.18872	-5.8756	0.54116
H	-1.88181	-5.4064	-0.72582

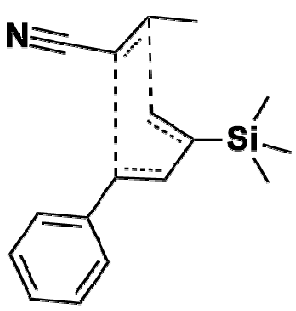
H	0.07526	-6.86719	-0.29381
C	0.70107	0.75552	-1.39269
C	0.96817	-0.60551	-1.48742
C	2.32426	-1.14853	-1.41839
C	4.52889	-0.77305	-0.68009
C	-0.60863	1.25665	-1.94772
O	2.6687	-2.23419	-1.82449
O	3.18403	-0.30663	-0.79316
H	1.55111	1.42736	-1.45487
H	0.23769	-1.28709	-1.90537
H	5.07245	0.01244	-0.1611
H	4.56367	-1.70232	-0.11012
H	4.95724	-0.94508	-1.66789
H	-1.41768	0.57774	-1.66763
H	-0.8523	2.25632	-1.58305
H	-0.56399	1.2929	-3.04012



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1140.930937
Gibbs's free energies (G)	-1140.983451

C	0.41847	1.44126	0.94973
C	-0.67821	0.67327	1.33627
C	-0.56845	-0.73216	1.33414
C	0.55091	-1.39366	0.87812
C	-2.56768	2.72613	0.08254
C	-3.7156	0.18107	1.38352
C	-2.48084	2.39201	3.13458
C	0.63741	-2.84053	0.64704
C	1.89642	-3.42887	0.47688
C	-0.49569	-3.65976	0.54967
C	2.02492	-4.79069	0.23215
C	-0.36953	-5.01999	0.30655
C	0.89119	-5.59257	0.14679
Si	-2.37618	1.49147	1.48487
H	1.42593	1.10568	1.17943
H	0.32105	2.52358	0.91678
H	-1.46952	-1.30981	1.51724
H	1.50779	-0.88456	0.88997
H	-3.53012	3.23994	0.15815
H	-1.78475	3.48962	0.09858
H	-2.52701	2.20163	-0.87486
H	-3.63353	-0.35699	0.43536
H	-3.64589	-0.53727	2.20492
H	-4.70451	0.64478	1.43412
H	-1.69495	3.14756	3.21807
H	-3.44581	2.89486	3.24453
H	-2.36504	1.69471	3.96827
H	2.7831	-2.8056	0.53823
H	-1.48564	-3.22935	0.65036
H	3.00949	-5.22599	0.10619
H	-1.25786	-5.63729	0.23564

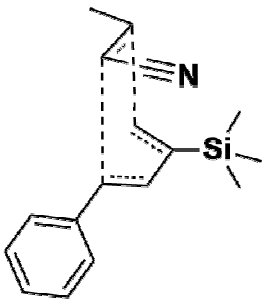
H	0.98714	-6.65433	-0.04679
C	0.72424	1.09469	-1.05363
C	0.60282	-0.26676	-1.31566
C	-0.71583	-0.80503	-1.61623
C	-1.9244	-2.66386	-2.39081
C	2.07471	1.75487	-1.2181
O	-1.76381	-0.21538	-1.43175
O	-0.6654	-2.05792	-2.10909
H	-0.14256	1.69531	-1.31205
H	1.4631	-0.88891	-1.53055
H	-1.70135	-3.68736	-2.68245
H	-2.56341	-2.65145	-1.50675
H	-2.42959	-2.13556	-3.20088
H	2.277	1.92965	-2.27796
H	2.12474	2.71682	-0.7058
H	2.86955	1.11475	-0.82702



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1005.349322
Gibbs's free energies (G)	-1005.400738

C	0.33596	1.27517	1.09257
C	-0.86696	0.59487	1.27206
C	-0.88524	-0.81294	1.16981
C	0.25684	-1.56573	0.99217
C	-3.68601	1.07379	0.02939
C	-3.28912	0.98277	3.0561
C	-2.20206	3.36964	1.44623
C	0.27643	-2.99367	0.65345
C	1.4183	-3.75006	0.94493
C	-0.79853	-3.62294	0.00971
C	1.47468	-5.10289	0.63074
C	-0.74284	-4.97463	-0.30052
C	0.39266	-5.72047	0.01171
Si	-2.51093	1.5175	1.43159
H	1.28018	0.8359	1.40073
H	0.33461	2.36168	1.12026
H	-1.84906	-1.31342	1.09545
H	1.19366	-1.18049	1.37912
H	-4.68849	1.44841	0.25502
H	-3.37033	1.51285	-0.91937
H	-3.76039	-0.00887	-0.10548
H	-3.45735	-0.09738	3.07282
H	-2.64377	1.23395	3.90119
H	-4.25413	1.47511	3.20412
H	-1.74433	3.72113	0.51776
H	-3.15034	3.90021	1.56765
H	-1.55173	3.65645	2.2766
H	2.26482	-3.26749	1.42156
H	-1.67578	-3.04721	-0.26452
H	2.36506	-5.67321	0.86744
H	-1.58176	-5.44818	-0.79708

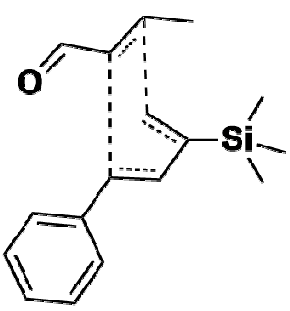
H	0.43502	-6.77454	-0.2358
C	0.77705	0.88843	-0.89519
C	1.15516	-0.45136	-0.97423
C	2.49343	-0.83343	-0.67796
C	-0.45959	1.30879	-1.64688
N	3.56918	-1.1374	-0.38824
H	1.57561	1.62008	-0.82101
H	0.55801	-1.17397	-1.51531
H	-1.24484	0.55934	-1.52162
H	-0.83878	2.27151	-1.29966
H	-0.23823	1.39079	-2.71473



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1005.349416
Gibbs's free energies (G)	-1005.400288

C	0.2649	1.42523	0.71774
C	-0.76995	0.68156	1.27838
C	-0.61266	-0.71074	1.42643
C	0.49417	-1.38992	0.95812
C	-2.91793	2.21952	-0.2294
C	-3.73619	0.14919	1.8891
C	-2.43053	2.81554	2.74699
C	0.58826	-2.85246	0.8699
C	1.84897	-3.46301	0.86186
C	-0.54947	-3.66253	0.75212
C	1.97237	-4.8436	0.7724
C	-0.42476	-5.04256	0.65928
C	0.83391	-5.63877	0.67375
Si	-2.48309	1.46853	1.43859
H	1.29908	1.14983	0.90233
H	0.12462	2.4898	0.54268
H	-1.4732	-1.29541	1.73888
H	1.44111	-0.86755	0.87049
H	-3.8869	2.7243	-0.18214
H	-2.17667	2.95856	-0.54696
H	-2.97954	1.44025	-0.99462
H	-3.78941	-0.61201	1.10554
H	-3.48982	-0.34259	2.83378
H	-4.72952	0.5935	1.99467
H	-1.68938	3.57781	2.49211
H	-3.40213	3.30835	2.83981
H	-2.16469	2.40227	3.72303
H	2.73796	-2.84446	0.93685
H	-1.53222	-3.20816	0.70273
H	2.9556	-5.29917	0.77779
H	-1.31357	-5.65539	0.56532

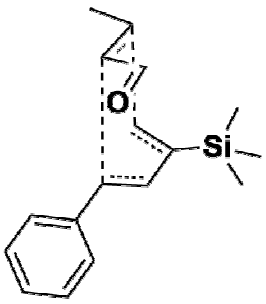
H	0.92685	-6.71591	0.60021
C	0.47497	0.77984	-1.26438
C	0.27966	-0.59989	-1.30472
C	-1.04867	-1.08884	-1.45196
C	1.84663	1.33009	-1.57209
N	-2.14845	-1.43356	-1.52679
H	-0.367	1.39681	-1.55918
H	1.08679	-1.28743	-1.52376
H	2.62343	0.70043	-1.13034
H	2.00766	1.35292	-2.65294
H	1.97003	2.34522	-1.19215



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1026.413395
Gibbs's free energies (G)	-1026.464263

C	0.39136	1.337	0.82796
C	-0.79158	0.64811	1.08862
C	-0.79147	-0.76196	1.04159
C	0.3457	-1.51589	0.83406
C	-3.66456	1.08032	-0.05897
C	-3.15404	1.02261	2.94952
C	-2.15643	3.40669	1.27917
C	0.34742	-2.95256	0.54852
C	1.47967	-3.71646	0.8534
C	-0.74738	-3.5882	-0.05492
C	1.50651	-5.08248	0.59844
C	-0.72053	-4.9513	-0.31001
C	0.40556	-5.70453	0.02031
Si	-2.44124	1.5505	1.2922
H	1.35073	0.9165	1.10997
H	0.37916	2.42388	0.82069
H	-1.74933	-1.27884	1.03717
H	1.3001	-1.11142	1.15508
H	-4.66751	1.41608	0.21968
H	-3.41167	1.54181	-1.01573
H	-3.70671	-0.00263	-0.20461
H	-3.31764	-0.05802	2.97893
H	-2.47787	1.28097	3.76784
H	-4.11468	1.51225	3.13142
H	-1.73971	3.75394	0.33011
H	-3.10605	3.92662	1.43211
H	-1.47785	3.70956	2.08072
H	2.34332	-3.23176	1.2949
H	-1.61565	-3.00627	-0.3444
H	2.39069	-5.65859	0.84406
H	-1.57274	-5.42856	-0.77955

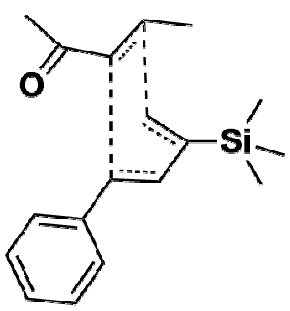
H	0.42648	-6.76817	-0.18546
C	0.74538	0.90191	-1.16804
C	1.04502	-0.45673	-1.26878
C	2.41372	-0.9113	-1.09657
C	-0.48837	1.41916	-1.86477
O	2.83636	-2.01333	-1.38361
H	1.59578	1.58005	-1.13416
H	0.3489	-1.15186	-1.72576
H	3.09676	-0.15728	-0.64809
H	-1.32068	0.73059	-1.70519
H	-0.78004	2.40905	-1.5087
H	-0.3085	1.48282	-2.9418



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1026.414342
Gibbs's free energies (G)	-1026.465894

C	0.39708	1.11673	1.38446
C	-0.81032	0.45312	1.59404
C	-0.89636	-0.92868	1.33589
C	0.16966	-1.66706	0.85695
C	-3.88271	0.37711	1.7902
C	-2.26801	2.33648	3.53878
C	-2.45302	2.78557	0.51083
C	0.09799	-3.04848	0.38291
C	1.2772	-3.80235	0.3013
C	-1.10207	-3.63854	-0.03559
C	1.25626	-5.11347	-0.15264
C	-1.12348	-4.95048	-0.48868
C	0.05267	-5.69302	-0.54635
Si	-2.36896	1.4847	1.86828
H	1.34378	0.61978	1.5734
H	0.43987	2.19357	1.53298
H	-1.87475	-1.40023	1.36822
H	1.17625	-1.30965	1.04457
H	-4.78691	0.96411	1.97202
H	-3.98334	-0.09499	0.80898
H	-3.84194	-0.4116	2.54623
H	-2.20381	1.60408	4.34716
H	-1.38342	2.97652	3.59523
H	-3.14807	2.96129	3.71361
H	-2.56807	2.32468	-0.47413
H	-3.30587	3.45103	0.67084
H	-1.55083	3.40376	0.49257
H	2.21575	-3.35002	0.60614
H	-2.01976	-3.06288	-0.03023
H	2.17679	-5.68304	-0.20205
H	-2.05865	-5.39033	-0.81435

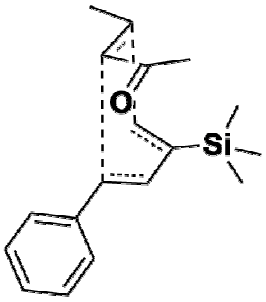
H	0.03336	-6.71474	-0.90672
C	0.77813	1.03977	-0.66131
C	0.61673	-0.26808	-1.11307
C	-0.66681	-0.70375	-1.63959
C	2.1591	1.65724	-0.66119
O	-0.85812	-1.68183	-2.3343
H	-0.03951	1.72441	-0.87107
H	1.47647	-0.89931	-1.31801
H	-1.51908	-0.05319	-1.34644
H	2.43857	1.94394	-1.67825
H	2.20843	2.55016	-0.03619
H	2.90215	0.942	-0.3002



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1065.698096
Gibbs's free energies (G)	-1065.750987

C	0.42757	1.2487	0.9456
C	-0.76173	0.57408	1.20483
C	-0.7751	-0.8361	1.15181
C	0.35072	-1.60074	0.92109
C	-3.62887	1.04869	0.06359
C	-3.1192	0.96569	3.07216
C	-2.09223	3.34665	1.41562
C	0.32798	-3.04276	0.65918
C	1.45587	-3.81599	0.95544
C	-0.78419	-3.67425	0.0854
C	1.46226	-5.186	0.72278
C	-0.77787	-5.0416	-0.14897
C	0.34395	-5.80382	0.17394
Si	-2.39915	1.49359	1.41774
H	1.37861	0.81356	1.23198
H	0.43123	2.3355	0.93332
H	-1.73724	-1.34481	1.16506
H	1.31623	-1.20481	1.22029
H	-4.62768	1.39612	0.34275
H	-3.36793	1.51243	-0.89002
H	-3.68469	-0.03274	-0.08882
H	-3.2968	-0.11287	3.09571
H	-2.43926	1.21045	3.8916
H	-4.07326	1.46666	3.25758
H	-1.67294	3.69364	0.46754
H	-3.0351	3.8774	1.57302
H	-1.40845	3.63673	2.2175
H	2.33374	-3.3347	1.37356
H	-1.64996	-3.08649	-0.19955
H	2.34383	-5.76881	0.96213
H	-1.64358	-5.51491	-0.5973

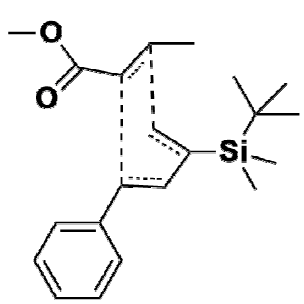
H	0.34877	-6.8706	-0.01572
C	0.79495	0.80191	-1.06505
C	1.0385	-0.56464	-1.18013
C	2.37795	-1.16254	-1.11668
C	3.51777	-0.34755	-0.53498
C	-0.43416	1.35915	-1.74249
O	2.58099	-2.29179	-1.52825
H	1.65826	1.4609	-1.0299
H	0.28876	-1.20601	-1.63199
H	3.80374	0.44021	-1.23714
H	3.24183	0.13751	0.40432
H	4.37231	-1.0022	-0.37448
H	-0.26885	1.42632	-2.8217
H	-1.28241	0.69194	-1.57563
H	-0.69483	2.35352	-1.37455



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1065.700649
Gibbs's free energies (G)	-1065.75352

C	0.50582	1.4315	1.38819
C	-0.57315	0.71625	1.90096
C	-0.47683	-0.68557	2.02024
C	0.64626	-1.3961	1.64571
C	-2.56011	2.71617	0.68977
C	-3.59424	0.34667	2.37258
C	-2.09074	2.67367	3.71535
C	0.73057	-2.85705	1.59171
C	1.98598	-3.47212	1.67624
C	-0.40078	-3.6675	1.43334
C	2.10692	-4.85479	1.6416
C	-0.28118	-5.04979	1.40029
C	0.97123	-5.64877	1.50813
Si	-2.21678	1.6086	2.17329
H	1.52357	1.11393	1.59159
H	0.4095	2.50505	1.24384
H	-1.37312	-1.24418	2.27778
H	1.60479	-0.88923	1.64274
H	-3.48953	3.27124	0.84533
H	-1.762	3.44881	0.54249
H	-2.66682	2.14063	-0.23353
H	-3.67829	-0.30309	1.4969
H	-3.43069	-0.28486	3.24998
H	-4.55272	0.85527	2.50579
H	-1.29824	3.41878	3.60572
H	-3.02894	3.20259	3.90387
H	-1.8597	2.06473	4.59279
H	2.87239	-2.85389	1.77762
H	-1.3782	-3.21435	1.3109
H	3.08593	-5.3135	1.71614
H	-1.16586	-5.66243	1.27306

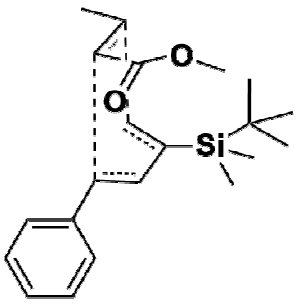
H	1.06246	-6.72806	1.47562
C	0.77667	0.82978	-0.59825
C	0.82649	-0.56141	-0.65293
C	-0.30386	-1.40314	-1.05898
C	-1.68835	-0.789	-1.07468
C	2.04307	1.61382	-0.87234
O	-0.13784	-2.56103	-1.40532
H	-0.1419	1.30679	-0.9272
H	1.79169	-1.05865	-0.70045
H	-1.84181	-0.1186	-0.22814
H	-1.811	-0.20317	-1.99105
H	-2.431	-1.58584	-1.06833
H	2.90302	1.13625	-0.39674
H	2.23371	1.64497	-1.94817
H	1.97787	2.6421	-0.51406



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1258.745749
Gibbs's free energies (G)	-1258.804702

C	0.81861	0.67876	2.46518
C	-0.5356	0.39305	2.31161
C	-0.90667	-0.75168	1.56897
C	0.00754	-1.64074	1.04324
C	-3.15612	2.269	1.87552
C	-2.78131	0.36531	4.27708
C	-1.0326	2.8845	4.03489
C	-4.43273	2.56615	2.68216
C	-2.6473	3.59503	1.29133
C	-3.51872	1.31872	0.72682
C	-0.3332	-2.71488	0.10433
C	0.48292	-3.84932	0.03375
C	-1.43438	-2.62854	-0.75869
C	0.1925	-4.88436	-0.84618
C	-1.72417	-3.66109	-1.6396
C	-0.91389	-4.79468	-1.68405
Si	-1.87213	1.49918	3.07703
H	1.5568	-0.11578	2.50737
H	1.11332	1.57873	2.9985
H	-1.95136	-0.88336	1.30128
H	0.96228	-1.75565	1.54638
H	-3.47935	0.92342	4.90567
H	-3.34666	-0.40544	3.74444
H	-2.06268	-0.14088	4.92632
H	-0.41341	2.48066	4.83997
H	-0.39707	3.50063	3.39257
H	-1.78138	3.54155	4.4865
H	-5.15674	3.09043	2.04721
H	-4.9075	1.65061	3.04372
H	-4.23114	3.2062	3.54779
H	-1.73264	3.46869	0.70932

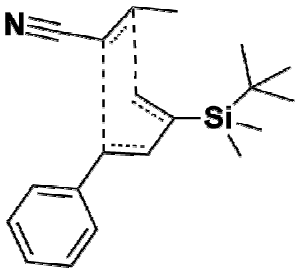
H	-3.40694	4.01986	0.62392
H	-2.44959	4.33168	2.07513
H	-3.92161	0.37027	1.0972
H	-4.289	1.7762	0.09408
H	-2.65524	1.09562	0.09316
H	1.35392	-3.91376	0.67763
H	-2.05335	-1.73726	-0.75408
H	0.83481	-5.75621	-0.88436
H	-2.5763	-3.5789	-2.30423
H	-1.13841	-5.5964	-2.37753
C	1.47639	1.09381	0.52304
C	1.39291	-0.08044	-0.21451
C	2.47996	-1.05798	-0.2577
C	4.37746	-1.90061	0.85325
C	0.60856	2.2552	0.1129
O	2.65345	-1.87709	-1.1301
O	3.28453	-0.98154	0.83098
H	2.44492	1.33283	0.95038
H	0.67117	-0.18384	-1.01528
H	4.90531	-1.71137	1.78456
H	4.01409	-2.92841	0.8224
H	5.03525	-1.73022	0.00046
H	-0.39661	1.89984	-0.12473
H	0.53526	3.00633	0.90149
H	1.01611	2.7348	-0.78197



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1258.750847
Gibbs's free energies (G)	-1258.807722

C	0.99031	0.98611	-1.63406
C	0.96647	-0.04394	-0.69866
C	-0.24731	-0.71607	-0.44612
C	-1.43803	-0.3689	-1.05004
C	3.8425	-1.19155	-0.47776
C	3.02084	1.4087	1.02679
C	1.91556	-1.3206	1.93554
C	5.01481	-1.44567	0.48069
C	3.32532	-2.53488	-1.01142
C	4.33595	-0.34481	-1.65843
C	-2.74948	-0.90772	-0.67536
C	-3.80052	-0.85627	-1.59961
C	-3.00076	-1.45417	0.58984
C	-5.05476	-1.36237	-1.28443
C	-4.25304	-1.96259	0.90495
C	-5.28377	-1.92212	-0.03062
Si	2.44225	-0.2882	0.45261
H	0.35853	0.94226	-2.51631
H	1.90918	1.54632	-1.78727
H	-0.28164	-1.42134	0.37985
H	-1.41411	0.12929	-2.013
H	3.89472	1.33252	1.6792
H	3.28742	2.05419	0.18572
H	2.2178	1.89882	1.58381
H	1.03011	-0.88985	2.40807
H	1.67779	-2.34965	1.65339
H	2.71187	-1.35541	2.68372
H	5.82528	-1.96363	-0.04645
H	5.42499	-0.51176	0.87709
H	4.71839	-2.07268	1.32669
H	2.4873	-2.39722	-1.70137

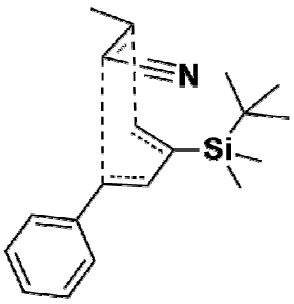
H	4.12396	-3.05642	-1.55296
H	2.99333	-3.19328	-0.20327
H	4.71417	0.62898	-1.33174
H	5.15637	-0.86093	-2.17212
H	3.54267	-0.17637	-2.3925
H	-3.62378	-0.42002	-2.57785
H	-2.21861	-1.46148	1.33994
H	-5.8542	-1.31798	-2.01474
H	-4.43095	-2.3788	1.88961
H	-6.26243	-2.31365	0.22042
C	-0.20508	2.52292	-0.89135
C	-1.389	1.98548	-0.39909
C	-1.56388	1.63605	1.00802
C	-0.49465	1.24948	3.06311
C	-0.25651	3.38752	-2.13131
O	-2.62701	1.45291	1.55837
O	-0.38468	1.53714	1.67059
H	0.54677	2.78526	-0.15506
H	-2.31763	2.08257	-0.94926
H	0.52411	1.22928	3.44531
H	-1.07511	2.02262	3.56766
H	-0.97958	0.28414	3.21966
H	-0.59883	4.39208	-1.86935
H	0.72143	3.48151	-2.60617
H	-0.95722	2.97736	-2.86298



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1123.172554
Gibbs's free energies (G)	-1123.227876

C	-0.14634	1.57307	0.13596
C	-1.02636	0.9977	1.05093
C	-0.74742	-0.29266	1.55118
C	0.41878	-0.97328	1.26505
C	-2.58078	2.41899	3.28861
C	-2.93236	3.32969	0.36043
C	-4.09699	0.62607	1.25649
C	-3.8035	3.29456	3.6024
C	-2.57001	1.2132	4.23755
C	-1.30505	3.24314	3.50999
C	0.65593	-2.38947	1.57152
C	1.97189	-2.85552	1.68033
C	-0.39491	-3.30504	1.72128
C	2.23128	-4.19164	1.96253
C	-0.13515	-4.63846	2.00569
C	1.17901	-5.0858	2.13128
Si	-2.66946	1.83606	1.47308
H	0.92083	1.37677	0.17996
H	-0.39176	2.54065	-0.29478
H	-1.53856	-0.82687	2.07273
H	1.31575	-0.39931	1.06055
H	-3.92767	3.74754	0.53387
H	-2.20139	4.11775	0.55929
H	-2.86718	3.07065	-0.69892
H	-4.27903	0.42757	0.1972
H	-3.90273	-0.32974	1.74966
H	-5.01823	1.03649	1.67938
H	-3.77827	3.60661	4.6535
H	-3.82035	4.20098	2.9904
H	-4.74441	2.75879	3.44293
H	-1.69833	0.57456	4.06829
H	-2.52894	1.55738	5.27799

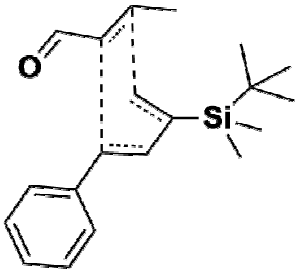
H	-3.47152	0.60276	4.12728
H	-1.26942	4.12146	2.85765
H	-1.26531	3.60141	4.54579
H	-0.40634	2.64789	3.32555
H	2.79215	-2.15965	1.53968
H	-1.42025	-2.97395	1.59813
H	3.25546	-4.53499	2.0469
H	-0.95724	-5.3352	2.12016
H	1.37979	-6.12814	2.34908
C	-0.32009	0.29102	-1.49875
C	0.34519	-0.88354	-1.15074
C	1.75909	-0.97202	-1.28868
C	-1.7999	0.19169	-1.76347
N	2.91088	-1.01721	-1.35687
H	0.23572	1.02283	-2.07619
H	-0.18563	-1.82164	-1.05131
H	-2.27628	-0.41768	-0.99118
H	-2.27796	1.17142	-1.77904
H	-1.97422	-0.29086	-2.72933



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1123.172343
Gibbs's free energies (G)	-1123.227248

C	0.03005	1.55509	0.67294
C	-0.89068	0.82528	1.42113
C	-0.60893	-0.52338	1.72148
C	0.49853	-1.18471	1.23012
C	-2.63402	2.77534	3.09128
C	-3.18338	2.28906	0.05667
C	-3.80024	0.07878	2.08627
C	-4.04758	3.34565	3.27968
C	-2.18595	2.0932	4.39147
C	-1.66875	3.92499	2.77285
C	0.69199	-2.63787	1.31468
C	1.98865	-3.16627	1.26843
C	-0.38996	-3.52473	1.40326
C	2.20379	-4.53674	1.34086
C	-0.1737	-4.89499	1.47122
C	1.12165	-5.40621	1.44576
Si	-2.64145	1.49882	1.67682
H	1.09412	1.36918	0.78871
H	-0.2044	2.57595	0.38233
H	-1.38719	-1.11877	2.19039
H	1.39153	-0.62069	0.98236
H	-4.17495	2.73872	0.15622
H	-2.49692	3.06739	-0.28657
H	-3.24651	1.52112	-0.72047
H	-3.74762	-0.68151	1.30134
H	-3.55687	-0.39504	3.04056
H	-4.83299	0.43253	2.14341
H	-4.05552	4.05726	4.11424
H	-4.39162	3.88026	2.38901
H	-4.77583	2.56169	3.50804
H	-1.19206	1.64637	4.2885

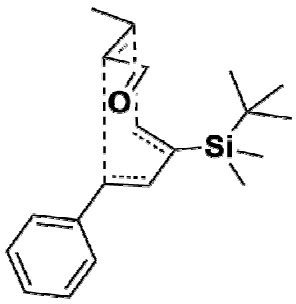
H	-2.13979	2.82723	5.20522
H	-2.88172	1.30645	4.69737
H	-1.93202	4.43098	1.83841
H	-1.70235	4.67328	3.5741
H	-0.6364	3.57242	2.69267
H	2.83361	-2.48966	1.18707
H	-1.40399	-3.14244	1.38922
H	3.21452	-4.92664	1.31378
H	-1.02047	-5.56837	1.53343
H	1.28583	-6.47593	1.49788
C	0.11098	0.6853	-1.22622
C	0.02154	-0.69833	-1.08393
C	-1.27265	-1.2876	-1.0391
C	1.40068	1.2846	-1.73327
N	-2.34534	-1.70941	-0.96593
H	-0.79952	1.20372	-1.50641
H	0.85659	-1.35323	-1.29847
H	2.26328	0.77518	-1.29588
H	1.46226	1.17632	-2.81928
H	1.47281	2.34715	-1.49716



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1144.236924
Gibbs's free energies (G)	-1144.293159

C	-0.08294	1.54253	0.55479
C	-1.05455	0.90258	1.32082
C	-0.83689	-0.42987	1.73297
C	0.33323	-1.12198	1.49551
C	-2.5939	2.542	3.40174
C	-3.17324	2.99648	0.3975
C	-4.0665	0.38243	1.73696
C	-3.97897	3.03244	3.84767
C	-2.05853	1.54829	4.4418
C	-1.63699	3.7382	3.3076
C	0.50195	-2.56138	1.70895
C	1.78422	-3.08244	1.91553
C	-0.58457	-3.44747	1.68012
C	1.97445	-4.44317	2.1248
C	-0.39497	-4.80546	1.88873
C	0.88567	-5.30778	2.11645
Si	-2.7276	1.7044	1.69198
H	0.96941	1.31926	0.69493
H	-0.26731	2.55141	0.19427
H	-1.67877	-0.9834	2.14214
H	1.25807	-0.56184	1.40187
H	-3.95928	3.65139	0.7836
H	-2.32496	3.62906	0.12475
H	-3.55534	2.5265	-0.51125
H	-4.0549	-0.2183	0.8234
H	-3.94933	-0.294	2.58751
H	-5.05291	0.84715	1.81795
H	-3.90178	3.53463	4.81956
H	-4.40798	3.75032	3.14202
H	-4.68346	2.20327	3.95985
H	-1.05122	1.20558	4.19103
H	-2.01524	2.02631	5.42798

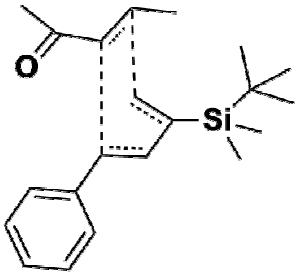
H	-2.70218	0.6673	4.53254
H	-2.00969	4.49855	2.61434
H	-1.52583	4.21124	4.29086
H	-0.64139	3.43016	2.9727
H	2.63662	-2.41221	1.91035
H	-1.58068	-3.07198	1.47344
H	2.97416	-4.82925	2.28431
H	-1.24421	-5.47811	1.86183
H	1.03301	-6.36986	2.27298
C	-0.09144	0.44652	-1.22489
C	0.35342	-0.84367	-0.94128
C	1.774	-1.14341	-1.00245
C	-1.49749	0.64359	-1.73459
O	2.2649	-2.25375	-1.03472
H	0.65545	1.13347	-1.61796
H	-0.32884	-1.68679	-0.94787
H	2.43205	-0.24728	-1.00965
H	-2.20847	0.09911	-1.10765
H	-1.77763	1.69713	-1.74941
H	-1.58229	0.25119	-2.75211



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1144.234682
Gibbs's free energies (G)	-1144.289871

C	0.8992	1.45729	-1.08944
C	0.92311	0.27253	-0.32746
C	-0.26635	-0.46713	-0.15635
C	-1.47922	-0.14295	-0.7386
C	3.63969	-1.2753	-0.51706
C	3.39742	1.3504	1.18263
C	2.021	-1.2094	2.16924
C	4.90734	-1.69303	0.25945
C	2.89864	-2.54507	-0.98494
C	4.06033	-0.45854	-1.75608
C	-2.75755	-0.78818	-0.47614
C	-3.81064	-0.60939	-1.3936
C	-2.99896	-1.58231	0.66111
C	-5.04184	-1.22511	-1.20419
C	-4.23055	-2.19721	0.85015
C	-5.25545	-2.02599	-0.08187
Si	2.49615	-0.21949	0.62825
H	0.25803	1.51211	-1.96469
H	1.83389	1.99121	-1.22796
H	-0.25441	-1.2902	0.55131
H	-1.48044	0.52437	-1.59137
H	4.30881	1.09448	1.73076
H	3.68611	1.99278	0.34662
H	2.76838	1.9403	1.85606
H	1.32332	-0.64231	2.79285
H	1.5505	-2.16678	1.92999
H	2.90561	-1.42136	2.77673
H	5.56298	-2.29116	-0.38618
H	5.48718	-0.82889	0.59776
H	4.67165	-2.30397	1.136
H	1.99352	-2.30501	-1.55037

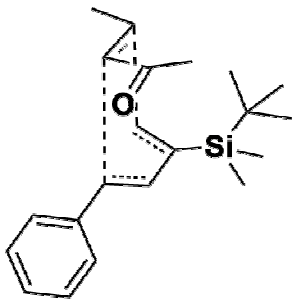
H	3.54758	-3.14094	-1.63946
H	2.61012	-3.18515	-0.14564
H	4.61585	0.44421	-1.48396
H	4.71356	-1.06098	-2.40018
H	3.1981	-0.15533	-2.35722
H	-3.6499	0.01494	-2.26646
H	-2.22549	-1.70648	1.40909
H	-5.83641	-1.0779	-1.92689
H	-4.39838	-2.80183	1.73422
H	-6.21677	-2.50265	0.07264
C	-0.14682	2.85841	-0.10822
C	-1.46404	2.42083	0.12655
C	-1.87829	1.88669	1.39862
C	0.06101	4.03736	-1.04729
O	-3.038	1.73059	1.77365
H	0.491	2.87983	0.77173
H	-2.24983	2.65831	-0.585
H	-1.04151	1.62587	2.08216
H	-0.28024	4.95778	-0.5638
H	1.11114	4.17254	-1.3137
H	-0.51436	3.91701	-1.96898



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1183.521293
Gibbs's free energies (G)	-1222.861151

C	0.82909	1.61266	-0.90063
C	1.08457	0.40033	-0.26796
C	0.01886	-0.5055	-0.07269
C	-1.26282	-0.28567	-0.53455
C	3.70274	-1.13233	-0.73416
C	3.77257	1.56449	0.77921
C	2.53946	-0.89927	2.12801
C	4.98688	-1.65714	-0.07573
C	2.82793	-2.32757	-1.13663
C	4.06582	-0.32895	-1.99036
C	-2.41709	-1.11868	-0.18577
C	-3.50832	-1.18344	-1.05879
C	-2.47731	-1.83837	1.01525
C	-4.61166	-1.97477	-0.76409
C	-3.57998	-2.62627	1.31193
C	-4.64898	-2.702	0.42063
Si	2.77017	-0.00187	0.48846
H	0.07261	1.67895	-1.67513
H	1.62734	2.34262	-1.00489
H	0.18129	-1.35852	0.58241
H	-1.39826	0.33736	-1.41356
H	4.81803	1.30484	0.9687
H	3.75413	2.24229	-0.07749
H	3.40676	2.10653	1.65393
H	1.8852	-0.3328	2.79606
H	2.10794	-1.89516	1.99766
H	3.50434	-1.0188	2.62809
H	5.54458	-2.27903	-0.78633
H	5.64974	-0.84537	0.23899
H	4.76642	-2.27438	0.80027
H	1.92315	-2.0087	-1.66056
H	3.3891	-2.98997	-1.80692

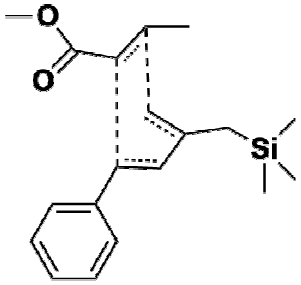
H	2.52442	-2.9213	-0.26817
H	4.74421	0.49817	-1.75941
H	4.56817	-0.9754	-2.72013
H	3.17442	0.0861	-2.47168
H	-3.48656	-0.607	-1.97801
H	-1.66519	-1.76233	1.72987
H	-5.44618	-2.01536	-1.45389
H	-3.61408	-3.17481	2.24595
H	-5.51148	-3.31359	0.65797
C	-0.46381	2.60051	0.44329
C	-1.63081	1.85251	0.56888
C	-2.84036	2.10057	-0.22598
C	-2.72258	2.90755	-1.50564
C	0.42872	2.75783	1.65129
O	-3.92579	1.67793	0.13218
H	-0.49061	3.44886	-0.23487
H	-1.80449	1.27773	1.47316
H	-2.6237	3.96854	-1.26017
H	-1.84871	2.62627	-2.09797
H	-3.62896	2.76869	-2.09214
H	-0.05339	3.40266	2.39178
H	0.60668	1.7864	2.12024
H	1.38966	3.20044	1.38744



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1183.523707
Gibbs's free energies (G)	-1222.861591

C	0.97536	1.25046	-1.28288
C	0.98009	0.1289	-0.45612
C	-0.21702	-0.59331	-0.26953
C	-1.40796	-0.24272	-0.87275
C	3.78953	-1.16872	-0.51375
C	3.25155	1.38605	1.16818
C	2.05896	-1.31201	2.0527
C	5.12134	-1.28778	0.24116
C	3.25823	-2.57243	-0.83554
C	4.02668	-0.41164	-1.82738
C	-2.7058	-0.85335	-0.5787
C	-3.72367	-0.78793	-1.53855
C	-2.97957	-1.48142	0.64303
C	-4.9649	-1.36347	-1.30294
C	-4.21964	-2.05879	0.87888
C	-5.21466	-2.00663	-0.09369
Si	2.52202	-0.24594	0.57156
H	0.34852	1.27901	-2.16899
H	1.88401	1.83965	-1.37654
H	-0.23935	-1.36816	0.49304
H	-1.3762	0.32379	-1.79666
H	4.08332	1.20344	1.85369
H	3.62905	1.99515	0.34253
H	2.50186	1.97407	1.70541
H	1.36327	-0.7896	2.7148
H	1.59213	-2.25166	1.74714
H	2.95021	-1.55934	2.6359
H	5.83546	-1.87396	-0.34969
H	5.56966	-0.30637	0.42187
H	5.00278	-1.79035	1.20604
H	2.27813	-2.53034	-1.32208

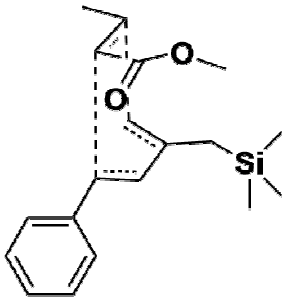
H	3.94657	-3.08839	-1.51585
H	3.16488	-3.18447	0.06612
H	4.36883	0.61388	-1.65311
H	4.80012	-0.92057	-2.41523
H	3.11889	-0.3684	-2.43526
H	-3.5303	-0.28581	-2.4812
H	-2.22693	-1.49585	1.42339
H	-5.7386	-1.30714	-2.05966
H	-4.41678	-2.5369	1.8311
H	-6.18412	-2.45269	0.09483
C	-0.28091	2.68409	-0.425
C	-1.50147	2.09265	-0.10916
C	-1.86633	1.64875	1.24007
C	-0.7633	1.49501	2.2673
C	-0.23111	3.69479	-1.5513
O	-3.02879	1.4365	1.54348
H	0.40464	2.87508	0.39499
H	-2.34458	2.21514	-0.78359
H	0.14396	1.07774	1.82774
H	-0.5149	2.47932	2.67641
H	-1.11833	0.86017	3.0783
H	0.78318	3.84977	-1.92226
H	-0.85875	3.3741	-2.38623
H	-0.61104	4.65795	-1.20082



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1180.207612
Gibbs's free energies (G)	-1180.265105

C	0.2393	1.13436	0.99261
C	-0.96596	0.46183	1.16698
C	-0.99118	-0.94783	1.12002
C	0.14653	-1.71127	0.99361
C	-2.26315	1.21392	1.20588
C	-4.47162	2.44171	2.94239
C	-3.17355	-0.22272	3.78107
C	-1.55746	2.39492	3.95125
C	0.15567	-3.15364	0.72914
C	1.28462	-3.90631	1.07212
C	-0.92063	-3.80657	0.11187
C	1.32845	-5.2752	0.83616
C	-0.87778	-5.17309	-0.12356
C	0.24571	-5.91374	0.24151
Si	-2.87195	1.45573	2.99396
H	1.17326	0.70216	1.33055
H	0.22034	2.221	0.99051
H	-1.9623	-1.42881	1.03249
H	1.08499	-1.30868	1.36028
H	-2.1488	2.20741	0.76028
H	-3.04517	0.68797	0.64673
H	-5.24001	1.91491	2.3705
H	-4.86001	2.60627	3.95095
H	-4.31639	3.4194	2.47862
H	-3.9267	-0.788	3.22502
H	-2.25694	-0.81744	3.8074
H	-3.53287	-0.10733	4.80716
H	-0.62047	1.83267	3.97785
H	-1.35563	3.36632	3.49125
H	-1.87648	2.57071	4.98199
H	2.13419	-3.40832	1.52689
H	-1.7876	-3.23661	-0.20304

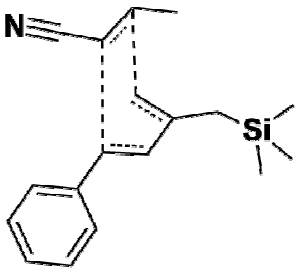
H	2.21116	-5.84134	1.10907
H	-1.71643	-5.66313	-0.6044
H	0.27912	-6.97981	0.05068
C	0.71048	0.69521	-0.96677
C	1.04877	-0.65397	-1.05731
C	2.38143	-1.15295	-0.75446
C	4.41731	-0.70825	0.34589
C	-0.49848	1.17686	-1.73111
O	2.8352	-2.22273	-1.0974
O	3.09185	-0.29126	0.02254
H	1.53526	1.39528	-0.87801
H	0.41974	-1.34998	-1.59791
H	4.85282	0.1035	0.92364
H	4.39817	-1.62616	0.9352
H	4.99504	-0.88299	-0.56219
H	-1.34415	0.50356	-1.56623
H	-0.79595	2.18294	-1.43196
H	-0.28386	1.1875	-2.80335



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1180.206607
Gibbs's free energies (G)	-1180.262557

C	1.24856	1.28648	-1.3347
C	1.26164	0.28534	-0.36655
C	0.11809	-0.51532	-0.17935
C	-1.04871	-0.30845	-0.8798
C	2.40563	0.17464	0.59527
C	5.10883	-1.13313	1.24138
C	2.92222	-2.75029	-0.21042
C	4.3772	-0.46612	-1.67605
C	-2.32688	-0.97015	-0.60363
C	-3.31018	-0.9887	-1.60102
C	-2.61904	-1.56473	0.63044
C	-4.5347	-1.60748	-1.38721
C	-3.84221	-2.18484	0.84501
C	-4.80317	-2.21207	-0.16247
Si	3.71764	-1.05983	-0.01981
H	0.70606	1.12705	-2.25875
H	2.13775	1.90142	-1.44242
H	0.11106	-1.18799	0.67457
H	-1.00194	0.18548	-1.84326
H	2.89127	1.14872	0.71988
H	2.05779	-0.14741	1.58233
H	4.74208	-1.47487	2.21281
H	5.89139	-1.8242	0.91699
H	5.56627	-0.14995	1.38019
H	2.54137	-3.117	0.74686
H	2.08536	-2.71026	-0.91253
H	3.64501	-3.47975	-0.58565
H	3.57426	-0.3975	-2.4146
H	4.83755	0.52174	-1.5843
H	5.13363	-1.15458	-2.06212
H	-3.10337	-0.51591	-2.55601

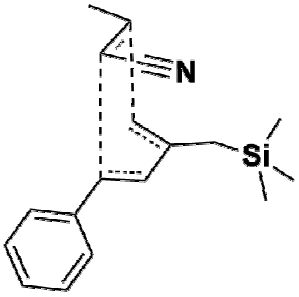
H	-1.89608	-1.52242	1.43611
H	-5.28	-1.61644	-2.17385
H	-4.05288	-2.6367	1.80717
H	-5.75942	-2.69183	0.00987
C	-0.11158	2.69672	-0.73863
C	-1.28434	2.09007	-0.28748
C	-1.47469	1.7088	1.10293
C	-0.38577	1.25615	3.13854
C	-0.17183	3.51837	-2.00824
O	-2.52458	1.39277	1.62197
O	-0.3066	1.72051	1.7958
H	0.55893	3.06453	0.03071
H	-2.18715	2.09556	-0.88681
H	0.61931	1.34355	3.54546
H	-1.08444	1.86082	3.71775
H	-0.71613	0.21537	3.16351
H	-0.63742	4.48612	-1.80501
H	0.82039	3.70319	-2.42315
H	-0.77269	3.01287	-2.76876



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1044.631020
Gibbs's free energies (G)	-1044.685545

C	-1.42921	-0.01413	0.8735
C	-0.71983	-1.19111	1.10444
C	0.69098	-1.1744	1.07661
C	1.41664	-0.01696	0.91855
C	-1.43387	-2.50591	1.18247
C	-2.648	-4.66335	2.98648
C	-0.00487	-3.30303	3.79927
C	-2.6441	-1.71273	3.89001
C	2.85791	0.04788	0.65056
C	3.53365	1.25468	0.87104
C	3.57995	-1.04167	0.14394
C	4.89605	1.36376	0.61803
C	4.94088	-0.93303	-0.10458
C	5.60493	0.26922	0.13423
Si	-1.68171	-3.05154	2.99234
H	-1.03513	0.93941	1.20459
H	-2.51454	-0.06837	0.86661
H	1.20065	-2.13339	1.02809
H	0.97985	0.92159	1.2387
H	-2.42616	-2.43687	0.72545
H	-0.88003	-3.2939	0.66013
H	-2.11091	-5.44307	2.44004
H	-2.81177	-5.02225	4.006
H	-3.62593	-4.53292	2.51568
H	0.57311	-4.06761	3.27266
H	0.5781	-2.37857	3.80025
H	-0.12329	-3.62909	4.83601
H	-2.08985	-0.77061	3.89304
H	-3.61099	-1.5342	3.41126
H	-2.83161	-1.99755	4.92864
H	2.97789	2.11227	1.23504
H	3.07234	-1.97515	-0.07063

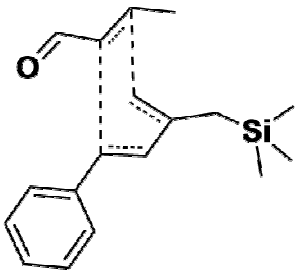
H	5.402	2.30538	0.79506
H	5.48583	-1.78463	-0.49486
H	6.66668	0.3525	-0.06523
C	-0.98848	0.38684	-1.08764
C	0.34178	0.80923	-1.16081
C	0.679	2.1589	-0.88415
C	-1.36442	-0.88315	-1.80934
N	0.9479	3.24785	-0.60335
H	-1.74341	1.16733	-1.06996
H	1.1001	0.20869	-1.64574
H	-0.63345	-1.66892	-1.59969
H	-2.35047	-1.24117	-1.51158
H	-1.37189	-0.71015	-2.88879



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1044.629111
Gibbs's free energies (G)	-1044.683095

C	-0.00524	1.21472	1.18074
C	-1.15632	0.45344	1.36094
C	-1.06804	-0.95292	1.34269
C	0.11409	-1.61787	1.10678
C	-2.50543	1.10488	1.36932
C	-4.80207	2.24627	3.04785
C	-3.34784	-0.30699	3.97866
C	-1.90335	2.40915	4.08531
C	0.21921	-3.05859	0.85031
C	1.44191	-3.70686	1.06955
C	-0.85707	-3.8072	0.35565
C	1.57984	-5.06839	0.83272
C	-0.71719	-5.16786	0.11585
C	0.49782	-5.80442	0.35765
Si	-3.14694	1.36328	3.14395
H	0.94093	0.85774	1.56964
H	-0.1024	2.29652	1.16729
H	-1.99845	-1.51332	1.322
H	1.05358	-1.13004	1.34054
H	-2.45739	2.08894	0.89121
H	-3.23788	0.50421	0.82064
H	-5.52662	1.66161	2.47517
H	-5.21598	2.40715	4.04688
H	-4.69878	3.22181	2.56557
H	-4.03956	-0.94414	3.42069
H	-2.39094	-0.83021	4.05162
H	-3.74535	-0.18617	4.98993
H	-0.93535	1.90497	4.14693
H	-1.75057	3.37656	3.59887
H	-2.25038	2.59779	5.10479
H	2.28708	-3.13333	1.43734

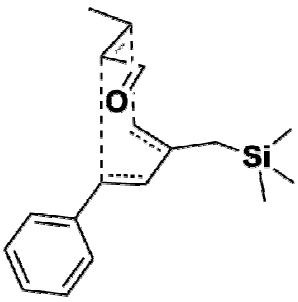
H	-1.79555	-3.31669	0.12749
H	2.53078	-5.55495	1.01546
H	-1.55683	-5.73229	-0.27229
H	0.60339	-6.86595	0.16752
C	0.62667	0.86064	-0.75283
C	0.58034	-0.50744	-1.03397
C	-0.58249	-1.06402	-1.62857
C	1.98085	1.52927	-0.67621
N	-1.55095	-1.49638	-2.08805
H	-0.1738	1.46337	-1.16984
H	1.48372	-1.10301	-1.08274
H	2.69359	0.89602	-0.14153
H	2.37139	1.69561	-1.68332
H	1.93133	2.49391	-0.1694



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1065.695400
Gibbs's free energies (G)	-1065.7493

C	1.11214	1.69484	-0.78715
C	1.26863	0.53218	-0.03461
C	0.17864	-0.34815	0.12923
C	-1.03666	-0.16493	-0.48805
C	2.51441	0.30704	0.76634
C	5.2541	-1.04945	0.92777
C	2.8776	-2.54947	-0.33807
C	4.13493	-0.1454	-1.80159
C	-2.25837	-0.90271	-0.16623
C	-3.29575	-0.95371	-1.10445
C	-2.44188	-1.53755	1.07124
C	-4.4695	-1.64612	-0.83097
C	-3.61273	-2.22801	1.34394
C	-4.62957	-2.28866	0.39142
Si	3.70932	-0.87969	-0.12777
H	0.45153	1.69898	-1.64428
H	1.96625	2.36048	-0.87914
H	0.27059	-1.11629	0.89268
H	-1.07377	0.39182	-1.41785
H	3.04712	1.24924	0.92856
H	2.2853	-0.11893	1.74956
H	5.01264	-1.44835	1.91656
H	5.97451	-1.72632	0.46105
H	5.74349	-0.08163	1.06499
H	2.57845	-2.96303	0.62906
H	1.98408	-2.47211	-0.96269
H	3.55975	-3.26192	-0.80975
H	3.23763	-0.03088	-2.41542
H	4.59813	0.83927	-1.69267
H	4.83438	-0.78743	-2.34337
H	-3.17852	-0.44231	-2.05327
H	-1.67206	-1.47058	1.83167

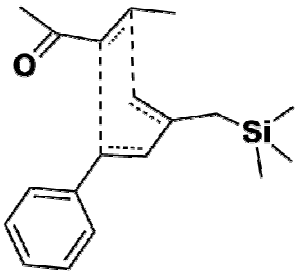
H	-5.26207	-1.67596	-1.56902
H	-3.74213	-2.7102	2.3059
H	-5.54637	-2.82345	0.60971
C	-0.17327	2.8034	0.34501
C	-1.42364	2.17633	0.38684
C	-2.40388	2.43744	-0.63939
C	0.59158	2.98634	1.6344
O	-3.57502	2.09952	-0.61858
H	-0.08069	3.61885	-0.37031
H	-1.76084	1.66027	1.27939
H	-2.0086	2.98818	-1.52189
H	0.60961	2.05313	2.20304
H	1.62051	3.3044	1.45942
H	0.10008	3.74365	2.25129



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1065.695025
Gibbs's free energies (G)	-1065.748714

C	1.21041	1.67073	-0.7842
C	1.2567	0.49137	-0.04339
C	0.12611	-0.34672	0.01766
C	-1.05146	-0.0531	-0.63305
C	2.42347	0.20698	0.85341
C	5.08953	-1.266	1.21026
C	2.78323	-2.62174	-0.31835
C	4.25845	-0.23005	-1.57383
C	-2.31583	-0.76406	-0.45896
C	-3.30035	-0.64368	-1.44894
C	-2.59893	-1.53568	0.67561
C	-4.51619	-1.302	-1.33028
C	-3.81429	-2.19554	0.79416
C	-4.77424	-2.08509	-0.2083
Si	3.6528	-0.99485	0.03032
H	0.6324	1.71379	-1.69962
H	2.09807	2.29638	-0.79117
H	0.14476	-1.16631	0.73106
H	-1.02333	0.60567	-1.49295
H	2.96776	1.12855	1.08423
H	2.09713	-0.23446	1.8013
H	4.74283	-1.68283	2.15949
H	5.81683	-1.96246	0.78456
H	5.6088	-0.32796	1.42313
H	2.38084	-3.05976	0.5993
H	1.95566	-2.48437	-1.0188
H	3.47983	-3.3423	-0.75556
H	3.43129	-0.07658	-2.27169
H	4.7355	0.73778	-1.39669
H	4.99122	-0.88123	-2.05805
H	-3.09899	-0.03001	-2.32123

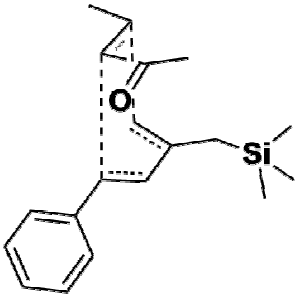
H	-1.87594	-1.60308	1.47973
H	-5.26427	-1.20078	-2.10766
H	-4.02217	-2.78398	1.67992
H	-5.72517	-2.59495	-0.1081
C	-0.11052	2.89433	0.18102
C	-1.34807	2.26262	0.33409
C	-1.68582	1.58632	1.56703
C	-0.0179	4.09032	-0.74521
O	-2.80122	1.23992	1.91474
H	0.50156	2.95892	1.07818
H	-2.15754	2.45627	-0.36433
H	-0.81333	1.38434	2.22586
H	-0.48938	4.95708	-0.27545
H	1.0145	4.35374	-0.97819
H	-0.5439	3.89286	-1.68218



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1104.979393
Gibbs's free energies (G)	-1105.035232

C	1.10963	1.73279	-0.55772
C	1.36769	0.51031	0.05498
C	0.34395	-0.45528	0.13697
C	-0.90353	-0.28355	-0.4212
C	2.64779	0.28369	0.80358
C	5.45838	-0.93992	0.78196
C	3.11687	-2.46527	-0.51891
C	4.20227	0.09359	-1.83827
C	-2.04824	-1.16131	-0.16477
C	-3.09171	-1.22783	-1.09434
C	-2.15059	-1.91795	1.011
C	-4.18814	-2.0536	-0.87663
C	-3.24489	-2.74082	1.22973
C	-4.26607	-2.81593	0.28355
Si	3.86921	-0.77375	-0.20658
H	0.43482	1.78058	-1.4022
H	1.9001	2.47819	-0.57303
H	0.50806	-1.30087	0.80017
H	-1.0076	0.36183	-1.28724
H	3.14041	1.23574	1.02495
H	2.46572	-0.22395	1.75757
H	5.27595	-1.4215	1.74624
H	6.19238	-1.5426	0.24067
H	5.90509	0.0394	0.97279
H	2.9036	-2.98328	0.42013
H	2.182	-2.38247	-1.07897
H	3.80299	-3.08972	-1.09743
H	3.27653	0.21698	-2.40629
H	4.63621	1.0847	-1.67928
H	4.89986	-0.48434	-2.45028
H	-3.04122	-0.62242	-1.99317
H	-1.37919	-1.84156	1.769

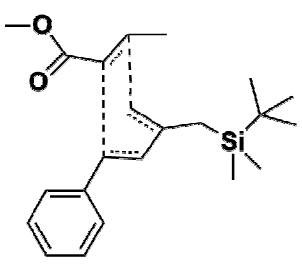
H	-4.9863	-2.09402	-1.60826
H	-3.31084	-3.31657	2.14552
H	-5.12318	-3.45524	0.45921
C	-0.2777	2.59219	0.7215
C	-1.46199	1.85245	0.69592
C	-2.56941	2.1201	-0.21771
C	-2.32915	3.03466	-1.40622
C	0.49792	2.65057	2.01689
O	-3.67392	1.62666	-0.04391
H	-0.24762	3.49702	0.11992
H	-1.71825	1.22308	1.54194
H	-2.24643	4.06973	-1.06356
H	-1.40417	2.79234	-1.93503
H	-3.17411	2.95751	-2.088
H	-0.04158	3.26021	2.74707
H	0.60876	1.64779	2.43793
H	1.49215	3.07926	1.8813



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1104.980014
Gibbs's free energies (G)	-1105.035228

C	0.08007	1.14648	1.38174
C	-1.08938	0.39917	1.49423
C	-1.02525	-1.00694	1.45287
C	0.15835	-1.69519	1.29837
C	-2.42788	1.07807	1.47406
C	-4.73382	2.26324	3.111
C	-3.32806	-0.30424	4.07451
C	-1.85138	2.39572	4.19392
C	0.26333	-3.13629	1.06279
C	1.46341	-3.79134	1.3653
C	-0.78442	-3.88343	0.51016
C	1.60287	-5.15694	1.15748
C	-0.64697	-5.2489	0.30366
C	0.54442	-5.89137	0.63017
Si	-3.09109	1.35989	3.23752
H	1.00055	0.77385	1.81457
H	-0.00575	2.22937	1.38419
H	-1.96387	-1.55036	1.37813
H	1.08256	-1.22074	1.6072
H	-2.3562	2.05629	0.98606
H	-3.16967	0.48711	0.92575
H	-5.45864	1.68352	2.53354
H	-5.15892	2.43686	4.10317
H	-4.61209	3.234	2.62333
H	-4.02336	-0.93208	3.51038
H	-2.38018	-0.84184	4.15847
H	-3.73485	-0.17543	5.08111
H	-0.88889	1.88339	4.27079
H	-1.68347	3.36104	3.70838
H	-2.21241	2.58892	5.2077
H	2.29045	-3.21871	1.77305

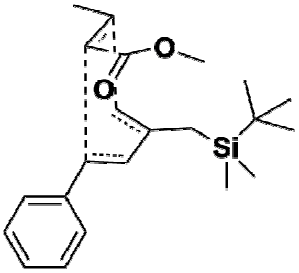
H	-1.70287	-3.38903	0.21473
H	2.53717	-5.64848	1.40168
H	-1.46475	-5.8114	-0.13108
H	0.65239	-6.95614	0.46042
C	0.8428	0.81677	-0.51029
C	0.9536	-0.55358	-0.75621
C	-0.01197	-1.32362	-1.53539
C	-1.37032	-0.70839	-1.81568
C	2.11742	1.62186	-0.35625
O	0.26302	-2.42766	-1.98217
H	0.02934	1.34052	-1.00453
H	1.91411	-1.04306	-0.61906
H	-1.73761	-0.1097	-0.98113
H	-1.28929	-0.05267	-2.6883
H	-2.07597	-1.50509	-2.04906
H	2.83991	1.08333	0.26175
H	2.57412	1.78227	-1.33627
H	1.93835	2.59869	0.09507



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1298.030438
Gibbs's free energies (G)	-1298.091452

C	-0.46968	-1.83253	0.12459
C	-0.86438	-0.57287	0.56534
C	0.0342	0.50953	0.45815
C	1.25372	0.40685	-0.17091
C	-3.9032	-0.04765	-1.24598
C	-4.98034	0.64426	1.57514
C	-2.84326	2.43298	0.28626
C	-5.22632	0.5771	-1.71626
C	-2.81133	0.27424	-2.27743
C	-4.07629	-1.56966	-1.15236
C	2.29417	1.44053	-0.14469
C	3.24258	1.48072	-1.1726
C	2.39173	2.37786	0.89295
C	4.24111	2.44666	-1.18491
C	3.38959	3.34193	0.88215
C	4.31552	3.38272	-0.15923
C	-2.13469	-0.39274	1.34521
Si	-3.45872	0.66437	0.46481
H	0.1938	-1.94788	-0.72387
H	-1.15082	-2.66478	0.27752
H	-0.19519	1.41151	1.02007
H	1.37031	-0.33718	-0.9525
H	-5.73198	1.3559	1.22381
H	-5.44172	-0.34691	1.60214
H	-4.71329	0.91754	2.59959
H	-2.61661	2.86399	1.26575
H	-1.94119	2.48911	-0.32725
H	-3.60886	3.05877	-0.18154
H	-5.46604	0.225	-2.72683
H	-6.05921	0.30243	-1.06297
H	-5.17118	1.66995	-1.75387
H	-1.83902	-0.13045	-1.98293

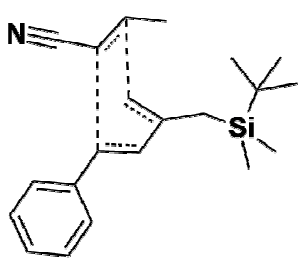
H	-3.07817	-0.16187	-3.24824
H	-2.69897	1.35287	-2.41979
H	-4.81778	-1.85159	-0.39744
H	-4.41793	-1.96947	-2.11492
H	-3.13217	-2.06254	-0.90515
H	3.19047	0.74559	-1.9688
H	1.69475	2.33711	1.72255
H	4.96504	2.46371	-1.99088
H	3.45543	4.05789	1.69313
H	5.09737	4.133	-0.16211
H	-1.93632	0.11079	2.30026
H	-2.58263	-1.3633	1.58105
C	1.0716	-2.29435	1.41929
C	2.15982	-1.47192	1.13197
C	3.11762	-1.77496	0.07845
C	3.50044	-2.98309	-1.90792
C	0.42776	-2.17252	2.77857
O	4.22899	-1.30508	-0.02863
O	2.61367	-2.63673	-0.84503
H	1.08454	-3.28581	0.97762
H	2.49343	-0.72274	1.83908
H	2.95146	-3.67767	-2.53916
H	3.78371	-2.09537	-2.47508
H	4.40177	-3.45489	-1.51543
H	0.26271	-1.1204	3.02683
H	-0.53134	-2.69076	2.82313
H	1.08414	-2.59685	3.54349



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1298.029203
Gibbs's free energies (G)	-1298.088919

C	0.60523	1.54984	-1.28938
C	0.68862	0.61878	-0.2563
C	-0.35206	-0.31502	-0.08503
C	-1.48011	-0.32467	-0.87467
C	4.07122	-0.63189	-0.83081
C	4.19163	-0.32515	2.25087
C	2.22538	-2.32598	1.00279
C	5.34977	-1.45857	-0.62664
C	3.26747	-1.2404	-1.98923
C	4.45931	0.80968	-1.18568
C	-2.66891	-1.14615	-0.62624
C	-3.54801	-1.4112	-1.68419
C	-2.97481	-1.66232	0.63913
C	-4.67981	-2.19282	-1.49441
C	-4.10463	-2.44494	0.82978
C	-4.95949	-2.7166	-0.23547
C	1.74304	0.72979	0.8048
Si	3.05695	-0.65276	0.78451
H	0.15698	1.2598	-2.23245
H	1.39799	2.28551	-1.38521
H	-0.33811	-0.9202	0.81796
H	-1.42687	0.09486	-1.8727
H	4.91452	-1.13448	2.37999
H	4.74884	0.60749	2.12583
H	3.61057	-0.24575	3.17378
H	1.67926	-2.36695	1.94963
H	1.51974	-2.53557	0.19547
H	2.97056	-3.12663	1.01637
H	5.91902	-1.50478	-1.563
H	5.99943	-1.01831	0.13505
H	5.12585	-2.48776	-0.3278
H	2.33532	-0.69763	-2.16976

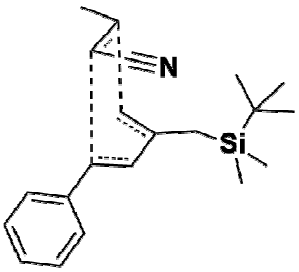
H	3.86029	-1.20644	-2.9118
H	3.01655	-2.28752	-1.79651
H	5.00404	1.29895	-0.37144
H	5.10791	0.81961	-2.07005
H	3.57713	1.41352	-1.41509
H	-3.33212	-1.00234	-2.66631
H	-2.33902	-1.43142	1.48518
H	-5.34494	-2.39189	-2.32645
H	-4.3287	-2.83271	1.81651
H	-5.84425	-3.32305	-0.08186
H	1.27949	0.69473	1.79822
H	2.26492	1.68912	0.72838
C	-0.97999	2.78064	-0.88022
C	-2.09026	2.035	-0.48019
C	-2.34923	1.72014	0.91613
C	-1.40522	1.57605	3.06634
C	-1.04997	3.51829	-2.19982
O	-3.38929	1.29462	1.3728
O	-1.26028	1.93978	1.6981
H	-0.43401	3.28036	-0.08735
H	-2.93145	1.88201	-1.14581
H	-0.46506	1.83762	3.54726
H	-2.23101	2.11947	3.5267
H	-1.5939	0.5043	3.15976
H	-1.66219	4.41737	-2.09237
H	-0.06324	3.82465	-2.55046
H	-1.50939	2.89257	-2.96941



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1162.453468
Gibbs's free energies (G)	-1162.512539

C	-0.38213	1.94617	0.39246
C	-0.58616	0.75764	-0.30668
C	0.44147	-0.20901	-0.34912
C	1.60889	-0.0867	0.36733
C	-3.74579	-0.31018	1.08774
C	-4.40482	-0.74696	-1.91197
C	-2.1961	-2.41403	-0.58278
C	-5.02099	-1.1378	1.31364
C	-2.73563	-0.64467	2.19532
C	-4.1012	1.18107	1.16198
C	2.80161	-0.92294	0.18799
C	3.75229	-0.97666	1.21486
C	3.05039	-1.63465	-0.99395
C	4.90698	-1.73754	1.0764
C	4.20254	-2.39618	-1.13036
C	5.13419	-2.45244	-0.09497
C	-1.77568	0.5916	-1.20458
Si	-3.03081	-0.73012	-0.62693
H	0.2049	1.95696	1.30359
H	-1.16624	2.69722	0.36155
H	0.35428	-0.99614	-1.09408
H	1.60144	0.48914	1.28567
H	-5.10173	-1.56862	-1.72872
H	-4.97489	0.18599	-1.90526
H	-3.98949	-0.8781	-2.91491
H	-1.83118	-2.69342	-1.57526
H	-1.34955	-2.42915	0.10744
H	-2.90481	-3.18335	-0.26263
H	-5.4095	-0.9554	2.3228
H	-5.80793	-0.87224	0.602
H	-4.83185	-2.21246	1.22447
H	-1.79326	-0.10483	2.06597

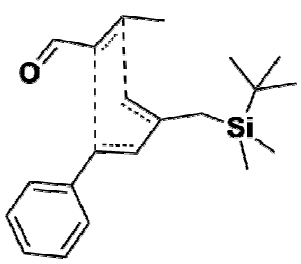
H	-3.14988	-0.36704	3.17239
H	-2.51051	-1.71452	2.22321
H	-4.78117	1.48147	0.35809
H	-4.59848	1.40198	2.11411
H	-3.20671	1.80704	1.10428
H	3.58059	-0.41059	2.12409
H	2.34809	-1.57715	-1.81797
H	5.6307	-1.76837	1.88216
H	4.38232	-2.93966	-2.05057
H	6.03574	-3.04316	-0.20616
H	-1.46126	0.28149	-2.20933
H	-2.31517	1.5376	-1.31329
C	1.11394	2.84229	-0.6804
C	2.30251	2.15283	-0.42608
C	3.04865	2.42553	0.74916
C	0.59723	2.85114	-2.09703
N	3.61679	2.61656	1.73776
H	0.94435	3.74735	-0.10477
H	2.8038	1.58513	-1.19893
H	0.64176	1.84438	-2.52173
H	-0.43342	3.2037	-2.15167
H	1.21879	3.50344	-2.7164



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1162.451142
Gibbs's free energies (G)	-1162.508279

C	0.12263	1.15948	1.739
C	-1.05969	0.43085	1.83768
C	-1.01073	-0.97569	1.75906
C	0.16103	-1.66911	1.55546
C	-2.4776	1.89199	4.84813
C	-5.02292	1.90831	3.07804
C	-3.7348	-0.76829	3.86178
C	-3.46515	2.13354	5.99998
C	-1.32244	1.01997	5.36223
C	-1.92033	3.24207	4.37679
C	0.23473	-3.10202	1.24731
C	1.42467	-3.79627	1.50172
C	-0.83732	-3.79809	0.67254
C	1.53477	-5.15166	1.21912
C	-0.72502	-5.15252	0.38689
C	0.45725	-5.83516	0.66253
C	-2.39445	1.1133	1.79353
Si	-3.39474	1.02715	3.41779
H	1.03672	0.75805	2.16055
H	0.06511	2.24361	1.75364
H	-1.95506	-1.50366	1.66241
H	1.10116	-1.22362	1.86121
H	-5.71277	1.80199	3.91889
H	-4.87104	2.97625	2.89879
H	-5.50712	1.48688	2.19297
H	-4.30232	-1.26193	3.06778
H	-2.81217	-1.33163	4.01874
H	-4.32708	-0.82787	4.77943
H	-2.94292	2.58793	6.85064
H	-4.27243	2.81016	5.70629
H	-3.91599	1.20003	6.35218
H	-0.59314	0.80356	4.57659

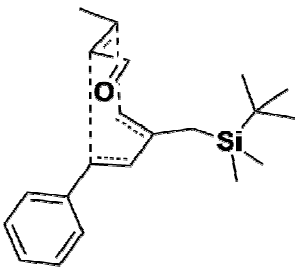
H	-0.79759	1.5384	6.17439
H	-1.68402	0.06693	5.75877
H	-2.70373	3.88845	3.96788
H	-1.45965	3.77403	5.21804
H	-1.15273	3.11158	3.60883
H	2.26555	-3.26461	1.93612
H	-1.74982	-3.27196	0.4196
H	2.46002	-5.67433	1.43119
H	-1.56009	-5.6753	-0.0644
H	0.54074	-6.89165	0.43681
H	-3.03074	0.65593	1.02636
H	-2.27958	2.16939	1.5301
C	0.84816	0.85173	-0.16924
C	0.76906	-0.50252	-0.50518
C	-0.37818	-0.99151	-1.18411
C	2.21982	1.46383	0.00666
N	-1.33457	-1.36825	-1.7124
H	0.09438	1.49959	-0.60485
H	1.65344	-1.12732	-0.53353
H	2.87471	0.78714	0.56179
H	2.67517	1.64391	-0.97045
H	2.17758	2.41443	0.53989



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1183.517507
Gibbs's free energies (G)	-1183.575685

C	0.10314	1.20586	1.09281
C	-1.06949	0.45078	1.05466
C	-0.98964	-0.95796	1.02478
C	0.19381	-1.64866	1.14039
C	-2.881	1.84086	3.84176
C	-5.16357	1.92913	1.74057
C	-4.03427	-0.7788	2.64411
C	-4.01787	2.11819	4.83798
C	-1.8489	0.92062	4.50961
C	-2.20998	3.16972	3.46998
C	0.36205	-3.07998	0.88541
C	1.4903	-3.73363	1.39427
C	-0.55204	-3.81926	0.11994
C	1.6865	-5.09205	1.17513
C	-0.35656	-5.17451	-0.09801
C	0.76186	-5.8171	0.43281
C	-2.39522	1.10703	0.81122
Si	-3.60955	1.0178	2.28542
H	0.96641	0.84239	1.63598
H	0.01517	2.28822	1.07499
H	-1.89024	-1.50056	0.74952
H	1.02077	-1.18231	1.66392
H	-5.96348	1.81056	2.47587
H	-4.97983	2.99945	1.61219
H	-5.52538	1.5354	0.78686
H	-4.49081	-1.25145	1.76973
H	-3.15139	-1.35923	2.92218
H	-4.75204	-0.84428	3.467
H	-3.60716	2.53522	5.7653
H	-4.73806	2.83885	4.44011
H	-4.56226	1.20548	5.10137
H	-1.02778	0.66966	3.83221

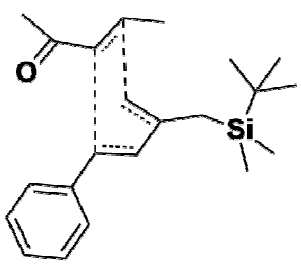
H	-1.41962	1.41792	5.38813
H	-2.30421	-0.01422	4.84865
H	-2.89962	3.84621	2.95464
H	-1.86071	3.68176	4.37478
H	-1.34232	3.01034	2.8242
H	2.22113	-3.16624	1.95896
H	-1.41034	-3.32753	-0.32319
H	2.56617	-5.58022	1.57696
H	-1.07043	-5.73281	-0.69221
H	0.91492	-6.87514	0.25558
H	-2.91658	0.62878	-0.02783
H	-2.26486	2.16219	0.55145
C	0.94865	0.83481	-0.7201
C	1.37479	-0.49757	-0.773
C	2.67303	-0.86075	-0.2583
C	-0.10749	1.29932	-1.69388
O	3.22661	-1.93863	-0.39252
H	1.72224	1.56597	-0.49079
H	0.84803	-1.23324	-1.37063
H	3.17469	-0.05718	0.32527
H	-0.9328	0.58373	-1.73184
H	-0.51009	2.27758	-1.42663
H	0.32019	1.3675	-2.69794



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1183.517722
Gibbs's free energies (G)	-1183.57593

C	0.05502	1.17811	1.06615
C	-1.11032	0.41278	1.075
C	-1.02158	-0.99311	1.05039
C	0.18186	-1.66221	1.0319
C	-2.8961	1.85876	3.87541
C	-5.21996	1.83277	1.82138
C	-4.00894	-0.8199	2.78117
C	-4.02221	2.14594	4.88102
C	-1.83521	0.98036	4.55462
C	-2.25646	3.1871	3.45055
C	0.35168	-3.09723	0.81259
C	1.55337	-3.70372	1.20212
C	-0.62523	-3.88704	0.19267
C	1.76136	-5.06268	1.01259
C	-0.41837	-5.24657	0.00414
C	0.77199	-5.83964	0.41576
C	-2.44914	1.05501	0.86031
Si	-3.63388	0.97381	2.3576
H	0.93876	0.82589	1.5851
H	-0.04688	2.25846	1.0488
H	-1.93681	-1.55071	0.87177
H	1.06382	-1.16039	1.41285
H	-6.00378	1.7112	2.57333
H	-5.06495	2.90413	1.66639
H	-5.58834	1.40916	0.88316
H	-4.48078	-1.32958	1.93626
H	-3.10685	-1.37319	3.05222
H	-4.70107	-0.87259	3.62669
H	-3.60424	2.59081	5.792
H	-4.75746	2.84725	4.47614
H	-4.55103	1.23319	5.17461
H	-1.02203	0.72235	3.87032

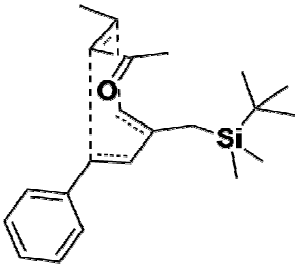
H	-1.39955	1.51468	5.40802
H	-2.26594	0.04901	4.93314
H	-2.96289	3.82875	2.91366
H	-1.9137	3.74044	4.33326
H	-1.3889	3.0216	2.80599
H	2.32595	-3.09725	1.66404
H	-1.54161	-3.43466	-0.16756
H	2.69478	-5.51555	1.32539
H	-1.1812	-5.84269	-0.48231
H	0.93349	-6.89974	0.2597
H	-2.98157	0.56478	0.03513
H	-2.33334	2.10912	0.58861
C	0.92337	0.8716	-0.75604
C	1.13323	-0.4919	-0.98118
C	0.18687	-1.26398	-1.75621
C	2.12984	1.77124	-0.57902
O	0.38206	-2.36473	-2.2405
H	0.09467	1.31847	-1.30121
H	2.10386	-0.94161	-0.79081
H	-0.79648	-0.76487	-1.89741
H	2.62008	1.92244	-1.54397
H	1.86024	2.75066	-0.18214
H	2.85737	1.31373	0.09554



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1222.801374
Gibbs's free energies (G)	-1222.861151

C	-0.462	1.86066	0.32556
C	-0.73241	0.65859	-0.32292
C	0.24353	-0.35877	-0.32459
C	1.43855	-0.26365	0.35251
C	-3.97079	-0.17322	1.08685
C	-4.59253	-0.78777	-1.89261
C	-2.47627	-2.44034	-0.41529
C	-5.27832	-0.93789	1.34757
C	-2.9895	-0.46657	2.23173
C	-4.27284	1.33104	1.05267
C	2.55575	-1.19778	0.19501
C	3.50646	-1.31302	1.21533
C	2.72735	-1.96058	-0.96858
C	4.57629	-2.19201	1.09658
C	3.7967	-2.83507	-1.08924
C	4.72252	-2.95856	-0.05386
C	-1.93277	0.51002	-1.21188
Si	-3.24261	-0.73087	-0.58277
H	0.1324	1.86153	1.23011
H	-1.20218	2.65401	0.27678
H	0.10181	-1.18254	-1.01918
H	1.49357	0.36686	1.23422
H	-5.31898	-1.57429	-1.67308
H	-5.13242	0.16037	-1.96215
H	-4.16019	-0.99794	-2.87483
H	-2.10737	-2.79598	-1.38166
H	-1.64174	-2.44796	0.28942
H	-3.22241	-3.15806	-0.0618
H	-5.67907	-0.66457	2.33109
H	-6.042	-0.70268	0.60074
H	-5.12466	-2.02179	1.34551
H	-2.02671	0.03052	2.08189

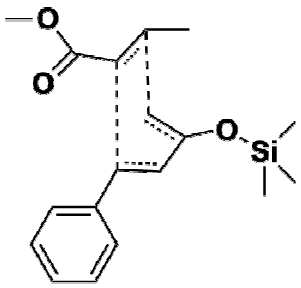
H	-3.40812	-0.11007	3.1811
H	-2.80224	-1.53925	2.33472
H	-4.93307	1.59736	0.22082
H	-4.77205	1.63621	1.98033
H	-3.35587	1.91975	0.96152
H	3.40292	-0.70571	2.10838
H	2.03119	-1.85099	-1.79236
H	5.30131	-2.27015	1.898
H	3.91834	-3.41436	-1.99703
H	5.55994	-3.63911	-0.1522
H	-1.6329	0.14859	-2.20375
H	-2.42772	1.47494	-1.35946
C	1.07239	2.66379	-0.79532
C	2.20767	1.8565	-0.69359
C	3.25318	2.04151	0.30775
C	2.96838	2.93331	1.50409
C	0.41676	2.80647	-2.14974
O	4.34327	1.49956	0.19945
H	1.04514	3.55454	-0.17245
H	2.49186	1.22689	-1.53033
H	2.97829	3.98138	1.19193
H	1.98906	2.73526	1.94684
H	3.747	2.78318	2.24986
H	1.03801	3.42832	-2.80035
H	0.31238	1.82825	-2.62596
H	-0.572	3.26327	-2.08175



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1222.802438
Gibbs's free energies (G)	-1222.861591

C	-0.04497	1.17707	0.91786
C	-1.20774	0.4095	0.95093
C	-1.10873	-0.99514	0.91575
C	0.09945	-1.65669	0.86878
C	-2.78817	1.83685	3.88282
C	-5.25172	1.80897	1.9989
C	-3.95683	-0.84334	2.84723
C	-3.83701	2.07095	4.98125
C	-1.65066	0.98048	4.4586
C	-2.22532	3.19166	3.43317
C	0.25969	-3.0972	0.66076
C	1.44272	-3.71768	1.08097
C	-0.71318	-3.87684	0.02303
C	1.63632	-5.0807	0.90233
C	-0.52133	-5.23998	-0.15475
C	0.65105	-5.8476	0.28665
C	-2.56139	1.04957	0.82943
Si	-3.62483	0.95654	2.41367
H	0.84321	0.82768	1.43046
H	-0.14437	2.25782	0.89023
H	-2.02414	-1.56003	0.75914
H	0.97909	-1.16038	1.26234
H	-5.98315	1.67904	2.80039
H	-5.11278	2.88194	1.83948
H	-5.68078	1.38932	1.08489
H	-4.48578	-1.34772	2.03346
H	-3.0337	-1.39316	3.04395
H	-4.58486	-0.90859	3.74049
H	-3.36451	2.53311	5.85625
H	-4.63451	2.73828	4.64309
H	-4.29606	1.13385	5.31291
H	-0.87856	0.77269	3.7127

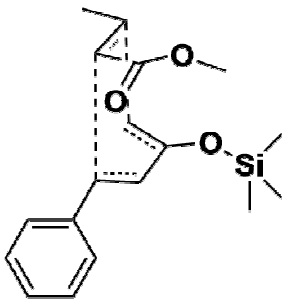
H	-1.17532	1.50669	5.29583
H	-2.02017	0.02342	4.83773
H	-2.99752	3.82809	2.98859
H	-1.80824	3.73083	4.29239
H	-1.42367	3.0668	2.70007
H	2.21305	-3.11993	1.55787
H	-1.61391	-3.41188	-0.36139
H	2.55616	-5.54432	1.23894
H	-1.28095	-5.82779	-0.6563
H	0.8017	-6.91051	0.13906
H	-3.15969	0.55898	0.05113
H	-2.46902	2.10344	0.54808
C	0.90721	0.83107	-0.88903
C	1.04034	-0.54118	-1.11212
C	0.15098	-1.31401	-1.97667
C	-1.16879	-0.69286	-2.39195
C	2.15997	1.637	-0.61246
O	0.46142	-2.42307	-2.38492
H	0.14665	1.35228	-1.4627
H	1.98538	-1.02842	-0.88807
H	-1.61881	-0.10431	-1.59177
H	-0.99443	-0.02403	-3.24053
H	-1.84692	-1.4837	-2.71006
H	2.82342	1.09563	0.06658
H	2.70499	1.8049	-1.54482
H	1.93745	2.61063	-0.17339



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1216.184301
Gibbs's free energies (G)	-1216.240311

C	-0.78888	-2.03203	-0.94364
C	-1.36971	-0.77909	-0.81065
C	-0.58062	0.38045	-0.6436
C	0.79006	0.34287	-0.70425
C	-5.43084	-0.32858	-0.17017
C	-3.34983	1.08408	1.58534
C	-3.69041	1.89429	-1.38207
C	1.66591	1.4586	-0.33603
C	2.9747	1.49263	-0.82983
C	1.24801	2.48446	0.52335
C	3.83235	2.53642	-0.50371
C	2.10327	3.52656	0.84894
C	3.3979	3.55878	0.33246
O	-2.70771	-0.74334	-0.60216
Si	-3.76289	0.49585	-0.14313
H	0.16363	-2.1382	-1.44339
H	-1.46467	-2.87598	-1.02511
H	-1.06779	1.29058	-0.3128
H	1.26888	-0.45131	-1.26638
H	-5.44238	-1.19606	0.49368
H	-6.20942	0.3634	0.16136
H	-5.6836	-0.6672	-1.17741
H	-3.48389	0.27622	2.30907
H	-2.32715	1.45637	1.68062
H	-4.02536	1.89749	1.86613
H	-2.76974	2.47808	-1.32545
H	-3.78312	1.50603	-2.39952
H	-4.52752	2.57651	-1.2079
H	3.31841	0.68939	-1.4723
H	0.25467	2.45485	0.95721
H	4.84232	2.54649	-0.8956
H	1.76664	4.31087	1.51671

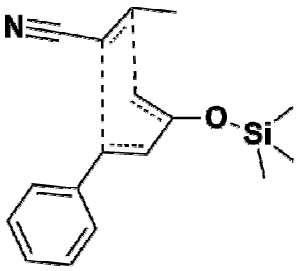
H	4.06613	4.3709	0.59305
C	0.07067	-2.30566	0.90665
C	1.15134	-1.43782	1.05806
C	2.46995	-1.71234	0.5203
C	3.71036	-2.99602	-1.02041
C	-1.10341	-2.14353	1.84102
O	3.5009	-1.15569	0.83395
O	2.4436	-2.66319	-0.45617
H	0.30389	-3.31938	0.59603
H	1.10916	-0.6156	1.76127
H	3.51394	-3.76586	-1.76293
H	4.16387	-2.12199	-1.48999
H	4.38528	-3.37301	-0.25123
H	-1.37038	-1.08663	1.92815
H	-1.9814	-2.69105	1.49581
H	-0.8391	-2.50339	2.83919



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1216.183292
Gibbs's free energies (G)	-1216.237802

C	1.00014	1.22785	1.99215
C	-0.27812	0.75278	2.24648
C	-0.63395	-0.58697	1.99813
C	0.26433	-1.50106	1.50434
C	-3.47484	3.22181	3.15064
C	-2.2014	3.18861	0.3546
C	-3.74987	0.71588	1.40703
C	-0.09655	-2.84639	1.05103
C	0.88793	-3.84007	0.9969
C	-1.39375	-3.16576	0.63054
C	0.58022	-5.12503	0.56997
C	-1.70259	-4.44975	0.2052
C	-0.71865	-5.43497	0.17739
O	-1.23687	1.6442	2.60525
Si	-2.65496	2.16706	1.85209
H	1.84306	0.57171	2.15961
H	1.17933	2.27867	2.18887
H	-1.68242	-0.84924	2.07536
H	1.32448	-1.33868	1.65437
H	-2.82897	4.05341	3.44115
H	-4.41279	3.63746	2.77257
H	-3.69999	2.63673	4.04527
H	-1.59932	4.05062	0.65439
H	-1.63403	2.60143	-0.36984
H	-3.10271	3.56548	-0.13794
H	-3.26187	0.03654	0.70707
H	-4.0268	0.15279	2.30252
H	-4.67143	1.07671	0.9404
H	1.9016	-3.59764	1.29961
H	-2.16073	-2.39862	0.61526
H	1.35338	-5.88366	0.53879

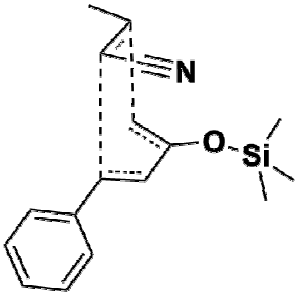
H	-2.70981	-4.68106	-0.12066
H	-0.96071	-6.43537	-0.16115
C	1.29635	1.09345	-0.05271
C	1.01627	-0.19307	-0.51017
C	-0.2202	-0.55484	-1.1784
C	-2.39579	0.13548	-1.75164
C	2.73832	1.55831	-0.06035
O	-0.38974	-1.53653	-1.86957
O	-1.21984	0.34838	-0.97262
H	0.55891	1.8559	-0.28047
H	1.81867	-0.90707	-0.65793
H	-3.06537	0.96009	-1.51265
H	-2.1526	0.13914	-2.81483
H	-2.86236	-0.81864	-1.50023
H	3.03895	1.799	-1.08327
H	2.88923	2.44756	0.55266
H	3.40196	0.77042	0.30425



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1080.607433
Gibbs's free energies (G)	-1080.661897

C	0.11445	1.58623	0.5693
C	-0.98781	0.94535	1.12611
C	-0.97655	-0.42779	1.4326
C	0.16264	-1.18572	1.30632
C	-4.41883	3.17406	1.72915
C	-2.78571	1.6948	3.91427
C	-1.54557	4.07274	2.41933
C	0.21744	-2.6493	1.38265
C	1.45928	-3.26903	1.57096
C	-0.92013	-3.45534	1.23582
C	1.56051	-4.65376	1.63252
C	-0.81827	-4.83746	1.30164
C	0.42198	-5.44194	1.50232
O	-2.20154	1.56675	1.09405
Si	-2.73256	2.63341	2.30098
H	1.11133	1.29096	0.86947
H	-0.00209	2.63317	0.30991
H	-1.94163	-0.89187	1.60852
H	1.1266	-0.69696	1.38429
H	-5.09363	2.32036	1.63621
H	-4.85816	3.87886	2.43984
H	-4.35711	3.66826	0.75681
H	-3.46823	0.84369	3.8518
H	-1.79412	1.31613	4.17674
H	-3.12306	2.34122	4.72878
H	-0.54738	3.7453	2.72094
H	-1.46094	4.59813	1.46471
H	-1.90084	4.78879	3.16592
H	2.34889	-2.65472	1.65898
H	-1.88788	-3.0007	1.05674
H	2.52947	-5.11635	1.77836
H	-1.70655	-5.44787	1.18863

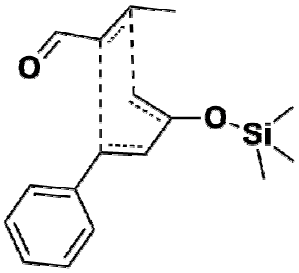
H	0.49857	-6.52184	1.54867
C	0.25126	0.68257	-1.25095
C	0.69476	-0.63194	-1.07176
C	2.07531	-0.90535	-0.90432
C	-1.12105	0.88962	-1.84236
N	3.1966	-1.11003	-0.70852
H	1.00666	1.41192	-1.52926
H	0.05095	-1.47759	-1.27475
H	-1.84877	0.23786	-1.35107
H	-1.46002	1.91954	-1.72957
H	-1.10821	0.64041	-2.90673



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1080.604779
Gibbs's free energies (G)	-1080.657879

C	0.04926	1.28076	1.50887
C	-1.03253	0.52334	1.95939
C	-1.00056	-0.88384	1.90799
C	0.0887	-1.56553	1.42806
C	-4.54248	2.53819	2.76956
C	-1.77561	3.5368	3.68709
C	-2.51592	3.5323	0.68164
C	0.11305	-3.00146	1.13718
C	1.34818	-3.65807	1.06041
C	-1.05558	-3.73662	0.89769
C	1.41725	-5.01669	0.78284
C	-0.9849	-5.0947	0.61614
C	0.2481	-5.73993	0.56219
O	-2.23908	1.0662	2.2178
Si	-2.74077	2.68131	2.3337
H	1.04186	0.89095	1.69024
H	-0.01315	2.36148	1.56185
H	-1.94291	-1.39275	2.07641
H	1.06329	-1.09229	1.44454
H	-4.67095	1.99299	3.7072
H	-4.99344	3.52703	2.88609
H	-5.08722	2.00481	1.98738
H	-1.89332	3.00683	4.63535
H	-0.70828	3.60641	3.46854
H	-2.15528	4.55356	3.82251
H	-1.46895	3.72232	0.43375
H	-2.9569	2.9341	-0.12014
H	-3.03039	4.49766	0.69524
H	2.25963	-3.09365	1.23029
H	-2.01793	-3.23966	0.90225
H	2.38039	-5.51091	0.73469

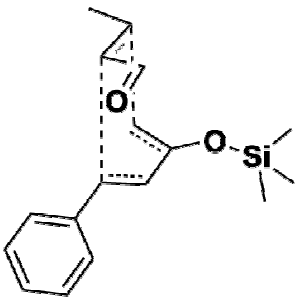
H	-1.89581	-5.64961	0.42547
H	0.29739	-6.79939	0.34016
C	0.17836	0.9693	-0.49054
C	0.12964	-0.39651	-0.8011
C	-1.09972	-1.00373	-1.15533
C	1.47753	1.70446	-0.74508
N	-2.1166	-1.48519	-1.42487
H	-0.72328	1.53475	-0.70822
H	1.03119	-0.94786	-1.03889
H	2.32896	1.10994	-0.40361
H	1.59973	1.87839	-1.81682
H	1.50831	2.671	-0.2401



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1101.671726
Gibbs's free energies (G)	-1101.725499

C	0.97274	1.98937	-1.3141
C	1.26458	0.67181	-0.97497
C	0.23985	-0.2651	-0.70784
C	-1.08784	0.03569	-0.86875
C	5.10597	-0.50014	-0.01035
C	2.70388	-1.15476	1.79572
C	2.96497	-2.47699	-0.99173
C	-2.19768	-0.79044	-0.39665
C	-3.47656	-0.57373	-0.92278
C	-2.03498	-1.77658	0.58838
C	-4.55653	-1.34252	-0.50561
C	-3.1122	-2.54368	1.00352
C	-4.3767	-2.33281	0.45322
O	2.54994	0.39558	-0.66953
Si	3.30169	-0.951	0.03425
H	0.09456	2.19627	-1.9078
H	1.81958	2.64346	-1.48916
H	0.51169	-1.19466	-0.22124
H	-1.37143	0.83457	-1.54272
H	5.28077	0.44107	0.51584
H	5.71018	-1.27482	0.46866
H	5.45445	-0.38519	-1.03908
H	3.01342	-0.30521	2.40958
H	1.61688	-1.24384	1.86665
H	3.14007	-2.058	2.23188
H	1.94776	-2.85787	-0.88359
H	3.13878	-2.27041	-2.05084
H	3.65065	-3.2746	-0.6915
H	-3.62114	0.20818	-1.6594
H	-1.06422	-1.93108	1.04668
H	-5.53938	-1.16233	-0.92428
H	-2.97254	-3.3012	1.76583

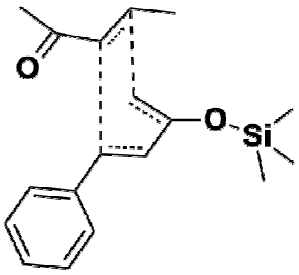
H	-5.21838	-2.93093	0.78202
C	0.18074	2.71857	0.40722
C	-1.0642	2.12898	0.66382
C	-2.25941	2.65967	0.06749
C	1.30165	2.50017	1.39529
O	-3.40588	2.30994	0.30499
H	0.14573	3.70822	-0.04549
H	-1.17768	1.36996	1.43037
H	-2.07929	3.45303	-0.69199
H	1.36038	1.44384	1.67091
H	2.26989	2.80616	0.99705
H	1.10363	3.06999	2.30719



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1101.671612
Gibbs's free energies (G)	-1101.724664

C	1.16692	1.98563	-1.30619
C	1.31016	0.63288	-1.01679
C	0.19062	-0.20862	-0.84365
C	-1.09312	0.25915	-0.97524
C	4.94512	-0.89043	0.22631
C	2.32137	-1.38199	1.75276
C	2.78733	-2.67272	-1.0293
C	-2.29945	-0.4838	-0.62396
C	-3.52424	-0.0892	-1.1784
C	-2.28714	-1.55066	0.28365
C	-4.69639	-0.76416	-0.86853
C	-3.45884	-2.22642	0.59352
C	-4.665	-1.83893	0.01632
O	2.54865	0.21585	-0.6737
Si	3.11672	-1.19772	0.07056
H	0.34751	2.30409	-1.93532
H	2.08495	2.55143	-1.41247
H	0.34666	-1.20677	-0.45061
H	-1.26766	1.16903	-1.53598
H	5.14239	-0.00159	0.82971
H	5.44036	-1.74086	0.70187
H	5.39689	-0.74134	-0.75714
H	2.47805	-0.47934	2.34952
H	1.24727	-1.57412	1.70664
H	2.78505	-2.21695	2.28624
H	3.18128	-2.49352	-2.03295
H	3.29749	-3.55118	-0.62367
H	1.7278	-2.91908	-1.12157
H	-3.54858	0.75334	-1.86184
H	-1.36352	-1.83406	0.77469
H	-5.6345	-0.4493	-1.30994

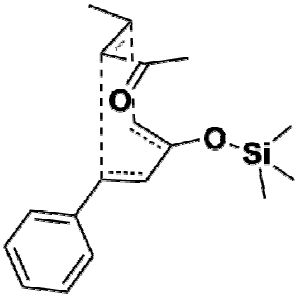
H	-3.43536	-3.0455	1.30219
H	-5.57942	-2.36349	0.26694
C	0.36289	2.81586	0.37417
C	-0.84881	2.20932	0.72049
C	-0.89309	1.165	1.71274
C	0.34153	4.25594	-0.09824
O	-1.89184	0.71878	2.255
H	1.21747	2.55085	0.99427
H	-1.79423	2.63891	0.40008
H	0.10584	0.75592	1.98127
H	0.12791	4.91397	0.74768
H	1.29294	4.56333	-0.53329
H	-0.44421	4.40608	-0.84237



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1140.955501
Gibbs's free energies (G)	-1141.011056

C	0.91581	1.96862	-1.19365
C	1.3338	0.67355	-0.91271
C	0.40194	-0.36144	-0.68107
C	-0.95186	-0.16702	-0.80345
C	5.28076	-0.19183	-0.04644
C	2.97215	-1.15347	1.74461
C	3.31712	-2.29698	-1.11414
C	-1.97723	-1.12296	-0.3855
C	-3.27533	-0.98514	-0.89004
C	-1.7193	-2.15882	0.52468
C	-4.28083	-1.87181	-0.52522
C	-2.72253	-3.04328	0.88943
C	-4.00656	-2.90598	0.362
O	2.64581	0.50298	-0.63275
Si	3.52361	-0.8036	-0.00872
H	0.02336	2.11054	-1.7847
H	1.69093	2.7145	-1.32912
H	0.76344	-1.28918	-0.25305
H	-1.31136	0.63363	-1.4391
H	5.38204	0.72778	0.53446
H	5.9613	-0.93676	0.37387
H	5.59663	0.01646	-1.0712
H	3.21	-0.31017	2.39787
H	1.89967	-1.34825	1.82148
H	3.49828	-2.03199	2.1293
H	2.33255	-2.76245	-1.03881
H	3.48191	-2.02164	-2.15902
H	4.0623	-3.05231	-0.84795
H	-3.49486	-0.17081	-1.57146
H	-0.73405	-2.2634	0.96555
H	-5.2796	-1.74818	-0.92635
H	-2.50997	-3.8373	1.59566

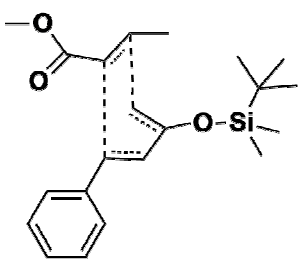
H	-4.78965	-3.59561	0.65402
C	0.02873	2.53836	0.57202
C	-1.13214	1.79553	0.80906
C	-2.45247	2.16731	0.32688
C	-2.56614	3.28346	-0.69918
C	1.17916	2.38299	1.53921
O	-3.46561	1.60265	0.72032
H	-0.10244	3.5366	0.1619
H	-1.1236	1.0111	1.5589
H	-2.36504	4.24721	-0.22349
H	-1.84959	3.16815	-1.5161
H	-3.57882	3.29385	-1.09797
H	0.94076	2.8803	2.48334
H	1.34537	1.32409	1.755
H	2.10773	2.80254	1.14962



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1140.963029
Gibbs's free energies (G)	-1141.016765

C	1.254	1.00087	-1.28226
C	1.01727	-0.31476	-0.87234
C	-0.2992	-0.83214	-0.75721
C	-1.40675	-0.08055	-1.00473
C	4.1009	-2.44144	0.81557
C	4.59393	-0.62998	-1.62164
C	3.74813	0.60789	1.09231
C	-2.78826	-0.47332	-0.71263
C	-3.82714	0.37726	-1.11256
C	-3.11816	-1.64325	-0.0142
C	-5.15246	0.07297	-0.82887
C	-4.44247	-1.94991	0.26584
C	-5.46515	-1.09371	-0.13751
O	1.9877	-1.13333	-0.44598
Si	3.61375	-0.86592	-0.04562
H	0.57586	1.40782	-2.02091
H	2.28519	1.30842	-1.41919
H	-0.37403	-1.80774	-0.29117
H	-1.31055	0.84912	-1.55223
H	3.93214	-3.30584	0.1694
H	5.1585	-2.42288	1.0914
H	3.51221	-2.57464	1.72599
H	4.45745	-1.48316	-2.29057
H	4.308	0.27438	-2.16329
H	5.65988	-0.55384	-1.38838
H	3.72601	1.55824	0.55318
H	2.92004	0.59014	1.8066
H	4.68958	0.563	1.64692
H	-3.58456	1.28975	-1.64789
H	-2.33766	-2.3135	0.32565
H	-5.94077	0.74517	-1.14663

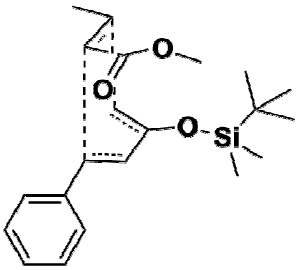
H	-4.67921	-2.85769	0.80832
H	-6.49748	-1.33424	0.08768
C	0.65384	2.28242	0.12787
C	-0.59292	1.92142	0.65258
C	-0.64861	0.89817	1.66212
C	-1.96789	0.62206	2.3528
C	0.7776	3.58138	-0.63771
O	0.35443	0.24302	1.96328
H	1.49026	2.03624	0.7741
H	-1.49902	2.43668	0.35272
H	-1.92305	1.03474	3.36446
H	-2.81608	1.06287	1.82731
H	-2.11364	-0.45625	2.438
H	1.72422	3.65242	-1.17647
H	-0.03745	3.69172	-1.35764
H	0.72475	4.4222	0.05835



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1334.006537
Gibbs's free energies (G)	-1334.068046

C	-0.47962	-1.81256	-0.03645
C	-0.86283	-0.5127	0.26021
C	0.04561	0.56054	0.17748
C	1.31181	0.4045	-0.33495
C	-4.07705	-0.02065	-1.14317
C	-4.5305	0.50501	1.89673
C	-2.79059	2.42727	0.24818
C	-5.44588	0.63825	-1.37774
C	-3.15576	0.29853	-2.33071
C	-4.25847	-1.54129	-1.04061
C	2.36745	1.41892	-0.25101
C	3.4357	1.37452	-1.15314
C	2.36032	2.42079	0.72939
C	4.45131	2.3219	-1.10233
C	3.37415	3.36582	0.78126
C	4.42165	3.3229	-0.13788
O	-2.03653	-0.32398	0.9302
Si	-3.34171	0.65118	0.46812
H	0.24937	-2.00094	-0.81272
H	-1.21318	-2.5944	0.12674
H	-0.22199	1.47424	0.69684
H	1.4846	-0.3819	-1.06257
H	-5.38107	1.17859	1.76512
H	-4.91322	-0.51264	2.00076
H	-4.02903	0.77374	2.82956
H	-2.38793	2.82827	1.1822
H	-2.03002	2.53386	-0.52824
H	-3.6477	3.04535	-0.03554
H	-5.87166	0.2821	-2.32321
H	-6.15536	0.39319	-0.5819
H	-5.36997	1.72844	-1.44295
H	-2.16034	-0.13758	-2.20208

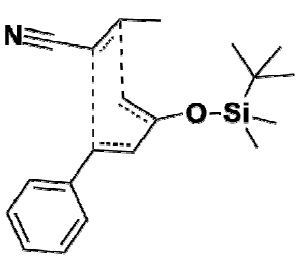
H	-3.58298	-0.11291	-3.25314
H	-3.03751	1.3765	-2.4736
H	-4.89944	-1.82116	-0.19917
H	-4.72578	-1.92413	-1.95569
H	-3.29771	-2.04746	-0.9177
H	3.46857	0.58481	-1.89605
H	1.56679	2.44838	1.46765
H	5.27064	2.27154	-1.80949
H	3.35588	4.13281	1.54673
H	5.21581	4.05865	-0.09103
C	0.93511	-2.18069	1.42381
C	2.06982	-1.41319	1.16155
C	3.08766	-1.81565	0.20502
C	3.56865	-3.17787	-1.65776
C	0.17401	-1.91489	2.69879
O	4.21436	-1.37482	0.13341
O	2.62397	-2.73651	-0.68402
H	0.95382	-3.2085	1.07511
H	2.36718	-0.61517	1.83001
H	3.04866	-3.91561	-2.26414
H	3.90042	-2.34247	-2.27609
H	4.43642	-3.62661	-1.17337
H	-0.00006	-0.84203	2.82002
H	-0.79308	-2.41841	2.70803
H	0.75423	-2.25927	3.55939



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1334.004292
Gibbs's free energies (G)	-1334.064094

C	0.45057	1.77659	-1.55829
C	0.70798	0.73706	-0.67126
C	-0.25889	-0.24994	-0.39941
C	-1.49661	-0.2259	-0.99435
C	3.78632	-1.0917	-0.80921
C	4.07478	0.71223	1.72144
C	2.0876	-1.61592	1.73717
C	4.81452	-2.11349	-0.29977
C	2.77873	-1.80548	-1.7232
C	4.50297	0.00133	-1.61422
C	-2.61461	-1.10375	-0.64029
C	-3.67651	-1.24245	-1.54258
C	-2.67699	-1.79547	0.57588
C	-4.75449	-2.0693	-1.25607
C	-3.75255	-2.62433	0.8622
C	-4.79331	-2.76695	-0.05233
O	1.81193	0.83866	0.1085
Si	2.9143	-0.308	0.67687
H	-0.14384	1.56696	-2.43711
H	1.23783	2.50959	-1.69422
H	-0.07524	-0.91605	0.43558
H	-1.6215	0.30284	-1.93129
H	4.88089	0.10081	2.13461
H	4.51977	1.52185	1.13928
H	3.53048	1.15989	2.55696
H	1.39997	-1.15782	2.45349
H	1.53611	-2.35801	1.15572
H	2.85339	-2.1477	2.30964
H	5.34992	-2.55749	-1.14705
H	5.55996	-1.65189	0.35528
H	4.33568	-2.92954	0.25029
H	2.06018	-1.10684	-2.16027

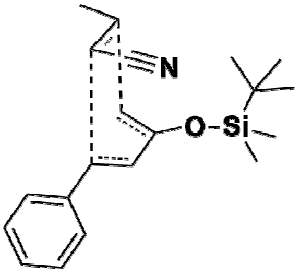
H	3.31134	-2.29379	-2.54835
H	2.21613	-2.5795	-1.19223
H	5.27502	0.50085	-1.02204
H	4.99091	-0.43923	-2.49169
H	3.79981	0.76177	-1.96759
H	-3.64739	-0.69681	-2.48038
H	-1.8926	-1.66993	1.31314
H	-5.56425	-2.16813	-1.96929
H	-3.78822	-3.15055	1.80873
H	-5.63457	-3.40996	0.1779
C	-1.04717	2.90519	-0.75056
C	-2.08001	2.10358	-0.25712
C	-2.0885	1.61292	1.10913
C	-0.75445	1.21119	3.0077
C	-1.33783	3.7902	-1.94368
O	-3.0256	1.1008	1.68703
O	-0.87673	1.76536	1.70447
H	-0.3743	3.32031	-0.0079
H	-3.01823	2.00416	-0.78982
H	0.27409	1.39318	3.31278
H	-1.44787	1.68968	3.70073
H	-0.96182	0.13874	2.99024
H	-1.93962	4.64768	-1.632
H	-0.42424	4.17038	-2.40319
H	-1.90403	3.2444	-2.70307



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1198.429519
Gibbs's free energies (G)	-1198.48674

C	0.63667	1.18686	1.09201
C	-0.27752	0.51992	1.90113
C	-0.31335	-0.8907	1.96305
C	0.59737	-1.66995	1.29696
C	-2.4277	0.79843	5.03453
C	-3.74662	2.50428	2.78354
C	-3.63352	-0.55179	2.51277
C	-3.73265	0.42218	5.75267
C	-1.37829	-0.29574	5.27757
C	-1.9038	2.13225	5.58578
C	0.48304	-3.12045	1.11849
C	1.61711	-3.84708	0.73432
C	-0.73045	-3.80457	1.27899
C	1.54775	-5.22168	0.54048
C	-0.79746	-5.17718	1.0888
C	0.34236	-5.89153	0.7219
O	-1.28196	1.25894	2.41664
Si	-2.76403	0.97086	3.18437
H	1.62667	0.77197	0.95934
H	0.57768	2.26943	1.08438
H	-1.17406	-1.35559	2.42801
H	1.56843	-1.25995	1.04937
H	-4.68185	2.53616	3.34885
H	-3.17267	3.40318	3.01842
H	-3.99482	2.52781	1.7192
H	-3.469	-0.67466	1.43922
H	-3.32907	-1.47355	3.01462
H	-4.70991	-0.43513	2.67012
H	-3.55393	0.33884	6.83092
H	-4.51153	1.17739	5.60706
H	-4.12339	-0.53999	5.40754
H	-0.42816	-0.06076	4.78899

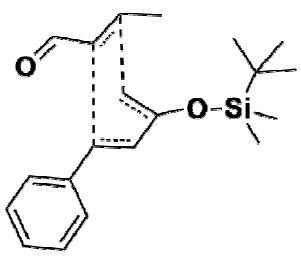
H	-1.18543	-0.39424	6.35217
H	-1.71349	-1.27337	4.91633
H	-2.64476	2.92977	5.47955
H	-1.67327	2.03201	6.65269
H	-0.98984	2.44556	5.07278
H	2.55431	-3.32304	0.58113
H	-1.63215	-3.25925	1.53566
H	2.4351	-5.76861	0.24476
H	-1.74225	-5.69234	1.21658
H	0.28636	-6.9628	0.56945
C	0.00575	0.68362	-0.77509
C	0.30835	-0.65926	-1.02519
C	1.61201	-1.04017	-1.42224
C	-1.44787	1.0888	-0.76488
N	2.69683	-1.34416	-1.68702
H	0.69812	1.41623	-1.17997
H	-0.4658	-1.41163	-1.09841
H	-2.03727	0.35603	-0.20644
H	-1.59553	2.06726	-0.306
H	-1.83404	1.1191	-1.78701



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1198.427802
Gibbs's free energies (G)	-1198.483819

C	0.10215	2.3331	-1.26874
C	0.52868	1.09648	-0.79529
C	-0.37538	0.02322	-0.63816
C	-1.71143	0.15598	-0.91649
C	3.52086	-1.22558	-0.6622
C	3.91455	0.97245	1.50385
C	1.64101	-1.07459	1.80921
C	4.26809	-2.34321	0.08067
C	2.46929	-1.84679	-1.59262
C	4.51678	-0.41337	-1.50241
C	-2.73169	-0.82782	-0.5446
C	-3.95826	-0.82953	-1.22142
C	-2.53845	-1.7414	0.5007
C	-4.95422	-1.7373	-0.88816
C	-3.53681	-2.64669	0.83509
C	-4.74433	-2.65178	0.1407
O	1.76994	1.03807	-0.27579
Si	2.68261	-0.09569	0.59984
H	-0.67369	2.3589	-2.0214
H	0.85354	3.11047	-1.34556
H	-0.03459	-0.85953	-0.11141
H	-2.04421	0.92479	-1.60331
H	4.69346	0.36635	1.97418
H	4.39392	1.67727	0.8209
H	3.41404	1.54472	2.28881
H	0.8194	-0.47802	2.21692
H	1.21984	-1.98216	1.36857
H	2.27599	-1.38362	2.6449
H	4.78513	-2.98932	-0.63841
H	5.02314	-1.94471	0.7658
H	3.58457	-2.97235	0.65871
H	1.92432	-1.08083	-2.15231

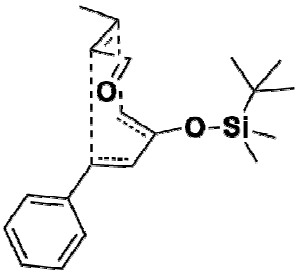
H	2.95807	-2.50614	-2.31963
H	1.73922	-2.4505	-1.04411
H	5.32047	-0.00035	-0.88607
H	4.97648	-1.05572	-2.26267
H	4.02316	0.41589	-2.01808
H	-4.12304	-0.11328	-2.02006
H	-1.62141	-1.71592	1.07814
H	-5.8942	-1.73021	-1.42712
H	-3.37838	-3.34267	1.6503
H	-5.52186	-3.3577	0.4076
C	-1.14237	3.09841	0.1694
C	-2.06099	2.14379	0.61708
C	-1.75275	1.33843	1.73942
C	-1.67453	4.2828	-0.60731
N	-1.46375	0.67649	2.64365
H	-0.3103	3.31038	0.83421
H	-3.09293	2.15483	0.28864
H	-2.42941	3.96057	-1.32927
H	-2.14697	4.99098	0.07793
H	-0.88467	4.80803	-1.14542



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1219.493517
Gibbs's free energies (G)	-1219.550699

C	0.41092	1.93055	-0.84607
C	0.66034	0.76296	-0.13126
C	-0.33952	-0.21105	0.06652
C	-1.56455	-0.13658	-0.54902
C	3.76471	-0.65748	-1.00127
C	4.18174	0.19554	1.96848
C	2.25763	-2.10355	1.29311
C	5.08118	-1.43833	-0.86175
C	2.82805	-1.41589	-1.95384
C	4.05808	0.7321	-1.58385
C	-2.72421	-0.96196	-0.21487
C	-3.78038	-1.05362	-1.12849
C	-2.83222	-1.64273	1.00701
C	-4.89929	-1.82874	-0.84721
C	-3.94861	-2.41463	1.28767
C	-4.98496	-2.5137	0.35916
O	1.77865	0.72017	0.63873
Si	2.97904	-0.47587	0.71245
H	-0.24959	1.89183	-1.70002
H	1.22259	2.64654	-0.91521
H	-0.17459	-0.92969	0.86153
H	-1.65195	0.41518	-1.47802
H	4.96573	-0.53432	2.18538
H	4.65712	1.11333	1.61471
H	3.66309	0.42224	2.90296
H	1.76334	-1.98569	2.26123
H	1.53753	-2.519	0.58502
H	3.06014	-2.83635	1.4196
H	5.53386	-1.58235	-1.84977
H	5.80508	-0.90322	-0.24045
H	4.92548	-2.43028	-0.42531
H	1.86711	-0.90634	-2.07383

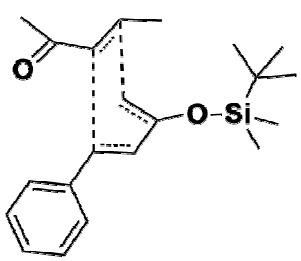
H	3.28981	-1.49187	-2.94558
H	2.63044	-2.43279	-1.60336
H	4.70602	1.32287	-0.92928
H	4.56528	0.63195	-2.55068
H	3.13608	1.2965	-1.74684
H	-3.72221	-0.50742	-2.06293
H	-2.04781	-1.55148	1.74978
H	-5.70766	-1.88856	-1.56591
H	-4.02051	-2.93276	2.23672
H	-5.85926	-3.11282	0.58498
C	-0.94309	2.88288	0.33179
C	-2.15241	2.17437	0.34654
C	-3.13804	2.39438	-0.67993
C	-0.18246	3.04833	1.62563
O	-4.27622	1.9539	-0.69519
H	-0.90913	3.73778	-0.34153
H	-2.45258	1.6005	1.21667
H	-2.7825	3.01621	-1.53161
H	-0.08382	2.08632	2.13519
H	0.81802	3.45151	1.4651
H	-0.72864	3.72471	2.28866



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1219.493263
Gibbs's free energies (G)	-1219.551177

C	0.50912	1.91471	-0.83747
C	0.6588	0.72413	-0.13363
C	-0.38137	-0.21932	-0.03616
C	-1.57658	-0.03676	-0.69049
C	3.78932	-0.68976	-0.87134
C	4.04353	0.03402	2.14823
C	2.14899	-2.22089	1.26876
C	5.0934	-1.48157	-0.68527
C	2.90817	-1.40754	-1.90495
C	4.12023	0.71891	-1.38341
C	-2.78092	-0.84358	-0.51722
C	-3.79963	-0.73826	-1.47348
C	-2.97925	-1.68757	0.58278
C	-4.96829	-1.47662	-1.35524
C	-4.14683	-2.42877	0.70015
C	-5.14234	-2.32914	-0.26853
O	1.71614	0.62656	0.71686
Si	2.9085	-0.57505	0.80118
H	-0.07233	1.91867	-1.74916
H	1.35267	2.59515	-0.82133
H	-0.27811	-0.99815	0.71153
H	-1.60319	0.62739	-1.54596
H	4.80684	-0.71241	2.3819
H	4.54779	0.9586	1.85777
H	3.47463	0.23236	3.05964
H	1.61018	-2.14173	2.21678
H	1.45934	-2.59641	0.50977
H	2.93814	-2.96769	1.39817
H	5.59613	-1.60226	-1.65201
H	5.78615	-0.96721	-0.01287
H	4.91042	-2.4835	-0.28361
H	1.95206	-0.89608	-2.05236

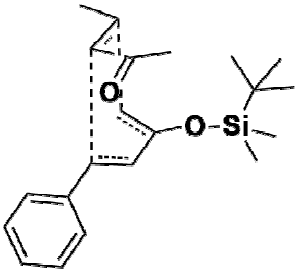
H	3.42267	-1.43759	-2.87294
H	2.69813	-2.43969	-1.61086
H	4.7221	1.28533	-0.66641
H	4.69177	0.6524	-2.31676
H	3.21108	1.28991	-1.58834
H	-3.66489	-0.06867	-2.31686
H	-2.22819	-1.7514	1.36131
H	-5.74451	-1.38416	-2.10559
H	-4.28879	-3.07516	1.55793
H	-6.05592	-2.90342	-0.16971
C	-0.9018	2.98322	0.16618
C	-2.08782	2.25396	0.30491
C	-2.37042	1.53215	1.52379
C	-0.90848	4.21133	-0.72202
O	-3.44979	1.07091	1.85479
H	-0.29457	3.06955	1.06514
H	-2.9067	2.39184	-0.39597
H	-1.49029	1.41104	2.19178
H	-1.44775	5.02063	-0.22359
H	0.0983	4.56561	-0.94606
H	-1.41992	4.00204	-1.66455



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1258.778288
Gibbs's free energies (G)	-1258.838175

C	0.17251	1.95659	-1.17683
C	0.59045	0.66778	-0.86928
C	-0.33974	-0.36872	-0.63742
C	-1.69208	-0.18247	-0.78311
C	4.53569	-0.11551	0.10133
C	2.18522	-1.59452	1.4773
C	2.73265	-2.0917	-1.52167
C	5.55243	-1.23706	0.36115
C	4.9449	0.65823	-1.15975
C	4.50958	0.84314	1.3013
C	-2.71899	-1.13413	-0.35964
C	-4.00497	-1.02697	-0.90103
C	-2.47462	-2.13301	0.5944
C	-5.01062	-1.91145	-0.53164
C	-3.47831	-3.01503	0.96411
C	-4.74892	-2.91118	0.39799
O	1.89379	0.50892	-0.54798
Si	2.81432	-0.85055	-0.12741
H	-0.71214	2.08586	-1.78237
H	0.9465	2.70391	-1.3115
H	0.02035	-1.28294	-0.17897
H	-2.04623	0.60521	-1.438
H	3.0014	-2.10759	1.99423
H	1.80414	-0.82099	2.14899
H	1.39316	-2.32936	1.31629
H	1.70049	-2.38841	-1.72527
H	3.15165	-1.68134	-2.44332
H	3.29335	-2.99414	-1.26311
H	6.54882	-0.80626	0.51277
H	5.3074	-1.81703	1.25622
H	5.61757	-1.92793	-0.48479
H	4.23917	1.46362	-1.37683

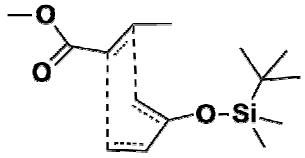
H	5.9371	1.10252	-1.01841
H	4.99784	0.00561	-2.03636
H	4.25932	0.32084	2.22975
H	5.49525	1.304	1.43509
H	3.7799	1.64473	1.15451
H	-4.21387	-0.23912	-1.61631
H	-1.50084	-2.20703	1.06599
H	-6.0001	-1.81227	-0.9617
H	-3.27769	-3.77999	1.70515
H	-5.53252	-3.59851	0.69406
C	-0.74128	2.55045	0.56724
C	-1.89457	1.79679	0.80642
C	-3.21554	2.14615	0.30932
C	-3.33426	3.24223	-0.73784
C	0.40432	2.43346	1.54575
O	-4.22562	1.57897	0.70675
H	-0.88257	3.53861	0.13642
H	-1.88208	1.02311	1.56732
H	-3.15639	4.21742	-0.27629
H	-2.6055	3.12572	-1.54378
H	-4.34197	3.22795	-1.14901
H	0.14645	2.93593	2.48192
H	0.59872	1.38201	1.77472
H	1.32453	2.87207	1.15755



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1258.778623
Gibbs's free energies (G)	-1258.837907

C	0.5784	1.75219	-1.0601
C	0.6999	0.60642	-0.28382
C	-0.35167	-0.31878	-0.16327
C	-1.54381	-0.149	-0.83099
C	4.01339	-0.62056	-0.80299
C	3.88361	-0.12004	2.26885
C	2.15283	-2.32572	0.99678
C	5.27861	-1.45098	-0.53693
C	3.25648	-1.22271	-1.99644
C	4.41493	0.82274	-1.1364
C	-2.74398	-0.95984	-0.62063
C	-3.72893	-0.9863	-1.61563
C	-2.96546	-1.68005	0.55975
C	-4.88641	-1.73509	-1.45332
C	-4.12179	-2.42996	0.72246
C	-5.08413	-2.46288	-0.2832
O	1.73122	0.546	0.609
Si	2.9315	-0.64014	0.75261
H	0.02981	1.69656	-1.9901
H	1.41189	2.445	-1.05085
H	-0.26772	-1.06561	0.61876
H	-1.55627	0.44881	-1.73488
H	4.65143	-0.85672	2.51791
H	4.37147	0.84648	2.12284
H	3.20993	-0.03243	3.1246
H	1.52575	-2.33833	1.8923
H	1.54031	-2.62567	0.14343
H	2.93402	-3.07997	1.12943
H	5.90185	-1.4782	-1.43852
H	5.88165	-1.02258	0.26893
H	5.04098	-2.48612	-0.27181
H	2.33783	-0.67047	-2.21758

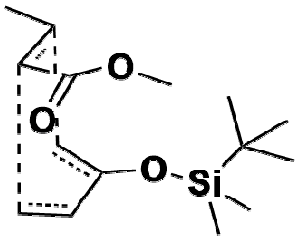
H	3.88794	-1.18898	-2.89248
H	2.98948	-2.26854	-1.82022
H	4.94462	1.30171	-0.30746
H	5.08092	0.83417	-2.00728
H	3.53944	1.43154	-1.37587
H	-3.57705	-0.41501	-2.52589
H	-2.24458	-1.63063	1.36783
H	-5.63592	-1.74812	-2.23577
H	-4.28304	-2.97511	1.6448
H	-5.99017	-3.04206	-0.14978
C	-0.9167	2.89258	-0.218
C	-2.06206	2.12718	0.01799
C	-2.39962	1.56162	1.32156
C	-1.32311	1.5129	2.39098
C	-0.97942	3.96286	-1.2886
O	-3.52684	1.15826	1.57075
H	-0.31109	3.14671	0.64716
H	-2.88779	2.16923	-0.68725
H	-0.34198	1.24581	1.99422
H	-1.23574	2.5021	2.85144
H	-1.6254	0.8023	3.1594
H	-1.49024	3.58686	-2.17858
H	-1.54567	4.82185	-0.91981
H	0.01092	4.31389	-1.58182



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1103.065161
Gibbs's free energies (G)	-1103.120164

C	0.77737	0.33418	-1.00903
C	-0.02116	-0.15958	0.00442
C	0.46813	-0.27386	1.32542
C	1.70591	0.20175	1.66289
C	-3.27809	1.16495	-0.22226
C	-3.72073	-1.87948	-0.71221
C	-2.83512	-0.88586	2.05829
C	-4.80302	1.26442	-0.06168
C	-2.60586	2.18592	0.7081
C	-2.89883	1.48114	-1.67564
O	-1.15318	-0.83894	-0.34234
Si	-2.72977	-0.59633	0.20991
H	1.52028	1.09242	-0.80589
H	0.38483	0.30166	-2.01931
H	-0.05333	-0.95123	1.99351
H	2.13777	1.04958	1.14673
H	-4.75396	-1.91041	-0.3578
H	-3.73331	-1.67786	-1.7857
H	-3.28288	-2.86942	-0.5631
H	-2.4919	-1.89197	2.31348
H	-2.24009	-0.16661	2.62501
H	-3.87285	-0.79709	2.39303
H	-5.13436	2.28829	-0.27136
H	-5.32711	0.59896	-0.75391
H	-5.12445	1.01914	0.95583
H	-1.51451	2.13208	0.6513
H	-2.90519	3.20188	0.42388
H	-2.89847	2.03578	1.75111
H	-3.33822	0.76676	-2.37855
H	-3.26103	2.47936	-1.94859
H	-1.8147	1.4685	-1.81388
C	2.32278	-1.13059	-1.02804
C	3.06154	-1.00951	0.14432

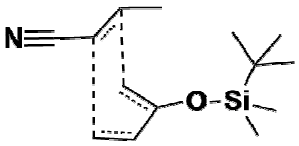
C	4.16597	-0.06114	0.28364
C	5.13931	1.91219	-0.54513
C	1.53732	-2.39606	-1.25637
O	5.0385	-0.10841	1.11641
O	4.08714	0.95237	-0.61947
H	2.70078	-0.61589	-1.90458
H	3.07544	-1.81549	0.86621
H	4.94104	2.63411	-1.33379
H	5.14377	2.40097	0.43008
H	6.10558	1.43118	-0.70067
H	0.97408	-2.66006	-0.35675
H	0.8277	-2.29511	-2.078
H	2.21613	-3.2239	-1.48094
H	2.14236	-0.02987	2.62738



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1103.063414
Gibbs's free energies (G)	-1103.118803

C	0.50593	1.39133	1.00866
C	-0.61421	0.67326	1.38831
C	-0.58103	-0.73949	1.43751
C	0.55047	-1.43015	1.10323
C	-2.83085	1.47062	4.15191
C	-4.34609	2.43563	1.60603
C	-3.9667	-0.56266	2.10927
C	-4.08986	1.1892	4.98625
C	-1.69137	0.56095	4.63479
C	-2.41255	2.93675	4.332
O	-1.79519	1.33683	1.43852
Si	-3.2143	1.14158	2.32956
H	1.48288	1.02272	1.28517
H	0.40751	2.46747	0.92578
H	-1.52556	-1.26892	1.49484
H	1.53741	-1.00234	1.21083
H	-5.27725	2.50895	2.174
H	-3.86618	3.41655	1.60414
H	-4.60021	2.18189	0.57373
H	-3.93483	-0.87013	1.06089
H	-3.47266	-1.33016	2.70953
H	-5.01702	-0.52946	2.41397
H	-3.89557	1.41399	6.04152
H	-4.93793	1.80506	4.67011
H	-4.39035	0.13898	4.92227
H	-0.75466	0.77443	4.11295
H	-1.52034	0.7206	5.70624
H	-1.92102	-0.49978	4.49212
H	-3.22213	3.62284	4.06677
H	-2.1468	3.12594	5.37877
H	-1.54222	3.18318	3.71588
C	0.89367	0.81876	-0.98494

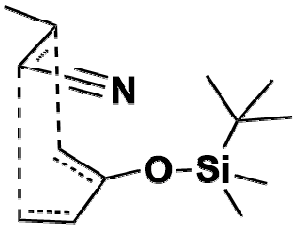
C	0.85047	-0.56813	-1.11316
C	-0.35807	-1.27313	-1.52696
C	-2.69558	-1.13284	-1.72773
C	2.22332	1.52107	-1.1428
O	-0.41818	-2.42334	-1.90885
O	-1.45966	-0.49541	-1.4207
H	0.0201	1.36324	-1.3253
H	1.76495	-1.13995	-1.21701
H	-3.46443	-0.37742	-1.58018
H	-2.70217	-1.48511	-2.75974
H	-2.86109	-1.98335	-1.0633
H	2.48944	1.57647	-2.20185
H	2.19891	2.53837	-0.75027
H	3.0175	0.97252	-0.62964
H	0.51487	-2.50684	0.98329



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-967.487451
Gibbs's free energies (G)	-967.538887

C	0.06296	1.24941	1.96646
C	-1.08265	0.50429	2.19219
C	-1.07013	-0.90371	2.05947
C	0.09158	-1.58612	1.83056
C	-2.73949	1.78616	5.02926
C	-4.81049	2.21368	2.74065
C	-4.09103	-0.64076	3.65064
C	-3.88614	2.09304	6.00572
C	-1.79638	0.75677	5.67016
C	-1.95925	3.07697	4.7435
O	-2.27825	1.15336	2.2132
Si	-3.47038	1.1102	3.41817
H	1.02829	0.84631	2.23961
H	-0.02664	2.32952	1.99719
H	-2.02662	-1.39787	1.92323
H	1.04838	-1.21531	2.1717
H	-4.4687	3.24828	2.66101
H	-5.10794	1.87858	1.74432
H	-5.69555	2.19485	3.38134
H	-4.50212	-1.03322	2.71672
H	-3.30273	-1.31603	3.99013
H	-4.88994	-0.65735	4.39783
H	-3.47719	2.46195	6.95358
H	-4.55846	2.86181	5.6141
H	-4.48206	1.20268	6.23115
H	-0.97272	0.48569	5.00267
H	-1.35904	1.1732	6.58542
H	-2.32619	-0.15965	5.94469
H	-2.58562	3.83764	4.26772
H	-1.57965	3.49868	5.68162
H	-1.10252	2.88753	4.09168
C	0.39462	0.85393	-0.05383
C	0.84484	-0.4622	-0.18205

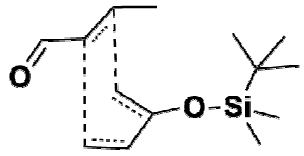
C	2.22143	-0.76029	0.01013
C	-0.92347	1.2181	-0.68602
N	3.33303	-0.99641	0.2187
H	1.15311	1.62993	-0.02948
H	0.25766	-1.20159	-0.70931
H	-1.67619	0.45791	-0.45838
H	-1.29408	2.17894	-0.32872
H	-0.81305	1.267	-1.77285
H	0.06413	-2.63878	1.5727



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-967.485302
Gibbs's free energies (G)	-967.535596

C	0.49673	1.51969	1.24308
C	-0.4437	0.8827	2.03773
C	-0.36601	-0.51424	2.25844
C	0.60618	-1.27084	1.67105
C	-2.74746	1.31733	4.99694
C	-4.10721	2.6631	2.5501
C	-3.74581	-0.38799	2.59213
C	-4.05299	0.93137	5.70861
C	-1.63895	0.33591	5.40268
C	-2.3387	2.73756	5.4119
O	-1.54334	1.58489	2.37454
Si	-3.02826	1.25508	3.12775
H	1.51937	1.17115	1.26774
H	0.36068	2.57984	1.06465
H	-1.21567	-1.01202	2.71083
H	1.55626	-0.85859	1.36234
H	-5.05748	2.67723	3.09064
H	-3.61134	3.6241	2.70295
H	-4.32796	2.55914	1.48497
H	-3.48702	-0.62316	1.55576
H	-3.42154	-1.22264	3.21852
H	-4.83638	-0.33284	2.66058
H	-3.91637	0.98501	6.79509
H	-4.87391	1.60648	5.44746
H	-4.36166	-0.08938	5.46373
H	-0.68322	0.58835	4.93391
H	-1.4949	0.36569	6.48931
H	-1.88653	-0.69619	5.13427
H	-3.13115	3.46166	5.20245
H	-2.13534	2.76929	6.48877
H	-1.43389	3.06282	4.88985
C	0.24513	0.72927	-0.67764
C	0.10398	-0.65983	-0.64191

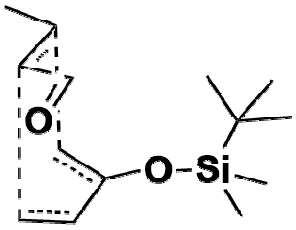
C	-1.19745	-1.22677	-0.58937
C	1.49397	1.30535	-1.30484
N	-2.26943	-1.65406	-0.52389
H	-0.665	1.30371	-0.81663
H	0.90729	-1.31042	-0.96374
H	2.37517	0.73236	-1.00416
H	1.41843	1.25503	-2.39414
H	1.64949	2.34785	-1.02518
H	0.55656	-2.35228	1.72817



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-988.551975
Gibbs's free energies (G)	-988.602601

C	0.17991	1.22485	1.23789
C	-0.94874	0.43192	1.36478
C	-0.85592	-0.97741	1.30266
C	0.35412	-1.60798	1.22537
C	-2.99177	1.90583	3.8674
C	-4.8271	1.87739	1.3507
C	-3.97132	-0.7753	2.66253
C	-4.26282	2.19552	4.68134
C	-2.03299	1.05563	4.71524
C	-2.30598	3.23217	3.51086
O	-2.16794	1.0161	1.20905
Si	-3.47846	0.99041	2.28333
H	1.11929	0.87924	1.64362
H	0.04167	2.29949	1.20651
H	-1.76508	-1.52341	1.07324
H	1.24745	-1.17646	1.65565
H	-5.77069	1.84013	1.90081
H	-4.5735	2.92602	1.17922
H	-4.9844	1.4049	0.37816
H	-4.27508	-1.30051	1.75328
H	-3.15928	-1.33752	3.12924
H	-4.82233	-0.78315	3.35001
H	-3.99751	2.69788	5.61896
H	-4.94971	2.85057	4.13772
H	-4.80067	1.27845	4.94146
H	-1.12009	0.8009	4.16777
H	-1.73743	1.6138	5.61169
H	-2.50135	0.12414	5.04546
H	-2.94075	3.86645	2.88496
H	-2.07661	3.79124	4.42568
H	-1.36705	3.06228	2.97796
C	0.77269	0.76637	-0.71703
C	1.17401	-0.57157	-0.78761

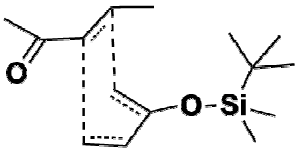
C	2.55306	-0.9274	-0.51748
C	-0.43559	1.20971	-1.50329
O	3.06798	-2.00873	-0.73067
H	1.56828	1.50037	-0.60926
H	0.57158	-1.29974	-1.3186
H	3.15655	-0.11319	-0.05994
H	-1.26687	0.51782	-1.34385
H	-0.76668	2.20905	-1.21999
H	-0.20155	1.21069	-2.57169
H	0.41326	-2.66533	0.99512



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-988.551281
Gibbs's free energies (G)	-988.602575

C	-1.11058	1.4467	-0.25371
C	-0.51536	0.19784	-0.23039
C	-1.07296	-0.88903	-0.93986
C	-2.19241	-0.73606	-1.70926
C	3.00279	0.57231	-0.44866
C	2.58758	-0.80272	2.31972
C	1.95098	-2.33894	-0.26704
C	4.48319	0.16437	-0.38518
C	2.54532	0.57868	-1.91528
C	2.83919	1.98265	0.13486
O	0.41063	-0.05319	0.73457
Si	1.98285	-0.66131	0.56251
H	-1.60036	1.7844	-1.1559
H	-0.67805	2.21801	0.37233
H	-0.7459	-1.88532	-0.66223
H	-2.45056	0.20973	-2.16493
H	3.58023	-1.25798	2.35883
H	2.64077	0.17512	2.80353
H	1.9074	-1.42956	2.9013
H	1.34304	-3.04274	0.3076
H	1.55627	-2.29519	-1.28434
H	2.96554	-2.74472	-0.31976
H	5.08691	0.86075	-0.97889
H	4.86637	0.18518	0.63922
H	4.6478	-0.83886	-0.79085
H	1.49277	0.86108	-2.01205
H	3.13791	1.30446	-2.48516
H	2.679	-0.39902	-2.38681
H	3.1588	2.0317	1.17998
H	3.45049	2.69431	-0.43258
H	1.79983	2.3179	0.08241
C	-2.98206	1.14452	0.64468
C	-3.71234	0.18712	-0.06126

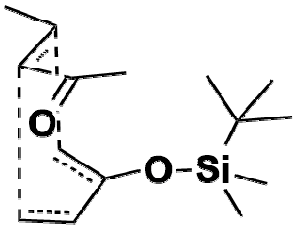
C	-3.84644	-1.16834	0.44553
C	-3.43948	2.5872	0.6072
O	-4.70201	-1.96898	0.11848
H	-2.54302	0.81814	1.58474
H	-4.44054	0.50278	-0.8038
H	-3.08513	-1.44733	1.20408
H	-4.33486	2.70294	1.22351
H	-2.68087	3.27255	0.98583
H	-3.69862	2.88385	-0.41184
H	-2.70871	-1.60437	-2.10186



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1027.837390
Gibbs's free energies (G)	-1027.891416

C	0.06163	1.18735	0.97303
C	-1.07226	0.41397	1.13888
C	-1.00462	-0.99576	1.06481
C	0.19285	-1.64258	0.92105
C	-2.96483	1.7957	3.77628
C	-4.89419	1.99458	1.33805
C	-4.12148	-0.76261	2.46646
C	-4.18928	2.11536	4.64853
C	-2.03438	0.84559	4.54561
C	-2.21162	3.09666	3.46518
O	-2.28895	1.02138	1.03943
Si	-3.55422	0.99596	2.16414
H	1.01036	0.82248	1.33766
H	-0.05604	2.26433	0.93757
H	-1.93151	-1.5276	0.87678
H	1.10855	-1.2289	1.32368
H	-5.81742	1.96834	1.92207
H	-4.59706	3.03855	1.21493
H	-5.10868	1.58548	0.34778
H	-4.47157	-1.22183	1.53818
H	-3.32791	-1.38786	2.8814
H	-4.95557	-0.76768	3.17441
H	-3.8626	2.54753	5.60178
H	-4.85238	2.83971	4.16658
H	-4.77409	1.21903	4.87872
H	-1.15098	0.57431	3.95925
H	-1.68656	1.33098	5.46549
H	-2.54724	-0.07679	4.83227
H	-2.82757	3.80063	2.89736
H	-1.91775	3.59093	4.39877
H	-1.3037	2.90012	2.88923
C	0.59525	0.68366	-1.03127
C	0.95006	-0.664	-1.09468

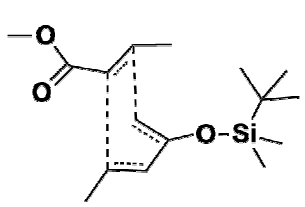
C	2.32124	-1.15456	-0.92035
C	3.36424	-0.21045	-0.35202
C	-0.64687	1.13501	-1.75818
O	2.62948	-2.29724	-1.21787
H	1.3959	1.41304	-0.95329
H	0.29004	-1.35883	-1.60243
H	3.62323	0.5446	-1.09894
H	2.99796	0.31778	0.53175
H	4.2564	-0.77932	-0.09808
H	-0.48124	1.09827	-2.83873
H	-1.48301	0.46958	-1.52583
H	-0.93645	2.15041	-1.48611
H	0.22465	-2.70072	0.68961



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1027.837361
Gibbs's free energies (G)	-1027.889925

C	0.06097	1.23815	0.99713
C	-1.05207	0.4429	1.19118
C	-0.96407	-0.96329	1.10607
C	0.22907	-1.58042	0.83234
C	-2.86409	1.74342	3.9197
C	-4.8786	1.98828	1.55425
C	-4.06088	-0.78947	2.59427
C	-4.05689	2.03908	4.84282
C	-1.90494	0.77859	4.63305
C	-2.12583	3.05364	3.61198
O	-2.28494	1.03011	1.1423
Si	-3.50837	0.97698	2.31148
H	1.02523	0.89108	1.33912
H	-0.07911	2.31238	0.9683
H	-1.89138	-1.516	0.99666
H	1.17304	-1.14539	1.13114
H	-5.77876	1.95366	2.17283
H	-4.58477	3.03387	1.43674
H	-5.13247	1.59605	0.56653
H	-4.42749	-1.23307	1.66466
H	-3.25617	-1.41828	2.9813
H	-4.88022	-0.81217	3.3189
H	-3.69654	2.4492	5.79365
H	-4.73866	2.7728	4.40293
H	-4.63154	1.13601	5.07254
H	-1.04499	0.52007	4.00768
H	-1.52213	1.24466	5.54903
H	-2.40678	-0.14979	4.9198
H	-2.76325	3.76846	3.08276
H	-1.8005	3.5272	4.54595
H	-1.23809	2.87384	3.00024
C	0.73848	0.80864	-0.99685
C	0.80123	-0.57004	-1.19123

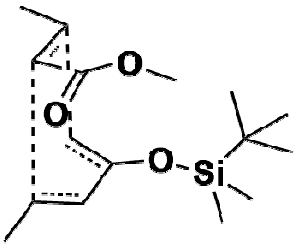
C	-0.23834	-1.33095	-1.90094
C	-1.59047	-0.67819	-2.10165
C	2.02646	1.59693	-0.91755
O	-0.0199	-2.44732	-2.3418
H	-0.10756	1.33899	-1.42181
H	1.76946	-1.06184	-1.15868
H	-1.9024	-0.09225	-1.23507
H	-1.52902	0.00139	-2.9573
H	-2.3271	-1.44911	-2.32241
H	2.7727	1.06032	-0.3261
H	2.43898	1.7372	-1.92044
H	1.8803	2.5833	-0.47488
H	0.25406	-2.63851	0.59877



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1142.348839
Gibbs's free energies (G)	-1142.404193

C	0.90198	-0.96879	-1.21045
C	0.0729	0.07918	-0.83923
C	0.60327	1.31769	-0.4006
C	1.94515	1.57545	-0.4077
C	-3.95237	-0.61664	-0.15737
C	-2.16966	0.86493	1.90181
C	-2.83797	2.21363	-0.79859
C	-5.15842	-0.15191	0.67261
C	-4.33965	-0.66744	-1.64232
C	-3.52481	-2.01739	0.30366
O	-1.2353	-0.21199	-0.66314
Si	-2.52422	0.59158	0.08225
H	1.85033	-0.76481	-1.68786
H	0.41604	-1.89446	-1.49821
H	-0.055	2.01002	0.1163
H	2.58533	1.01672	-1.08118
H	-2.94426	1.50527	2.33394
H	-2.16841	-0.07817	2.45395
H	-1.2064	1.35312	2.06798
H	-2.1307	2.9924	-0.50513
H	-2.76583	2.08057	-1.88091
H	-3.84362	2.57901	-0.57061
H	-6.00403	-0.83083	0.51327
H	-4.93415	-0.14839	1.74341
H	-5.48794	0.85329	0.39076
H	-3.48955	-0.95847	-2.26609
H	-5.13778	-1.40294	-1.79652
H	-4.70701	0.30036	-1.99631
H	-3.22643	-2.02754	1.35689
H	-4.35974	-2.71872	0.19005
H	-2.68521	-2.38779	-0.28953
C	1.77866	-1.44958	0.57298
C	2.63477	-0.42428	0.98088

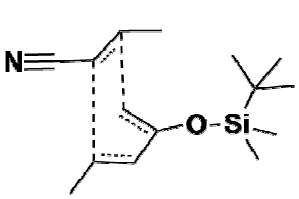
C	3.98598	-0.27487	0.48841
C	5.53721	-0.91664	-1.16787
C	0.58968	-1.76888	1.44735
O	4.84134	0.45261	0.9565
O	4.21768	-1.00882	-0.63456
H	2.24406	-2.29374	0.07369
H	2.39172	0.19104	1.838
H	5.54338	-1.54328	-2.05659
H	5.77667	0.11515	-1.42739
H	6.26814	-1.27842	-0.44372
H	0.09518	-0.84624	1.76328
H	-0.14571	-2.38835	0.93172
H	0.91878	-2.29579	2.34732
C	2.55944	2.78153	0.22558
H	3.44447	2.49085	0.79971
H	2.89572	3.48657	-0.54108
H	1.85449	3.29122	0.88411



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1142.345567
Gibbs's free energies (G)	-1142.401497

C	0.56109	1.87655	-0.27376
C	0.09455	0.62318	0.09777
C	0.71358	-0.11422	1.12955
C	1.78884	0.36947	1.82568
C	-3.43307	0.56793	0.3417
C	-2.84031	-1.35104	-2.04538
C	-2.04157	-2.16951	0.80224
C	-4.8542	-0.01391	0.40006
C	-2.99543	0.96682	1.75929
C	-3.42989	1.8149	-0.55411
O	-0.78301	-0.0005	-0.732
Si	-2.26394	-0.73509	-0.38229
H	0.94225	2.53732	0.49248
H	0.06275	2.36177	-1.10539
H	0.47295	-1.17066	1.20319
H	1.95148	1.43916	1.88401
H	-3.78322	-1.89681	-1.96102
H	-2.98187	-0.5266	-2.74757
H	-2.09551	-2.02911	-2.46938
H	-1.30738	-2.87972	0.41181
H	-1.71655	-1.8498	1.79437
H	-2.98956	-2.70338	0.91678
H	-5.54125	0.72338	0.83175
H	-5.22896	-0.27099	-0.59494
H	-4.90221	-0.91151	1.02485
H	-1.98658	1.38961	1.77002
H	-3.67941	1.72587	2.15776
H	-3.01306	0.11481	2.44483
H	-3.73644	1.58207	-1.57823
H	-4.1304	2.56036	-0.15934
H	-2.43801	2.27349	-0.5935
C	2.45082	1.58741	-1.01678

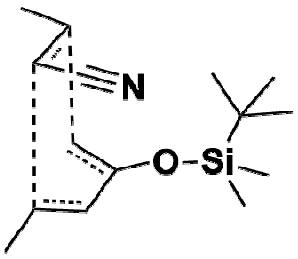
C	3.21448	0.80042	-0.15135
C	3.32262	-0.64001	-0.29721
C	2.33164	-2.5584	-1.23044
C	2.84056	3.03979	-1.19243
O	4.13164	-1.35728	0.25959
O	2.37996	-1.13983	-1.13312
H	2.07386	1.0903	-1.90408
H	3.96022	1.25233	0.49247
H	1.50743	-2.78244	-1.90389
H	3.26742	-2.95164	-1.6296
H	2.15309	-3.00223	-0.24873
H	3.73122	3.10914	-1.82228
H	2.0487	3.62269	-1.66495
H	3.07784	3.49776	-0.2287
C	2.57571	-0.46612	2.78524
H	2.37147	-1.52832	2.64457
H	3.64714	-0.31229	2.64165
H	2.3325	-0.19198	3.81681



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1006.769600
Gibbs's free energies (G)	-1006.823117

C	-1.09621	-0.73209	1.19401
C	-0.43074	-0.15295	0.12286
C	-1.0174	0.88559	-0.63411
C	-2.207	1.45853	-0.27297
C	2.94492	0.40474	0.93579
C	3.10773	-1.71531	-1.34567
C	2.15438	1.13418	-1.97493
C	4.44733	0.65243	0.72564
C	2.27539	1.71681	1.37142
C	2.7533	-0.64847	2.0363
O	0.64209	-0.81407	-0.38964
Si	2.20217	-0.2249	-0.68829
H	-1.72897	-0.12167	1.82391
H	-0.61323	-1.57095	1.68291
H	-0.61062	1.0726	-1.62403
H	-2.50877	1.44314	0.76789
H	3.194	-2.49819	-0.5888
H	2.57262	-2.13166	-2.20254
H	4.11411	-1.44583	-1.6754
H	1.67691	0.77805	-2.89172
H	1.61899	2.02141	-1.6303
H	3.17422	1.43723	-2.23026
H	4.89327	1.03598	1.65073
H	4.97694	-0.26699	0.45955
H	4.63347	1.39273	-0.05897
H	1.20143	1.59109	1.53787
H	2.71828	2.06442	2.31258
H	2.41347	2.50841	0.62959
H	3.21781	-1.60347	1.77312
H	3.21415	-0.30192	2.96884
H	1.69348	-0.82944	2.23449
C	-2.70222	-1.59997	0.24247
C	-3.5602	-0.59257	-0.21159

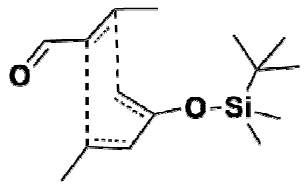
C	-4.52895	-0.02664	0.65574
C	-2.03804	-2.47967	-0.78643
N	-5.28225	0.47026	1.37908
H	-2.96699	-2.07685	1.18123
H	-3.6945	-0.41138	-1.27007
H	-1.62718	-1.8708	-1.59661
H	-1.22338	-3.06152	-0.35525
H	-2.7709	-3.16712	-1.21746
C	-2.95352	2.4202	-1.14376
H	-4.03117	2.25968	-1.05812
H	-2.76104	3.4485	-0.82189
H	-2.66047	2.32489	-2.19031



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1006.767851
Gibbs's free energies (G)	-1006.820557

C	1.53787	-1.38098	-1.30311
C	0.58996	-0.47225	-0.85244
C	0.88208	0.9107	-0.77857
C	2.10437	1.41359	-1.12392
C	-3.12492	0.21816	-0.53706
C	-2.36348	-1.8988	1.60484
C	-1.26506	0.96248	1.84827
C	-4.28425	0.82951	0.2641
C	-2.54506	1.28049	-1.48129
C	-3.64311	-0.96479	-1.36706
O	-0.50387	-0.98177	-0.25438
Si	-1.79891	-0.38764	0.66855
H	2.21526	-1.07902	-2.08948
H	1.25334	-2.42678	-1.30131
H	0.19959	1.5491	-0.22761
H	2.74699	0.85923	-1.7969
H	-3.31212	-1.7158	2.11629
H	-2.4948	-2.74716	0.92993
H	-1.623	-2.17527	2.35942
H	-0.24548	0.80321	2.21071
H	-1.3118	1.96074	1.40622
H	-1.93296	0.95713	2.71478
H	-5.07302	1.16814	-0.41791
H	-4.73305	0.10403	0.94979
H	-3.96022	1.69476	0.85031
H	-1.72499	0.88063	-2.08488
H	-3.32399	1.63325	-2.16761
H	-2.17172	2.15269	-0.93514
H	-4.12721	-1.71701	-0.7375
H	-4.3837	-0.61593	-2.09645
H	-2.83348	-1.45318	-1.91762
C	3.02205	-1.3494	0.12564

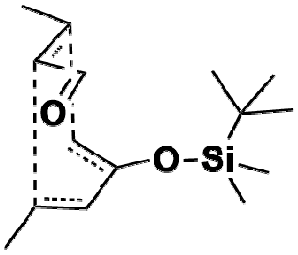
C	3.41333	-0.04209	0.43294
C	2.84786	0.63651	1.54074
C	4.01782	-2.23713	-0.58874
N	2.36192	1.18452	2.43672
H	2.39446	-1.8478	0.8585
H	4.32778	0.37178	0.02523
H	4.52607	-1.68419	-1.38294
H	4.77728	-2.58225	0.11745
H	3.54379	-3.11441	-1.03004
C	2.49843	2.83064	-0.84843
H	1.87162	3.27036	-0.07142
H	3.53967	2.88705	-0.52269
H	2.41058	3.43634	-1.75622



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1027.835942
Gibbs's free energies (G)	-1027.888945

C	0.98288	0.86593	1.21848
C	0.36084	0.15332	0.19926
C	0.98261	-0.96104	-0.40933
C	2.15758	-1.48423	0.05346
C	-3.08759	-0.29063	0.88947
C	-3.07363	1.46812	-1.68826
C	-2.09461	-1.442	-1.81763
C	-4.55537	-0.65234	0.61291
C	-2.40377	-1.4706	1.59699
C	-3.03093	0.94368	1.80083
O	-0.69595	0.73336	-0.42263
Si	-2.23092	0.0928	-0.7538
H	1.59116	0.33068	1.9331
H	0.45589	1.73044	1.6068
H	0.61329	-1.26657	-1.38369
H	2.43754	-1.32235	1.08838
H	-4.07571	1.17169	-2.00761
H	-3.16031	2.36922	-1.077
H	-2.49734	1.72167	-2.58134
H	-1.5555	-1.22357	-2.74332
H	-1.58563	-2.26338	-1.30885
H	-3.09527	-1.78688	-2.09354
H	-5.06528	-0.8839	1.55526
H	-5.09488	0.17342	0.13969
H	-4.64317	-1.53227	-0.03204
H	-1.35419	-1.25866	1.8217
H	-2.91133	-1.67637	2.54701
H	-2.44404	-2.38431	0.99728
H	-3.52097	1.80899	1.34498
H	-3.5428	0.73333	2.7471
H	-1.99873	1.2206	2.03255
C	2.56636	1.68546	0.25867
C	3.44977	0.68638	-0.17973

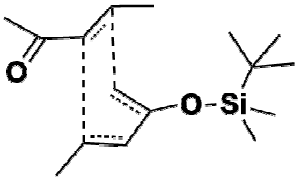
C	4.49166	0.1962	0.67795
C	1.89006	2.55446	-0.77565
O	5.394	-0.56486	0.35537
H	2.85537	2.19565	1.17605
H	3.49399	0.41055	-1.22803
H	4.42751	0.5477	1.73086
H	1.45744	1.93736	-1.56729
H	1.09189	3.15959	-0.34467
H	2.62548	3.2222	-1.23256
C	2.96403	-2.50095	-0.68131
H	4.01996	-2.21041	-0.66874
H	2.89573	-3.47337	-0.18369
H	2.62901	-2.60881	-1.71366



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1027.835827
Gibbs's free energies (G)	-1027.889537

C	-0.89193	1.3837	-0.69552
C	-0.40303	0.15399	-0.26429
C	-1.08791	-1.05677	-0.5124
C	-2.23944	-1.11506	-1.24533
C	3.2138	0.42214	-0.51186
C	2.66508	-0.41625	2.44207
C	1.97901	-2.34635	0.13202
C	4.65023	-0.11768	-0.43499
C	2.69916	0.2839	-1.95253
C	3.20877	1.90464	-0.1127
O	0.57374	0.16254	0.6754
Si	2.10853	-0.55876	0.66992
H	-1.41352	1.43229	-1.64193
H	-0.28222	2.24812	-0.45849
H	-0.77621	-1.93095	0.05134
H	-2.50183	-0.2912	-1.89798
H	3.66343	-0.83898	2.57952
H	2.6869	0.62637	2.76677
H	1.97776	-0.95861	3.09572
H	1.38032	-2.92608	0.83909
H	1.53018	-2.4464	-0.85909
H	2.97542	-2.79571	0.09583
H	5.29603	0.44777	-1.11698
H	5.06889	-0.01933	0.57095
H	4.70737	-1.1706	-0.72709
H	1.67807	0.66273	-2.05723
H	3.3381	0.86063	-2.63198
H	2.71174	-0.75631	-2.29097
H	3.60225	2.054	0.897
H	3.83846	2.48004	-0.80147
H	2.2005	2.3263	-0.14854
C	-2.51317	1.71488	0.40451

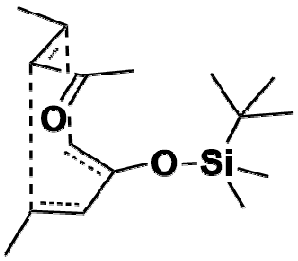
C	-3.49883	0.74289	0.17276
C	-3.69835	-0.3588	1.06861
C	-2.80067	3.13425	-0.05149
O	-4.64793	-1.13546	1.05627
H	-2.00561	1.64476	1.36531
H	-4.25477	0.90597	-0.59152
H	-2.90188	-0.48094	1.83222
H	-3.5738	3.56956	0.58586
H	-1.91894	3.77364	0.0011
H	-3.17334	3.14031	-1.07845
C	-3.08638	-2.33426	-1.35265
H	-4.06639	-2.14201	-0.89761
H	-3.25388	-2.59999	-2.39949
H	-2.63698	-3.18065	-0.83161



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1067.120153
Gibbs's free energies (G)	

C	-0.79307	-1.04334	0.85166
C	-0.12107	-0.13608	0.04386
C	-0.70874	1.09216	-0.33066
C	-1.91301	1.51404	0.16537
C	3.30356	-0.01207	1.00572
C	3.40308	-0.97507	-1.95822
C	2.44697	1.87315	-1.29843
C	4.80601	0.28757	0.88733
C	2.65822	1.00775	1.95602
C	3.11023	-1.42441	1.57493
C	-2.64759	2.70195	-0.36196
O	0.96583	-0.57767	-0.64539
Si	2.51904	0.09495	-0.71486
H	-1.42244	-0.66661	1.64518
H	-0.30372	-1.99038	1.05013
H	-0.28137	1.60566	-1.18669
H	-2.25345	1.13802	1.12438
H	4.40211	-0.58564	-2.16916
H	3.50394	-2.00249	-1.60134
H	2.84391	-0.99698	-2.89669
H	1.98681	1.94132	-2.28776
H	1.88665	2.51397	-0.6142
H	3.46138	2.2748	-1.37854
H	5.27094	0.25834	1.87989
H	5.31715	-0.44949	0.26119
H	4.99393	1.28071	0.46676
H	1.58127	0.84251	2.0598
H	3.10553	0.92064	2.95354
H	2.81246	2.03425	1.61212
H	3.542	-2.19013	0.92338
H	3.60119	-1.50501	2.55196
H	2.0503	-1.65411	1.71186
H	-3.7034	2.45287	-0.5081

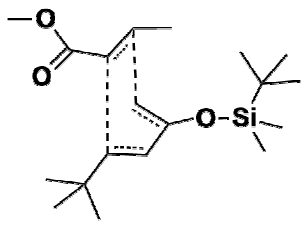
H	-2.60974	3.52428	0.35924
H	-2.22425	3.04493	-1.30711
C	-2.3756	-1.58373	-0.33459
C	-3.21265	-0.48715	-0.57275
C	-4.34446	-0.12874	0.26438
C	-4.49037	-0.79572	1.62137
C	-1.66004	-2.20048	-1.5143
O	-5.17267	0.70233	-0.09431
H	-2.6968	-2.28642	0.42997
H	-3.19642	-0.00946	-1.54681
H	-4.75564	-1.8485	1.49465
H	-3.55996	-0.76086	2.19415
H	-5.28105	-0.29527	2.17704
H	-2.37917	-2.72319	-2.15087
H	-1.18149	-1.42394	-2.11656
H	-0.89139	-2.90941	-1.20424



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1067.120382
Gibbs's free energies (G)	-1067.174384

C	0.6652	1.60057	0.44114
C	0.2149	0.29745	0.28108
C	0.90335	-0.79519	0.84563
C	2.03632	-0.63533	1.60123
C	-3.36991	0.50992	0.41903
C	-2.79771	-0.88435	-2.30559
C	-2.09292	-2.31066	0.33529
C	-4.82016	0.01483	0.30423
C	-2.96561	0.54736	1.90072
C	-3.27213	1.92512	-0.16687
O	-0.7087	0.05281	-0.69251
Si	-2.23669	-0.66279	-0.54212
H	1.1116	1.88339	1.38457
H	0.11384	2.38216	-0.06857
H	0.64813	-1.78716	0.48431
H	2.21471	0.30991	2.09975
H	-3.74709	-1.42384	-2.34835
H	-2.9288	0.07749	-2.8066
H	-2.05714	-1.45931	-2.86656
H	-1.48316	-3.00841	-0.2447
H	-1.64662	-2.20828	1.3271
H	-3.08403	-2.75728	0.45724
H	-5.48248	0.66991	0.88239
H	-5.17036	0.02215	-0.73216
H	-4.93997	-0.99959	0.6974
H	-1.93203	0.8822	2.03192
H	-3.613	1.24482	2.44582
H	-3.06663	-0.43421	2.37256
H	-3.5477	1.94872	-1.22549
H	-3.95195	2.59891	0.36803
H	-2.25981	2.32565	-0.07262
C	2.4839	1.69506	-0.50252

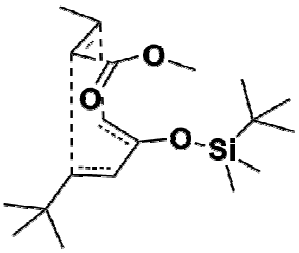
C	3.33755	0.68404	-0.04844
C	3.59473	-0.55343	-0.77174
C	2.67417	-0.93053	-1.91742
C	2.8235	3.1272	-0.13962
O	4.55061	-1.26978	-0.49467
H	2.055	1.56825	-1.49251
H	4.06691	0.91865	0.72261
H	1.63471	-0.65457	-1.73567
H	3.00625	-0.40718	-2.81954
H	2.75306	-2.00251	-2.09399
H	3.11593	3.19928	0.91084
H	3.66876	3.4681	-0.74285
H	1.98932	3.80805	-0.31389
C	2.88277	-1.78099	2.05075
H	3.93457	-1.59064	1.82137
H	2.79335	-1.91914	3.13262
H	2.59541	-2.70708	1.55059



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1260.175085
Gibbs's free energies (G)	-1067.175581

C	0.56479	-1.58989	-1.32837
C	-0.33799	-0.64678	-0.83777
C	0.09305	0.61784	-0.36733
C	1.39642	1.01464	-0.39929
C	-3.98748	0.579	-0.55946
C	-3.69921	-2.1871	0.84151
C	-2.22181	0.2657	1.96915
C	-5.07272	1.13265	0.37662
C	-3.1743	1.74555	-1.13933
C	-4.64707	-0.19626	-1.70932
O	-1.60108	-1.0577	-0.6176
Si	-2.85859	-0.5779	0.4176
H	1.43764	-1.23628	-1.86223
H	0.13111	-2.50831	-1.70874
H	-0.63517	1.23659	0.14233
H	2.0962	0.48475	-1.03543
H	-4.6374	-2.01523	1.37574
H	-3.91969	-2.75779	-0.06338
H	-3.05389	-2.79697	1.47918
H	-1.2571	-0.13258	2.29269
H	-2.1148	1.34628	1.84567
H	-2.93956	0.09739	2.77743
H	-5.75145	1.78503	-0.18479
H	-5.67693	0.3351	0.82047
H	-4.64257	1.72534	1.18987
H	-2.38763	1.39488	-1.81417
H	-3.83342	2.40965	-1.71077
H	-2.7056	2.34944	-0.35504
H	-5.28829	-1.00045	-1.33726
H	-5.27232	0.4781	-2.30597
H	-3.90025	-0.63751	-2.37586
C	1.51186	-2.20989	0.25001
C	2.30887	-1.20806	0.83198

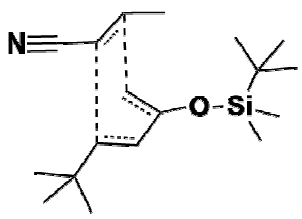
C	3.63211	-0.8893	0.36536
C	5.16783	-1.09987	-1.41662
C	0.42018	-2.81737	1.10558
O	4.47938	-0.24399	0.95872
O	3.86794	-1.3632	-0.8952
H	2.05766	-2.92558	-0.35973
H	2.02821	-0.76163	1.77705
H	5.19484	-1.56411	-2.39997
H	5.33923	-0.02552	-1.50078
H	5.93547	-1.5306	-0.77274
H	-0.15124	-2.03493	1.61145
H	-0.27482	-3.41951	0.51802
H	0.86457	-3.4528	1.8758
C	1.89357	2.31652	0.20427
C	2.12161	2.14251	1.716
C	3.21889	2.696	-0.4682
C	0.87136	3.44333	-0.01763
H	1.20266	1.80767	2.2063
H	2.91257	1.41517	1.90667
H	2.41765	3.10055	2.15396
H	3.08404	2.83113	-1.54561
H	3.60147	3.63254	-0.05367
H	3.96854	1.91876	-0.29959
H	1.28833	4.38746	0.34284
H	0.62919	3.55425	-1.07765
H	-0.05666	3.26401	0.53112



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1260.175455
Gibbs's free energies (G)	-1260.234823

C	0.38624	-1.14372	-2.05926
C	-0.22476	-0.46219	-1.01116
C	0.41199	0.62659	-0.37001
C	1.63874	1.08335	-0.75273
C	-3.6532	0.72661	-0.4538
C	-3.48055	-2.04816	0.95575
C	-1.93447	0.34782	2.09001
C	-4.70987	1.32836	0.48561
C	-2.79701	1.85922	-1.04
C	-4.35004	-0.02114	-1.59932
O	-1.33188	-1.01922	-0.48008
Si	-2.57485	-0.47491	0.53098
H	0.9789	-0.57052	-2.7589
H	-0.17845	-1.96064	-2.49392
H	-0.02348	0.9875	0.55369
H	2.02585	0.81943	-1.73169
H	-4.4081	-1.83553	1.49376
H	-3.72804	-2.61102	0.05328
H	-2.85918	-2.68348	1.59198
H	-1.02338	-0.13753	2.44586
H	-1.7263	1.41176	1.95301
H	-2.69108	0.25874	2.8752
H	-5.36622	2.00273	-0.07678
H	-5.34203	0.55865	0.93977
H	-4.25133	1.90986	1.2913
H	-2.06866	1.48342	-1.76368
H	-3.44175	2.57937	-1.55803
H	-2.24929	2.40666	-0.26558
H	-5.026	-0.7947	-1.22359
H	-4.94534	0.67844	-2.19779
H	-3.62473	-0.49809	-2.26554
C	1.96086	-2.0942	-1.29047

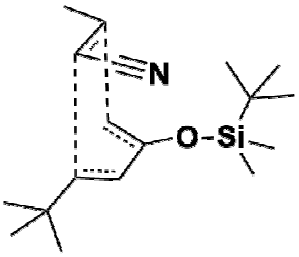
C	2.77493	-1.26083	-0.5107
C	2.63424	-1.16159	0.92345
C	1.26684	-1.63501	2.77757
C	2.552	-2.63172	-2.57975
O	3.45404	-0.70612	1.70248
O	1.44657	-1.65754	1.36605
H	1.34584	-2.79667	-0.73632
H	3.69944	-0.86365	-0.91216
H	0.306	-2.11116	2.96438
H	2.06528	-2.18498	3.27704
H	1.26253	-0.60866	3.15137
H	3.28868	-3.40598	-2.35203
H	1.79353	-3.06765	-3.23153
H	3.06298	-1.83678	-3.12917
C	2.37449	2.22668	-0.09177
C	1.99843	3.5009	-0.87519
C	1.99222	2.40214	1.38035
C	3.88878	2.00378	-0.20816
H	2.28026	3.41292	-1.9281
H	0.92268	3.68677	-0.82216
H	2.52326	4.36289	-0.45312
H	2.18846	1.48672	1.94409
H	2.59041	3.20495	1.81918
H	0.94009	2.67692	1.49576
H	4.42161	2.89252	0.14125
H	4.20233	1.15043	0.39525
H	4.17408	1.82688	-1.24992



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1124.598871
Gibbs's free energies (G)	-1260.233224

C	0.3232	-1.67401	-0.79589
C	-0.11893	-0.60143	-0.03042
C	0.72054	0.49249	0.26974
C	1.95222	0.66541	-0.30042
C	-3.44711	0.12702	-1.01535
C	-3.71111	-0.52784	2.02192
C	-2.18636	1.98964	1.10923
C	-4.85875	0.72927	-0.92983
C	-2.62304	0.91488	-2.04509
C	-3.54992	-1.33658	-1.4673
O	-1.25607	-0.76298	0.69883
Si	-2.63856	0.2195	0.69385
H	0.99525	-1.49157	-1.62415
H	-0.36985	-2.49729	-0.9297
H	0.42519	1.10498	1.11518
H	2.16528	0.20323	-1.26031
H	-4.60546	0.07751	2.18898
H	-4.02802	-1.53902	1.75648
H	-3.1597	-0.58273	2.96356
H	-1.73129	2.05851	2.10086
H	-1.49369	2.41865	0.38135
H	-3.08964	2.60705	1.11548
H	-5.32924	0.71352	-1.91992
H	-5.50007	0.16051	-0.25015
H	-4.84184	1.77022	-0.59172
H	-1.59867	0.5371	-2.12166
H	-3.08418	0.82552	-3.03595
H	-2.57548	1.97884	-1.79671
H	-4.10803	-1.94808	-0.75204
H	-4.07233	-1.39285	-2.4296
H	-2.56098	-1.78345	-1.59707
C	1.75394	-2.44662	0.38331
C	2.88702	-1.62152	0.32764

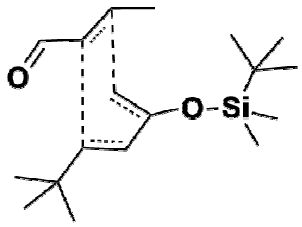
C	3.75989	-1.72967	-0.78243
C	1.08295	-2.6311	1.72181
N	4.42201	-1.8066	-1.72828
H	1.77306	-3.32426	-0.25679
H	3.24426	-1.09349	1.20129
H	0.95996	-1.66605	2.22146
H	0.09801	-3.08776	1.62114
H	1.70179	-3.26603	2.36122
C	2.89571	1.7876	0.08
C	2.50105	3.00857	-0.77636
C	2.79586	2.15508	1.56352
C	4.34299	1.40595	-0.25387
H	2.58741	2.78319	-1.8424
H	1.47081	3.3092	-0.56961
H	3.1631	3.84925	-0.54967
H	2.96288	1.27902	2.19698
H	3.55494	2.90249	1.8079
H	1.82238	2.58176	1.81587
H	4.99404	2.27297	-0.11457
H	4.7078	0.60618	0.39478
H	4.43569	1.06714	-1.2884



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1124.598482
Gibbs's free energies (G)	-1124.656543

C	0.63263	1.45859	1.33809
C	-0.37918	0.83693	2.06813
C	-0.39774	-0.56683	2.25261
C	0.55115	-1.39104	1.72501
C	-2.90156	1.21377	4.86234
C	-3.97748	2.76205	2.39277
C	-3.73962	-0.30648	2.28232
C	-4.27884	0.83419	5.42837
C	-1.86854	0.16831	5.30663
C	-2.48797	2.59025	5.40183
O	-1.45289	1.58286	2.37609
Si	-3.01724	1.27411	2.97601
H	1.63441	1.05813	1.42098
H	0.57331	2.53886	1.26785
H	-1.29241	-1.00235	2.67783
H	1.50457	-0.98447	1.40345
H	-4.97097	2.79271	2.84791
H	-3.4551	3.68687	2.64686
H	-4.10602	2.7296	1.30818
H	-3.39182	-0.50012	1.26342
H	-3.5035	-1.18477	2.88943
H	-4.82917	-0.21126	2.25422
H	-4.23942	0.81353	6.52372
H	-5.05151	1.55469	5.14198
H	-4.59722	-0.15632	5.08945
H	-0.86627	0.40575	4.93782
H	-1.82224	0.13563	6.4017
H	-2.12849	-0.83777	4.96118
H	-3.23469	3.35494	5.16938
H	-2.38306	2.54943	6.49238
H	-1.52947	2.91401	4.98521
C	0.35858	0.9258	-0.54671

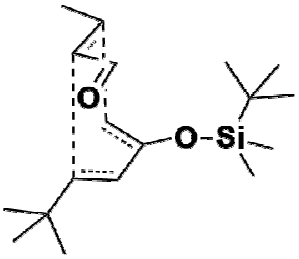
C	0.20435	-0.46124	-0.71314
C	-1.08471	-1.03626	-0.74277
C	1.60105	1.5547	-1.14798
N	-2.15392	-1.4838	-0.75589
H	-0.54944	1.51304	-0.65878
H	1.02822	-1.0754	-1.05288
H	2.48506	0.95848	-0.90694
H	1.50616	1.59078	-2.23564
H	1.76295	2.57046	-0.78574
C	0.51671	-2.89904	1.8224
C	1.51187	-3.30053	2.92857
C	-0.87713	-3.43168	2.16661
C	0.98199	-3.51465	0.49447
H	2.52364	-2.96041	2.6914
H	1.21942	-2.86872	3.88887
H	1.533	-4.38933	3.03004
H	-1.62037	-3.07958	1.44602
H	-0.86627	-4.52421	2.14433
H	-1.18734	-3.12644	3.17022
H	1.09118	-4.59664	0.60708
H	0.25565	-3.3262	-0.29907
H	1.95018	-3.10664	0.18966



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1145.664338
Gibbs's free energies (G)	-1145.721282

C	0.80467	1.34812	0.91505
C	-0.29102	0.74539	1.56018
C	-0.36332	-0.65329	1.82231
C	0.60839	-1.53248	1.47134
C	-3.43375	1.29945	3.7465
C	-3.77751	2.67859	0.96444
C	-3.56595	-0.38478	1.12859
C	-4.92822	1.01307	3.95741
C	-2.60082	0.24533	4.49075
C	-3.0945	2.69215	4.29765
O	-1.3654	1.50697	1.75464
Si	-3.04882	1.24301	1.90087
H	1.77933	0.92345	1.11844
H	0.78376	2.43319	0.93176
H	-1.28551	-1.02415	2.25195
H	1.56163	-1.16842	1.10476
H	-4.86038	2.73272	1.10335
H	-3.33992	3.62256	1.29626
H	-3.58067	2.56969	-0.10524
H	-2.95521	-0.6401	0.25867
H	-3.51876	-1.22192	1.82897
H	-4.60245	-0.2953	0.79052
H	-5.16827	1.05947	5.02579
H	-5.55975	1.74739	3.44802
H	-5.20725	0.01739	3.59982
H	-1.52729	0.42338	4.37554
H	-2.82987	0.28087	5.56197
H	-2.81838	-0.7713	4.14592
H	-3.70671	3.46962	3.83187
H	-3.28358	2.72296	5.37675
H	-2.04247	2.94347	4.13436
C	0.62539	0.96965	-0.88891
C	0.90247	-0.38872	-1.21346

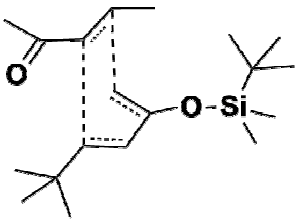
C	2.23864	-0.81459	-1.42181
C	-0.73529	1.51689	-1.27652
O	2.63013	-1.94717	-1.71771
H	1.43962	1.64033	-1.16865
H	0.09729	-1.10301	-1.35091
H	2.99711	-0.01046	-1.28775
H	-1.53006	0.83971	-0.95182
H	-0.92606	2.50095	-0.8435
H	-0.79566	1.59582	-2.36435
C	0.51243	-3.02918	1.61283
C	1.80404	-3.5184	2.28951
C	-0.70082	-3.46529	2.43699
C	0.42175	-3.64052	0.20189
H	2.67815	-3.24719	1.69211
H	1.91542	-3.08509	3.28714
H	1.78347	-4.60681	2.38792
H	-1.63841	-3.18393	1.94928
H	-0.69782	-4.55279	2.54094
H	-0.68247	-3.02782	3.43956
H	0.44551	-4.7314	0.28055
H	-0.51651	-3.34924	-0.27799
H	1.24826	-3.3136	-0.43386



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1145.664742
Gibbs's free energies (G)	-1145.72063

C	0.64917	1.39732	0.79621
C	-0.4515	0.79608	1.4049
C	-0.52101	-0.60435	1.60718
C	0.4851	-1.44616	1.24307
C	-3.21059	1.22532	3.92905
C	-4.02562	2.80299	1.37332
C	-3.8704	-0.26293	1.27877
C	-4.65026	0.90797	4.36344
C	-2.26974	0.13853	4.46898
C	-2.78961	2.58446	4.50629
O	-1.5475	1.55866	1.55712
Si	-3.15773	1.295	2.04047
H	1.63021	0.98487	0.99044
H	0.61111	2.47806	0.72407
H	-1.46662	-1.0213	1.92963
H	1.46612	-1.03998	1.01904
H	-5.06215	2.8488	1.7172
H	-3.51818	3.71709	1.68888
H	-4.0355	2.7804	0.28085
H	-3.4839	-0.42489	0.26917
H	-3.67274	-1.16393	1.86441
H	-4.9562	-0.15158	1.20409
H	-4.71471	0.89533	5.45755
H	-5.361	1.65762	4.00185
H	-4.97668	-0.07161	4.00127
H	-1.22642	0.33673	4.20627
H	-2.33641	0.10422	5.56279
H	-2.53216	-0.85683	4.09556
H	-3.47417	3.38131	4.20229
H	-2.79424	2.54286	5.60165
H	-1.7809	2.86207	4.18625
C	0.55182	0.87628	-1.0972

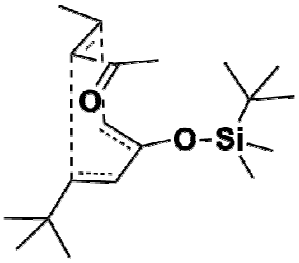
C	0.56692	-0.51591	-1.30633
C	-0.65794	-1.23006	-1.51292
C	1.74039	1.67074	-1.61055
O	-0.78966	-2.3645	-1.95987
H	-0.41062	1.35623	-1.27073
H	1.50029	-1.02607	-1.52699
H	-1.56599	-0.64664	-1.2423
H	1.73361	1.66923	-2.70283
H	1.72373	2.70725	-1.27166
H	2.67749	1.2144	-1.28275
C	0.45069	-2.94627	1.3929
C	1.08111	-3.26452	2.7642
C	-0.97325	-3.50725	1.34149
C	1.30633	-3.58454	0.2897
H	2.1025	-2.87974	2.82853
H	0.49471	-2.82236	3.57386
H	1.11548	-4.34814	2.90865
H	-1.4708	-3.22197	0.41165
H	-0.93653	-4.59852	1.3882
H	-1.57279	-3.16375	2.18952
H	1.37625	-4.6631	0.45442
H	0.86724	-3.41055	-0.69404
H	2.3208	-3.17432	0.30421



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1184.947061
Gibbs's free energies (G)	-1185.005353

C	0.6284	-1.54236	-1.62401
C	-0.19623	-0.58822	-1.02736
C	0.32622	0.62379	-0.51585
C	1.64753	0.95122	-0.58708
C	-3.77741	0.71177	-0.31931
C	-3.42277	-2.16388	0.83551
C	-1.762	0.15917	1.9814
C	-4.77278	1.18589	0.74991
C	-2.99043	1.91596	-0.85622
C	-4.54121	0.05275	-1.47708
O	-1.46135	-0.95202	-0.75352
Si	-2.59088	-0.54069	0.44851
H	1.47003	-1.18324	-2.20142
H	0.13205	-2.41434	-2.03458
H	-0.34097	1.2515	0.06406
H	2.29331	0.42149	-1.27757
H	-4.2904	-2.02078	1.4851
H	-3.75544	-2.65802	-0.07985
H	-2.72568	-2.83283	1.34701
H	-0.76913	-0.26736	2.14789
H	-1.65559	1.24628	1.94446
H	-2.37754	-0.08182	2.85307
H	-5.48021	1.89985	0.3125
H	-5.35653	0.35574	1.15954
H	-4.2672	1.68822	1.58027
H	-2.26967	1.61711	-1.62368
H	-3.67889	2.6392	-1.30861
H	-2.44686	2.43888	-0.062
H	-5.158	-0.78154	-1.13074
H	-5.20757	0.78396	-1.94926
H	-3.8591	-0.32445	-2.24464
C	1.62171	-2.31132	-0.12607
C	2.41758	-1.37309	0.56108

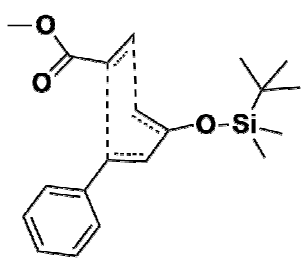
C	3.80594	-1.11711	0.26755
C	4.37683	-1.61489	-1.05231
C	0.52467	-3.00079	0.662
O	4.54541	-0.51663	1.04755
H	2.16231	-2.97998	-0.79369
H	2.05962	-0.97189	1.50429
H	4.61648	-2.67902	-0.97165
H	3.67748	-1.49706	-1.88367
H	5.29558	-1.07014	-1.26459
H	0.96793	-3.70759	1.3679
H	-0.04601	-2.27174	1.24228
H	-0.17165	-3.54257	0.0196
C	2.23163	2.19388	0.05996
C	1.36025	3.4164	-0.28006
C	2.28032	2.01944	1.58726
C	3.64924	2.42396	-0.47642
H	1.26563	3.54365	-1.36156
H	0.35694	3.3288	0.14411
H	1.82046	4.31753	0.1341
H	2.95828	1.20884	1.86089
H	2.63872	2.94359	2.05045
H	1.28407	1.80102	1.98384
H	4.0801	3.32386	-0.02976
H	4.29666	1.57959	-0.2306
H	3.63569	2.55881	-1.56224



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1184.949782
Gibbs's free energies (G)	-1185.009421

C	0.41339	1.54635	0.57154
C	-0.66763	0.86614	1.12116
C	-0.6245	-0.52845	1.33553
C	0.47828	-1.28362	1.04803
C	-3.05726	0.96924	3.81478
C	-4.27276	2.79163	1.61419
C	-4.21257	-0.22437	1.15474
C	-4.39039	1.2854	4.51753
C	-2.64696	-0.46633	4.17822
C	-1.98054	1.94401	4.31354
O	-1.84343	1.53276	1.1862
Si	-3.32455	1.22103	1.95217
H	1.40989	1.23389	0.85131
H	0.28622	2.61264	0.42349
H	-1.55641	-1.03081	1.56497
H	1.44324	-0.7974	0.94581
H	-5.31489	2.70169	1.92962
H	-3.82981	3.64433	2.13445
H	-4.25991	3.00668	0.543
H	-4.39134	-0.01551	0.09665
H	-3.68318	-1.1764	1.22441
H	-5.1887	-0.35289	1.63328
H	-4.28193	1.12919	5.59687
H	-4.69813	2.32253	4.36149
H	-5.20069	0.63434	4.17286
H	-1.64927	-0.71022	3.80727
H	-2.62639	-0.57612	5.26896
H	-3.35212	-1.20665	3.78687
H	-2.23827	2.98444	4.09293
H	-1.87024	1.8532	5.40063
H	-1.00807	1.73486	3.85839
C	0.60862	0.88417	-1.31933

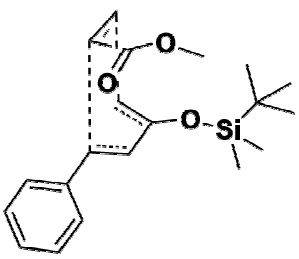
C	0.65487	-0.51586	-1.40728
C	-0.48871	-1.33151	-1.77762
C	-1.87732	-0.72257	-1.69702
C	1.87058	1.64715	-1.67761
O	-0.3662	-2.48057	-2.19305
H	-0.30979	1.35973	-1.65373
H	1.62098	-1.00369	-1.50234
H	-2.09977	-0.23435	-2.6513
H	-2.60277	-1.52277	-1.54898
H	-1.97651	0.02304	-0.90819
H	2.74345	1.18631	-1.20859
H	2.02198	1.62082	-2.75941
H	1.82402	2.69211	-1.3677
C	0.56208	-2.77846	1.26016
C	1.06886	-2.9836	2.70289
C	-0.79276	-3.47349	1.09625
C	1.58437	-3.38562	0.28984
H	2.03894	-2.5016	2.85258
H	0.36291	-2.56925	3.42715
H	1.18587	-4.05271	2.9024
H	-1.2128	-3.28479	0.10561
H	-0.66378	-4.55305	1.20954
H	-1.50795	-3.14909	1.858
H	1.73872	-4.44132	0.52915
H	1.2383	-3.31047	-0.74183
H	2.54882	-2.87584	0.38055



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1294.726551
Gibbs's free energies (G)	-1294.786017

C	0.50272	-1.93754	-0.08801
C	0.8916	-0.63739	-0.37402
C	-0.00246	0.44898	-0.25859
C	-1.26725	0.2955	0.24677
C	4.04103	-0.08	1.07523
C	4.61854	0.21163	-1.96853
C	2.88605	2.30785	-0.51995
C	5.44028	0.52079	1.28857
C	3.11892	0.37902	2.21529
C	4.14387	-1.61157	1.09501
C	-2.3132	1.32101	0.23634
C	-3.38799	1.19135	1.12286
C	-2.29874	2.41257	-0.64312
C	-4.40548	2.1363	1.15615
C	-3.31552	3.35575	-0.61171
C	-4.3704	3.22376	0.29054
O	2.0602	-0.45388	-1.05045
Si	3.38376	0.50454	-0.60268
H	-0.22467	-2.12186	0.69093
H	1.23344	-2.72129	-0.25034
H	0.28266	1.37706	-0.74214
H	-1.47129	-0.54991	0.89519
H	5.47185	0.88773	-1.87328
H	4.99282	-0.81477	-1.95232
H	4.1546	0.38678	-2.94201
H	2.49879	2.65167	-1.48273
H	2.1261	2.48982	0.24322
H	3.75802	2.92127	-0.27395
H	5.82152	0.23038	2.27452
H	6.15254	0.16251	0.53952
H	5.42841	1.61485	1.25118
H	2.10078	-0.00414	2.09695

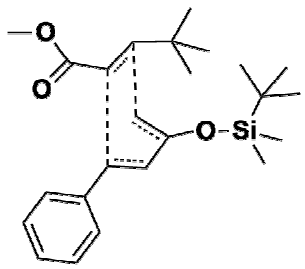
H	3.50394	0.01059	3.17383
H	3.06566	1.46954	2.27813
H	4.77252	-1.99036	0.28349
H	4.58879	-1.94275	2.04095
H	3.15967	-2.07827	1.00676
H	-3.41906	0.33855	1.79283
H	-1.49868	2.51407	-1.36777
H	-5.22811	2.01944	1.85136
H	-3.29354	4.19317	-1.29917
H	-5.16537	3.95984	0.30827
C	-0.9027	-2.32689	-1.52635
C	-1.99786	-1.47878	-1.42495
C	-3.14037	-1.78576	-0.57841
C	-3.92135	-3.07939	1.23076
O	-4.24155	-1.28754	-0.6591
O	-2.83646	-2.69703	0.38705
H	-0.24825	-2.21779	-2.38312
H	-1.00515	-3.33802	-1.1498
H	-2.15186	-0.66082	-2.11452
H	-3.51236	-3.79893	1.93597
H	-4.32219	-2.21327	1.75889
H	-4.71986	-3.5343	0.64353



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1294.728710
Gibbs's free energies (G)	-1294.788016

C	0.56059	1.57193	0.97015
C	-0.42448	0.95867	1.73059
C	-0.43801	-0.44022	1.93879
C	0.53751	-1.27637	1.47041
C	-3.16415	1.25369	4.40715
C	-3.98704	2.94554	1.93247
C	-3.74083	-0.10552	1.65187
C	-4.60649	0.92807	4.82389
C	-2.2325	0.13118	4.88541
C	-2.72929	2.57563	5.05628
C	0.42983	-2.7364	1.48044
C	1.58396	-3.5145	1.33771
C	-0.80753	-3.38718	1.57759
C	1.51095	-4.90131	1.32408
C	-0.88145	-4.77266	1.56317
C	0.27771	-5.53535	1.44007
O	-1.48515	1.71749	2.07893
Si	-3.09368	1.41971	2.52526
H	1.56125	1.1651	0.97683
H	0.48769	2.6463	0.84885
H	-1.33327	-0.86941	2.37082
H	1.5156	-0.88314	1.22324
H	-5.0292	2.95011	2.26234
H	-3.50466	3.85133	2.30577
H	-3.98024	2.98392	0.84031
H	-3.20433	-0.23738	0.7081
H	-3.62622	-1.02017	2.23947
H	-4.80476	0.01757	1.43202
H	-4.66901	0.84255	5.91502
H	-5.30645	1.71086	4.51593
H	-4.94875	-0.02049	4.39848
H	-1.18965	0.33028	4.6213

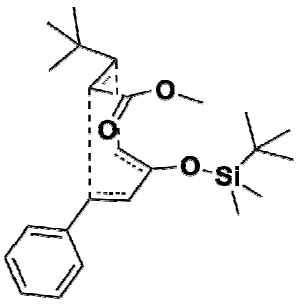
H	-2.28836	0.04294	5.9768
H	-2.5109	-0.84175	4.46692
H	-3.40587	3.395	4.79733
H	-2.73287	2.47522	6.14797
H	-1.71832	2.85916	4.74919
H	2.5452	-3.02162	1.23466
H	-1.7212	-2.80529	1.63806
H	2.41575	-5.4875	1.21535
H	-1.8463	-5.26139	1.63526
H	0.21777	-6.617	1.4217
C	0.15612	0.87515	-0.90669
C	0.4772	-0.46765	-1.0478
C	-0.48641	-1.53822	-1.22863
C	-2.74675	-2.1791	-1.23319
O	-0.21647	-2.64877	-1.63729
O	-1.76624	-1.18822	-0.9256
H	0.85456	1.60296	-1.3055
H	-0.88692	1.16755	-0.96197
H	1.49585	-0.76544	-1.26701
H	-3.69931	-1.77437	-0.89707
H	-2.77403	-2.36444	-2.308
H	-2.5247	-3.1146	-0.719



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1451.834911
Gibbs's free energies (G)	-1451.899882

C	-0.45109	1.29305	1.0411
C	-0.88495	0.26557	0.21197
C	-0.02088	-0.77202	-0.18278
C	1.23943	-0.9147	0.34972
C	-4.07349	-0.90629	1.21651
C	-4.5896	0.26873	-1.62581
C	-2.88275	-2.26518	-1.30599
C	-5.44263	-1.59604	1.10926
C	-3.1289	-1.78885	2.0464
C	-4.2387	0.44977	1.91645
C	2.25538	-1.82457	-0.18918
C	3.27913	-2.28839	0.64374
C	2.25415	-2.22019	-1.53413
C	4.25518	-3.1509	0.15897
C	3.22914	-3.07972	-2.0187
C	4.23042	-3.55308	-1.17192
O	-2.07148	0.42336	-0.44224
Si	-3.38649	-0.63838	-0.52762
H	0.27806	1.07818	1.8096
H	-1.16223	2.07507	1.27933
H	-0.30664	-1.35174	-1.05421
H	1.42105	-0.56161	1.35977
H	-5.45865	-0.3517	-1.8581
H	-4.94183	1.19066	-1.15733
H	-4.10358	0.53479	-2.5678
H	-2.43449	-2.10189	-2.28995
H	-2.17213	-2.82372	-0.69311
H	-3.76724	-2.89348	-1.44751
H	-5.84948	-1.77435	2.11156
H	-6.16496	-0.98136	0.56409
H	-5.3726	-2.56625	0.60685
H	-2.13686	-1.33896	2.14976

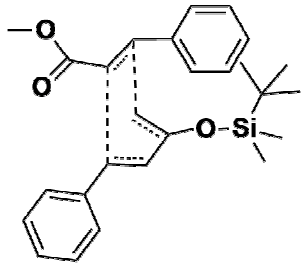
H	-3.53961	-1.92491	3.05415
H	-3.00636	-2.78081	1.60269
H	-4.89953	1.11995	1.3585
H	-4.67525	0.30676	2.91204
H	-3.27467	0.95029	2.04143
H	3.30715	-1.9661	1.67902
H	1.49886	-1.83247	-2.2091
H	5.03954	-3.50202	0.8188
H	3.21756	-3.37417	-3.06176
H	4.99348	-4.22115	-1.5535
C	1.03442	2.24592	-0.03441
C	2.10271	1.35214	-0.14753
C	3.09555	1.19179	0.9019
C	3.57273	1.48401	3.19204
O	4.19871	0.70679	0.76907
O	2.64303	1.60804	2.11708
H	1.10315	2.94415	0.79767
H	2.41081	0.95114	-1.1033
H	3.07112	1.88703	4.06861
H	3.83634	0.43748	3.35236
H	4.48064	2.04884	2.9789
C	0.4281	2.88335	-1.28914
C	1.42477	3.97125	-1.73452
C	0.23557	1.89003	-2.44033
C	-0.91415	3.55766	-0.9808
H	1.56976	4.7161	-0.94669
H	2.39718	3.53515	-1.97398
H	1.0442	4.48371	-2.6228
H	-0.46647	1.09932	-2.1736
H	-0.17344	2.42092	-3.3049
H	1.17859	1.43635	-2.75371
H	-1.21689	4.17917	-1.82797
H	-1.69827	2.81857	-0.80591
H	-0.83476	4.20488	-0.10145



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1451.832563
Gibbs's free energies (G)	-1451.897847

C	0.40119	1.64097	-0.66376
C	0.80119	0.40026	-0.17787
C	-0.02346	-0.73382	-0.28066
C	-1.2745	-0.65434	-0.84886
C	4.10965	-0.32926	-1.16196
C	4.33826	-0.03724	1.93016
C	2.83013	-2.42682	0.73518
C	5.53092	-0.911	-1.11277
C	3.32392	-1.01368	-2.29077
C	4.1857	1.17792	-1.44377
C	-2.27628	-1.72364	-0.83778
C	-3.32404	-1.6737	-1.76629
C	-2.2485	-2.77798	0.08312
C	-4.30047	-2.66012	-1.79551
C	-3.22418	-3.76486	0.05419
C	-4.25046	-3.71277	-0.88581
O	1.89918	0.35526	0.62539
Si	3.27337	-0.61966	0.51385
H	-0.1541	1.6743	-1.59031
H	1.08547	2.46319	-0.49593
H	0.2591	-1.61325	0.28805
H	-1.47709	0.13718	-1.56063
H	5.23173	-0.65892	2.02869
H	4.65573	0.99867	1.79098
H	3.7818	-0.0948	2.86885
H	2.29374	-2.57985	1.67587
H	2.21354	-2.81049	-0.08022
H	3.74318	-3.02858	0.77297
H	6.01878	-0.78523	-2.08661
H	6.14918	-0.40637	-0.36469
H	5.52643	-1.98172	-0.8843

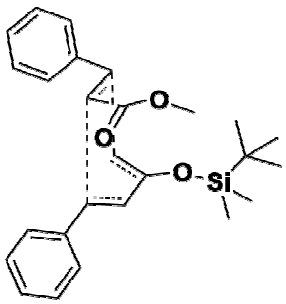
H	2.2964	-0.64324	-2.35363
H	3.80935	-0.8156	-3.25406
H	3.28602	-2.09847	-2.15729
H	4.72202	1.71503	-0.65564
H	4.71606	1.35581	-2.38687
H	3.18773	1.61558	-1.53264
H	-3.36391	-0.85064	-2.47331
H	-1.47802	-2.81246	0.8439
H	-5.10087	-2.60717	-2.52412
H	-3.19229	-4.57194	0.7765
H	-5.0126	-4.48294	-0.90217
C	-1.29386	2.22432	0.39108
C	-2.10773	1.11523	0.63515
C	-1.88282	0.24254	1.77697
C	-0.27777	-0.46992	3.34344
O	-2.64192	-0.60937	2.19163
O	-0.66727	0.45547	2.33703
H	-0.65912	2.52563	1.2198
H	-3.07013	0.98848	0.15721
H	0.7194	-0.16772	3.65522
H	-0.96939	-0.44176	4.18627
H	-0.2562	-1.48482	2.93845
C	-1.86034	3.40703	-0.40755
C	-2.59115	2.97082	-1.68281
C	-2.86702	4.11271	0.52214
C	-0.77005	4.42274	-0.77293
H	-1.92238	2.47414	-2.39128
H	-3.42651	2.30019	-1.46899
H	-2.99963	3.85088	-2.18696
H	-2.37883	4.43556	1.44573
H	-3.28106	4.99607	0.02742
H	-3.68862	3.44458	0.78811
H	-1.2318	5.3442	-1.13666
H	-0.16153	4.67379	0.10108
H	-0.10864	4.05467	-1.55914



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1525.667913
Gibbs's free energies (G)	-1525.731233

C	0.9736	1.32791	1.10548
C	-0.20341	0.79685	1.61832
C	-0.38998	-0.59512	1.7126
C	0.60817	-1.48929	1.39137
C	-2.85124	1.65706	4.15921
C	-3.61323	3.07752	1.48994
C	-3.73135	0.01069	1.6987
C	-4.2832	1.45049	4.67526
C	-1.93915	0.56255	4.73231
C	-2.33608	3.02995	4.61306
C	0.39305	-2.93539	1.26318
C	1.47744	-3.8066	1.41098
C	-0.86418	-3.47518	0.95728
C	1.30873	-5.18045	1.2866
C	-1.03274	-4.84652	0.83187
C	0.05307	-5.70461	0.99992
O	-1.23791	1.65072	1.76763
Si	-2.84895	1.5676	2.26956
H	1.91626	0.82459	1.26876
H	1.0166	2.40536	0.99273
H	-1.39421	-0.96294	1.88481
H	1.64176	-1.18749	1.52083
H	-4.64146	3.22498	1.83151
H	-3.0354	3.97108	1.73662
H	-3.61994	2.96883	0.40229
H	-3.41574	-0.28232	0.69565
H	-3.58021	-0.83458	2.37524
H	-4.806	0.21371	1.66321
H	-4.3041	1.54057	5.76781
H	-4.97447	2.19738	4.27141
H	-4.66807	0.45884	4.41875
H	-0.89932	0.70239	4.42281

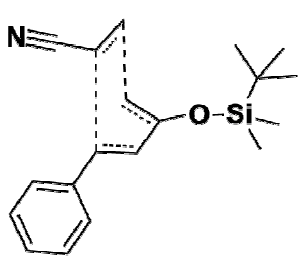
H	-1.9678	0.58891	5.82823
H	-2.25177	-0.43933	4.42053
H	-2.99435	3.83717	4.27905
H	-2.28852	3.07007	5.70781
H	-1.33206	3.22786	4.22592
H	2.45993	-3.39797	1.62121
H	-1.71142	-2.81613	0.79774
H	2.15937	-5.84112	1.40404
H	-2.00977	-5.24939	0.59163
H	-0.0799	-6.77506	0.89578
C	0.91066	0.64414	-0.86401
C	1.12665	-0.73806	-0.8697
C	2.46406	-1.30608	-0.80556
C	4.70828	-0.92877	-0.19333
C	-0.37717	1.20427	-1.33767
C	-0.43192	2.5256	-1.79374
C	-1.55964	0.45763	-1.31588
C	-1.62588	3.08061	-2.23548
C	-2.75727	1.01327	-1.75609
C	-2.7951	2.32315	-2.22249
O	2.77069	-2.43636	-1.11642
O	3.3718	-0.43617	-0.28655
H	1.77684	1.27167	-1.04863
H	0.3738	-1.42779	-1.22435
H	5.29067	-0.12701	0.25418
H	4.74396	-1.82199	0.43178
H	5.09442	-1.1738	-1.18341
H	0.47649	3.12001	-1.80254
H	-1.54596	-0.56591	-0.95575
H	-1.64502	4.10362	-2.593
H	-3.66437	0.41886	-1.74028
H	-3.72738	2.75151	-2.57205



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1525.663243
Gibbs's free energies (G)	-1525.728558

C	-0.00875	-1.57246	-0.38809
C	-0.80284	-0.46013	-0.12539
C	-0.3219	0.83941	-0.34761
C	0.96363	1.05763	-0.80135
C	-4.14864	-0.73171	-1.29752
C	-4.44598	-0.76854	1.80773
C	-3.55017	1.80382	0.40481
C	-5.66443	-0.49447	-1.37806
C	-3.46291	-0.02015	-2.47389
C	-3.86095	-2.23718	-1.38562
C	1.6032	2.37328	-0.91206
C	2.74347	2.50002	-1.71474
C	1.13851	3.50387	-0.22967
C	3.38889	3.72149	-1.85386
C	1.78162	4.72605	-0.36934
C	2.90583	4.84104	-1.1829
O	-1.93796	-0.64788	0.59749
Si	-3.50633	-0.06967	0.35699
H	0.64954	-1.55102	-1.24474
H	-0.41376	-2.54722	-0.14019
H	-0.89961	1.66349	0.05508
H	1.44786	0.28077	-1.38193
H	-4.44355	-1.86066	1.79608
H	-3.9849	-0.44203	2.7433
H	-5.48421	-0.42759	1.80718
H	-3.07302	2.17349	1.31703
H	-3.05647	2.26328	-0.45397
H	-4.58882	2.14741	0.41406
H	-6.04756	-0.85454	-2.34016
H	-6.20067	-1.02832	-0.58797
H	-5.91606	0.56842	-1.30244

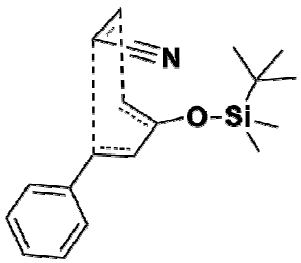
H	-2.37763	-0.1575	-2.45653
H	-3.83442	-0.42956	-3.42102
H	-3.66938	1.05376	-2.4758
H	-4.33473	-2.79082	-0.56941
H	-4.25086	-2.63807	-2.32878
H	-2.78653	-2.43885	-1.3532
H	3.1209	1.627	-2.23832
H	0.28232	3.42911	0.43008
H	4.26746	3.79935	-2.48334
H	1.41204	5.59135	0.16806
H	3.40683	5.79632	-1.28584
C	1.61019	-1.43485	0.90038
C	2.08865	-0.11832	0.96164
C	1.56478	0.82869	1.938
C	-0.26935	1.32566	3.32571
C	2.45026	-2.5005	0.29415
C	2.35511	-3.81062	0.76979
C	3.3218	-2.23753	-0.76775
C	3.12381	-4.82824	0.21497
C	4.08772	-3.25366	-1.32599
C	3.99407	-4.55347	-0.83507
O	2.05935	1.89554	2.23267
O	0.40013	0.39891	2.47908
H	0.99635	-1.75728	1.73383
H	3.04464	0.15704	0.53591
H	-1.18001	0.8271	3.65028
H	0.35117	1.58688	4.18362
H	-0.51151	2.23756	2.77474
H	1.67635	-4.02874	1.58808
H	3.4052	-1.23015	-1.16336
H	3.04273	-5.83639	0.60443
H	4.75983	-3.03095	-2.14656
H	4.59325	-5.34461	-1.26959



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1159.149913
Gibbs's free energies (G)	-1159.206959

C	-0.37713	2.14589	0.28306
C	-0.5989	0.85008	-0.16838
C	0.41742	-0.13087	-0.15874
C	1.65112	0.10451	0.38732
C	-3.72718	-0.27767	1.01488
C	-4.11826	-0.19155	-2.07704
C	-2.21786	-2.26409	-0.82525
C	-5.03536	-1.0829	1.07009
C	-2.79101	-0.75778	2.13449
C	-4.04038	1.21045	1.22338
C	2.82378	-0.76384	0.24975
C	3.92595	-0.5355	1.08341
C	2.90307	-1.79216	-0.70066
C	5.06774	-1.32113	0.98531
C	4.04202	-2.57838	-0.79483
C	5.12775	-2.34771	0.0492
O	-1.71512	0.62336	-0.9084
Si	-2.93111	-0.53868	-0.68339
H	0.29239	2.30964	1.11647
H	-1.20404	2.84208	0.20402
H	0.24449	-1.01641	-0.76029
H	1.76115	0.88732	1.12842
H	-4.5891	0.78786	-1.96444
H	-3.58933	-0.20441	-3.03293
H	-4.90625	-0.94749	-2.11693
H	-1.74167	-2.40924	-1.79866
H	-1.48299	-2.47408	-0.045
H	-3.01906	-3.00346	-0.73469
H	-5.49418	-0.9782	2.06019
H	-5.75933	-0.72772	0.33088
H	-4.86816	-2.15096	0.89773
H	-1.83715	-0.22126	2.12731

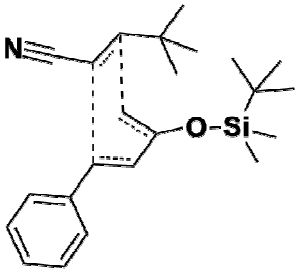
H	-3.26069	-0.58491	3.11013
H	-2.57925	-1.82769	2.05524
H	-4.69777	1.60377	0.44232
H	-4.5462	1.35296	2.18559
H	-3.12754	1.81137	1.23376
H	3.88396	0.27263	1.80517
H	2.07761	-1.97186	-1.37972
H	5.91056	-1.12813	1.63809
H	4.08966	-3.37012	-1.53327
H	6.01711	-2.96174	-0.02934
C	0.93762	2.8693	-1.06912
C	2.1619	2.20603	-1.00963
C	3.16089	2.63491	-0.10001
N	3.94943	2.96444	0.6796
H	0.32702	2.7222	-1.95194
H	0.8754	3.86136	-0.63542
H	2.45494	1.46452	-1.73853



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1159.150740
Gibbs's free energies (G)	-1159.205145

C	0.20519	2.38773	-1.6232
C	0.54477	1.18267	-1.01729
C	-0.43305	0.19932	-0.73243
C	-1.75677	0.37656	-1.02579
C	3.32602	-1.35206	-0.46719
C	3.91771	1.14205	1.29369
C	1.46095	-0.61167	1.90814
C	4.0174	-2.35582	0.46869
C	2.21722	-2.06996	-1.25012
C	4.35245	-0.78214	-1.45622
C	-2.82983	-0.50343	-0.56037
C	-4.05499	-0.50373	-1.2404
C	-2.68462	-1.32554	0.56565
C	-5.09557	-1.32675	-0.83189
C	-3.7276	-2.14567	0.97484
C	-4.93254	-2.15402	0.27602
O	1.78245	1.09141	-0.49935
Si	2.59334	0.0468	0.57021
H	-0.59492	2.39456	-2.34934
H	1.01274	3.08603	-1.80854
H	-0.138	-0.64668	-0.12395
H	-2.05122	1.10965	-1.76682
H	4.63384	0.56028	1.88003
H	4.46334	1.66424	0.50472
H	3.47276	1.89055	1.9538
H	0.68301	0.10807	2.17957
H	0.97244	-1.54761	1.62388
H	2.05547	-0.81455	2.80379
H	4.4523	-3.17391	-0.1172
H	4.82988	-1.89043	1.03549
H	3.31461	-2.79731	1.18218
H	1.70712	-1.39403	-1.94312

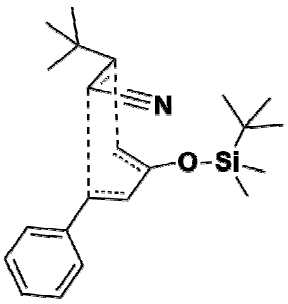
H	2.64876	-2.88769	-1.83932
H	1.46547	-2.50949	-0.58652
H	5.19002	-0.30613	-0.93834
H	4.76065	-1.58717	-2.07833
H	3.89847	-0.04155	-2.12117
H	-4.18225	0.14337	-2.10235
H	-1.76891	-1.29515	1.14484
H	-6.03336	-1.3217	-1.37461
H	-3.60604	-2.77062	1.85161
H	-5.74442	-2.79406	0.60057
C	-0.84092	3.3535	-0.18505
C	-1.92772	2.63276	0.30726
C	-1.79477	1.88072	1.49873
N	-1.65301	1.26632	2.46969
H	-1.05613	4.19077	-0.83921
H	0.01235	3.49881	0.46811
H	-2.92669	2.7544	-0.08877



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1316.258181
Gibbs's free energies (G)	-1316.320621

C	0.05714	1.26679	0.95501
C	-1.06718	0.51374	1.28092
C	-1.06726	-0.89099	1.19103
C	0.07837	-1.60379	0.93104
C	-2.48215	1.89588	4.23208
C	-4.75813	2.17713	2.11765
C	-3.88942	-0.6168	3.07389
C	-3.52811	2.10458	5.33919
C	-1.37556	0.96643	4.75274
C	-1.86702	3.25038	3.85422
C	0.10155	-3.02543	0.56856
C	1.27653	-3.7623	0.76019
C	-1.00665	-3.66393	-0.00561
C	1.33393	-5.10791	0.41669
C	-0.94877	-5.00776	-0.34626
C	0.22054	-5.73593	-0.13219
O	-2.2574	1.16238	1.41343
Si	-3.33475	1.13723	2.72244
H	1.03541	0.87102	1.19277
H	-0.03133	2.34468	1.02186
H	-2.0349	-1.38076	1.15128
H	1.03479	-1.19751	1.23786
H	-4.44386	3.20292	1.91252
H	-5.16085	1.75682	1.19265
H	-5.56583	2.20689	2.853
H	-4.36065	-1.05708	2.19105
H	-3.06322	-1.26256	3.37965
H	-4.63053	-0.61635	3.8784
H	-3.04739	2.52635	6.22941
H	-4.31434	2.79908	5.0288
H	-4.00163	1.16418	5.63792
H	-0.59686	0.80154	4.00203

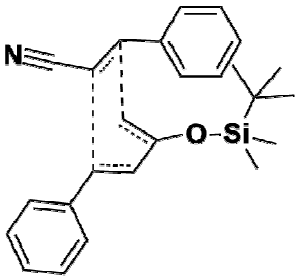
H	-0.89884	1.41417	5.63288
H	-1.77153	-0.00831	5.05109
H	-2.61805	3.9476	3.47119
H	-1.40645	3.71067	4.73628
H	-1.09069	3.13602	3.09296
H	2.14749	-3.26982	1.17904
H	-1.91142	-3.10006	-0.20537
H	2.24954	-5.66514	0.57533
H	-1.81276	-5.48876	-0.78978
H	0.26504	-6.78413	-0.40308
C	0.38177	0.89257	-1.04302
C	0.80199	-0.44026	-1.13819
C	2.15786	-0.765	-0.88135
N	3.25139	-1.02436	-0.60768
H	1.18439	1.62721	-1.00098
H	0.21458	-1.20081	-1.63254
C	-0.81282	1.38234	-1.86658
C	-0.29745	1.51332	-3.31346
C	-2.0013	0.41412	-1.84927
C	-1.28034	2.76306	-1.39223
H	0.55407	2.19775	-3.366
H	0.02115	0.54433	-3.70441
H	-1.0899	1.90467	-3.9577
H	-2.44744	0.34547	-0.85686
H	-2.76962	0.78365	-2.53433
H	-1.72275	-0.58829	-2.18391
H	-1.99408	3.1765	-2.10965
H	-1.77341	2.70277	-0.42042
H	-0.43722	3.45736	-1.31979



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1316.255588
Gibbs's free energies (G)	-1316.316343

C	0.39808	2.31372	-1.56597
C	0.67747	1.12654	-0.89613
C	-0.33069	0.17043	-0.65149
C	-1.63503	0.39793	-1.01067
C	3.42516	-1.41383	-0.42522
C	3.984	0.94352	1.52414
C	1.52484	-0.84982	1.96781
C	4.02828	-2.52586	0.44644
C	2.34378	-2.01465	-1.33469
C	4.52572	-0.79103	-1.29522
C	-2.76304	-0.43567	-0.58569
C	-3.94917	-0.41056	-1.33076
C	-2.70944	-1.22986	0.56802
C	-5.04134	-1.18277	-0.95744
C	-3.80397	-1.99858	0.94215
C	-4.9698	-1.98297	0.17949
O	1.88485	1.03075	-0.30441
Si	2.67179	-0.09136	0.69744
H	-0.31881	2.28525	-2.37427
H	1.22937	2.99471	-1.69461
H	-0.09899	-0.66447	-0.00222
H	-1.85854	1.10014	-1.80457
H	4.6817	0.31959	2.08906
H	4.55244	1.51137	0.78451
H	3.52641	1.65092	2.22003
H	0.76622	-0.13617	2.30179
H	1.01748	-1.74631	1.60107
H	2.11634	-1.14422	2.83995
H	4.49163	-3.28889	-0.19009
H	4.80355	-2.14469	1.11875
H	3.26601	-3.02163	1.05507

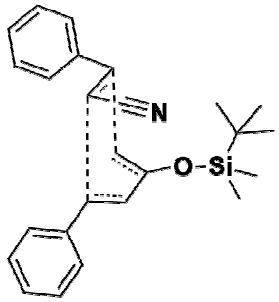
H	1.91426	-1.26339	-2.00397
H	2.77944	-2.80504	-1.95745
H	1.52675	-2.46421	-0.76117
H	5.3534	-0.41377	-0.68784
H	4.93313	-1.54277	-1.98161
H	4.14058	0.03792	-1.89662
H	-4.00401	0.21531	-2.21614
H	-1.82272	-1.21865	1.1922
H	-5.94787	-1.16009	-1.55078
H	-3.7532	-2.60369	1.83971
H	-5.82142	-2.58396	0.4759
C	-0.89	3.40219	-0.34616
C	-1.83585	2.55217	0.23855
C	-1.53433	1.90495	1.46066
N	-1.25305	1.36226	2.44311
H	-0.05446	3.68465	0.29059
H	-2.87612	2.5503	-0.05697
C	-1.37999	4.54616	-1.24644
C	-2.44209	4.09208	-2.25394
C	-2.00434	5.5974	-0.30785
C	-0.22493	5.21768	-2.00193
H	-2.06195	3.32513	-2.93438
H	-3.33912	3.70691	-1.76431
H	-2.74804	4.94511	-2.86543
H	-1.26951	5.95594	0.41817
H	-2.35596	6.45465	-0.88879
H	-2.84922	5.17786	0.24177
H	-0.5682	6.16439	-2.42655
H	0.61113	5.43315	-1.33026
H	0.14159	4.60281	-2.82538



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1390.090790
Gibbs's free energies (G)	-1390.153164

C	0.00378	0.98266	-2.15496
C	0.38278	0.05901	-1.18503
C	-0.58087	-0.68063	-0.47397
C	-1.9227	-0.60014	-0.77429
C	3.18957	-2.33569	-0.64887
C	4.08033	0.39576	0.57131
C	1.81771	-1.21272	1.88883
C	3.98576	-3.23636	0.30752
C	1.95117	-3.09428	-1.14807
C	4.069	-1.95837	-1.84904
C	-2.98502	-1.15967	0.07089
C	-4.23778	-1.42372	-0.49537
C	-2.80022	-1.40447	1.43876
C	-5.26957	-1.9454	0.2759
C	-3.83098	-1.92671	2.20765
C	-5.06809	-2.20325	1.62803
O	1.66382	0.11246	-0.77302
Si	2.6601	-0.77106	0.27067
H	-0.85875	0.78445	-2.77685
H	0.79671	1.56096	-2.61531
H	-0.26518	-1.18753	0.42961
H	-2.22401	-0.37347	-1.78967
H	4.88985	-0.09371	1.11966
H	4.47934	0.76704	-0.37534
H	3.73773	1.25473	1.15412
H	1.17915	-0.39524	2.23097
H	1.2197	-2.12548	1.8253
H	2.58661	-1.37582	2.64999
H	4.31492	-4.14015	-0.21846
H	4.88072	-2.73512	0.68996
H	3.38181	-3.55339	1.16322
H	1.38036	-2.50635	-1.87241

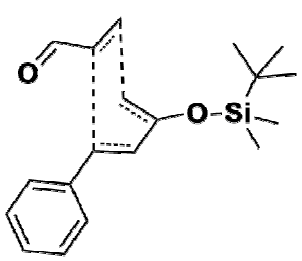
H	2.25875	-4.02349	-1.64232
H	1.27723	-3.3669	-0.32922
H	4.99424	-1.46869	-1.53137
H	4.34451	-2.85818	-2.41135
H	3.54486	-1.28357	-2.53241
H	-4.39757	-1.21425	-1.54768
H	-1.84929	-1.17408	1.90798
H	-6.23201	-2.14685	-0.17924
H	-3.67359	-2.11257	3.26366
H	-5.87175	-2.60857	2.23114
C	-1.01158	2.37071	-1.00454
C	-2.25154	1.81419	-0.65388
C	-3.3094	1.82006	-1.59707
C	-0.02115	2.6997	0.0478
C	1.01369	3.59806	-0.2345
C	-0.06129	2.10269	1.31103
C	1.97335	3.9031	0.72059
C	0.89973	2.40981	2.26998
C	1.91855	3.31055	1.98037
N	-4.14562	1.76209	-2.3936
H	-0.99779	3.03258	-1.86489
H	-2.53417	1.63892	0.37384
H	1.06304	4.05889	-1.21612
H	-0.84671	1.39554	1.55557
H	2.7648	4.60478	0.48461
H	0.84833	1.94644	3.24899
H	2.66403	3.55017	2.72963



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1390.086218
Gibbs's free energies (G)	-1390.148954

C	0.41245	1.66427	1.6871
C	-0.57112	0.96736	2.38272
C	-0.46939	-0.42496	2.56483
C	0.56659	-1.14778	2.01586
C	-2.99853	1.30679	5.24082
C	-4.33197	2.57989	2.73886
C	-3.8229	-0.45102	2.81043
C	-4.2972	0.82744	5.90655
C	-1.83781	0.40552	5.68552
C	-2.70584	2.75157	5.66837
C	0.61767	-2.61412	1.983
C	1.85773	-3.25041	1.84535
C	-0.54052	-3.40111	2.03801
C	1.9455	-4.63544	1.79423
C	-0.45148	-4.78592	1.98294
C	0.7894	-5.40777	1.866
O	-1.71085	1.6305	2.66648
Si	-3.20658	1.22969	3.36253
H	1.44128	1.35294	1.79392
H	0.25908	2.7258	1.53049
H	-1.32352	-0.95386	2.96889
H	1.51436	-0.65668	1.82728
H	-5.2962	2.5557	3.25391
H	-3.88396	3.56367	2.89447
H	-4.51853	2.45498	1.66948
H	-3.51765	-0.67512	1.78413
H	-3.48144	-1.26391	3.45681
H	-4.91647	-0.44888	2.84165
H	-4.20319	0.8903	6.99711
H	-5.15602	1.44059	5.61556
H	-4.52231	-0.21318	5.65364

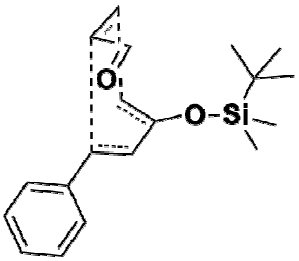
H	-0.88534	0.73323	5.25873
H	-1.74101	0.43592	6.77733
H	-1.99611	-0.63979	5.40118
H	-3.53915	3.41803	5.42839
H	-2.54451	2.79703	6.75181
H	-1.80788	3.14017	5.17883
H	2.75956	-2.64828	1.78864
H	-1.51465	-2.92793	2.09067
H	2.91357	-5.11227	1.69504
H	-1.3552	-5.38283	2.01848
H	0.85351	-6.48852	1.82144
C	0.35672	0.92036	-0.274
C	0.19931	-0.47305	-0.26827
C	-1.11217	-1.0127	-0.30046
C	1.63401	1.5149	-0.7426
C	1.63192	2.77594	-1.34297
C	2.85588	0.85522	-0.57366
C	2.81692	3.35651	-1.78198
C	4.04073	1.43618	-1.00813
C	4.02597	2.68831	-1.61687
N	-2.1904	-1.42891	-0.28988
H	-0.52747	1.50892	-0.49443
H	0.99599	-1.1364	-0.57693
H	0.69085	3.30071	-1.47193
H	2.88679	-0.11972	-0.09735
H	2.79444	4.33164	-2.25418
H	4.97877	0.91103	-0.8714
H	4.95017	3.13932	-1.9577



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1180.215449
Gibbs's free energies (G)	-1180.271589

C	-0.40317	2.17135	0.60903
C	-0.64959	0.92757	0.0369
C	0.34025	-0.07861	-0.03458
C	1.57721	0.06373	0.53303
C	-3.77	-0.4577	0.95276
C	-4.14011	0.21723	-2.06841
C	-2.24691	-2.04995	-1.2358
C	-5.09328	-1.23171	0.84277
C	-2.85265	-1.16847	1.95934
C	-4.05407	0.96676	1.44952
C	2.72446	-0.81241	0.30883
C	3.8553	-0.66091	1.12005
C	2.75415	-1.77764	-0.70974
C	4.97669	-1.46101	0.93659
C	3.87181	-2.57592	-0.89115
C	4.98707	-2.42181	-0.06691
O	-1.75772	0.80739	-0.73469
Si	-2.96222	-0.38694	-0.75707
H	0.26378	2.23452	1.45679
H	-1.22279	2.88075	0.60536
H	0.14856	-0.89965	-0.71552
H	1.71545	0.79543	1.32047
H	-4.92716	-0.51836	-2.25257
H	-4.61285	1.15809	-1.77747
H	-3.60725	0.38355	-3.00754
H	-1.71535	-1.98116	-2.18885
H	-1.56248	-2.45102	-0.48546
H	-3.05823	-2.77285	-1.36327
H	-5.55392	-1.32341	1.83321
H	-5.80724	-0.72089	0.19034
H	-4.94421	-2.24518	0.45618
H	-1.88204	-0.67123	2.05176

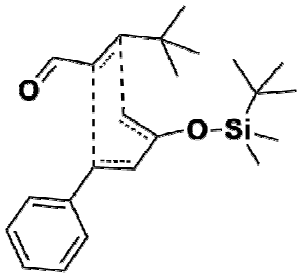
H	-3.32077	-1.1683	2.95095
H	-2.6736	-2.2102	1.67936
H	-4.68535	1.52613	0.75259
H	-4.57675	0.92839	2.41253
H	-3.12805	1.52974	1.59408
H	3.85498	0.09878	1.89335
H	1.90635	-1.89524	-1.37444
H	5.84394	-1.3257	1.57142
H	3.88228	-3.31507	-1.68349
H	5.86187	-3.04338	-0.2171
C	0.89231	3.00975	-0.67672
C	2.07983	2.28804	-0.8124
C	3.2091	2.58972	0.02801
O	4.32643	2.10593	-0.0637
H	0.2065	3.0464	-1.51548
H	0.93646	3.93016	-0.09952
H	2.23137	1.58223	-1.61971
H	2.99754	3.33	0.8315



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1180.217403
Gibbs's free energies (G)	-1180.273295

C	0.2563	2.35298	-1.62288
C	0.62523	1.16905	-0.99511
C	-0.31873	0.16201	-0.68289
C	-1.64338	0.26919	-1.00687
C	3.42276	-1.33052	-0.3974
C	4.06235	1.2349	1.23825
C	1.62332	-0.47473	1.99504
C	4.12741	-2.29398	0.57099
C	2.30465	-2.08282	-1.13306
C	4.43539	-0.80547	-1.42543
C	-2.69348	-0.63775	-0.55208
C	-3.91853	-0.64715	-1.2297
C	-2.53733	-1.47157	0.56306
C	-4.94442	-1.49488	-0.83494
C	-3.56156	-2.31961	0.95739
C	-4.76581	-2.33835	0.25724
O	1.86901	1.12535	-0.47644
Si	2.71842	0.11654	0.59096
H	-0.54985	2.33827	-2.34178
H	1.05059	3.06247	-1.82244
H	0.00555	-0.65701	-0.05263
H	-1.95134	0.97843	-1.76527
H	4.79811	0.67332	1.81978
H	4.58217	1.73384	0.41745
H	3.63673	2.00371	1.88772
H	0.87573	0.27908	2.25756
H	1.1019	-1.40842	1.77138
H	2.24218	-0.65026	2.87971
H	4.56115	-3.13152	0.01253
H	4.94253	-1.80513	1.11372
H	3.43208	-2.71181	1.30569
H	1.78522	-1.44006	-1.84984

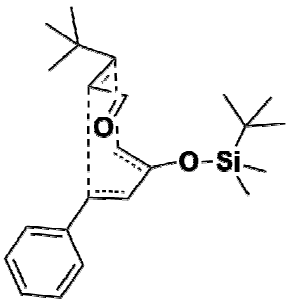
H	2.73136	-2.92544	-1.68971
H	1.56176	-2.49391	-0.4418
H	5.28378	-0.3133	-0.94151
H	4.82924	-1.63744	-2.0206
H	3.97423	-0.09029	-2.11296
H	-4.05958	0.01631	-2.07668
H	-1.62208	-1.43567	1.14376
H	-5.8843	-1.4929	-1.37379
H	-3.4301	-2.95478	1.82525
H	-5.56706	-2.99578	0.57321
C	-0.79825	3.3019	-0.18047
C	-2.00691	2.67974	0.12117
C	-2.14853	1.87357	1.30799
O	-3.19135	1.4355	1.76637
H	-0.82298	4.21189	-0.77027
H	-0.01528	3.28496	0.57331
H	-2.90655	2.89633	-0.4459
H	-1.18731	1.66757	1.82949



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1337.323432
Gibbs's free energies (G)	-1337.384072

C	0.13005	1.27643	-1.79194
C	0.44491	0.10476	-1.10764
C	-0.5618	-0.7583	-0.62943
C	-1.89085	-0.58031	-0.92499
C	4.31465	-0.66885	0.11834
C	1.90278	-2.07129	1.45052
C	2.5406	-2.7	-1.4965
C	5.3185	-1.79317	0.41261
C	4.76484	0.10134	-1.13073
C	4.25456	0.29312	1.3152
C	-2.98271	-1.27208	-0.24083
C	-4.22885	-1.37925	-0.86816
C	-2.83092	-1.80206	1.04946
C	-5.28435	-2.03309	-0.24301
C	-3.88474	-2.45175	1.67342
C	-5.11401	-2.57473	1.02606
O	1.72564	-0.04902	-0.69821
Si	2.59904	-1.39925	-0.15969
H	-0.737	1.27079	-2.4353
H	0.95786	1.88023	-2.14362
H	-0.28509	-1.47483	0.13566
H	-2.16791	-0.07568	-1.84284
H	2.6937	-2.59294	1.99804
H	1.53012	-1.27089	2.09517
H	1.09598	-2.78981	1.28747
H	3.05661	-3.60867	-1.17528
H	1.50452	-2.96725	-1.72306
H	3.00795	-2.34686	-2.41856
H	6.31005	-1.36575	0.60117
H	5.03971	-2.37429	1.29717
H	5.41172	-2.48308	-0.43152
H	4.07903	0.92101	-1.35865

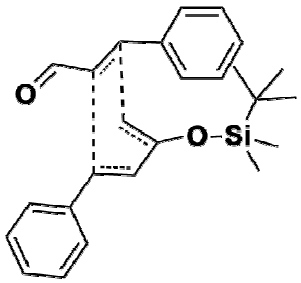
H	5.7622	0.52595	-0.96722
H	4.82268	-0.54806	-2.0097
H	3.98908	-0.2291	2.23943
H	5.23344	0.76248	1.46821
H	3.52202	1.09014	1.15352
H	-4.36761	-0.94076	-1.84981
H	-1.89012	-1.68216	1.57626
H	-6.24249	-2.10953	-0.74292
H	-3.75573	-2.85332	2.67169
H	-5.93789	-3.07823	1.51813
C	-0.85012	2.45217	-0.42633
C	-2.06556	1.82908	-0.10599
C	-3.22242	2.04249	-0.93773
O	-4.36747	1.70209	-0.68563
H	-0.92841	3.21934	-1.1991
H	-2.23392	1.35298	0.85229
H	-3.00714	2.55582	-1.90184
C	0.13423	2.85423	0.67805
C	-0.47375	4.09956	1.35226
C	0.32339	1.76349	1.7384
C	1.50294	3.23882	0.10475
H	-0.60707	4.90955	0.62927
H	-1.44772	3.86973	1.78957
H	0.19071	4.45565	2.1447
H	0.7337	0.85196	1.30301
H	1.02952	2.11868	2.49492
H	-0.61127	1.52201	2.24902
H	2.11043	3.70891	0.88323
H	2.0411	2.36214	-0.26033
H	1.39732	3.955	-0.71634



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1337.320329
Gibbs's free energies (G)	-1337.381835

C	0.51608	2.29184	-1.56344
C	0.79918	1.11191	-0.88247
C	-0.19517	0.14755	-0.63206
C	-1.50145	0.35415	-1.00698
C	3.52343	-1.42814	-0.32555
C	4.10277	0.97709	1.55889
C	1.62997	-0.78328	2.04792
C	4.14094	-2.5027	0.58286
C	2.43687	-2.07078	-1.19996
C	4.61196	-0.83539	-1.23139
C	-2.62601	-0.48855	-0.60878
C	-3.8031	-0.45374	-1.36888
C	-2.58423	-1.30558	0.52869
C	-4.89226	-1.24397	-1.03048
C	-3.67433	-2.096	0.86684
C	-4.82768	-2.07224	0.0874
O	1.99927	1.04355	-0.26217
Si	2.78278	-0.06391	0.75278
H	-0.19083	2.25484	-2.38009
H	1.34821	2.9718	-1.6881
H	0.04311	-0.68455	0.0185
H	-1.71861	1.05672	-1.8024
H	4.79429	0.36028	2.13888
H	4.67697	1.52251	0.80691
H	3.65262	1.70579	2.23749
H	0.88172	-0.05606	2.37425
H	1.10827	-1.68017	1.70415
H	2.21996	-1.06586	2.92477
H	4.59263	-3.2924	-0.02872
H	4.92812	-2.09413	1.22427
H	3.38922	-2.97208	1.2249

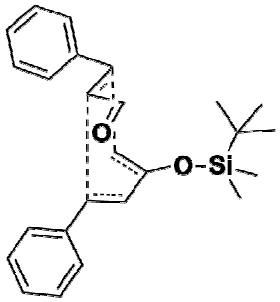
H	1.99118	-1.34892	-1.89056
H	2.87422	-2.87864	-1.79849
H	1.63205	-2.50887	-0.60095
H	5.44225	-0.42657	-0.64856
H	5.01826	-1.61368	-1.88788
H	4.21489	-0.03669	-1.86487
H	-3.85159	0.19416	-2.23845
H	-1.70815	-1.30341	1.1667
H	-5.79173	-1.21379	-1.634
H	-3.63217	-2.71952	1.75199
H	-5.67842	-2.68658	0.35808
C	-0.76559	3.37996	-0.34876
C	-1.78443	2.5638	0.15733
C	-1.59554	1.85625	1.40108
O	-2.45981	1.30146	2.05931
H	0.05028	3.58599	0.34479
H	-2.79499	2.60037	-0.23309
H	-0.54042	1.83753	1.75348
C	-1.13968	4.60063	-1.20629
C	-2.15145	4.26095	-2.30694
C	-1.782	5.6193	-0.24359
C	0.08854	5.26577	-1.84198
H	-1.75834	3.52215	-3.01055
H	-3.09142	3.88372	-1.89895
H	-2.38216	5.16372	-2.87898
H	-1.08647	5.89054	0.55555
H	-2.05041	6.52983	-0.78684
H	-2.68275	5.20716	0.21533
H	-0.18385	6.25587	-2.21607
H	0.89108	5.39225	-1.10918
H	0.47555	4.69293	-2.68625



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1411.154914
Gibbs's free energies (G)	-1411.214689

C	0.06869	1.01127	-2.13678
C	0.40344	0.02472	-1.21094
C	-0.59301	-0.70995	-0.54049
C	-1.93067	-0.56682	-0.83232
C	3.09484	-2.51022	-0.58385
C	4.09021	0.20311	0.5856
C	1.72983	-1.26684	1.90055
C	3.846	-3.41609	0.40325
C	1.83434	-3.23395	-1.07833
C	4.00126	-2.19767	-1.78272
C	-3.01308	-1.12866	-0.02255
C	-4.27341	-1.31413	-0.60188
C	-2.838	-1.46171	1.32851
C	-5.32229	-1.84974	0.13585
C	-3.88503	-1.99566	2.06421
C	-5.1302	-2.19638	1.46803
O	1.68467	-0.0034	-0.80167
Si	2.62011	-0.90047	0.28749
H	-0.79421	0.86814	-2.77079
H	0.88976	1.56716	-2.5751
H	-0.29996	-1.28239	0.33138
H	-2.22319	-0.25044	-1.82602
H	4.86402	-0.31195	1.16119
H	4.5251	0.52891	-0.36202
H	3.78311	1.09375	1.13956
H	1.11234	-0.42324	2.21635
H	1.10182	-2.15987	1.8488
H	2.47997	-1.43883	2.67849
H	4.1487	-4.3432	-0.0974
H	4.75384	-2.93898	0.78604
H	3.22043	-3.69114	1.25772
H	1.28495	-2.63713	-1.81197

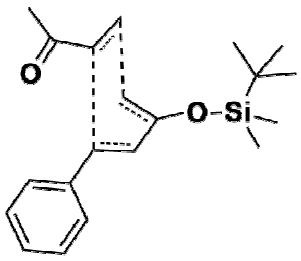
H	2.11348	-4.1787	-1.55982
H	1.14986	-3.47544	-0.25861
H	4.94365	-1.74195	-1.46513
H	4.24328	-3.12066	-2.32226
H	3.51471	-1.51558	-2.48639
H	-4.42881	-1.02984	-1.63624
H	-1.88217	-1.28462	1.81081
H	-6.29157	-1.98776	-0.32824
H	-3.73704	-2.24703	3.10784
H	-5.94804	-2.60969	2.04637
C	-0.86812	2.40341	-0.95397
C	-2.09319	1.89232	-0.49246
C	-3.26595	2.01334	-1.32298
C	0.21806	2.75846	-0.00688
C	1.16692	3.71807	-0.37085
C	0.33858	2.14047	1.24145
C	2.19652	4.06911	0.493
C	1.37075	2.48891	2.10696
C	2.2994	3.45789	1.73977
O	-4.41099	1.75686	-0.99106
H	-0.93019	3.06155	-1.81852
H	-2.25287	1.63512	0.54696
H	-3.06153	2.353	-2.3626
H	1.08976	4.19686	-1.34217
H	-0.37835	1.38204	1.53957
H	2.91611	4.82285	0.19539
H	1.44851	2.00509	3.07463
H	3.09823	3.73327	2.41827



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1411.151588
Gibbs's free energies (G)	-1411.213016

C	0.78162	-1.39968	-0.8933
C	-0.42736	-0.77722	-0.5913
C	-0.53155	0.62454	-0.53881
C	0.55617	1.43813	-0.76918
C	-4.19346	-1.12279	-0.81978
C	-3.21548	-2.93078	1.51487
C	-2.97486	0.12637	1.74978
C	-5.56846	-0.80747	-0.21126
C	-3.76911	0.02911	-1.74167
C	-4.28143	-2.4172	-1.6409
C	0.57845	2.88293	-0.55152
C	1.56081	3.65007	-1.1912
C	-0.32367	3.52733	0.30475
C	1.61876	5.02508	-1.01263
C	-0.26663	4.90262	0.48273
C	0.70012	5.65587	-0.17779
O	-1.40997	-1.56783	-0.10799
Si	-2.94287	-1.34076	0.57978
H	1.44284	-0.93886	-1.61332
H	0.79189	-2.48334	-0.88455
H	-1.44318	1.05791	-0.14555
H	1.38386	1.05696	-1.35496
H	-4.24207	-3.00419	1.88322
H	-3.01802	-3.7933	0.87457
H	-2.54519	-2.98713	2.37606
H	-2.02234	0.24276	2.27326
H	-3.20696	1.06918	1.2485
H	-3.74839	-0.04036	2.505
H	-6.31365	-0.70222	-1.00812
H	-5.91228	-1.60421	0.45584
H	-5.55644	0.12824	0.35555

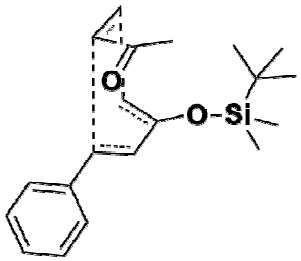
H	-2.80325	-0.16717	-2.21618
H	-4.5114	0.15988	-2.53781
H	-3.69685	0.98075	-1.20513
H	-4.63107	-3.25706	-1.03372
H	-4.98915	-2.28733	-2.46788
H	-3.31167	-2.68794	-2.06903
H	2.27846	3.15751	-1.83959
H	-1.05611	2.9497	0.85696
H	2.38114	5.60403	-1.52008
H	-0.96679	5.38647	1.15315
H	0.74612	6.72846	-0.03096
C	2.00416	-0.96806	0.69252
C	2.09286	0.41313	0.9238
C	1.25063	1.02395	1.92586
C	3.18995	-1.73627	0.22107
C	3.38123	-3.04513	0.66908
C	4.11507	-1.19427	-0.67639
C	4.47744	-3.79008	0.24802
C	5.20864	-1.93887	-1.10157
C	5.39631	-3.23909	-0.63915
O	1.38859	2.13524	2.40569
H	1.38397	-1.52062	1.39531
H	2.93862	0.99416	0.57211
H	0.40811	0.37938	2.25994
H	2.66588	-3.47891	1.36047
H	3.98144	-0.18328	-1.04779
H	4.61321	-4.80083	0.61468
H	5.91777	-1.50351	-1.79615
H	6.25136	-3.81721	-0.96862



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1219.499636
Gibbs's free energies (G)	-1219.558611

C	-0.4689	2.03354	0.29628
C	-0.75895	0.7551	-0.16178
C	0.19861	-0.28045	-0.14261
C	1.44408	-0.1168	0.40701
C	-3.96192	-0.18287	0.99011
C	-4.3085	-0.11516	-2.10523
C	-2.53213	-2.26577	-0.80831
C	-5.30295	-0.93186	1.04127
C	-3.06221	-0.68238	2.1307
C	-4.2136	1.32064	1.16828
C	2.55484	-1.06111	0.29469
C	3.65787	-0.9011	1.14096
C	2.57987	-2.09935	-0.64811
C	4.74311	-1.76546	1.07231
C	3.66331	-2.96159	-0.7176
C	4.74785	-2.80002	0.14449
O	-1.88156	0.59323	-0.91368
Si	-3.15515	-0.50318	-0.69357
H	0.19656	2.14881	1.14004
H	-1.25001	2.77988	0.20963
H	-0.02111	-1.15858	-0.73954
H	1.59255	0.66395	1.14492
H	-5.13134	-0.83297	-2.14603
H	-4.73315	0.88687	-2.0099
H	-3.76989	-0.16488	-3.05451
H	-2.04003	-2.44123	-1.76872
H	-1.82915	-2.5116	-0.0094
H	-3.37424	-2.96041	-0.73675
H	-5.77016	-0.79195	2.02318
H	-6.00221	-0.56092	0.2863
H	-5.17678	-2.00863	0.88941
H	-2.08724	-0.18559	2.12899

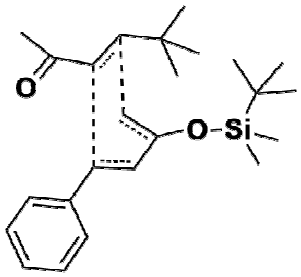
H	-3.53865	-0.47541	3.09648
H	-2.89292	-1.76105	2.07115
H	-4.85258	1.72445	0.37738
H	-4.71493	1.50428	2.12593
H	-3.2762	1.88283	1.16738
H	3.66249	-0.08565	1.85636
H	1.75696	-2.22455	-1.34219
H	5.58763	-1.62369	1.73578
H	3.67012	-3.75845	-1.452
H	5.59502	-3.47283	0.08293
C	0.91768	2.70121	-1.03845
C	2.05625	1.90006	-1.08632
C	3.25381	2.15937	-0.29809
C	3.17178	3.17219	0.83284
O	4.30857	1.58157	-0.52025
H	0.24862	2.68889	-1.89112
H	0.9817	3.66312	-0.53949
H	2.1724	1.15223	-1.86144
H	3.1503	4.18585	0.42343
H	2.26896	3.04448	1.43602
H	4.05392	3.06969	1.46249



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1219.502296
Gibbs's free energies (G)	-1219.559609

C	0.31562	1.97447	-1.75908
C	0.54649	0.7658	-1.11493
C	-0.50974	-0.1152	-0.79353
C	-1.81458	0.15935	-1.11287
C	4.35209	-0.3244	0.0527
C	1.92292	-1.04962	1.84706
C	2.16013	-2.26806	-0.9876
C	5.16471	-1.37544	0.82367
C	4.82713	-0.27928	-1.40701
C	4.55997	1.05295	0.69846
C	-2.96857	-0.60984	-0.64912
C	-4.17179	-0.52645	-1.36031
C	-2.92786	-1.39725	0.50838
C	-5.29138	-1.2379	-0.95113
C	-4.04588	-2.1097	0.91761
C	-5.22934	-2.03638	0.18731
O	1.7756	0.58406	-0.57524
Si	2.52265	-0.7831	0.09352
H	-0.47836	2.03278	-2.48907
H	1.17924	2.59951	-1.95381
H	-0.29573	-0.94675	-0.13057
H	-2.02668	0.86425	-1.90715
H	2.41827	-1.92443	2.27789
H	2.14962	-0.18742	2.47959
H	0.84547	-1.22566	1.89476
H	1.18949	-2.71921	-0.77182
H	2.1754	-1.98695	-2.04397
H	2.92279	-3.03741	-0.83579
H	6.23261	-1.13545	0.76555
H	4.89053	-1.40283	1.88245
H	5.03254	-2.38096	0.41144
H	4.24927	0.4417	-1.99267

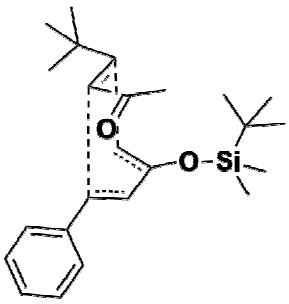
H	5.88075	0.02055	-1.44915
H	4.74134	-1.25737	-1.89018
H	4.24052	1.06284	1.74515
H	5.62361	1.31766	0.67576
H	4.00486	1.82869	0.16574
H	-4.22093	0.10051	-2.24472
H	-2.02674	-1.42651	1.11128
H	-6.21351	-1.16679	-1.51563
H	-4.00269	-2.70847	1.81966
H	-6.10364	-2.58769	0.51275
C	-0.71407	3.08143	-0.38002
C	-1.90477	2.48342	0.02223
C	-2.05993	1.77233	1.28518
C	-0.81134	1.45089	2.08962
O	-3.15975	1.4574	1.71916
H	-0.77775	3.91898	-1.06612
H	0.10674	3.15035	0.32532
H	-2.83005	2.69847	-0.50215
H	0.0392	1.18239	1.46076
H	-0.52724	2.33099	2.6751
H	-1.0385	0.63881	2.78012



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1376.606228
Gibbs's free energies (G)	-1376.669754

C	-0.52924	1.02106	1.11583
C	-0.71462	-0.02414	0.21716
C	0.33399	-0.89886	-0.11419
C	1.55507	-0.85726	0.51879
C	-4.24941	-0.69882	0.92646
C	-3.97308	-0.89225	-2.16427
C	-2.43461	-2.87282	-0.35146
C	-5.55711	-1.49831	0.81471
C	-3.56234	-1.04132	2.25673
C	-4.57452	0.80112	0.89054
C	2.74442	-1.58266	0.06941
C	3.77659	-1.8336	0.9798
C	2.90449	-2.00341	-1.25842
C	4.92298	-2.51413	0.5877
C	4.04865	-2.682	-1.65026
C	5.06044	-2.94405	-0.72704
O	-1.83507	-0.03396	-0.56082
Si	-3.11772	-1.13966	-0.5259
H	0.13539	0.85533	1.95084
H	-1.37483	1.66284	1.32952
H	0.20329	-1.50313	-1.00632
H	1.60684	-0.48314	1.53539
H	-4.39263	0.11304	-2.24856
H	-3.26253	-1.0309	-2.98263
H	-4.78404	-1.61291	-2.2957
H	-1.87794	-3.16549	-1.24539
H	-1.76332	-2.95719	0.50671
H	-3.24773	-3.59137	-0.2153
H	-6.20832	-1.2655	1.66545
H	-6.10658	-1.2515	-0.0985
H	-5.38014	-2.57838	0.8244
H	-2.6164	-0.5045	2.37651

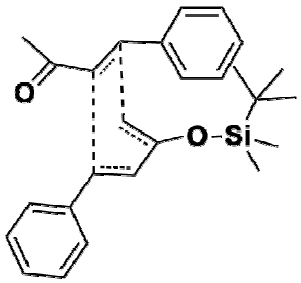
H	-4.2116	-0.76354	3.09564
H	-3.35527	-2.11219	2.33894
H	-5.08843	1.08282	-0.03332
H	-5.23186	1.0619	1.72838
H	-3.67098	1.41137	0.96932
H	3.67696	-1.48502	2.0019
H	2.13943	-1.77793	-1.99311
H	5.71226	-2.69804	1.3068
H	4.16058	-2.99867	-2.68056
H	5.956	-3.46935	-1.03733
C	0.8547	2.26431	0.22464
C	2.05828	1.56127	0.09188
C	3.11014	1.56681	1.10258
C	2.79138	2.07163	2.50031
O	4.24281	1.18141	0.84702
H	0.78621	2.9156	1.09602
H	2.388	1.21308	-0.87942
H	2.68847	3.16006	2.48562
H	1.85634	1.66278	2.89154
H	3.61285	1.80659	3.16343
C	0.19824	2.90114	-1.0097
C	1.00891	4.17918	-1.30103
C	0.24065	1.99738	-2.24698
C	-1.25541	3.30863	-0.73925
H	0.97402	4.86709	-0.4509
H	2.05505	3.93976	-1.5046
H	0.59283	4.69354	-2.17205
H	-0.27461	1.05212	-2.07154
H	-0.26439	2.50368	-3.07469
H	1.26412	1.7908	-2.56655
H	-1.60629	3.96868	-1.5371
H	-1.9127	2.43736	-0.71061
H	-1.3434	3.85245	0.20703



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1376.606061
Gibbs's free energies (G)	-1376.668829

C	0.16242	1.66849	-1.13054
C	0.65892	0.40782	-0.82403
C	-0.18489	-0.71385	-0.73173
C	-1.54291	-0.60438	-0.93228
C	4.67651	-0.15854	-0.02768
C	2.54395	-1.79426	1.52113
C	2.84651	-2.16759	-1.53339
C	5.71928	-1.19218	0.42317
C	5.04809	0.36888	-1.42105
C	4.65637	1.01021	0.96778
C	-2.50952	-1.67878	-0.70161
C	-3.74735	-1.62865	-1.35441
C	-2.25588	-2.74139	0.17438
C	-4.69051	-2.63065	-1.17097
C	-3.19787	-3.74421	0.35746
C	-4.41503	-3.69525	-0.31708
O	1.94313	0.34567	-0.38507
Si	2.97395	-0.96696	-0.10241
H	-0.63759	1.74751	-1.85201
H	0.88484	2.47452	-1.13399
H	0.21637	-1.63411	-0.32153
H	-1.91668	0.21576	-1.53293
H	3.20896	-2.64671	1.68755
H	2.65933	-1.10573	2.36203
H	1.51769	-2.16871	1.53591
H	1.9784	-2.82527	-1.4553
H	2.77756	-1.62809	-2.48153
H	3.73826	-2.80008	-1.57093
H	6.71671	-0.73759	0.42543
H	5.51957	-1.55285	1.43649
H	5.75648	-2.05867	-0.2449

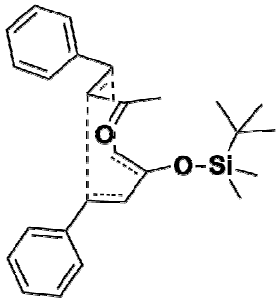
H	4.307	1.08489	-1.788
H	6.01804	0.87833	-1.38192
H	5.12909	-0.44209	-2.15082
H	4.39814	0.67959	1.97839
H	5.64819	1.47505	1.0164
H	3.9367	1.77495	0.66557
H	-3.96265	-0.7964	-2.01737
H	-1.33004	-2.77134	0.73738
H	-5.64043	-2.58042	-1.68988
H	-2.99058	-4.5576	1.04257
H	-5.15137	-4.47609	-0.16729
C	-1.18142	2.20931	0.40946
C	-1.9953	1.12174	0.73878
C	-1.69862	0.19474	1.82866
C	-0.31041	0.21203	2.44095
O	-2.54939	-0.56432	2.27177
H	-0.34919	2.40987	1.08112
H	-3.02684	1.08716	0.40587
H	0.478	0.34955	1.69958
H	-0.24788	1.04583	3.14764
H	-0.15355	-0.71673	2.98826
C	-1.83077	3.49841	-0.12157
C	-2.88416	3.23742	-1.20482
C	-2.52353	4.15336	1.09019
C	-0.79132	4.49049	-0.66008
H	-2.46253	2.728	-2.0756
H	-3.7212	2.64519	-0.83002
H	-3.28879	4.19202	-1.55206
H	-1.79793	4.37074	1.87917
H	-2.99546	5.0938	0.79132
H	-3.28831	3.49267	1.5033
H	-1.24929	5.47618	-0.77568
H	0.0517	4.58957	0.03037
H	-0.40589	4.19213	-1.63628



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1450.438686
Gibbs's free energies (G)	-1450.501504

C	0.05655	1.11104	-1.974
C	0.50828	0.09009	-1.14437
C	-0.39949	-0.77808	-0.51175
C	-1.75764	-0.71269	-0.74195
C	3.38022	-2.29154	-0.7677
C	4.2574	0.4065	0.51171
C	2.04743	-1.28507	1.83207
C	4.24645	-3.18743	0.13097
C	2.15028	-3.08149	-1.23789
C	4.19591	-1.85576	-1.99318
C	-2.74972	-1.4603	0.0357
C	-3.98811	-1.75985	-0.54064
C	-2.51083	-1.85527	1.35901
C	-4.95046	-2.46727	0.16931
C	-3.47339	-2.55657	2.07004
C	-4.69474	-2.87028	1.47496
O	1.80612	0.13408	-0.78098
Si	2.83989	-0.76473	0.211
H	-0.80971	0.93757	-2.59524
H	0.80149	1.78986	-2.37289
H	-0.03078	-1.40707	0.28985
H	-2.11101	-0.34713	-1.69975
H	5.07422	-0.08815	1.04447
H	4.64513	0.78824	-0.43547
H	3.92214	1.25944	1.10702
H	1.38317	-0.51195	2.22247
H	1.48476	-2.21872	1.7496
H	2.83933	-1.44449	2.57018
H	4.58467	-4.06495	-0.43252
H	5.13826	-2.6638	0.48984
H	3.69088	-3.5489	1.00172
H	1.52738	-2.49268	-1.91714

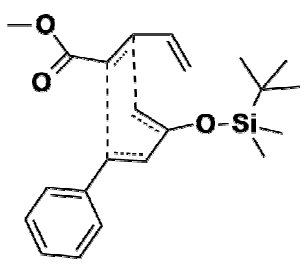
H	2.46933	-3.98289	-1.77463
H	1.52371	-3.40486	-0.40027
H	5.11595	-1.34049	-1.70238
H	4.47935	-2.73297	-2.58669
H	3.62017	-1.18562	-2.6385
H	-4.19535	-1.43233	-1.55375
H	-1.575	-1.59158	1.84102
H	-5.90392	-2.69222	-0.29339
H	-3.27864	-2.85024	3.09488
H	-5.44749	-3.41346	2.03391
C	-1.01111	2.30878	-0.62997
C	-2.1299	1.61499	-0.15068
C	-3.43934	1.67786	-0.79565
C	-3.53817	2.23107	-2.20687
C	0.09539	2.69838	0.27912
C	0.9259	3.76829	-0.06993
C	0.3626	2.00922	1.46554
C	1.983	4.15022	0.74538
C	1.42372	2.388	2.28212
C	2.23564	3.46096	1.92879
O	-4.44707	1.28811	-0.22498
H	-1.18127	3.01746	-1.43561
H	-2.16598	1.26978	0.87514
H	-2.7872	1.80101	-2.87436
H	-4.53378	2.02608	-2.5956
H	-3.38109	3.31297	-2.19386
H	0.73632	4.30549	-0.99406
H	-0.2622	1.17156	1.75691
H	2.60886	4.98757	0.45939
H	1.6154	1.84498	3.20125
H	3.05799	3.75798	2.56901



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1450.436568
Gibbs's free energies (G)	-1450.49965

C	-0.19712	-1.42786	-0.32724
C	-0.85913	-0.25291	0.01111
C	-0.2495	0.99888	-0.15854
C	1.02964	1.11404	-0.67114
C	-4.21094	-0.36579	-1.09231
C	-4.48726	-0.28762	2.01121
C	-3.43724	2.17793	0.51101
C	-5.71679	-0.06446	-1.1481
C	-3.52032	0.29491	-2.2952
C	-3.99462	-1.88423	-1.15673
C	1.78728	2.3669	-0.73782
C	2.84174	2.47444	-1.6527
C	1.51706	3.45301	0.10329
C	3.58494	3.64305	-1.74959
C	2.25847	4.62218	0.00632
C	3.29177	4.72292	-0.92132
O	-1.97464	-0.35029	0.79211
Si	-3.51466	0.30641	0.536
H	0.43899	-1.43718	-1.20078
H	-0.68544	-2.36868	-0.09949
H	-0.7215	1.85458	0.31149
H	1.39293	0.3374	-1.33471
H	-5.48684	0.15379	2.024
H	-4.59396	-1.3748	2.00782
H	-3.98025	-0.00107	2.93574
H	-2.97986	2.55807	1.42862
H	-2.87441	2.56404	-0.34169
H	-4.45036	2.58677	0.45308
H	-6.13182	-0.42	-2.09851
H	-6.25978	-0.5656	-0.3414
H	-5.92159	1.00886	-1.08172

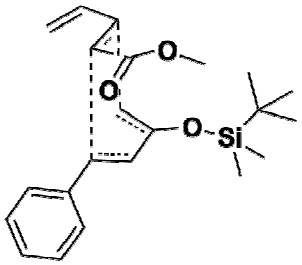
H	-2.43971	0.12351	-2.29029
H	-3.91914	-0.12277	-3.22737
H	-3.69247	1.3746	-2.31742
H	-4.46647	-2.3999	-0.31483
H	-4.43224	-2.28539	-2.07857
H	-2.93073	-2.13594	-1.15449
H	3.07311	1.63129	-2.29631
H	0.74041	3.37555	0.85571
H	4.39434	3.71152	-2.46674
H	2.04119	5.45211	0.66805
H	3.87331	5.63473	-0.98926
C	1.48903	-1.50696	0.90486
C	2.16271	-0.27758	0.90202
C	1.9991	0.71355	1.96907
C	0.814	0.58943	2.90744
C	2.10719	-2.70314	0.27234
C	2.91307	-2.60434	-0.8666
C	1.86204	-3.97016	0.80745
C	3.4689	-3.7397	-1.44315
C	2.42146	-5.10731	0.2343
C	3.22808	-4.99639	-0.89333
O	2.81087	1.61246	2.12145
H	0.89321	-1.73797	1.78256
H	3.08089	-0.16462	0.33586
H	-0.09753	0.26203	2.4049
H	1.05285	-0.14984	3.67874
H	0.65197	1.55064	3.39388
H	3.10819	-1.6328	-1.30984
H	1.23145	-4.0611	1.6862
H	4.09275	-3.64465	-2.32432
H	2.22797	-6.08041	0.67064
H	3.66449	-5.88065	-1.34198



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1372.078821
Gibbs's free energies (G)	-1372.142266

C	-0.49848	-1.81374	-0.07888
C	-0.87951	-0.50938	0.1953
C	0.03817	0.54877	0.10712
C	1.31298	0.36484	-0.40031
C	-4.11112	-0.05496	-1.22383
C	-4.54368	0.56013	1.8001
C	-2.79956	2.42498	0.08878
C	-5.48231	0.59578	-1.46485
C	-3.19941	0.23069	-2.42681
C	-4.28907	-1.57244	-1.07655
C	2.35518	1.40139	-0.35626
C	3.3806	1.38987	-1.30673
C	2.37121	2.3905	0.63582
C	4.37859	2.35695	-1.28856
C	3.36813	3.35557	0.65526
C	4.37332	3.34496	-0.31013
O	-2.06178	-0.30943	0.84291
Si	-3.36065	0.65945	0.3623
H	0.24711	-2.02496	-0.83238
H	-1.21754	-2.60068	0.11966
H	-0.2223	1.47654	0.60408
H	1.4515	-0.39022	-1.16786
H	-5.38836	1.23899	1.65809
H	-4.93587	-0.45102	1.92974
H	-4.03269	0.84456	2.72309
H	-2.39399	2.85002	1.0108
H	-2.03738	2.50255	-0.68962
H	-3.65184	3.04083	-0.21368
H	-5.91448	0.21699	-2.39859
H	-6.18553	0.36878	-0.65818
H	-5.40854	1.6843	-1.55628
H	-2.20306	-0.20188	-2.29289

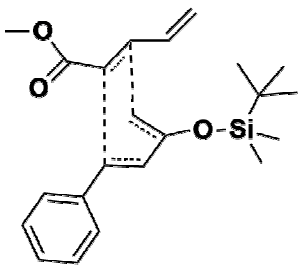
H	-3.63306	-0.20647	-3.33431
H	-3.08231	1.30417	-2.60057
H	-4.92221	-1.82934	-0.22188
H	-4.76327	-1.98255	-1.97616
H	-3.32606	-2.0728	-0.94664
H	3.39451	0.61122	-2.06197
H	1.60689	2.3948	1.40555
H	5.16513	2.33296	-2.03341
H	3.3687	4.11332	1.43008
H	5.15379	4.09636	-0.29018
C	1.02831	-2.07573	1.39993
C	2.12679	-1.30453	1.00518
C	3.10251	-1.79778	0.03728
C	3.48437	-3.28175	-1.75158
O	4.23223	-1.38512	-0.09491
O	2.58659	-2.75555	-0.77384
H	1.02153	-3.11993	1.10947
H	2.51084	-0.51878	1.64011
H	2.92089	-4.03299	-2.29922
H	3.82252	-2.49226	-2.42378
H	4.3514	-3.73287	-1.26828
C	0.27602	-1.72722	2.614
C	0.36453	-0.56607	3.26565
H	-0.44514	-2.46564	2.95337
H	-0.25948	-0.3657	4.12801
H	1.05574	0.21524	2.96878



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1372.075230
Gibbs's free energies (G)	-1372.139432

C	0.4759	1.90956	-0.96373
C	0.74821	0.70869	-0.31763
C	-0.20682	-0.31744	-0.277
C	-1.46454	-0.13604	-0.82399
C	3.90127	-0.63885	-1.15211
C	4.23925	0.16448	1.83801
C	2.40113	-2.176	1.09295
C	5.24575	-1.36711	-0.99694
C	3.01634	-1.41892	-2.13627
C	4.14775	0.77122	-1.70676
C	-2.56885	-1.09958	-0.71929
C	-3.62472	-1.00929	-1.63457
C	-2.62575	-2.087	0.27102
C	-4.69577	-1.89136	-1.58115
C	-3.69591	-2.96999	0.32495
C	-4.73253	-2.87816	-0.60053
O	1.84751	0.64385	0.48146
Si	3.07501	-0.51365	0.54792
H	-0.11062	1.89214	-1.86988
H	1.22118	2.69461	-0.8987
H	-0.01805	-1.1591	0.38007
H	-1.5763	0.573	-1.63796
H	3.69869	0.36449	2.76629
H	5.03844	-0.54757	2.0583
H	4.696	1.10031	1.50724
H	1.84772	-2.07682	2.03105
H	1.74228	-2.62901	0.3493
H	3.22872	-2.86963	1.26908
H	5.71959	-1.48767	-1.9782
H	5.93718	-0.80677	-0.3609
H	5.12279	-2.36681	-0.56736
H	2.03758	-0.94755	-2.26659

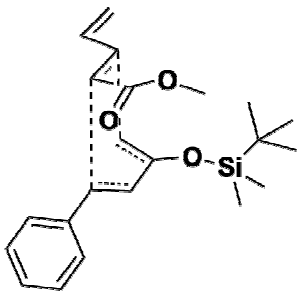
H	3.50096	-1.45819	-3.11932
H	2.85529	-2.4493	-1.80699
H	4.76135	1.37556	-1.0318
H	4.67418	0.70811	-2.66661
H	3.20682	1.30214	-1.87497
H	-3.59576	-0.23976	-2.40008
H	-1.84261	-2.1557	1.01662
H	-5.50069	-1.80819	-2.30187
H	-3.72887	-3.72606	1.10053
H	-5.56782	-3.56661	-0.55145
C	-1.19881	2.74051	0.05106
C	-2.09619	1.72951	0.41293
C	-1.95914	1.02522	1.68595
C	-0.45119	0.4292	3.38893
O	-2.80249	0.32621	2.20373
O	-0.73281	1.20108	2.22667
H	-0.52826	3.09193	0.82481
H	-3.08181	1.6632	-0.02842
H	0.57503	0.666	3.66025
H	-1.13254	0.68911	4.19991
H	-0.55129	-0.63629	3.17034
C	-1.55576	3.73016	-0.98943
C	-2.52708	3.59989	-1.89323
H	-0.92754	4.61669	-1.02217
H	-2.70228	4.36868	-2.63555
H	-3.18243	2.73481	-1.91978



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1372.077206
Gibbs's free energies (G)	-1372.139613

C	0.49125	-1.66104	0.53967
C	0.88262	-0.47138	-0.06388
C	-0.02095	0.59022	-0.23963
C	-1.29533	0.54646	0.28289
C	3.96656	0.49963	1.26698
C	4.64544	-0.03018	-1.72622
C	2.86179	2.35618	-0.954
C	5.3555	1.15302	1.35598
C	3.00686	1.23661	2.21374
C	4.07137	-0.96999	1.69732
C	-2.34434	1.52927	-0.00978
C	-3.39351	1.69381	0.90057
C	-2.3528	2.28922	-1.1872
C	-4.40931	2.61086	0.66004
C	-3.36705	3.20472	-1.42842
C	-4.39716	3.37149	-0.50382
O	2.06337	-0.45653	-0.74334
Si	3.36577	0.60306	-0.52703
H	-0.23568	-1.64497	1.34091
H	1.21544	-2.46705	0.5656
H	0.25253	1.36759	-0.94518
H	-1.46908	-0.05229	1.17104
H	5.50998	0.63689	-1.76735
H	4.99494	-1.02596	-1.44362
H	4.21991	-0.09581	-2.73038
H	2.48168	2.41226	-1.97752
H	2.09515	2.74367	-0.27954
H	3.73021	3.01828	-0.88639
H	5.70267	1.14624	2.39594
H	6.09524	0.61486	0.75642
H	5.34025	2.19572	1.02252
H	1.99493	0.8222	2.17601

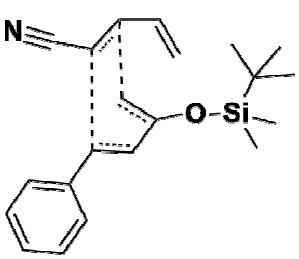
H	3.3654	1.14743	3.24629
H	2.94524	2.30241	1.97653
H	4.72989	-1.54395	1.03834
H	4.48059	-1.03371	2.7126
H	3.09134	-1.45381	1.70001
H	-3.40878	1.09366	1.80432
H	-1.57299	2.14772	-1.92745
H	-5.21319	2.72577	1.37722
H	-3.36311	3.78343	-2.34469
H	-5.19088	4.08323	-0.69751
C	-0.93692	-2.39117	-0.7613
C	-2.03166	-1.51724	-0.7733
C	-3.12806	-1.64426	0.175
C	-3.78061	-2.47395	2.28272
O	-4.24545	-1.19977	0.03388
O	-2.75192	-2.29398	1.30982
H	-1.02287	-3.27605	-0.13744
H	-2.26367	-0.93276	-1.65393
H	-3.31794	-3.0069	3.10983
H	-4.16448	-1.50959	2.61793
H	-4.60255	-3.05679	1.86573
C	-0.15322	-2.55646	-2.00048
C	0.43584	-3.69229	-2.36638
H	-0.07493	-1.67442	-2.63333
H	0.9974	-3.76446	-3.28951
H	0.37074	-4.58431	-1.75075



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1372.076656
Gibbs's free energies (G)	-1372.1381

C	0.29391	1.99679	-1.51237
C	0.73087	0.83078	-0.89542
C	-0.13305	-0.26517	-0.71829
C	-1.44246	-0.22908	-1.1395
C	3.81671	-1.27292	-0.70258
C	4.07869	0.91597	1.49443
C	1.92384	-1.26104	1.76043
C	4.65533	-2.32457	0.03921
C	2.80774	-1.98168	-1.61787
C	4.73806	-0.39195	-1.55808
C	-2.43665	-1.26144	-0.83147
C	-3.58451	-1.3532	-1.62678
C	-2.30228	-2.13793	0.25244
C	-4.55694	-2.31012	-1.36947
C	-3.27195	-3.09746	0.5087
C	-4.40031	-3.18977	-0.30252
O	1.92897	0.88761	-0.27161
Si	2.91199	-0.20337	0.56549
H	-0.4145	1.92531	-2.32525
H	0.99101	2.82356	-1.57095
H	0.19409	-1.07537	-0.07922
H	-1.71855	0.43573	-1.94817
H	4.87713	0.34672	1.97785
H	4.53606	1.6437	0.82032
H	3.53892	1.46543	2.26967
H	1.06357	-0.70199	2.13624
H	1.56076	-2.18875	1.31026
H	2.55249	-1.53177	2.61331
H	5.2007	-2.94385	-0.68245
H	5.39498	-1.86311	0.70088
H	4.03041	-2.99187	0.64086

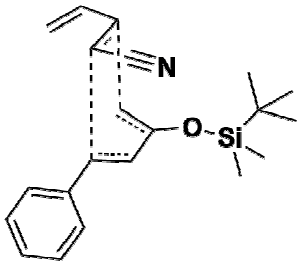
H	2.21255	-1.26774	-2.19409
H	3.34048	-2.62332	-2.32979
H	2.11884	-2.61966	-1.05501
H	5.51551	0.08387	-0.95354
H	5.23643	-1.00069	-2.32157
H	4.17664	0.39483	-2.0706
H	-3.70878	-0.66493	-2.45658
H	-1.44587	-2.05646	0.91354
H	-5.43782	-2.36753	-1.99795
H	-3.15647	-3.76686	1.35296
H	-5.15904	-3.93538	-0.09607
C	-1.14258	2.76577	-0.22412
C	-2.12464	1.80652	0.05053
C	-2.17444	1.06141	1.29761
C	-1.03787	0.47625	3.26727
O	-3.14571	0.47552	1.72615
O	-0.99727	1.08413	1.97747
H	-0.42248	2.97082	0.56178
H	-3.06437	1.82338	-0.48896
H	-0.05982	0.64855	3.71179
H	-1.81694	0.93266	3.87865
H	-1.23645	-0.59398	3.18527
C	-1.51823	3.92267	-1.06388
C	-0.95328	5.12498	-0.97853
H	-2.32014	3.75146	-1.77974
H	-1.27715	5.94736	-1.60431
H	-0.15378	5.32017	-0.27042



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1236.501110
Gibbs's free energies (G)	-1236.560381

C	0.40795	1.88104	-0.83197
C	0.63872	0.70044	-0.13796
C	-0.3819	-0.24539	0.04876
C	-1.60862	-0.12029	-0.57758
C	3.83317	-0.56021	-1.05854
C	4.09012	-0.06898	2.00956
C	2.20234	-2.25819	0.95726
C	5.10937	-1.41181	-0.96785
C	2.91915	-1.13752	-2.15002
C	4.21206	0.88113	-1.42704
C	-2.77624	-0.95792	-0.26288
C	-3.801	-1.08477	-1.20767
C	-2.92047	-1.59793	0.97528
C	-4.92835	-1.85072	-0.93384
C	-4.04519	-2.3647	1.24677
C	-5.05208	-2.49627	0.29219
O	1.76271	0.62115	0.62177
Si	2.95745	-0.57811	0.61915
H	-0.26511	1.89313	-1.67798
H	1.20366	2.61741	-0.84671
H	-0.238	-0.97983	0.83305
H	-1.64676	0.35442	-1.55178
H	4.56997	0.89068	1.80502
H	3.52127	0.02931	2.93735
H	4.87214	-0.81523	2.17095
H	1.688	-2.26624	1.92194
H	1.49009	-2.55742	0.18511
H	2.99035	-3.01604	0.99678
H	5.61329	-1.43125	-1.94128
H	5.81605	-1.00647	-0.23787
H	4.89067	-2.44841	-0.69228
H	1.98529	-0.57423	-2.2401

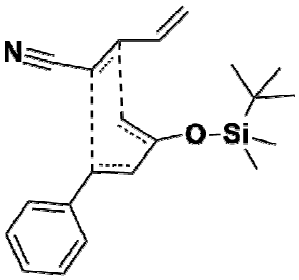
H	3.42756	-1.09513	-3.12068
H	2.66625	-2.18348	-1.95456
H	4.86482	1.33561	-0.67562
H	4.74843	0.89416	-2.38316
H	3.32559	1.51235	-1.53166
H	-3.70866	-0.57521	-2.16098
H	-2.15509	-1.48637	1.73574
H	-5.71057	-1.94186	-1.67807
H	-4.14309	-2.85476	2.20842
H	-5.93087	-3.09198	0.50877
C	-1.11187	2.7378	0.3849
C	-2.2809	2.0057	0.13051
C	-3.05122	2.31366	-1.02436
N	-3.63597	2.51741	-1.99948
H	-0.96004	3.65176	-0.17784
H	-2.80917	1.49394	0.92241
C	-0.4796	2.67929	1.71062
C	-0.76206	1.78061	2.65528
H	0.31597	3.39772	1.88517
H	-0.22043	1.77548	3.59308
H	-1.53612	1.03029	2.53234



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1236.498273
Gibbs's free energies (G)	-1236.556476

C	-0.0093	2.30014	-1.03619
C	0.54089	1.08407	-0.64556
C	-0.26314	-0.06642	-0.55016
C	-1.62675	-0.00152	-0.75163
C	3.73168	-0.94168	-0.81079
C	4.02499	1.11111	1.50984
C	1.96591	-1.16201	1.74249
C	4.67238	-1.9874	-0.19456
C	2.69831	-1.64709	-1.7004
C	4.54306	0.04116	-1.66597
C	-2.5469	-1.11483	-0.48345
C	-3.78131	-1.14909	-1.14316
C	-2.25019	-2.12264	0.44339
C	-4.68536	-2.17722	-0.90984
C	-3.15619	-3.14919	0.67765
C	-4.37269	-3.1832	0.00008
O	1.80102	1.10581	-0.16573
Si	2.85431	0.00054	0.57485
H	-0.79876	2.30206	-1.77222
H	0.64245	3.16628	-1.03798
H	0.1668	-0.96289	-0.12037
H	-2.03119	0.77304	-1.39509
H	4.85437	0.54339	1.93976
H	4.43916	1.88022	0.85419
H	3.49923	1.60938	2.32811
H	1.12377	-0.67096	2.23836
H	1.59378	-2.06324	1.24788
H	2.66863	-1.48211	2.51753
H	5.1964	-2.53235	-0.98861
H	5.43256	-1.52582	0.4435
H	4.12519	-2.72093	0.40529
H	2.01297	-0.93369	-2.16777

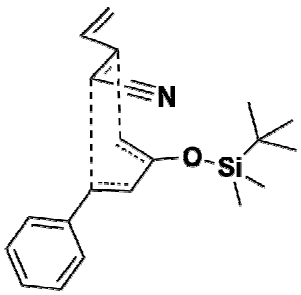
H	3.20728	-2.19368	-2.50317
H	2.10162	-2.37305	-1.13884
H	5.32607	0.53253	-1.08151
H	5.0296	-0.49111	-2.49185
H	3.90325	0.81683	-2.09709
H	-4.02443	-0.36346	-1.85196
H	-1.32378	-2.0859	1.00574
H	-5.63266	-2.1936	-1.43561
H	-2.91808	-3.92007	1.40101
H	-5.07723	-3.98476	0.18774
C	-1.43382	2.76865	0.48816
C	-2.12503	1.61645	0.88233
C	-1.62465	0.8523	1.9697
N	-1.18392	0.22003	2.83044
H	-0.62664	3.10015	1.13042
H	-3.17396	1.47853	0.65733
C	-2.1176	3.83368	-0.27737
C	-3.29086	3.72212	-0.89938
H	-1.57185	4.77028	-0.35203
H	-3.70407	4.55402	-1.45571
H	-3.88196	2.81231	-0.87321



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1236.498938
Gibbs's free energies (G)	-1236.557146

C	-0.38315	1.65622	1.0108
C	-0.5988	0.55492	0.18608
C	0.43208	-0.3556	-0.10412
C	1.66475	-0.26872	0.50378
C	-3.7105	-0.88451	1.02146
C	-4.11788	0.03598	-1.92977
C	-2.17206	-2.26112	-1.29018
C	-5.01614	-1.67828	0.85562
C	-2.76907	-1.65333	1.96081
C	-4.02631	0.4861	1.63653
C	2.85086	-1.03265	0.09917
C	3.90487	-1.17923	1.00893
C	2.98478	-1.58978	-1.18033
C	5.05098	-1.88468	0.66118
C	4.12807	-2.29642	-1.52536
C	5.16387	-2.44931	-0.60494
O	-1.72255	0.54472	-0.57698
Si	-2.91671	-0.65389	-0.68267
H	0.28177	1.56273	1.85934
H	-1.20201	2.35705	1.12467
H	0.28572	-1.01309	-0.95426
H	1.73123	0.17065	1.49232
H	-4.5998	0.94327	-1.55836
H	-3.59572	0.28625	-2.85619
H	-4.89647	-0.69357	-2.16611
H	-1.69976	-2.12726	-2.26711
H	-1.42788	-2.66141	-0.59807
H	-2.95894	-3.01275	-1.40382
H	-5.47382	-1.84822	1.83725
H	-5.74231	-1.13845	0.24103
H	-4.8458	-2.65878	0.39941
H	-1.81531	-1.13436	2.09723

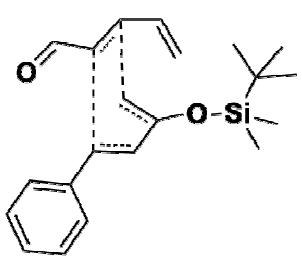
H	-3.23389	-1.75788	2.94848
H	-2.5573	-2.65917	1.58739
H	-4.67267	1.08741	0.99015
H	-4.54344	0.35463	2.59426
H	-3.11284	1.05572	1.82576
H	3.82071	-0.72974	1.99242
H	2.19912	-1.45683	-1.91569
H	5.8559	-1.99006	1.37865
H	4.21875	-2.72213	-2.51786
H	6.05664	-2.9989	-0.87886
C	0.98962	2.75246	-0.05001
C	2.1985	2.03791	-0.08175
C	3.12578	2.17784	0.98159
N	3.84721	2.25279	1.88193
H	0.90852	3.55121	0.68201
H	2.57802	1.62089	-1.00492
C	0.28298	2.98808	-1.32367
C	-0.4433	4.07211	-1.58166
H	0.38444	2.20681	-2.07458
H	-0.94113	4.20321	-2.53433
H	-0.55744	4.8619	-0.84563



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1236.499414
Gibbs's free energies (G)	-1236.556233

C	0.03348	2.18643	-1.19856
C	0.5197	0.955	-0.7664
C	-0.33921	-0.15234	-0.63125
C	-1.69008	-0.04982	-0.8744
C	3.61784	-1.23895	-0.69009
C	3.9161	0.93191	1.51865
C	1.73252	-1.21892	1.77935
C	4.41273	-2.33659	0.03267
C	2.5919	-1.88788	-1.63008
C	4.57716	-0.36906	-1.51439
C	-2.66585	-1.09337	-0.54333
C	-3.89916	-1.10562	-1.2072
C	-2.4237	-2.05756	0.44481
C	-4.85436	-2.07061	-0.91825
C	-3.38129	-3.02058	0.73487
C	-4.59559	-3.03437	0.05271
O	1.76969	0.93735	-0.2631
Si	2.73166	-0.17058	0.5921
H	-0.74811	2.20343	-1.94472
H	0.73236	3.01314	-1.23895
H	0.04164	-1.04035	-0.14265
H	-2.05434	0.71399	-1.55074
H	4.7147	0.34958	1.98624
H	4.37288	1.66297	0.84778
H	3.39007	1.47479	2.30778
H	0.88829	-0.66664	2.20253
H	1.34716	-2.13235	1.31816
H	2.38137	-1.52166	2.60659
H	4.95309	-2.94974	-0.69794
H	5.15331	-1.91759	0.72129
H	3.75787	-3.00211	0.60332

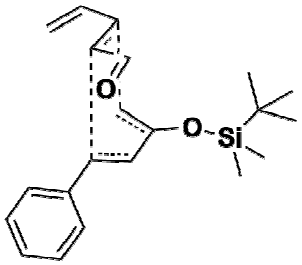
H	2.01425	-1.13659	-2.17681
H	3.10637	-2.51477	-2.36789
H	1.88894	-2.53029	-1.08996
H	5.3616	0.06656	-0.88894
H	5.06525	-0.97579	-2.2861
H	4.04825	0.44759	-2.01471
H	-4.10056	-0.35291	-1.96291
H	-1.50038	-2.0324	1.01232
H	-5.79965	-2.07099	-1.44783
H	-3.18559	-3.75665	1.50568
H	-5.3401	-3.7872	0.28325
C	-1.23768	2.81822	0.30398
C	-2.10568	1.78617	0.69616
C	-1.76882	0.97177	1.80543
N	-1.45942	0.30268	2.69654
H	-0.41061	3.04701	0.96935
H	-3.14549	1.78784	0.39349
C	-1.82281	3.97549	-0.4035
C	-1.31457	5.20491	-0.37738
H	-2.73161	3.77484	-0.96819
H	-1.79141	6.02303	-0.90277
H	-0.41032	5.42847	0.18016



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1257.564878
Gibbs's free energies (G)	-1257.623087

C	0.45026	1.77241	-1.07759
C	0.69085	0.68587	-0.24179
C	-0.32047	-0.23935	0.0557
C	-1.54456	-0.21307	-0.58776
C	3.82567	-0.74719	-1.00835
C	4.19795	0.27837	1.91245
C	2.28612	-2.06387	1.33658
C	5.13805	-1.5212	-0.80712
C	2.89903	-1.55542	-1.92903
C	4.13244	0.60594	-1.66584
C	-2.70067	-1.01968	-0.18172
C	-3.69609	-1.31279	-1.11917
C	-2.8596	-1.47823	1.1335
C	-4.80755	-2.06811	-0.76321
C	-3.96865	-2.23207	1.48851
C	-4.94505	-2.53259	0.5397
O	1.81382	0.71543	0.52119
Si	3.01423	-0.46785	0.68073
H	-0.20839	1.66118	-1.92652
H	1.24572	2.50083	-1.18961
H	-0.17578	-0.87061	0.92536
H	-1.58129	0.15278	-1.60795
H	4.98151	-0.4332	2.184
H	4.67479	1.17647	1.51321
H	3.66233	0.55682	2.82317
H	1.80308	-1.90417	2.30422
H	1.55355	-2.4968	0.65176
H	3.08247	-2.80008	1.48089
H	5.60743	-1.71523	-1.77878
H	5.85232	-0.95538	-0.20188
H	4.9735	-2.4894	-0.32353
H	1.93972	-1.05231	-2.0848

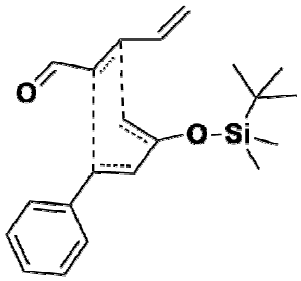
H	3.37029	-1.68423	-2.91083
H	2.69746	-2.55183	-1.52584
H	4.77069	1.23243	-1.03537
H	4.65628	0.44844	-2.61605
H	3.21511	1.1617	-1.87755
H	-3.59775	-0.93963	-2.1321
H	-2.11992	-1.22862	1.88666
H	-5.5699	-2.28411	-1.50212
H	-4.0799	-2.57908	2.50903
H	-5.8135	-3.11667	0.82081
C	-1.04027	2.77188	0.00192
C	-2.21818	2.00849	-0.05357
C	-3.09838	2.16146	-1.19379
O	-4.23334	1.73221	-1.28085
H	-0.9556	3.58041	-0.71969
H	-2.64951	1.5654	0.83451
H	-2.64881	2.70196	-2.05589
C	-0.33272	2.99007	1.27588
C	-0.54316	2.30277	2.3988
H	0.45798	3.73513	1.25575
H	0.05207	2.49514	3.2831
H	-1.30911	1.53922	2.47844



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1257.563509
Gibbs's free energies (G)	-1257.621921

C	0.70751400	1.12960200	1.27198600
C	-0.32261200	0.41974800	1.88619400
C	-0.31619300	-0.98496700	1.92314800
C	0.70090500	-1.71520700	1.34756100
C	-2.76315900	0.56243300	4.73948000
C	-3.95833000	2.26696900	2.43199700
C	-3.69809800	-0.77758600	2.09593200
C	-4.11864500	0.14525200	5.33080100
C	-1.71557200	-0.51098900	5.06660100
C	-2.32509800	1.89838300	5.35634900
C	0.69405000	-3.16760700	1.18766000
C	1.91310600	-3.83505500	1.01185200
C	-0.49051300	-3.91489100	1.16639200
C	1.95368800	-5.21369500	0.85839900
C	-0.45003000	-5.29382500	1.01399300
C	0.77011200	-5.94741700	0.86453000
O	-1.42901000	1.12217500	2.21446100
Si	-2.95022600	0.75998800	2.86899800
H	1.71736600	0.75128200	1.33813000
H	0.61328500	2.20941400	1.26419800
H	-1.20699500	-1.49737600	2.26514500
H	1.67039100	-1.25165700	1.21020400
H	-4.92255600	2.25834400	2.94709700
H	-3.42856400	3.18009300	2.71123300
H	-4.15073800	2.30090600	1.35698700
H	-3.42322200	-0.86890700	1.04169800
H	-3.40796300	-1.69899400	2.60677500
H	-4.78835300	-0.70477100	2.14807700
H	-4.03686200	0.05236900	6.42006200
H	-4.90018300	0.88275900	5.12249100
H	-4.45190500	-0.82161900	4.94153300
H	-0.72542900	-0.23800200	4.69080000

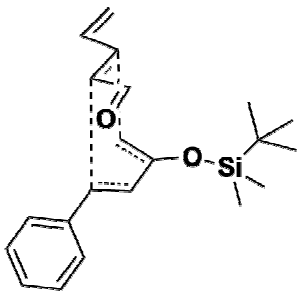
H	-1.63722800	-0.63393500	6.15326100
H	-1.98116300	-1.48676300	4.64678800
H	-3.07600700	2.67863900	5.20251900
H	-2.18267500	1.78286900	6.43722100
H	-1.37975200	2.24714700	4.92992900
H	2.83406300	-3.26081100	1.00386700
H	-1.44901800	-3.41379500	1.24118400
H	2.90528000	-5.71566300	0.73007500
H	-1.37373400	-5.85960500	0.99352700
H	0.79720900	-7.02334400	0.73877900
C	0.55165800	0.65007300	-0.72900800
C	0.57622400	-0.73625300	-0.93179300
C	-0.66350600	-1.45594800	-1.10936300
O	-0.78377800	-2.59167800	-1.53408200
H	-0.42738900	1.11846000	-0.80743800
H	1.48809600	-1.25691100	-1.20184100
H	-1.56664800	-0.88036200	-0.80941600
C	1.66924700	1.52471300	-1.16964700
C	2.80000000	1.12752800	-1.74954400
H	1.52599000	2.58575200	-0.98242800
H	3.56110200	1.84833100	-2.02231000
H	2.99986800	0.08854800	-1.98509700



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1257.564490
Gibbs's free energies (G)	-1257.623652

C	0.44366	1.60623	-1.08746
C	0.64487	0.52513	-0.2304
C	-0.38895	-0.37905	0.06476
C	-1.61526	-0.31669	-0.55894
C	3.78368	-0.9169	-0.96167
C	4.11539	0.07015	1.97772
C	2.19651	-2.2509	1.33914
C	5.08289	-1.70972	-0.74694
C	2.86366	-1.70203	-1.90863
C	4.1196	0.43977	-1.59682
C	-2.80041	-1.0691	-0.14725
C	-3.85049	-1.23205	-1.05752
C	-2.94029	-1.60363	1.14213
C	-4.99619	-1.93565	-0.70522
C	-4.08315	-2.3052	1.49347
C	-5.1137	-2.47741	0.56924
O	1.75264	0.53862	0.55521
Si	2.94829	-0.65254	0.7173
H	-0.20649	1.48131	-1.9422
H	1.27063	2.29414	-1.21856
H	-0.25372	-1.01424	0.93326
H	-1.67543	0.11397	-1.55202
H	4.8905	-0.65021	2.25051
H	4.60288	0.97109	1.59832
H	3.56881	0.33884	2.88476
H	1.70855	-2.10354	2.30629
H	1.46402	-2.66342	0.64167
H	2.98306	-2.99902	1.47602
H	5.5645	-1.90085	-1.71309
H	5.79476	-1.15818	-0.12595
H	4.89926	-2.68007	-0.27472
H	1.91317	-1.18545	-2.07421

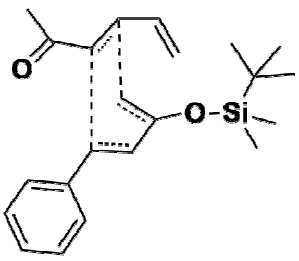
H	3.35019	-1.82285	-2.88393
H	2.64351	-2.70146	-1.52312
H	4.7488	1.05367	-0.9454
H	4.66411	0.28608	-2.53595
H	3.21356	1.00704	-1.82466
H	-3.76572	-0.79731	-2.04704
H	-2.16014	-1.45409	1.87996
H	-5.79883	-2.05161	-1.42344
H	-4.17976	-2.71134	2.4935
H	-6.00768	-3.0221	0.84912
C	-0.90677	2.74935	-0.08576
C	-2.10977	2.039	0.07974
C	-3.14935	2.15504	-0.91419
O	-4.29605	1.75658	-0.80514
H	-0.89688	3.48751	-0.88666
H	-2.38065	1.61618	1.04017
H	-2.82599	2.64264	-1.8604
C	-0.12461	3.12942	1.1087
C	0.55927	4.26509	1.22095
H	-0.13383	2.4155	1.92962
H	1.1115	4.50526	2.12103
H	0.5811	4.99141	0.41412



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1257.565531
Gibbs's free energies (G)	-1257.62443

C	0.15071	2.12307	-1.27565
C	0.61146	0.90644	-0.77493
C	-0.25822	-0.18192	-0.58499
C	-1.59921	-0.09093	-0.88655
C	3.60693	-1.38808	-0.58804
C	4.08356	0.94218	1.41658
C	1.82968	-1.07785	1.94693
C	4.44976	-2.40497	0.19644
C	2.52631	-2.13421	-1.38425
C	4.50752	-0.61853	-1.56486
C	-2.60187	-1.1035	-0.56315
C	-3.813	-1.10057	-1.26694
C	-2.4151	-2.0554	0.44749
C	-4.79452	-2.04403	-0.99951
C	-3.39572	-3.00071	0.71396
C	-4.5849	-3.00151	-0.01042
O	1.85529	0.90636	-0.24827
Si	2.81736	-0.1777	0.62986
H	-0.62005	2.12037	-2.03365
H	0.87318	2.92624	-1.35364
H	0.10504	-1.04486	-0.03993
H	-1.92665	0.64967	-1.60552
H	4.87974	0.36887	1.89854
H	4.53577	1.59825	0.66992
H	3.61399	1.57005	2.17792
H	1.05695	-0.43265	2.37361
H	1.35007	-1.98856	1.58056
H	2.50303	-1.36672	2.75912
H	4.92239	-3.11008	-0.49721
H	5.24795	-1.92008	0.76674
H	3.83862	-2.98715	0.89299

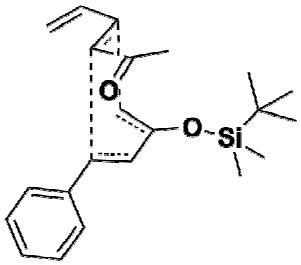
H	1.91314	-1.44965	-1.97725
H	2.99859	-2.8412	-2.0764
H	1.86098	-2.71158	-0.73405
H	5.33385	-0.12197	-1.0481
H	4.94104	-1.30966	-2.29717
H	3.94464	0.14188	-2.11434
H	-3.97607	-0.35186	-2.03552
H	-1.51131	-2.04099	1.04635
H	-5.72273	-2.03222	-1.55819
H	-3.24073	-3.72924	1.5008
H	-5.351	-3.73727	0.20405
C	-1.08672	2.84525	0.18417
C	-2.1081	1.93279	0.49452
C	-1.99413	1.07388	1.64985
O	-2.8965	0.44351	2.17261
H	-0.28307	2.94046	0.91194
H	-3.09115	2.03411	0.04417
H	-0.96516	1.01313	2.06732
C	-1.45986	4.10892	-0.49
C	-0.81061	5.26049	-0.33787
H	-2.33437	4.06088	-1.13587
H	-1.13631	6.1627	-0.84045
H	0.06235	5.33326	0.30362



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1296.850798
Gibbs's free energies (G)	-1296.910519

C	0.17857	1.9234	-1.25366
C	0.59051	0.64204	-0.91231
C	-0.34837	-0.37104	-0.65187
C	-1.70634	-0.17002	-0.81327
C	4.56515	-0.14448	-0.09729
C	2.33473	-1.48293	1.57224
C	2.61068	-2.19088	-1.4147
C	5.53355	-1.1872	0.48069
C	4.99642	0.21693	-1.52584
C	4.59419	1.1185	0.77649
C	-2.72437	-1.13635	-0.38618
C	-3.96979	-1.14572	-1.02146
C	-2.50293	-2.02903	0.67095
C	-4.95668	-2.04626	-0.63964
C	-3.4885	-2.92652	1.05465
C	-4.71755	-2.94158	0.39667
O	1.89405	0.48816	-0.59521
Si	2.81599	-0.84888	-0.12498
H	-0.70897	2.05584	-1.85329
H	0.94567	2.68148	-1.36401
H	-0.00731	-1.27772	-0.1653
H	-2.04221	0.54239	-1.55918
H	2.83347	-2.44013	1.75287
H	2.64269	-0.78985	2.35803
H	1.25975	-1.64422	1.67455
H	1.63782	-2.68262	-1.34144
H	2.70419	-1.77574	-2.42116
H	3.37894	-2.95974	-1.29203
H	6.55448	-0.78814	0.48007
H	5.28172	-1.44643	1.51337
H	5.54239	-2.10901	-0.10959
H	4.31297	0.94212	-1.97663

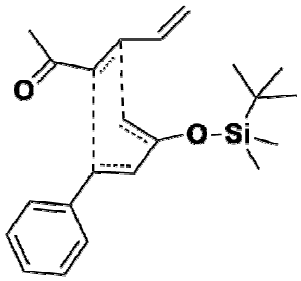
H	5.99915	0.66012	-1.514
H	5.03183	-0.66587	-2.17131
H	4.31702	0.9022	1.81307
H	5.6061	1.54032	0.78773
H	3.90988	1.88002	0.39402
H	-4.16312	-0.43723	-1.81967
H	-1.5624	-2.00328	1.21136
H	-5.91528	-2.04062	-1.1444
H	-3.30558	-3.60908	1.87623
H	-5.48821	-3.63929	0.70226
C	-0.87035	2.47032	0.52109
C	-2.01765	1.67904	0.65126
C	-3.31773	2.06998	0.10434
C	-3.37537	3.17456	-0.93558
O	-4.34569	1.51625	0.46154
H	-0.99086	3.45875	0.08917
H	-2.08328	0.93952	1.43928
H	-2.62528	3.04456	-1.71946
H	-4.36987	3.19026	-1.37734
H	-3.18618	4.14071	-0.45997
C	0.25722	2.33838	1.46244
C	0.43743	1.34225	2.33052
H	1.02266	3.10647	1.38492
H	1.31979	1.31492	2.95864
H	-0.27978	0.53792	2.45526



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1296.849891
Gibbs's free energies (G)	-1296.910085

C	0.21892	2.00573	-1.2418
C	0.57927	0.70421	-0.9073
C	-0.39002	-0.30416	-0.78185
C	-1.73453	-0.03829	-0.95348
C	4.49741	-0.25716	0.01472
C	2.1609	-1.69986	1.44604
C	2.53853	-2.06535	-1.59873
C	5.4198	-1.3967	0.47254
C	4.97627	0.27405	-1.34411
C	4.54231	0.87869	1.04714
C	-2.80473	-0.99945	-0.67482
C	-4.04511	-0.84188	-1.30515
C	-2.64324	-2.05451	0.23138
C	-5.08345	-1.73207	-1.0658
C	-3.68051	-2.94471	0.47125
C	-4.9016	-2.78987	-0.17937
O	1.84649	0.51229	-0.46152
Si	2.73061	-0.89872	-0.14916
H	-0.59092	2.15937	-1.93994
H	1.01301	2.74308	-1.27458
H	-0.0931	-1.25858	-0.36153
H	-2.02811	0.7921	-1.58498
H	2.7534	-2.60069	1.63135
H	2.29377	-1.02904	2.29851
H	1.1106	-1.99919	1.41813
H	1.55797	-2.54578	-1.61769
H	2.67106	-1.53267	-2.54365
H	3.29237	-2.85641	-1.54846
H	6.45404	-1.03827	0.52812
H	5.14514	-1.76562	1.46497
H	5.40255	-2.24267	-0.22181
H	4.31782	1.06263	-1.71936

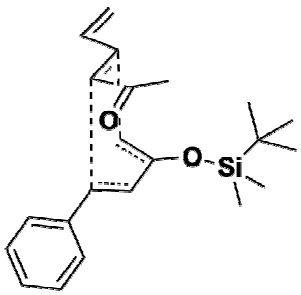
H	5.98387	0.69472	-1.24648
H	5.02043	-0.52047	-2.09478
H	4.22137	0.54115	2.03711
H	5.56797	1.25376	1.14306
H	3.90315	1.71302	0.74823
H	-4.18798	-0.01556	-1.99418
H	-1.71214	-2.16441	0.77606
H	-6.03521	-1.59948	-1.56655
H	-3.54283	-3.75117	1.18152
H	-5.71185	-3.48279	0.01409
C	-0.97779	2.68129	0.33886
C	-1.97191	1.74771	0.65399
C	-1.8585	0.81688	1.77474
C	-0.49341	0.59044	2.39832
O	-2.83668	0.23771	2.2227
H	-0.11894	2.73049	1.00154
H	-2.98439	1.88341	0.29074
H	0.31475	0.58765	1.66494
H	-0.29252	1.39648	3.11118
H	-0.50817	-0.35299	2.94313
C	-1.31268	3.98105	-0.29746
C	-2.53148	4.4286	-0.59404
H	-0.45857	4.60845	-0.54018
H	-2.66149	5.39214	-1.07181
H	-3.43074	3.87155	-0.35833



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1296.847943
Gibbs's free energies (G)	-1296.907436

C	-0.45905	1.63869	0.9295
C	-0.76295	0.51945	0.16047
C	0.19934	-0.47004	-0.09955
C	1.45581	-0.4291	0.46637
C	-3.90649	-0.80531	1.0516
C	-4.35144	0.17761	-1.87298
C	-2.50692	-2.22134	-1.32872
C	-5.2507	-1.53743	0.91299
C	-2.97767	-1.62667	1.95851
C	-4.14145	0.57258	1.68633
C	2.56221	-1.31697	0.10094
C	3.61748	-1.49054	1.00258
C	2.62186	-1.97519	-1.13493
C	4.68763	-2.3227	0.69787
C	3.69119	-2.80358	-1.44125
C	4.72596	-2.98384	-0.52412
O	-1.90073	0.55215	-0.58447
Si	-3.14938	-0.58845	-0.67169
H	0.21361	1.53051	1.7691
H	-1.2227	2.40114	1.02796
H	-0.00778	-1.16463	-0.90596
H	1.57836	0.07449	1.41937
H	-5.17099	-0.50911	-2.09851
H	-4.77782	1.10159	-1.4758
H	-3.84297	0.41668	-2.81
H	-2.02813	-2.08528	-2.30222
H	-1.78811	-2.68926	-0.65254
H	-3.33879	-2.91872	-1.46458
H	-5.69341	-1.69249	1.90389
H	-5.96542	-0.96215	0.31738
H	-5.13435	-2.52206	0.44859
H	-2.0007	-1.14942	2.08144

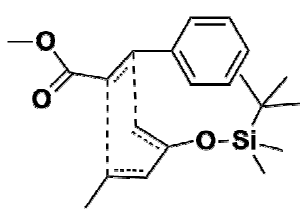
H	-3.42599	-1.72833	2.95418
H	-2.81539	-2.63424	1.5654
H	-4.78572	1.20412	1.06724
H	-4.62769	0.45663	2.66222
H	-3.19819	1.10252	1.84295
H	3.59573	-0.96362	1.9508
H	1.83858	-1.8233	-1.86908
H	5.495	-2.44499	1.40979
H	3.72691	-3.30319	-2.4022
H	5.56302	-3.62652	-0.76995
C	0.97656	2.60628	-0.20734
C	2.08467	1.76708	-0.39798
C	3.28049	1.82779	0.43652
C	3.18966	2.51529	1.78821
O	4.33801	1.33564	0.07424
H	1.06715	3.38621	0.54505
H	2.22628	1.28101	-1.35706
H	3.18342	3.60001	1.65028
H	2.27862	2.24932	2.33069
H	4.06301	2.24432	2.37888
C	0.1567	2.97891	-1.37788
C	-0.41641	4.16935	-1.53758
H	0.0403	2.21168	-2.14064
H	-1.00158	4.40166	-2.41873
H	-0.31019	4.94946	-0.7897



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1296.851763
Gibbs's free energies (G)	-1296.911998

C	0.26502	1.9213	-1.3207
C	0.55216	0.61675	-0.93198
C	-0.47116	-0.33296	-0.77561
C	-1.79742	-0.00938	-0.98322
C	4.40838	-0.52784	0.02657
C	2.00046	-1.76239	1.53615
C	2.32832	-2.27968	-1.49598
C	5.2752	-1.70901	0.48788
C	4.88995	-0.04784	-1.3501
C	4.53463	0.62046	1.03859
C	-2.91945	-0.90132	-0.67907
C	-4.14332	-0.70545	-1.33021
C	-2.82205	-1.92869	0.26728
C	-5.2279	-1.53318	-1.07208
C	-3.90478	-2.75764	0.52486
C	-5.10945	-2.56593	-0.14617
O	1.8007	0.37833	-0.45531
Si	2.60536	-1.06863	-0.09643
H	-0.52353	2.08713	-2.0407
H	1.0874	2.6255	-1.36071
H	-0.23199	-1.27584	-0.29635
H	-2.03841	0.8024	-1.65846
H	2.55697	-2.67212	1.7792
H	2.1512	-1.04774	2.34914
H	0.93981	-2.02366	1.51483
H	1.32773	-2.71664	-1.47337
H	2.46076	-1.78871	-2.46335
H	3.04892	-3.10005	-1.43239
H	6.32714	-1.40355	0.52832
H	4.9939	-2.05345	1.48718
H	5.2075	-2.55963	-0.19749

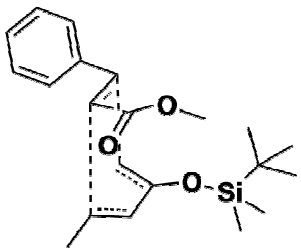
H	4.27797	0.77957	-1.72015
H	5.92629	0.30319	-1.28301
H	4.86021	-0.85279	-2.0905
H	4.22385	0.31268	2.0415
H	5.57939	0.9465	1.10259
H	3.92884	1.48059	0.74262
H	-4.23726	0.1011	-2.05041
H	-1.90287	-2.06697	0.82544
H	-6.16632	-1.37118	-1.58896
H	-3.81435	-3.54466	1.26409
H	-5.95567	-3.20981	0.06228
C	-0.8896	2.72204	0.21478
C	-1.95075	1.86325	0.54045
C	-1.92501	0.96516	1.69266
C	-0.59016	0.66982	2.35161
O	-2.9494	0.47296	2.14092
H	-0.04639	2.76597	0.89836
H	-2.9439	2.07782	0.15715
H	0.23507	0.61589	1.63989
H	-0.36489	1.47167	3.06213
H	-0.66978	-0.2655	2.90531
C	-1.20899	4.00293	-0.44997
C	-0.47393	5.1079	-0.34523
H	-2.11642	4.01165	-1.05108
H	-0.76108	6.02623	-0.84194
H	0.43343	5.125	0.25096



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1334.009555
Gibbs's free energies (G)	-1334.068679

C	-0.9936	-0.29812	-1.56945
C	-0.18664	-0.9269	-0.63318
C	-0.74664	-1.67121	0.42868
C	-2.09763	-1.88429	0.53691
C	3.89318	-0.35864	-0.68824
C	2.45925	-0.75347	2.01874
C	2.45632	-3.05933	-0.03082
C	5.21135	-0.68746	0.02703
C	3.96007	-0.84965	-2.14098
C	3.66409	1.16031	-0.67024
O	1.11611	-0.57108	-0.61678
Si	2.45662	-1.20077	0.19703
H	-1.93719	-0.73892	-1.85915
H	-0.49819	0.31384	-2.31446
H	-0.11452	-1.91252	1.27864
H	-2.6996	-1.88035	-0.36534
H	3.17145	-1.39343	2.54841
H	2.76455	0.28474	2.16475
H	1.48149	-0.88205	2.48807
H	1.73089	-3.55015	0.6222
H	2.21293	-3.32098	-1.06366
H	3.44289	-3.47153	0.20001
H	6.04675	-0.19641	-0.48552
H	5.20826	-0.33599	1.06335
H	5.41704	-1.76256	0.03293
H	3.02938	-0.64013	-2.67574
H	4.77486	-0.34268	-2.67126
H	4.14899	-1.92618	-2.19388
H	3.66164	1.55716	0.34932
H	4.46691	1.66548	-1.22072
H	2.70811	1.42854	-1.12912
C	-1.96884	1.10639	-0.37747
C	-2.81706	0.44074	0.51436

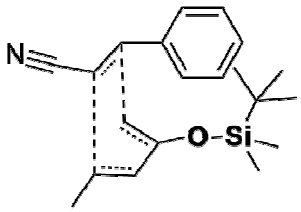
C	-4.15605	0.03129	0.13085
C	-5.62137	-0.39271	-1.66687
O	-5.0421	-0.30197	0.89162
O	-4.32366	-0.00511	-1.21663
H	-2.4293	1.48398	-1.28449
H	-2.64947	0.47243	1.58183
H	-5.58355	-0.34993	-2.75263
H	-5.85696	-1.40385	-1.33316
H	-6.37786	0.29339	-1.28506
C	-2.7299	-2.5115	1.73951
H	-3.66635	-2.00318	1.98415
H	-2.9769	-3.55815	1.53515
H	-2.06487	-2.47499	2.60389
C	-0.82971	1.91675	0.11528
C	-0.35418	2.97336	-0.66786
C	-0.19631	1.65242	1.3335
C	0.70637	3.76121	-0.23957
H	-0.83115	3.18079	-1.62071
C	0.86599	2.44136	1.76379
H	-0.53542	0.82835	1.95263
C	1.31898	3.49998	0.98321
H	1.05287	4.58118	-0.8579
H	1.33686	2.2317	2.71762
H	2.14396	4.11531	1.32265



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1334.004540
Gibbs's free energies (G)	-1334.06438

C	-0.5634	-0.95573	0.16206
C	0.48888	-0.05694	0.25787
C	0.41423	1.0549	1.11665
C	-0.70892	1.31566	1.86905
C	3.59413	-1.71075	0.50002
C	3.76282	-0.27453	-2.26265
C	3.78363	1.3826	0.32109
C	5.10766	-1.94907	0.38394
C	3.22547	-1.52507	1.9796
C	2.84369	-2.92962	-0.05463
O	1.46332	-0.1061	-0.69156
Si	3.1407	-0.17031	-0.50729
H	-1.13491	-1.19154	1.04791
H	-0.49081	-1.74747	-0.57505
H	1.15062	1.84253	0.98582
H	-1.3486	0.49142	2.16493
H	4.85285	-0.20921	-2.30025
H	3.45806	-1.20989	-2.73755
H	3.35405	0.55007	-2.85192
H	3.46402	2.27236	-0.22853
H	3.44634	1.47766	1.35527
H	4.87756	1.37224	0.32697
H	5.39447	-2.82205	0.982
H	5.4077	-2.14314	-0.64997
H	5.68537	-1.09505	0.75216
H	2.15434	-1.34669	2.11262
H	3.48413	-2.43022	2.54224
H	3.76763	-0.68948	2.43124
H	3.07193	-3.10474	-1.11025
H	3.13281	-3.82991	0.50067
H	1.76118	-2.80936	0.0425
C	-2.18595	0.18365	-0.56526

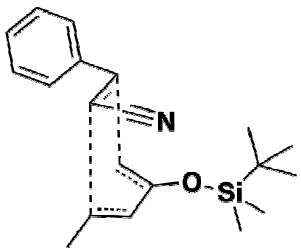
C	-2.26138	1.40449	0.1151
C	-1.62114	2.60584	-0.41069
C	0.065	3.42368	-1.82812
O	-1.84431	3.74184	-0.04682
O	-0.69821	2.31855	-1.35391
H	-1.74627	0.21093	-1.55551
H	-3.06283	1.6009	0.81539
H	0.76245	3.01329	-2.55454
H	-0.58238	4.16621	-2.29562
H	0.6048	3.89332	-1.00341
C	-0.86164	2.57458	2.6675
H	-0.19631	3.35795	2.30266
H	-1.88395	2.95314	2.61314
H	-0.63247	2.38114	3.72026
C	-3.23586	-0.84805	-0.37414
C	-3.54637	-1.7194	-1.42148
C	-3.91344	-0.99769	0.84065
C	-4.52077	-2.70005	-1.26887
H	-3.02168	-1.61985	-2.36624
C	-4.88473	-1.97926	0.99612
H	-3.6799	-0.34389	1.67489
C	-5.19496	-2.83335	-0.05915
H	-4.75361	-3.35998	-2.09645
H	-5.40055	-2.0788	1.94416
H	-5.9538	-3.59706	0.06277



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1198.429256
Gibbs's free energies (G)	-1198.484329

C	-1.17468	-0.63279	-1.75048
C	-0.26666	-0.8113	-0.71502
C	-0.59737	-1.60229	0.40754
C	-1.77743	-2.29988	0.47633
C	3.44425	-1.0814	-0.38704
C	2.7319	1.9502	-0.20103
C	1.92109	0.04231	2.06127
C	4.6988	-1.03143	0.49791
C	2.81888	-2.48171	-0.30761
C	3.83249	-0.78475	-1.84251
O	0.79392	0.0189	-0.69636
Si	2.20398	0.21284	0.21395
H	-1.84224	-1.43698	-2.02624
H	-0.89216	0.04909	-2.544
H	0.00014	-1.49326	1.30704
H	-2.25181	-2.62854	-0.44044
H	2.77141	2.09335	-1.28316
H	2.01023	2.66232	0.20754
H	3.71693	2.17851	0.21491
H	0.9808	0.51019	2.36077
H	1.91902	-0.99608	2.40156
H	2.73076	0.55849	2.58616
H	5.43777	-1.75769	0.13968
H	5.17274	-0.04479	0.47736
H	4.47049	-1.27745	1.53936
H	1.94425	-2.5705	-0.9585
H	3.54947	-3.23436	-0.62745
H	2.50864	-2.7372	0.71095
H	4.33945	0.18013	-1.93468
H	4.51638	-1.5567	-2.21434
H	2.95539	-0.77088	-2.49641
C	-2.69849	0.39878	-0.74289
C	-3.32925	-0.49942	0.12986

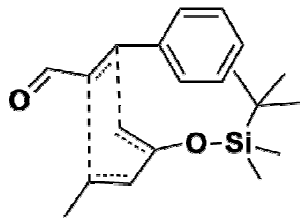
C	-4.35282	-1.34768	-0.36586
N	-5.14248	-2.08309	-0.78056
H	-3.17023	0.55791	-1.70713
H	-3.31746	-0.35196	1.20038
C	-2.23479	-2.99938	1.71975
H	-3.32407	-2.97239	1.80024
H	-1.94492	-4.05438	1.68819
H	-1.80081	-2.55002	2.61466
C	-1.96149	1.56895	-0.2139
C	-1.72878	2.66873	-1.04649
C	-1.45518	1.59941	1.08899
C	-1.02997	3.77656	-0.58712
H	-2.10485	2.65145	-2.06453
C	-0.75399	2.70982	1.55027
H	-1.60466	0.75277	1.75066
C	-0.54259	3.80338	0.71746
H	-0.86747	4.62168	-1.24574
H	-0.37471	2.72156	2.56608
H	-0.00167	4.66966	1.08005



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1198.425548
Gibbs's free energies (G)	-1198.482705

C	0.95184	-0.81243	-0.69009
C	-0.27499	-0.18085	-0.54829
C	-0.40829	1.19788	-0.81888
C	0.66773	1.9745	-1.17125
C	-4.00919	-0.71135	-0.79147
C	-3.07131	-1.87302	1.93592
C	-2.93747	1.15652	1.449
C	-5.42168	-0.32946	-0.32372
C	-3.58987	0.2144	-1.94243
C	-4.00859	-2.16314	-1.28994
O	-1.2504	-0.86759	0.08294
Si	-2.81024	-0.53613	0.6606
H	1.61871	-0.4951	-1.4779
H	1.02329	-1.85433	-0.40068
H	-1.32123	1.69711	-0.51161
H	1.51981	1.51693	-1.66053
H	-4.10466	-1.88063	2.29273
H	-2.8425	-2.85805	1.52361
H	-2.41993	-1.70404	2.79699
H	-2.00862	1.44249	1.94994
H	-3.19234	1.94326	0.73446
H	-3.73069	1.13113	2.20232
H	-6.13237	-0.44061	-1.151
H	-5.76816	-0.96962	0.49364
H	-5.4685	0.70963	0.01593
H	-2.59497	-0.03711	-2.32153
H	-4.29799	0.11716	-2.77403
H	-3.583	1.26689	-1.64079
H	-4.36752	-2.85275	-0.52071
H	-4.66986	-2.26158	-2.159
H	-3.00687	-2.4823	-1.5925
C	2.19271	0.13414	0.76445

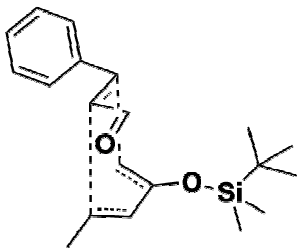
C	2.00246	1.52163	0.73666
C	1.07162	2.11442	1.63185
N	0.29443	2.58498	2.34594
H	1.70241	-0.41195	1.56282
H	2.77274	2.18133	0.35937
C	0.56725	3.46594	-1.27994
H	-0.19411	3.85729	-0.60291
H	1.51998	3.94372	-1.04304
H	0.30395	3.75574	-2.30228
C	3.4752	-0.45029	0.30211
C	3.93216	-1.64755	0.85953
C	4.23885	0.15406	-0.7021
C	5.13026	-2.21564	0.44035
H	3.3449	-2.13163	1.63329
C	5.43408	-0.41448	-1.12374
H	3.89816	1.07494	-1.16461
C	5.88701	-1.60074	-0.55196
H	5.47321	-3.13986	0.8907
H	6.01294	0.06872	-1.9022
H	6.82011	-2.04261	-0.88031



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1219.496734
Gibbs's free energies (G)	-1219.55226

C	-1.10133	-0.45956	-1.84134
C	-0.20927	-0.75688	-0.81404
C	-0.56555	-1.65179	0.21903
C	-1.74295	-2.35401	0.19879
C	3.47617	-1.11796	-0.34201
C	2.81539	1.91381	-0.04051
C	1.87272	-0.08091	2.0959
C	4.6962	-1.1324	0.59133
C	2.82667	-2.50934	-0.35111
C	3.92504	-0.76326	-1.76654
O	0.85991	0.04964	-0.70172
Si	2.23724	0.17165	0.27282
H	-1.75719	-1.23321	-2.21241
H	-0.7787	0.27792	-2.56736
H	0.01797	-1.63552	1.13437
H	-2.2115	-2.57086	-0.7539
H	3.78442	2.10239	0.42957
H	2.90903	2.10223	-1.1123
H	2.09031	2.62404	0.36498
H	0.9262	0.38444	2.37847
H	1.84498	-1.13346	2.38822
H	2.66507	0.40023	2.67746
H	5.43577	-1.85491	0.22689
H	5.18746	-0.15512	0.63658
H	4.42396	-1.42299	1.6104
H	1.98076	-2.55654	-1.04277
H	3.55989	-3.25957	-0.67062
H	2.46743	-2.80292	0.64058
H	4.45161	0.19494	-1.79635
H	4.60938	-1.53059	-2.14706
H	3.07386	-0.70408	-2.45151
C	-2.59617	0.49939	-0.80902
C	-3.25375	-0.41162	0.03718

C	-4.34	-1.20677	-0.47091
O	-5.07592	-1.91995	0.19487
H	-3.09302	0.707	-1.75443
H	-3.15418	-0.36095	1.11382
H	-4.47499	-1.16295	-1.57353
C	-2.25104	-3.14643	1.35807
H	-3.32922	-2.99396	1.46749
H	-2.09597	-4.21577	1.18371
H	-1.74897	-2.86654	2.28541
C	-1.8583	1.65988	-0.24873
C	-1.64389	2.7952	-1.03592
C	-1.33716	1.6414	1.04851
C	-0.94813	3.88928	-0.53762
H	-2.03222	2.81933	-2.04941
C	-0.63845	2.73533	1.5488
H	-1.47608	0.76553	1.67287
C	-0.44529	3.86524	0.76077
H	-0.80073	4.76349	-1.161
H	-0.24674	2.70609	2.55969
H	0.09275	4.72003	1.15365



Charge	0
Number of imaginary frequencies	1
Optimized potential energies (E)	-1219.493340
Gibbs's free energies (G)	-1219.550823

C	0.60972	-0.47246	-0.48242
C	-0.46534	0.34415	-0.14846
C	-0.48221	1.70929	-0.49069
C	0.53306	2.29552	-1.20754
C	-3.54407	-1.24362	-0.75675
C	-3.45244	-1.04284	2.35351
C	-3.77796	1.50436	0.66083
C	-5.0106	-1.6682	-0.57867
C	-3.41032	-0.43108	-2.05368
C	-2.66175	-2.49584	-0.85321
O	-1.33489	-0.11591	0.78871
Si	-3.02655	-0.20801	0.74269
H	1.11972	-0.31581	-1.42258
H	0.58222	-1.49876	-0.13469
H	-1.20843	2.34468	0.00738
H	1.16015	1.67932	-1.84137
H	-4.53294	-1.05412	2.51596
H	-3.09245	-2.07412	2.37561
H	-2.99132	-0.50668	3.18646
H	-3.44123	2.11844	1.50009
H	-3.53116	2.02252	-0.26801
H	-4.868	1.42995	0.72033
H	-5.34122	-2.23665	-1.45584
H	-5.14298	-2.30707	0.29932
H	-5.67811	-0.80628	-0.47655
H	-2.38541	-0.08209	-2.21329
H	-3.6865	-1.05451	-2.91245
H	-4.06877	0.44217	-2.05361
H	-2.7007	-3.09649	0.06046
H	-3.00225	-3.12908	-1.68108
H	-1.61733	-2.23394	-1.04164
C	2.15627	0.29927	0.60611

C	2.39678	1.64151	0.27001
C	1.9327	2.70085	1.13653
O	2.31176	3.86031	1.10849
H	1.6663	0.14033	1.56425
H	3.16815	1.90529	-0.4465
H	1.16543	2.3862	1.87442
C	0.61958	3.76757	-1.44031
H	1.62404	4.13429	-1.21193
H	0.41124	3.99523	-2.4901
H	-0.08524	4.31364	-0.81211
C	3.14913	-0.76009	0.2705
C	3.33258	-1.82522	1.15498
C	3.89107	-0.7382	-0.91398
C	4.24556	-2.83596	0.87456
H	2.75579	-1.85646	2.07365
C	4.80097	-1.74989	-1.19761
H	3.75626	0.07211	-1.62318
C	4.98356	-2.80233	-0.30386
H	4.37961	-3.64938	1.57801
H	5.36963	-1.71734	-2.11971
H	5.6946	-3.58909	-0.52564