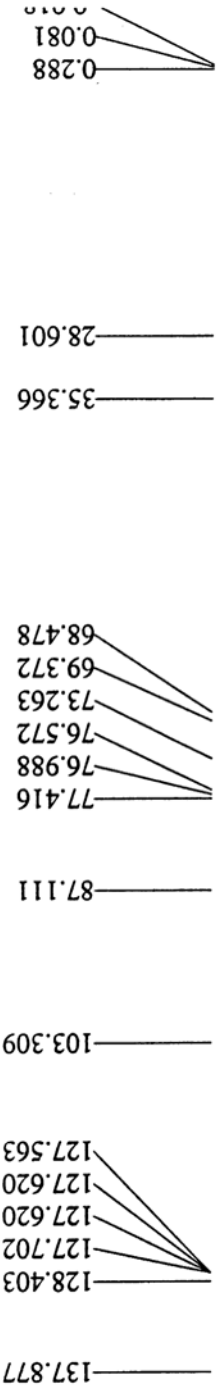
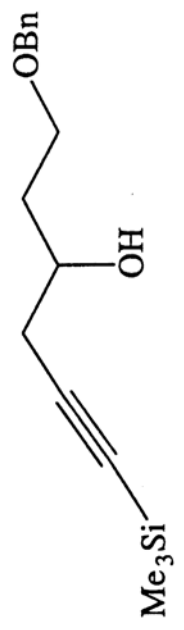
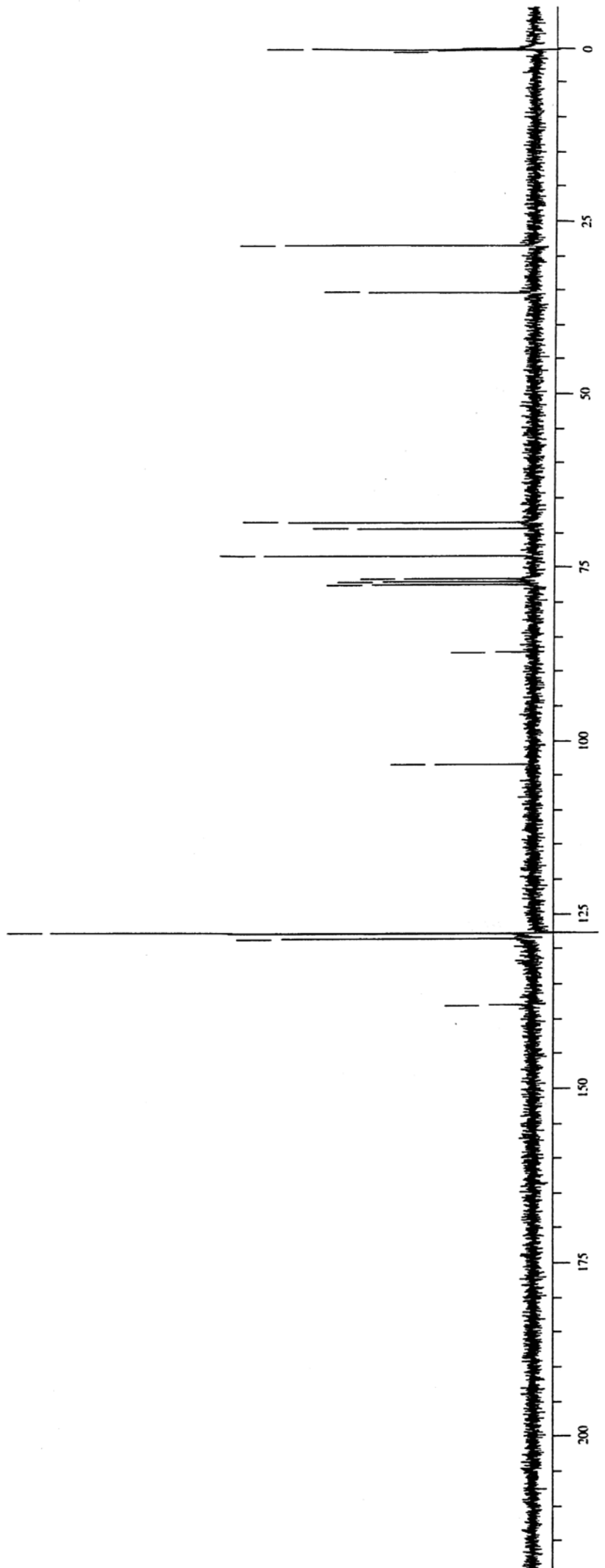


**Experimental and quantum-mechanical investigation
of the vinylsilane-iminium ion cyclization**

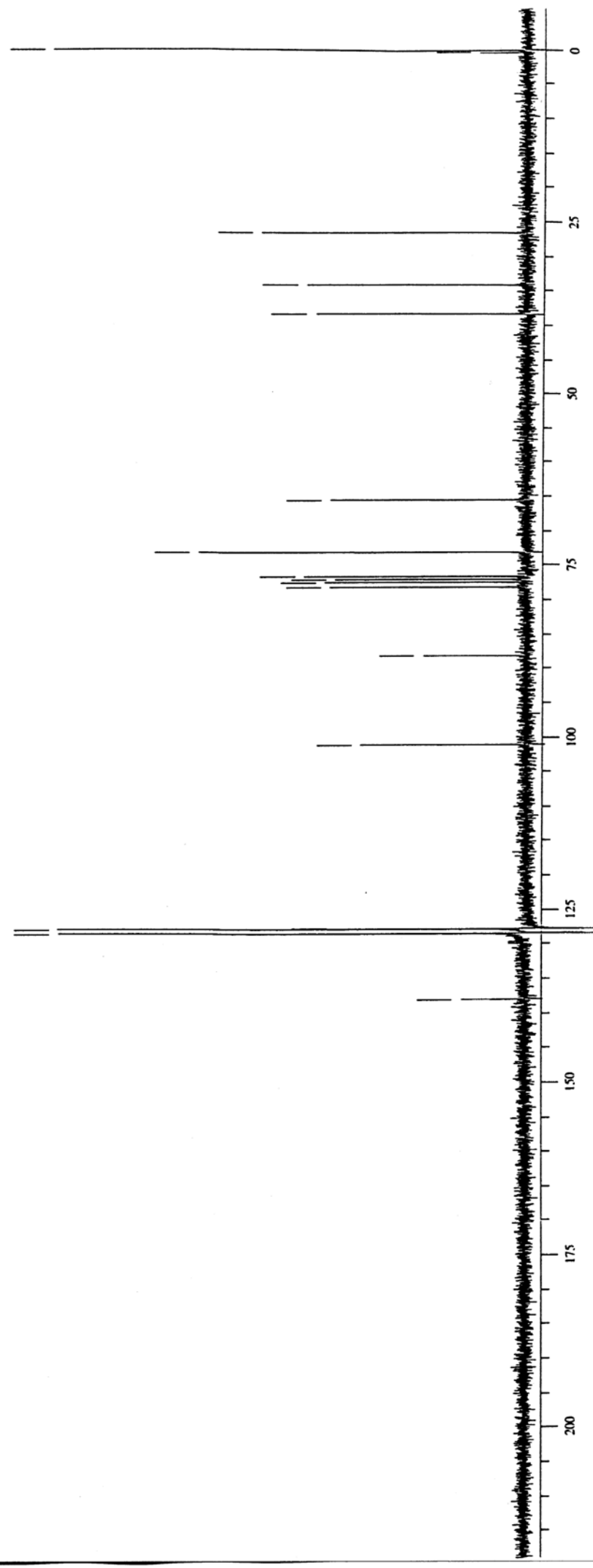
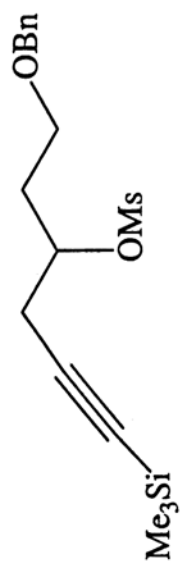
Lisbet Kværnø, Per-Ola Norrby and David Tanner*

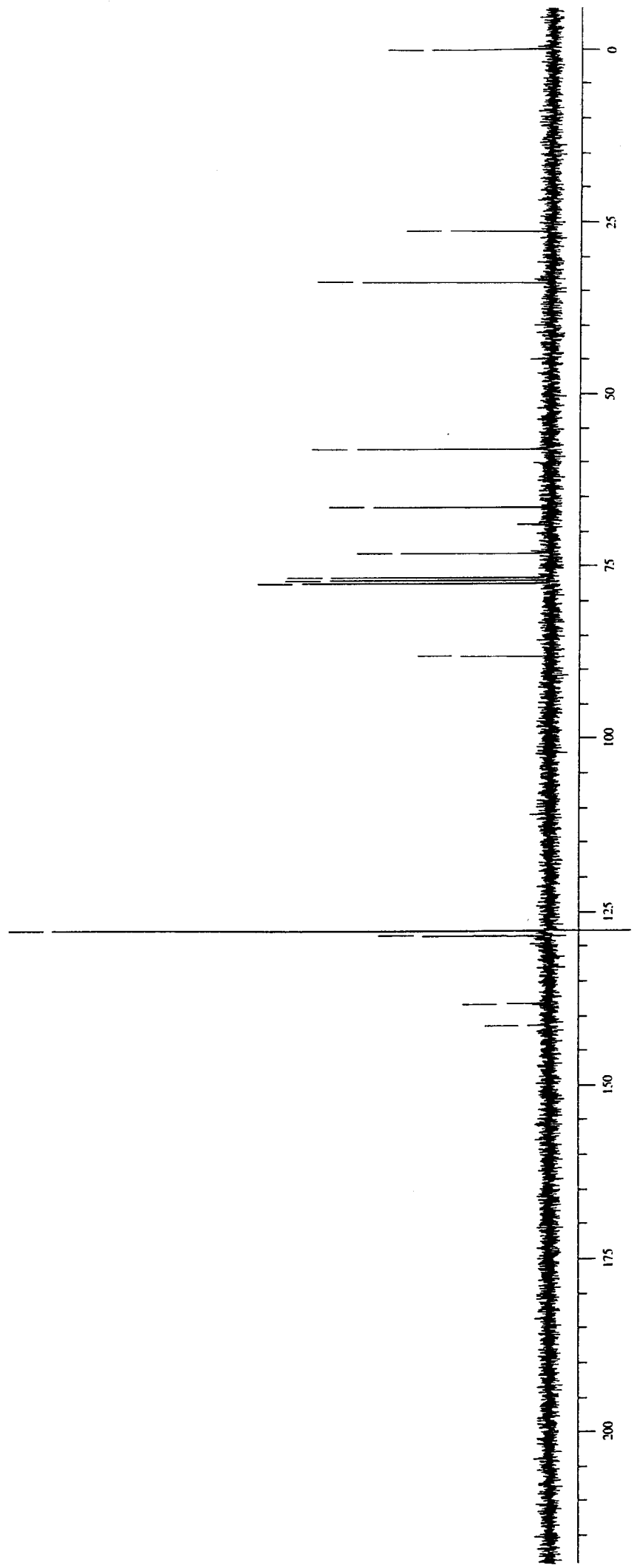
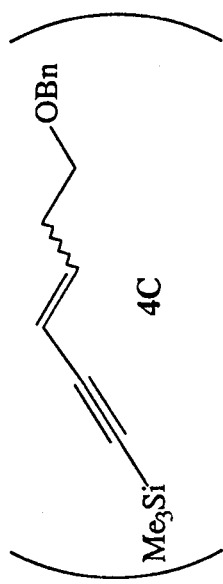
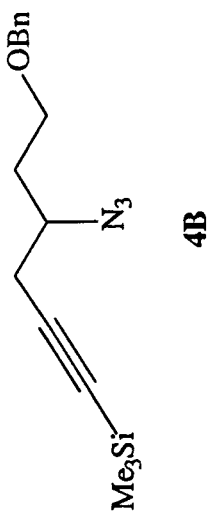
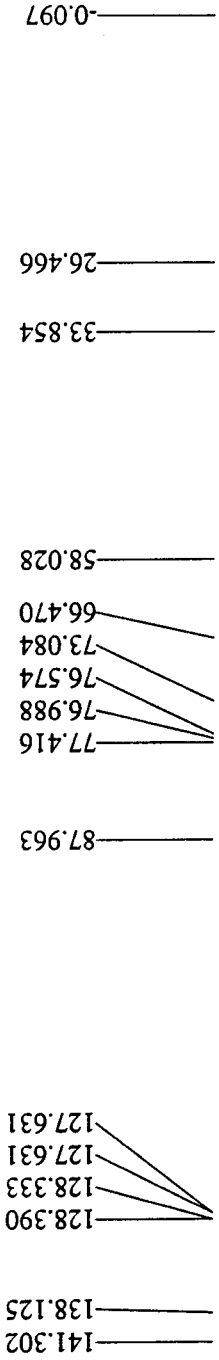
Electronic Supplementary Information

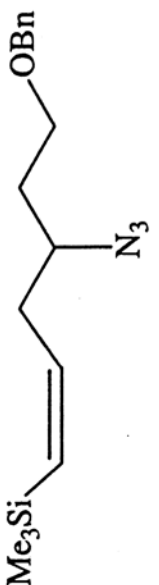
Copies of ^{13}C NMR spectra for compounds **4-16**



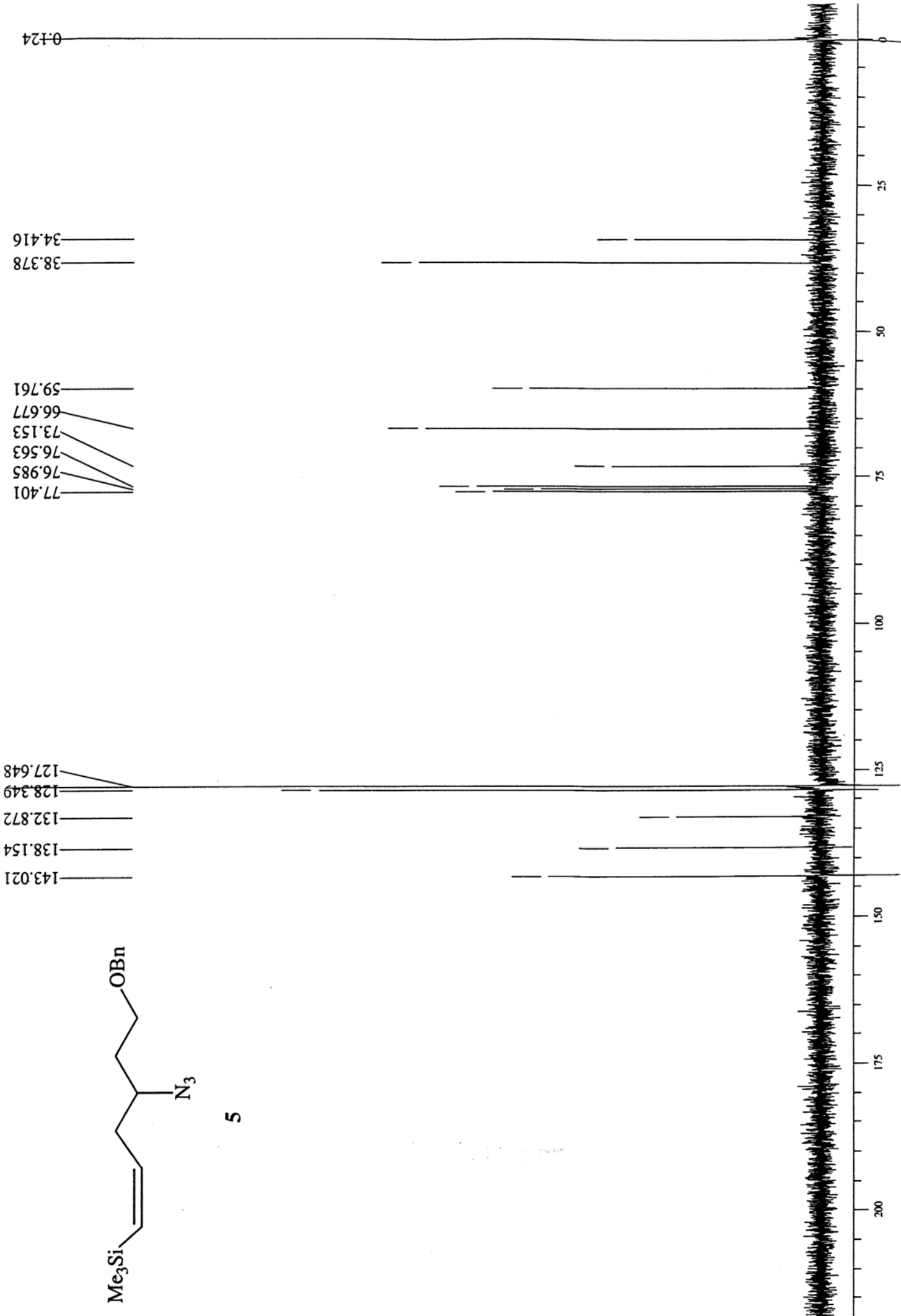
0.247
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 26.663
 34.171
 38.350
 65.480
 73.030
 76.563
 76.987
 77.400
 78.104
 88.101
 101.013
 127.675
 127.675
 127.715
 128.376
 128.376
 128.376
 137.920

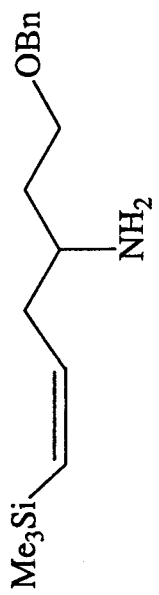






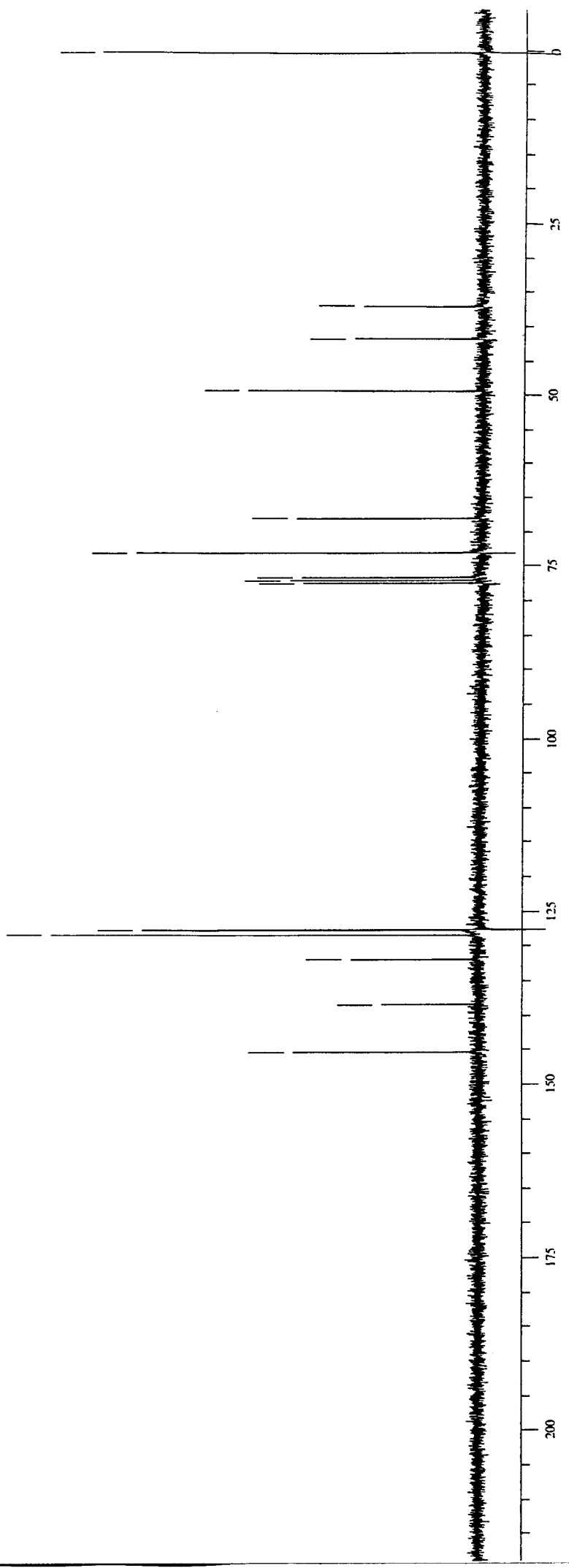
5

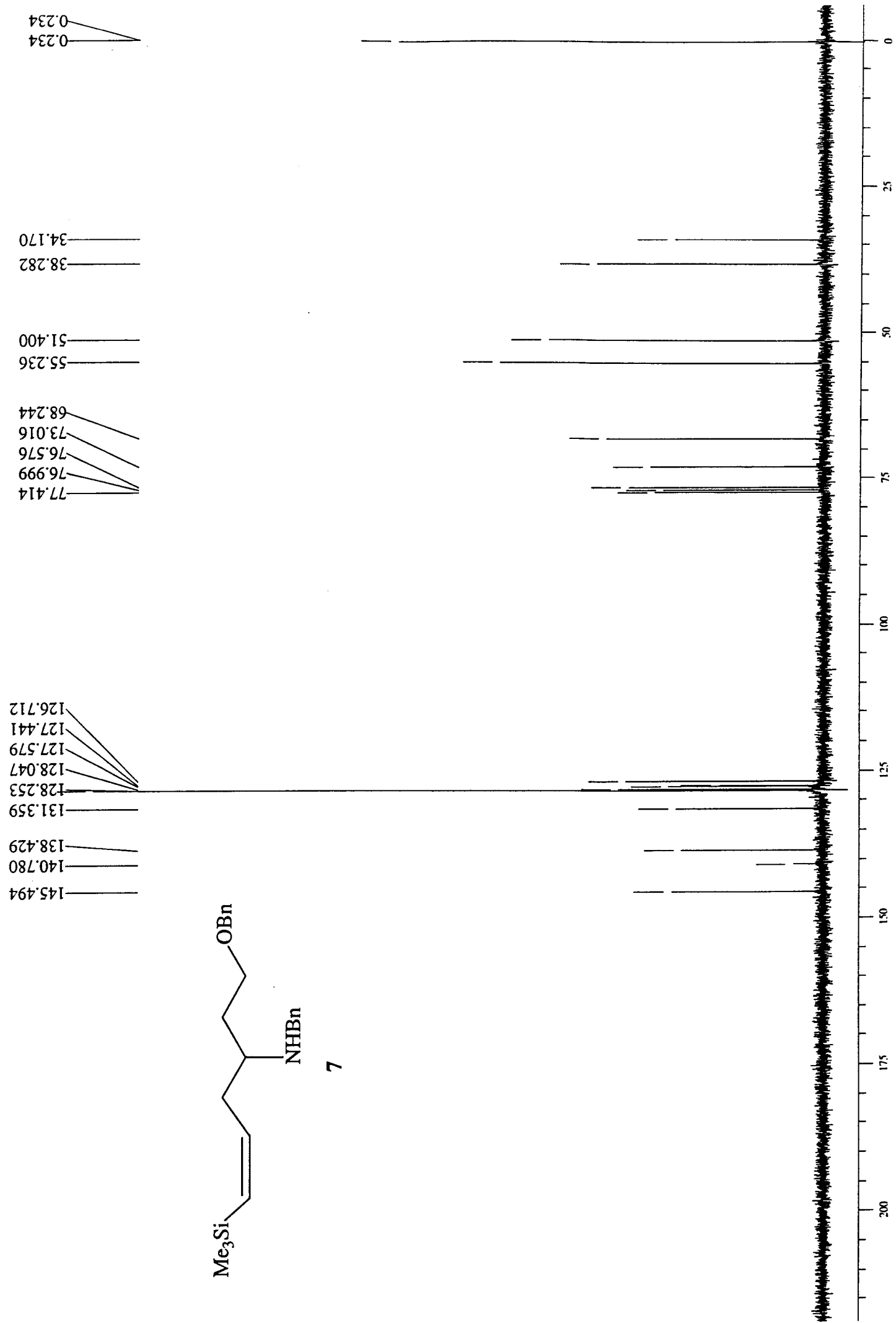
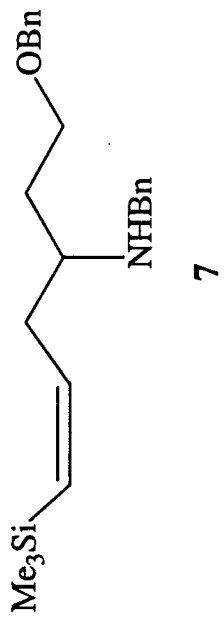


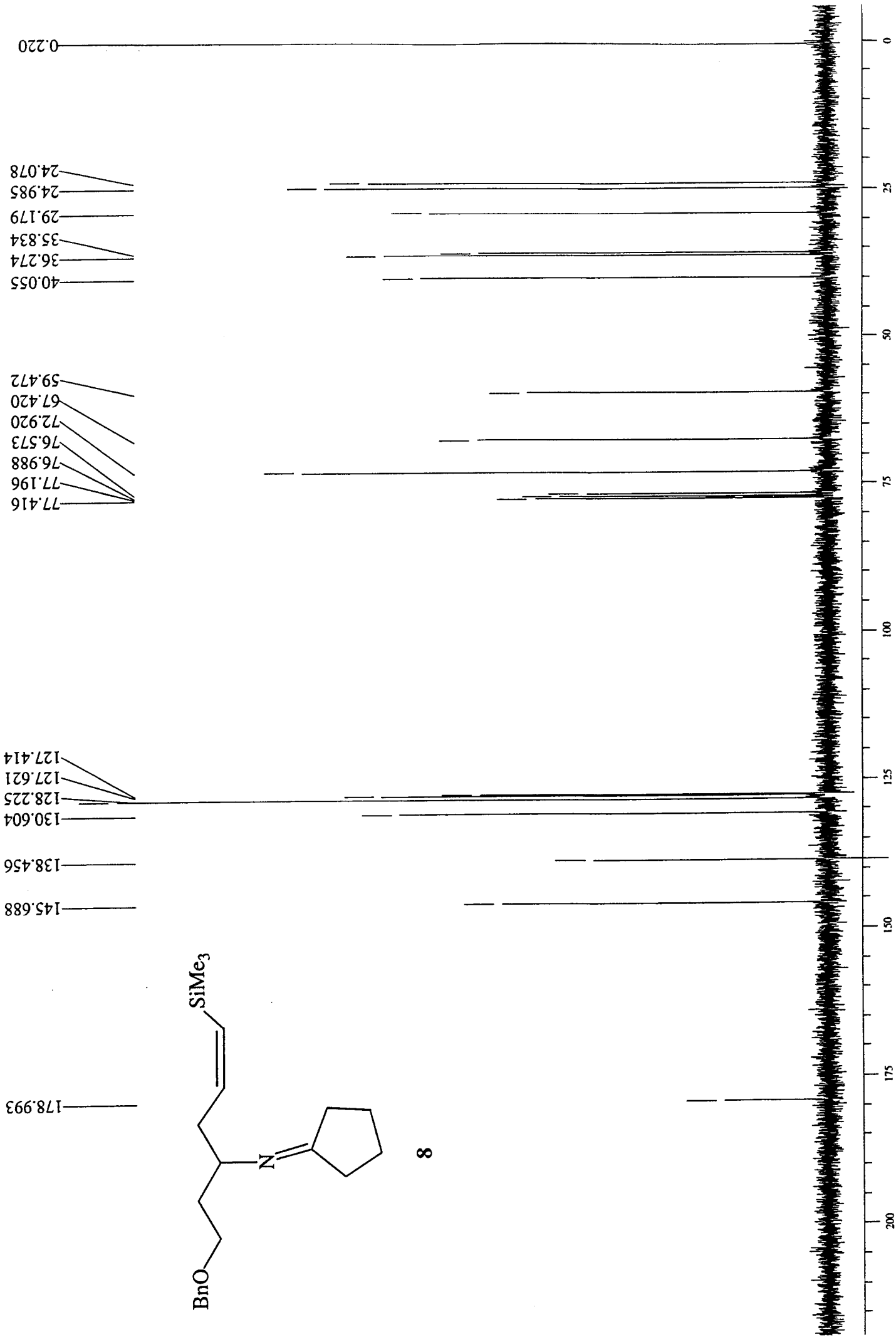


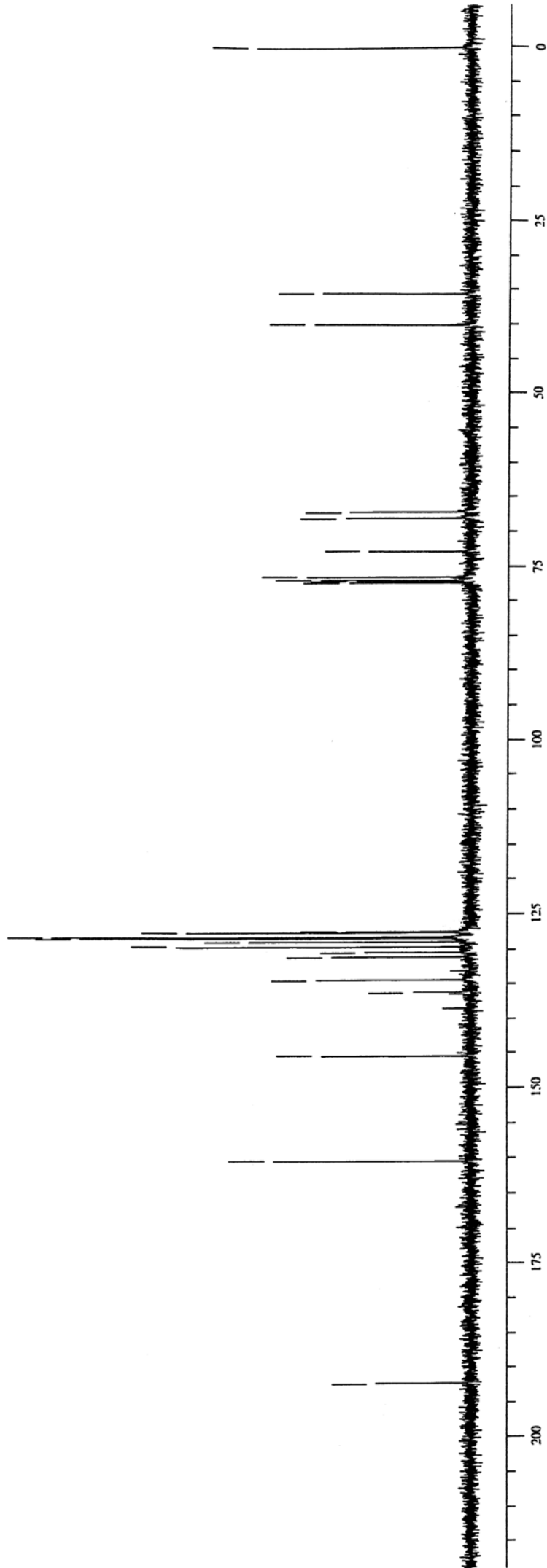
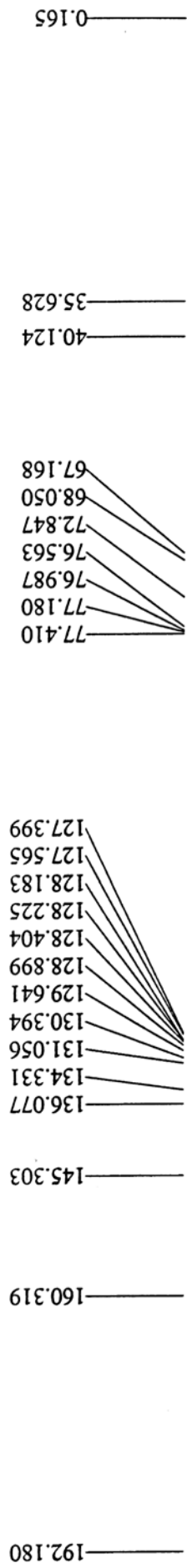
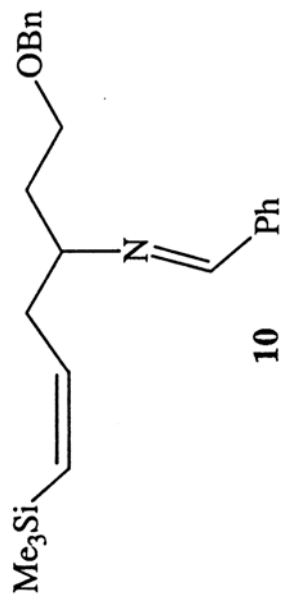
9

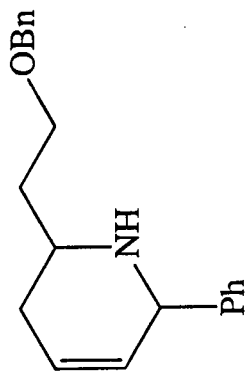
- 145.262
- 138.360
- 131.839
- 128.308
- 127.565
- 127.497
- 77.415
- 76.989
- 76.564
- 73.003
- 68.037
- 49.392
- 41.801
- 37.122
- 0.275











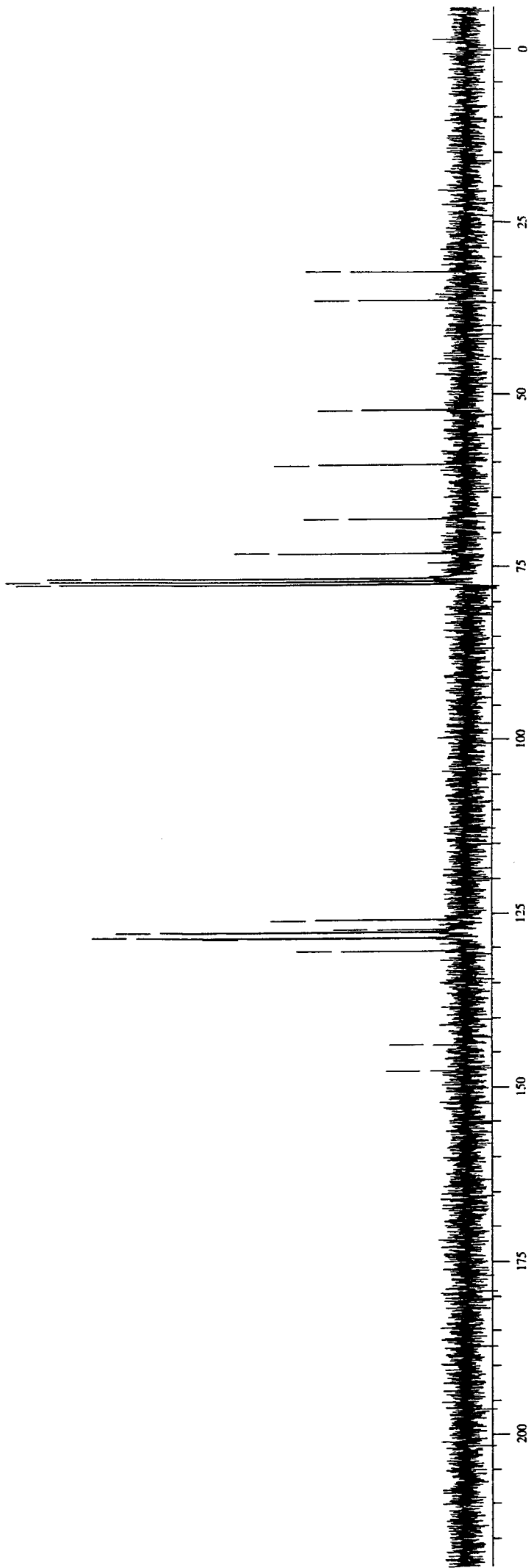
11A

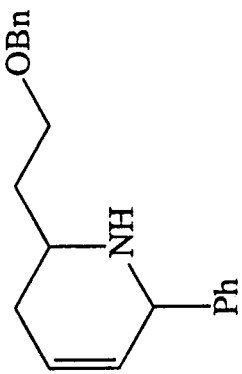
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36.356

52.238
60.145
67.996
72.947
76.561
76.867
76.990
77.345
77.415

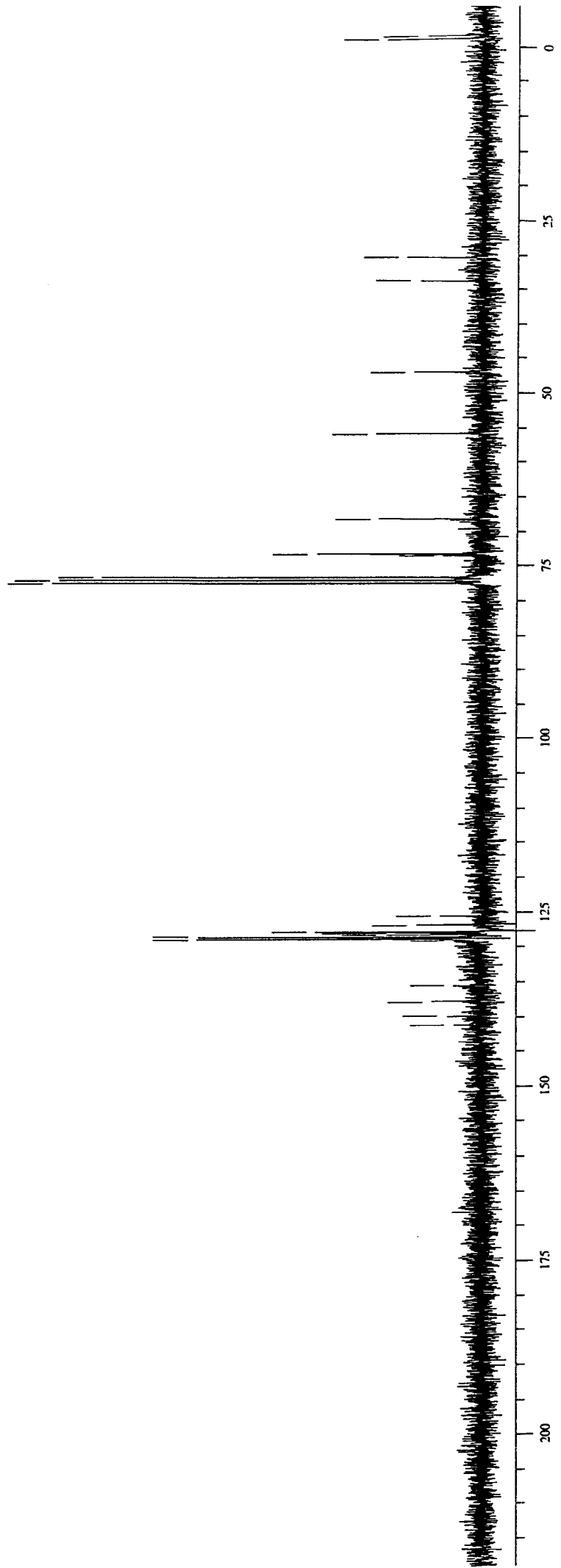
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127.234
127.522
127.592
127.662
128.335
128.445
130.302

143.831
147.531

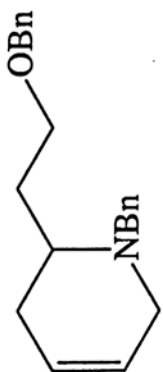




11B



- 1.320
- 1.789
- 30.414
- 33.826
- 46.926
- 55.745
- 68.134
- 68.217
- 73.194
- 73.345
- 73.511
- 76.560
- 76.990
- 77.416
- 125.446
- 126.616
- 126.642
- 127.561
- 127.633
- 127.661
- 127.756
- 127.854
- 127.990
- 128.101
- 128.361
- 128.498
- 128.564
- 128.665
- 128.772
- 129.045
- 135.443
- 137.672
- 139.856
- 141.103



12

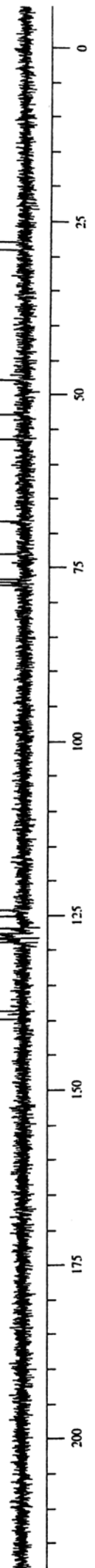
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27.940

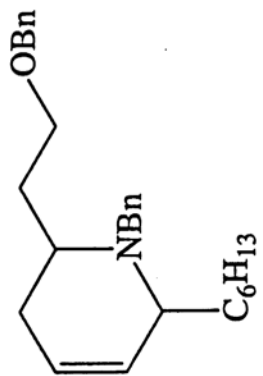
56.377
52.803
47.797

77.416
76.988
76.571
72.934
68.203

128.720
128.267
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127.538
127.414
126.685
125.008
124.141

139.694
138.552





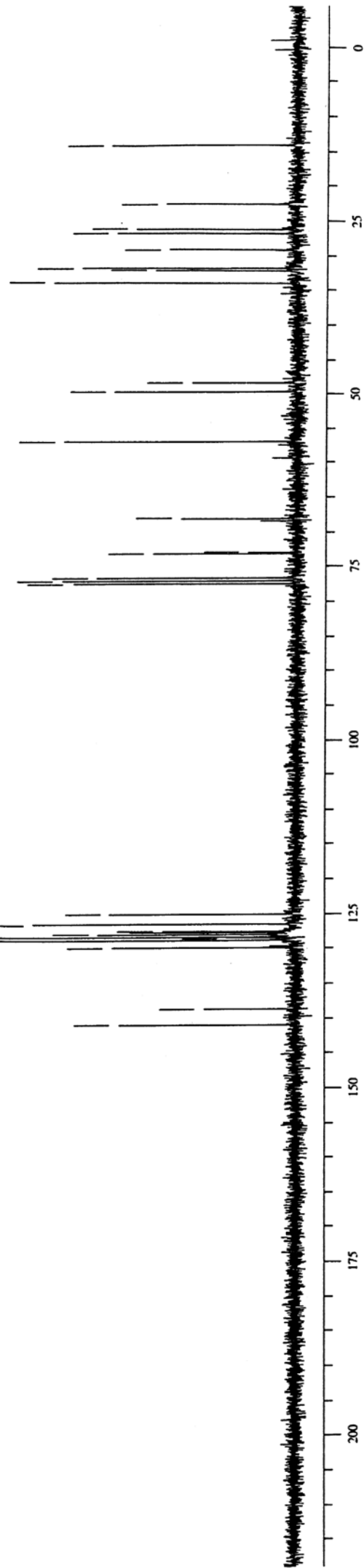
14.108
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 26.291
 26.828
 26.910
 29.219
 31.846
 31.887
 32.245
 34.019

 48.316
 49.626

 56.859
 68.060
 72.865
 73.057
 76.562
 76.990
 77.416

 124.994
 126.383
 127.414
 127.565
 127.632
 127.892
 128.266
 128.404
 128.720
 129.779

 138.621
 140.917



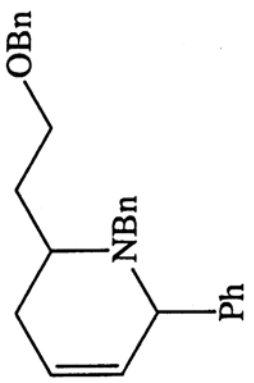
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28.226

51.314
48.512

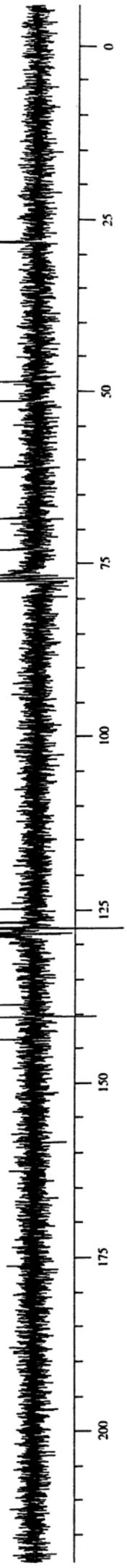
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68.410
72.891
76.563
76.988
77.411

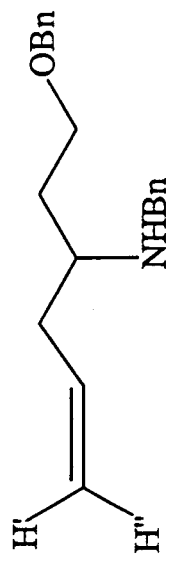
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126.738
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128.170
128.225
128.390
128.596
128.734

138.511
140.312
143.557



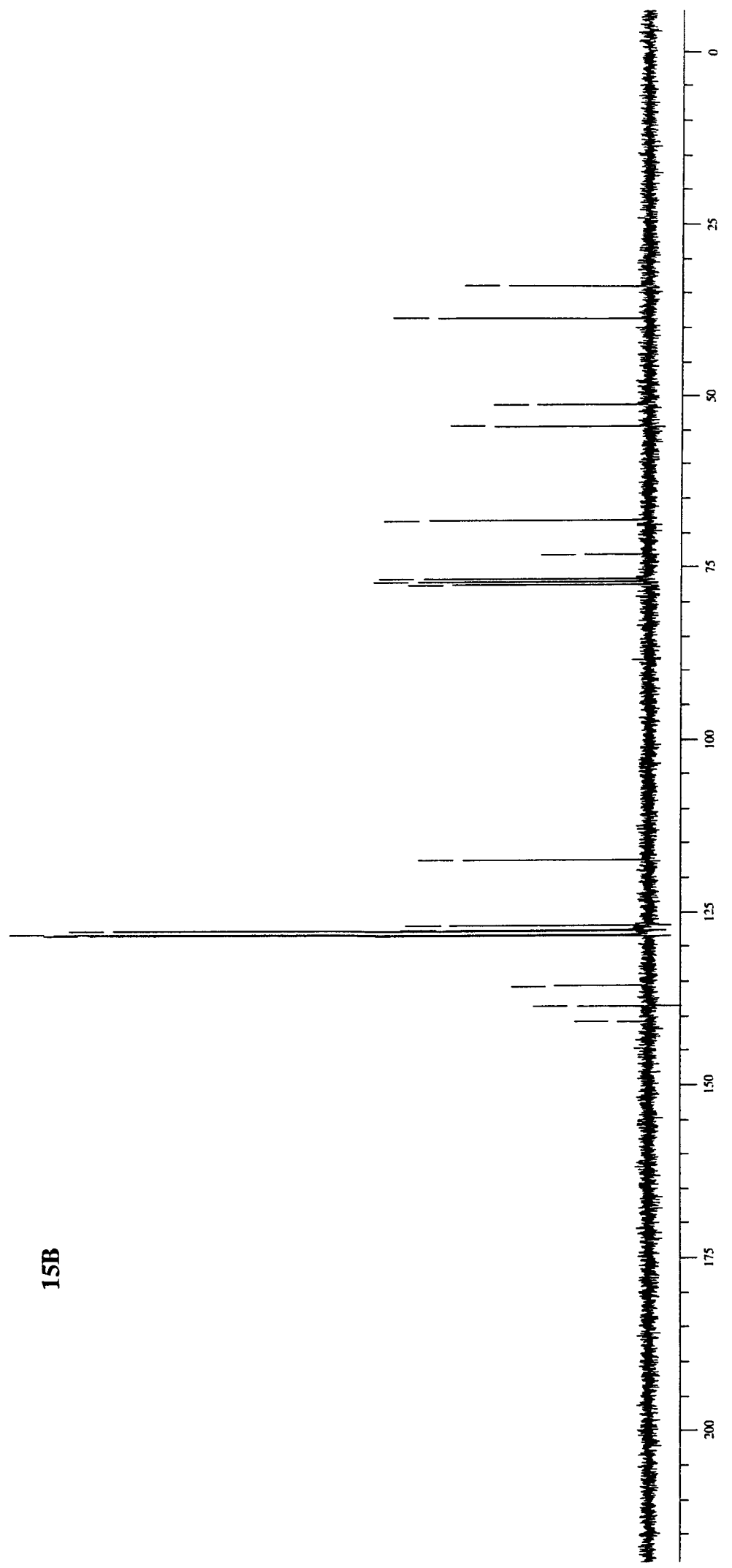
14

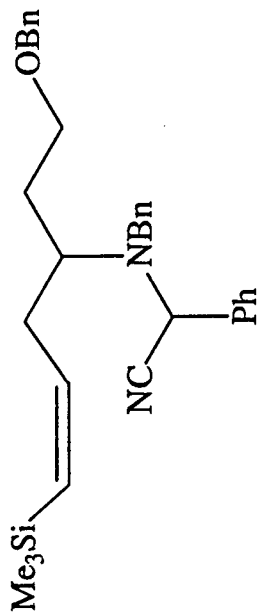




15B

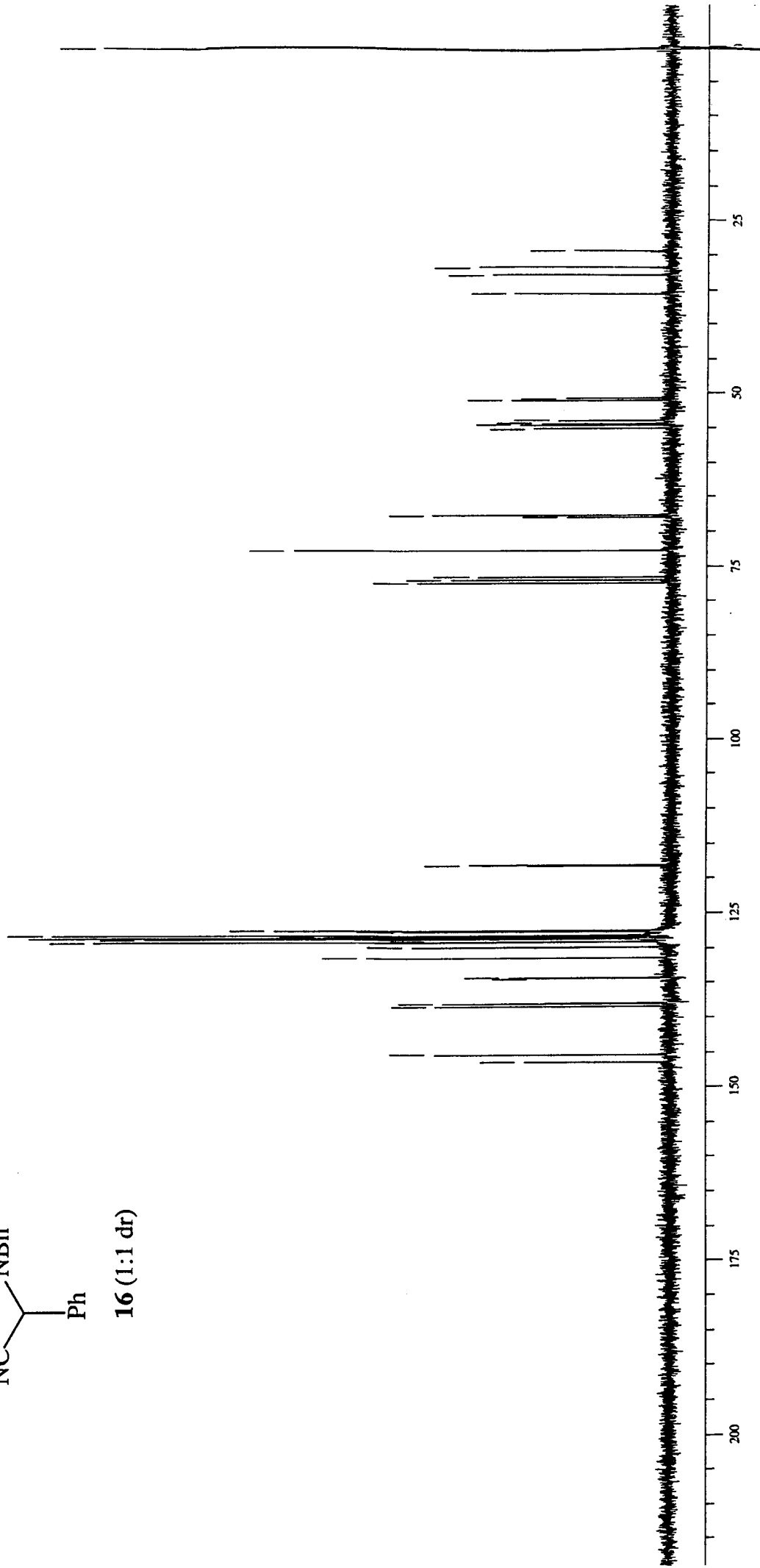
- 140.697
- 138.455
- 135.444
- 128.267
- 128.102
- 127.566
- 127.441
- 126.740
- 117.279
- 77.414
- 76.989
- 76.564
- 72.984
- 68.079
- 54.356
- 51.166
- 38.639
- 33.992





16 (1:1 dr)

146.390	0.220
145.317	0.041
138.356	
137.961	
137.823	
134.276	
134.193	
131.319	
129.807	
129.064	
128.965	
128.596	
128.569	
128.432	
128.363	
128.267	
128.196	
128.033	
127.552	
127.442	
127.387	
127.359	
118.146	
117.967	
77.417	
76.988	
76.572	
72.727	
67.950	
67.626	
54.988	
54.519	
54.302	
53.872	
50.932	
50.612	
35.669	
32.946	
31.792	
29.435	



**Experimental and quantum-mechanical investigation
of the vinylsilane-iminium ion cyclization**

Lisbet Kværnø, Per-Ola Norrby and David Tanner*

Electronic Supplementary Information: Selected bond lengths in geometry optimized structures of α -substituted (*Z*)-vinylsilanes. Cartesian coordinates, raw energies and lower frequencies of computationally characterized species **17A-32H**.

Table. α -Substituted (*Z*)-Vinylsilanes. Selected Bond Lengths in Geometry Optimized Structures, in Å

	R=H				R=Me			
	A	B	C	D	E	F	G	H
27 C2-C3	4.617	4.619	4.504	4.505	3.659	3.603	4.259	4.693
28 C2-C3	1.796	1.827	1.922	1.947	1.856	1.867	1.915	1.942
29 C2-C3	1.504 ^a	1.507 ^a	1.554	1.554	1.599	1.592	1.577	1.563
30 C2-C3	1.671	1.668	1.646	1.601	1.652	1.647	1.608	1.586
27 C5-C6	1.559	1.550	1.553	1.553	1.550	1.554	1.547	1.554
28 C5-C6	1.663	1.652	1.637	1.631	1.663	1.646	1.648	1.630
29 C5-C6	1.552 ^a	1.558 ^a	1.654	1.573	1.609	1.600	1.608	1.598
30 C5-C6	1.930	1.969	1.961	2.034	1.912	1.964	1.935	1.985
27 C3-Si	1.912	1.912	1.913	1.913	1.902	1.909	1.902	1.902
28 C3-Si	1.981	1.981	1.960	1.961	1.980	1.985	1.965	1.964
29 C3-Si	2.625 ^a	2.582 ^a	2.164	2.151	2.102	2.113	2.085	2.105
30 C3-Si	1.972	1.973	1.970	1.992	1.989	1.991	1.993	2.000

^a The trimethylsilyl group had partly migrated to give a π -silyl complex in the geometry optimization.

Cartesian coordinates, raw energies and lower frequencies of computationally characterized species
17A-32H.

17A

Filename: reac_minTMS_f.out

B3LYP/6-31g*: -659.69612375 Hartree

ZPE: 650.788 kJ/mol

DeltaG (excl. ZPE): -108.193 kJ/mol

Low frequencies: 28.72 58.29 88.50

Cartesian coordinates:

C	-1.02529	0.17881	0.26663
H	-2.02686	-0.13780	-0.03424
H	-1.10326	0.82877	1.14592
C	-0.23827	0.88003	-0.85964
H	-0.80185	1.78466	-1.11902
H	-0.22007	0.24164	-1.74805
C	1.15487	1.23128	-0.39209
C	2.30226	0.66142	-0.80815
H	3.20035	1.05474	-0.32330
H	1.18690	2.00962	0.37507
N	-0.26816	-1.02143	0.69523
C	-0.73220	-2.15599	1.05090
H	-1.80730	-2.31622	1.08556
H	-0.04847	-2.95743	1.31780
H	0.75313	-0.87755	0.64662
Si	2.65966	-0.60675	-2.19767
C	4.51354	-0.92590	-2.15157
H	5.08330	-0.00603	-2.32746
H	4.83395	-1.33543	-1.18601
H	4.80495	-1.64455	-2.92628
C	1.73989	-2.23993	-1.86657
H	1.99797	-2.67028	-0.88938
H	0.64911	-2.14700	-1.93754
H	2.03951	-2.97883	-2.61959
C	2.12107	0.10116	-3.86126
H	2.37267	-0.59497	-4.67048
H	1.04238	0.28955	-3.91434
H	2.63211	1.04778	-4.06992

17B

Filename: reac_minTMS_eqMe.out

B3LYP/6-31g*: -699.03193535 Hartree

ZPE: 724.234 kJ/mol

DeltaG (excl. ZPE): -114.516 kJ/mol

Low frequencies: 23.35 48.02 72.61

Cartesian coordinates:

C	0.15263	-0.11390	0.54974
H	0.01899	0.78238	1.16628
H	1.21075	-0.21404	0.29553
C	-0.75902	-0.05945	-0.69025
H	-0.57463	-0.93366	-1.32191
H	-0.45515	0.82580	-1.26347
C	-2.21149	0.04208	-0.28740
C	-3.16493	-0.88494	-0.49503
H	-4.15195	-0.61073	-0.11155
H	-2.46660	0.96943	0.23327
N	-0.23215	-1.27423	1.38868
C	0.54791	-2.05466	2.04762
H	1.61438	-1.83378	1.99451
Si	-3.12783	-2.53875	-1.45307

C	-4.87219	-3.24103	-1.36071
H	-5.19031	-3.40913	-0.32469
H	-5.60046	-2.56637	-1.82584
H	-4.93538	-4.20207	-1.88428
C	-2.60671	-2.24877	-3.24363
H	-3.27521	-1.53406	-3.73687
H	-1.58483	-1.86271	-3.33543
H	-2.65357	-3.18768	-3.80862
C	-1.92153	-3.75100	-0.61977
H	-1.96490	-4.72130	-1.12911
H	-0.87721	-3.41732	-0.66571
H	-2.18800	-3.93355	0.42973
H	-1.24578	-1.45155	1.39073
C	0.08560	-3.20453	2.85620
H	0.43132	-3.07774	3.89077
H	-0.99989	-3.32606	2.84285
H	0.56189	-4.12094	2.48295

17C

Filename: reac_minTMS_axMe.out

B3LYP/6-31g*: -699.03020820 Hartree

ZPE: 724.786 kJ/mol

DeltaG (excl. ZPE): -114.840 kJ/mol

Low frequencies: 27.18 37.47 72.57

Cartesian coordinates:

C	1.02125	-1.02162	1.48397
H	0.99783	-1.08709	2.57300
H	1.43799	-0.05008	1.19488
C	-0.37550	-1.22895	0.86180
H	-1.00250	-0.39969	1.21145
H	-0.81370	-2.15331	1.25040
C	-0.29998	-1.24267	-0.64613
C	-0.47675	-2.31508	-1.44189
H	-0.35657	-2.10806	-2.50923
H	-0.04678	-0.27725	-1.09247
N	1.93134	-2.06629	0.95573
C	2.98051	-2.58909	1.48739
Si	-1.04371	-4.10150	-1.05579
C	-0.95374	-5.04606	-2.68173
H	-1.60139	-4.59748	-3.44398
H	0.06598	-5.06992	-3.08474
H	-1.27782	-6.08463	-2.54691
C	0.12121	-4.93020	0.20082
H	-0.18890	-5.97261	0.34306
H	1.15984	-4.96141	-0.15566
H	0.10297	-4.45996	1.19160
C	-2.80116	-4.07006	-0.37066
H	-3.16290	-5.09037	-0.19510
H	-2.87257	-3.52740	0.57927
H	-3.49011	-3.59200	-1.07604
H	1.63362	-2.39811	0.02745
C	3.57089	-2.23204	2.79630
H	3.58145	-3.12603	3.43516
H	4.62395	-1.96011	2.64261
H	3.05894	-1.41881	3.31049
H	3.46491	-3.36804	0.89925

17D

Filename: reac_minTMS_MeMe.out

B3LYP/6-31g*: -738.36101972 Hartree

ZPE: 797.496 kJ/mol

DeltaG (excl. ZPE): -120.518 kJ/mol

Low frequencies: 24.80 38.82 57.71

Cartesian coordinates:

C	2.33206	-1.85616	1.97877
H	2.19252	-1.50049	3.00209
H	3.20525	-1.34999	1.54948
C	1.07827	-1.61535	1.11497
H	0.94290	-0.52841	1.05109
H	0.20015	-2.02054	1.62695
C	1.23722	-2.21368	-0.26194
C	0.53675	-3.24709	-0.76566
H	0.82089	-3.53324	-1.78245
H	2.02010	-1.74777	-0.86696
N	2.62644	-3.30620	2.01312
C	3.30021	-3.96873	2.89909
Si	-0.95735	-4.21338	-0.06654
C	-1.37757	-5.53285	-1.34280
H	-1.64239	-5.08702	-2.30869
H	-0.53868	-6.21862	-1.51295
H	-2.23289	-6.13512	-1.01486
C	-0.49918	-5.06312	1.57262
H	-1.35366	-5.65129	1.92902
H	0.33534	-5.76613	1.44932
H	-0.24636	-4.35778	2.37391
C	-2.41100	-3.04131	0.20525
H	-3.29006	-3.59711	0.55345
H	-2.19686	-2.26559	0.94966
H	-2.68793	-2.53612	-0.72702
H	2.24362	-3.80912	1.20362
C	3.89469	-3.27442	4.08417
H	3.09624	-2.93892	4.75987
H	4.54958	-3.94714	4.63989
H	4.46227	-2.38734	3.78274
C	3.47780	-5.44106	2.74202
H	4.54922	-5.67142	2.68504
H	3.09748	-5.94828	3.63781
H	2.97290	-5.84154	1.86006

17E

Filename: reac_minMeTMS_f.out

B3LYP/6-31g*: -699.01291359 Hartree

ZPE: 724.836 kJ/mol

DeltaG (excl. ZPE): -106.838 kJ/mol

Low frequencies: -12.66 56.33 84.01

Cartesian coordinates:

C	-1.57029	0.64648	0.54233
H	-2.60254	0.65085	0.18772
H	-1.53879	1.10796	1.53289
C	-0.62674	1.38664	-0.44145
H	-1.08594	2.37299	-0.59509
H	-0.62839	0.88188	-1.41198
C	0.76947	1.53567	0.09999
C	1.90577	1.06517	-0.45272
H	2.81345	1.31288	0.10532
H	0.82586	2.11662	1.02636
N	-1.15785	-0.77532	0.70704
C	-0.17046	-1.08474	1.46810
H	0.30419	-0.31975	2.07191
H	0.17869	-2.11144	1.51487
C	-1.84478	-1.80071	-0.11246
H	-1.42342	-2.78333	0.09588
H	-2.90931	-1.78555	0.13795
H	-1.72675	-1.54408	-1.16891
Si	2.21727	0.15907	-2.10909

C	4.08609	0.06774	-2.31028
H	4.53028	1.06862	-2.36357
H	4.56043	-0.46376	-1.47578
H	4.35741	-0.46046	-3.23206
C	1.50713	-1.59319	-1.97194
H	2.02857	-2.17390	-1.20052
H	0.44195	-1.57652	-1.70721
H	1.62231	-2.13397	-2.91842
C	1.44784	1.10604	-3.55006
H	1.72842	0.63418	-4.49994
H	0.35266	1.13828	-3.51405
H	1.80938	2.13922	-3.57725

17F

Filename: reac_minMeTMS_eqMe.out

B3LYP/6-31g*: -738.34332927 Hartree

ZPE: 798.198 kJ/mol

DeltaG (excl. ZPE): -121.212 kJ/mol

Low frequencies: 15.29 44.77 66.28

Cartesian coordinates:

C	0.18485	0.21281	0.73703
H	-0.12206	1.08766	1.31640
H	1.22542	0.35174	0.43622
C	-0.73854	0.00921	-0.48434
H	-0.46654	-0.91104	-1.01161
H	-0.51503	0.84135	-1.16660
C	-2.19844	0.02732	-0.11228
C	-3.10417	-0.94209	-0.33423
H	-4.11641	-0.69827	0.00158
H	-2.51978	0.95925	0.36401
N	0.15315	-0.96976	1.64715
C	-0.79799	-1.08675	2.51493
H	-1.49096	-0.24965	2.55183
Si	-2.96473	-2.62118	-1.23180
C	-4.70566	-3.33858	-1.28010
H	-5.11576	-3.48427	-0.27346
H	-5.39382	-2.68343	-1.82707
H	-4.71350	-4.31316	-1.78208
C	-2.29269	-2.38481	-2.98106
H	-2.92142	-1.69407	-3.55433
H	-1.26916	-1.99238	-3.00025
H	-2.28464	-3.34267	-3.51544
C	-1.82779	-3.79308	-0.25981
H	-1.82531	-4.78438	-0.72897
H	-0.78626	-3.44937	-0.23825
H	-2.17017	-3.92766	0.77373
C	1.21539	-1.96863	1.41324
H	0.96726	-2.92382	1.86843
H	1.32724	-2.10192	0.33567
H	2.15190	-1.58527	1.82852
C	-1.04047	-2.19887	3.46470
H	-1.03965	-1.78997	4.48410
H	-2.05336	-2.58534	3.29240
H	-0.32804	-3.02059	3.41018

17G

Filename: reac_minMeTMS_axMe.out

B3LYP/6-31g*: -738.34249371 Hartree

ZPE: 799.558 kJ/mol

DeltaG (excl. ZPE): -119.759 kJ/mol

Low frequencies: 12.74 42.55 53.41

Cartesian coordinates:

C	-0.21941	0.33064	1.02889
H	-0.85687	1.13298	1.40916
H	0.81402	0.58888	1.26264
C	-0.41829	0.14526	-0.49137
H	0.16548	-0.71151	-0.83777
H	0.03028	1.04058	-0.94626
C	-1.86064	0.04318	-0.92141
C	-2.43755	-0.95151	-1.61712
H	-3.49316	-0.77459	-1.84828
H	-2.46017	0.91754	-0.65019
N	-0.57783	-0.88825	1.81545
C	0.24895	-1.84608	2.07372
Si	-1.81352	-2.58106	-2.37515
C	-3.23158	-3.81378	-2.19716
H	-3.47129	-4.01813	-1.14652
H	-4.14539	-3.44712	-2.67927
H	-2.97568	-4.77043	-2.66804
C	-1.41228	-2.27452	-4.19237
H	-2.28051	-1.87828	-4.73114
H	-0.59176	-1.55802	-4.31341
H	-1.11620	-3.20855	-4.68519
C	-0.28667	-3.29305	-1.49325
H	-0.09047	-4.30066	-1.87978
H	0.62451	-2.70669	-1.66087
H	-0.44951	-3.39330	-0.41199
C	-1.98639	-0.95946	2.26619
H	-2.16275	-1.90244	2.78481
H	-2.18097	-0.11939	2.93770
H	-2.62637	-0.88661	1.38384
C	1.67490	-1.93988	1.67958
H	1.79929	-2.83864	1.06024
H	2.05742	-1.07947	1.13239
H	2.27970	-2.10268	2.58127
H	-0.15987	-2.67695	2.64706

17H

Filename: reac_minMeTMS_MeMe.out

B3LYP/6-31g*: -777.66608881 Hartree

ZPE: 872.833 kJ/mol

DeltaG (excl. ZPE): -123.587 kJ/mol

Low frequencies: 24.97 42.42 50.56

Cartesian coordinates:

C	0.04684	-0.05933	0.59839
H	-0.16479	0.87130	1.13245
H	1.10140	-0.04055	0.32396
C	-0.85695	-0.18450	-0.64695
H	-0.72683	-1.17086	-1.10371
H	-0.46201	0.54948	-1.36467
C	-2.31428	0.11397	-0.38987
C	-3.36009	-0.69306	-0.63455
H	-4.33466	-0.25416	-0.40284
H	-2.49337	1.11900	0.00435
N	-0.15396	-1.15456	1.59739
C	0.52496	-2.26547	1.58718
Si	-3.44917	-2.44390	-1.37911
C	-5.25713	-2.96729	-1.30548
H	-5.63273	-2.98895	-0.27536
H	-5.89479	-2.28196	-1.87630
H	-5.39405	-3.96978	-1.72747
C	-2.82280	-2.43657	-3.16126
H	-3.40154	-1.73997	-3.77843
H	-1.76845	-2.14484	-3.23746
H	-2.92187	-3.43339	-3.60810

C	-2.40889	-3.65785	-0.34584
H	-2.56758	-4.68387	-0.69896
H	-1.33323	-3.45498	-0.42280
H	-2.69691	-3.62921	0.71274
C	-1.19052	-0.85619	2.61184
H	-0.78416	-0.14708	3.33958
H	-2.03901	-0.40942	2.09160
H	-1.52015	-1.76190	3.11420
C	0.33798	-3.30698	2.65371
H	1.16216	-4.02217	2.62235
H	0.28480	-2.87652	3.65707
H	-0.59020	-3.86460	2.46900
C	1.53665	-2.58006	0.52879
H	1.42526	-3.63122	0.24174
H	1.47545	-1.96418	-0.36606
H	2.54216	-2.48274	0.96231

18A

Filename: TS1_TMS_f.out

B3LYP/6-31g*: -659.68901955 Hartree

ZPE: 652.687 kJ/mol

DeltaG (excl. ZPE): -101.357 kJ/mol

Low frequencies: -225.64 32.95 109.39

Cartesian coordinates:

C	0.00000	0.00000	0.00000
C	0.00000	0.00000	1.61715
N	1.36176	0.00000	2.06905
C	2.14783	-1.04804	1.72840
C	2.18980	-1.20455	-0.27232
C	0.80747	-1.15731	-0.40274
H	0.41967	0.95759	-0.31669
H	-1.04041	-0.07047	-0.32737
H	-0.52065	-0.88945	1.97835
H	-0.52470	0.88828	1.97224
H	1.81571	0.90865	2.07881
H	3.20988	-0.93484	1.92709
H	1.74957	-2.03438	1.94426
H	2.59276	-2.20886	-0.44343
H	0.26165	-2.08437	-0.59206
Si	3.49127	0.12398	-0.87416
C	5.16889	-0.67723	-0.58769
H	5.38128	-0.86899	0.47103
H	5.25928	-1.62814	-1.12538
H	5.96339	-0.01880	-0.95901
C	3.13624	0.38600	-2.70290
H	3.16990	-0.55571	-3.26205
H	2.15390	0.84213	-2.87151
H	3.88912	1.05387	-3.13901
C	3.37460	1.75910	0.06968
H	4.08244	2.46034	-0.39052
H	2.39088	2.24003	0.01513
H	3.67687	1.67850	1.12183

18B

Filename: TS1_TMS_eqMe_f.out

B3LYP/6-31g*: -699.00705902 Hartree

ZPE: 726.665 kJ/mol

DeltaG (excl. ZPE): -103.313 kJ/mol

Low frequencies: -141.93 60.33 102.69

Cartesian coordinates:

C	0.00000	0.00000	0.00000
C	0.00000	0.00000	1.63847

N	1.33592	0.00000	2.12462
C	2.16041	-1.06196	1.75128
C	2.19603	-1.20236	-0.03373
C	0.83267	-1.13235	-0.38150
H	0.42082	0.96878	-0.27871
H	-1.03087	-0.07359	-0.35201
H	-0.53949	-0.88503	1.98178
H	-0.53831	0.89206	1.96316
H	1.78813	0.90931	2.15247
H	1.67804	-2.01154	1.99027
H	2.61176	-2.19523	-0.24028
H	0.32553	-2.02137	-0.76241
Si	3.40130	0.13075	-0.88629
C	5.13544	-0.59380	-0.81940
H	5.56649	-0.61407	0.18565
H	5.16436	-1.61199	-1.22434
H	5.79530	0.01953	-1.44597
C	2.81615	0.26221	-2.67078
H	2.81981	-0.71209	-3.17275
H	1.80682	0.68144	-2.75459
H	3.48975	0.92005	-3.23348
C	3.30703	1.82347	-0.05140
H	3.94636	2.50508	-0.62793
H	2.30442	2.26683	-0.06132
H	3.68764	1.84126	0.97556
C	3.56615	-1.02934	2.32400
H	4.17153	-1.83815	1.90883
H	4.07400	-0.08009	2.13698
H	3.50123	-1.17653	3.40741

18C

Filename: TS1_TMS_axMe_f.out

B3LYP/6-31g*: -699.00702989 Hartree

ZPE: 726.836 kJ/mol

DeltaG (excl. ZPE): -104.944 kJ/mol

Low frequencies: -253.27 37.39 87.50

Cartesian coordinates:

C	0.00000	0.00000	0.00000
C	0.00000	0.00000	1.62145
N	1.35457	0.00000	2.07997
C	2.18344	-1.05535	1.76495
C	2.15514	-1.27890	-0.13938
C	0.78793	-1.16947	-0.39175
H	0.44789	0.95107	-0.29888
H	-1.03600	-0.04281	-0.34395
H	-0.54296	-0.87373	1.98336
H	-0.51727	0.89871	1.96193
H	1.80205	0.91013	2.03398
H	3.22767	-0.79722	1.93567
H	2.52181	-2.29425	-0.32182
H	0.22859	-2.05732	-0.69320
Si	3.52038	-0.03495	-0.80874
C	5.14892	-0.92539	-0.50291
H	5.34748	-1.10847	0.55985
H	5.18187	-1.89059	-1.02154
H	5.98114	-0.32293	-0.88639
C	3.16646	0.18391	-2.64223
H	3.14505	-0.77734	-3.16784
H	2.20851	0.68631	-2.81948
H	3.95010	0.79476	-3.10661
C	3.48285	1.62748	0.08913
H	4.22735	2.28004	-0.38462
H	2.52383	2.15335	0.01286

H	3.77122	1.56056	1.14574
C	1.83676	-2.43323	2.30316
H	2.50784	-3.18929	1.88893
H	1.97563	-2.41917	3.39074
H	0.80822	-2.73171	2.08877

18D

Filename: TS1_TMS_MeMe_f.out

B3LYP/6-31g*: -738.32068892 Hartree

ZPE: 799.671 kJ/mol

DeltaG (excl. ZPE): -106.820 kJ/mol

Low frequencies: -191.62 56.36 87.01

Cartesian coordinates:

C	0.00000	0.00000	0.00000
C	0.00000	0.00000	1.63135
N	1.33320	0.00000	2.12835
C	2.21637	-1.03401	1.75433
C	2.23806	-1.13119	-0.02151
C	0.88584	-1.08152	-0.41613
H	0.38094	0.98861	-0.26963
H	-1.02276	-0.10972	-0.36606
H	-0.55627	-0.87371	1.97231
H	-0.52839	0.89765	1.95704
H	1.76365	0.91894	2.16543
H	2.68928	-2.09532	-0.28063
H	0.43310	-1.94312	-0.91055
Si	3.38287	0.24850	-0.90401
C	5.15627	-0.37155	-0.80924
H	5.59760	-0.30228	0.18866
H	5.24140	-1.40959	-1.15082
H	5.77091	0.23894	-1.48303
C	2.81172	0.28269	-2.69769
H	2.87472	-0.70723	-3.16411
H	1.78208	0.64266	-2.80676
H	3.45508	0.95555	-3.27776
C	3.17733	1.96129	-0.13378
H	3.78420	2.65468	-0.73136
H	2.15149	2.34514	-0.17300
H	3.54075	2.04286	0.89584
C	3.62439	-0.79109	2.28906
H	4.32341	-1.52645	1.88477
H	3.99882	0.20909	2.05885
H	3.60916	-0.90441	3.37849
C	1.72647	-2.42877	2.18322
H	2.41120	-3.20199	1.82514
H	1.70565	-2.47293	3.27729
H	0.72786	-2.66605	1.80785

18E

Filename: TS1_MeTMS_f.out

B3LYP/6-31g*: -698.99937570 Hartree

ZPE: 726.137 kJ/mol

DeltaG (excl. ZPE): -105.506 kJ/mol

Low frequencies: -263.78 35.48 110.41

Cartesian coordinates:

C	0.00000	0.00000	0.00000
C	0.00000	0.00000	1.62682
N	1.36190	0.00000	2.07194
C	2.09226	-1.10129	1.74166
C	2.08829	-1.37885	-0.18207
C	0.71674	-1.21630	-0.38167
H	0.49674	0.92367	-0.30555

H	-1.04160	0.01034	-0.32931
H	-0.53135	-0.88470	1.98330
H	-0.52398	0.89364	1.96950
H	3.15375	-1.04316	1.96226
H	1.63996	-2.05320	2.00549
H	2.39266	-2.42722	-0.28351
H	0.10073	-2.09623	-0.58033
C	2.00279	1.30806	2.25744
H	1.51230	1.83051	3.08259
H	3.05436	1.16840	2.50971
H	1.92584	1.92457	1.35379
Si	3.49519	-0.30596	-1.03685
C	5.00004	-0.23003	0.09445
H	4.86868	0.43090	0.95877
H	5.29831	-1.22020	0.45926
H	5.84949	0.16551	-0.47627
C	3.87184	-1.32035	-2.57753
H	4.21419	-2.33288	-2.33564
H	2.99790	-1.40618	-3.23328
H	4.66894	-0.83448	-3.15373
C	2.91469	1.41721	-1.53507
H	3.71133	1.87640	-2.13472
H	2.02115	1.38916	-2.16881
H	2.72602	2.09596	-0.69720

18F

Filename: TS1_MeTMS_eqMe5_f.out

B3LYP/6-31g*: -738.31286136 Hartree

ZPE: 800.734 kJ/mol

DeltaG (excl. ZPE): -108.798 kJ/mol

Low frequencies: -250.05 38.83 91.45

Cartesian coordinates:

C	0.00000	0.00000	0.00000
C	0.00000	0.00000	1.63789
N	1.34943	0.00000	2.09396
C	2.08234	-1.14248	1.78373
C	2.00271	-1.49964	-0.03135
C	0.65299	-1.25486	-0.33621
H	0.55778	0.89555	-0.28593
H	-1.03258	0.06995	-0.34741
H	-0.54447	-0.87842	1.98994
H	-0.52727	0.89850	1.96204
H	1.53231	-2.03198	2.09300
H	2.23045	-2.57049	-0.10625
H	0.00042	-2.08974	-0.60009
C	1.96952	1.31704	2.27425
H	1.34040	1.90681	2.94440
H	2.94978	1.21302	2.73693
H	2.07901	1.85737	1.32578
Si	3.38322	-0.63871	-1.17110
C	4.99702	-1.56436	-0.88353
H	5.48905	-1.31557	0.06099
H	4.86262	-2.65136	-0.92400
H	5.69120	-1.29800	-1.69086
C	2.76154	-0.96202	-2.91975
H	2.59044	-2.02855	-3.10511
H	1.82675	-0.42903	-3.12957
H	3.50598	-0.62028	-3.64916
C	3.59681	1.21447	-0.90087
H	4.30205	1.57373	-1.66198
H	2.67157	1.78469	-1.04042
H	4.02360	1.47171	0.07325
C	3.52198	-1.21598	2.24978

H	3.95652	-2.17374	1.95533
H	4.14754	-0.41804	1.84639
H	3.54700	-1.16058	3.34452

18G

Filename: TS1_MeTMS_axMe_f.out

B3LYP/6-31g*: -738.31521112 Hartree

ZPE: 799.889 kJ/mol

DeltaG (excl. ZPE): -110.355 kJ/mol

Low frequencies: -273.52 23.95 96.80

Cartesian coordinates:

C	0.00000	0.00000	0.00000
C	0.00000	0.00000	1.62818
N	1.35927	0.00000	2.07135
C	2.13016	-1.10415	1.76576
C	2.07121	-1.41032	-0.11461
C	0.71203	-1.21678	-0.38027
H	0.50798	0.92225	-0.29335
H	-1.03733	0.02082	-0.34108
H	-0.54964	-0.87080	1.98545
H	-0.51533	0.90170	1.96303
H	3.18593	-0.90395	1.93300
H	2.35000	-2.46303	-0.23411
H	0.09540	-2.07415	-0.65728
C	1.98187	1.32039	2.22343
H	1.52339	1.83663	3.07143
H	3.04780	1.20556	2.42431
H	1.84883	1.93733	1.32584
Si	3.51180	-0.41255	-1.01515
C	5.05730	-0.47095	0.06124
H	5.01590	0.19641	0.92962
H	5.27841	-1.48444	0.41676
H	5.91722	-0.15125	-0.54050
C	3.75833	-1.42345	-2.58425
H	4.03294	-2.46254	-2.36958
H	2.85745	-1.43403	-3.20839
H	4.56854	-0.98846	-3.18230
C	3.03418	1.35605	-1.45425
H	3.83477	1.77207	-2.07954
H	2.11389	1.40694	-2.04683
H	2.93229	2.02220	-0.59214
C	1.71569	-2.45369	2.33998
H	2.37111	-3.24545	1.96948
H	1.82498	-2.41014	3.42993
H	0.68475	-2.72672	2.10468

18H

Filename: TS1_MeTMS_MeMe_f.out

B3LYP/6-31g*: -777.62381123 Hartree

ZPE: 874.414 kJ/mol

DeltaG (excl. ZPE): -111.177 kJ/mol

Low frequencies: -252.83 44.94 89.74

Cartesian coordinates:

C	0.00000	0.00000	0.00000
C	0.00000	0.00000	1.63870
N	1.34795	0.00000	2.09952
C	2.13209	-1.13191	1.79718
C	2.02520	-1.46633	-0.01829
C	0.67539	-1.23917	-0.34204
H	0.54658	0.90516	-0.27796
H	-1.03183	0.05613	-0.35196
H	-0.56495	-0.86337	1.98704

H	-0.51896	0.90524	1.95576
H	2.26721	-2.53085	-0.12064
H	0.04515	-2.07560	-0.65082
C	1.94867	1.32988	2.26976
H	1.22120	1.97284	2.76839
H	2.82934	1.26949	2.90817
H	2.23137	1.79159	1.31526
Si	3.37003	-0.60886	-1.20732
C	5.00799	-1.49729	-0.93388
H	5.52937	-1.19653	-0.02093
H	4.88988	-2.58697	-0.91907
H	5.66760	-1.25945	-1.77829
C	2.72107	-1.00115	-2.93262
H	2.56678	-2.07648	-3.07893
H	1.77275	-0.49265	-3.14286
H	3.44536	-0.67155	-3.68747
C	3.55155	1.25629	-1.00265
H	4.20416	1.61015	-1.81170
H	2.60608	1.80058	-1.10483
H	4.02527	1.55099	-0.06123
C	1.56849	-2.44013	2.38589
H	2.17969	-3.29172	2.07762
H	1.60972	-2.37355	3.47884
H	0.53773	-2.64556	2.09162
C	3.60374	-0.99942	2.16864
H	4.13954	-1.90288	1.87164
H	4.09449	-0.14253	1.70623
H	3.69475	-0.90591	3.25767

19A

Filename: ts_minTMS.out

B3LYP/6-31g*: -659.69818599 Hartree

ZPE: 653.997 kJ/mol

DeltaG (excl. ZPE): -103.517 kJ/mol

Low frequencies: 31.86 88.12 105.58

Cartesian coordinates:

C	-0.59475	0.66875	1.25246
C	-0.31619	-0.86563	1.28773
N	0.73122	-1.26246	0.36856
C	0.53036	-0.89543	-1.01172
C	-0.09467	0.50566	-1.21970
C	-0.73309	1.12298	-0.15898
H	0.23967	1.19609	1.73947
H	-1.49171	0.95332	1.81618
H	-1.23852	-1.39761	1.02715
H	-0.04270	-1.17292	2.29988
H	1.66025	-1.04366	0.71063
H	1.47040	-1.01127	-1.55780
H	-0.17951	-1.59121	-1.48538
H	-0.52265	0.70688	-2.20755
H	-1.40605	1.95453	-0.36736
Si	1.48115	1.99426	-1.39834
C	1.99252	1.61191	-3.16048
H	2.29709	0.57044	-3.30322
H	1.19985	1.84663	-3.87847
H	2.85683	2.24438	-3.40477
C	0.76573	3.71379	-1.20889
H	-0.10501	3.87816	-1.85346
H	0.48666	3.95149	-0.17712
H	1.53104	4.43927	-1.51493
C	2.78210	1.56423	-0.12362
H	3.61397	2.26912	-0.26014
H	2.44227	1.67518	0.91086

H 3.19495 0.55938 -0.25858

19B

Filename: ts_minTMS_eqMe.out

B3LYP/6-31g*: -699.01394682 Hartree

ZPE: 727.602 kJ/mol

DeltaG (excl. ZPE): -108.371 kJ/mol

Low frequencies: 26.91 73.61 94.35

Cartesian coordinates:

C	-0.44438	0.92158	0.76793
C	-0.51214	-0.56804	1.18088
N	0.54145	-1.37873	0.58310
C	0.58306	-1.35365	-0.86145
C	0.13484	-0.06574	-1.48159
C	-0.29833	1.02612	-0.75276
H	0.38892	1.40034	1.29564
H	-1.34895	1.45912	1.07381
H	-1.47883	-0.98379	0.86857
H	-0.45672	-0.66593	2.26812
H	1.45372	-1.20653	0.99692
H	-0.22806	-2.01975	-1.23720
H	0.02890	-0.05909	-2.56691
H	-0.96920	1.71319	-1.27763
Si	1.42072	2.28005	-1.28291
C	1.52251	2.33968	-3.15060
H	1.95033	1.43036	-3.58475
H	0.54817	2.52557	-3.61670
H	2.17580	3.17517	-3.43463
C	0.77090	3.86954	-0.53193
H	-0.15254	4.21002	-1.01160
H	0.59834	3.79280	0.54570
H	1.53137	4.64657	-0.68943
C	2.95877	1.63983	-0.43050
H	3.70340	2.44725	-0.43739
H	2.79064	1.37417	0.61814
H	3.40352	0.78405	-0.94598
C	1.89164	-1.93860	-1.41546
H	1.86827	-2.00286	-2.50726
H	2.75455	-1.33389	-1.12005
H	2.02444	-2.94528	-1.01115

19C

Filename: ts_minTMS_axMeOK.out

B3LYP/6-31g*: -699.01451118 Hartree

ZPE: 728.100 kJ/mol

DeltaG (excl. ZPE): -107.625 kJ/mol

Low frequencies: 33.92 72.48 99.91

Cartesian coordinates:

C	-0.58804	0.70288	1.26948
C	-0.32879	-0.83194	1.31283
N	0.70272	-1.24915	0.38269
C	0.50848	-0.90035	-1.01579
C	-0.10867	0.51259	-1.20636
C	-0.73029	1.14487	-0.14479
H	0.25751	1.22473	1.74361
H	-1.47639	1.00470	1.83776
H	-1.26239	-1.35412	1.07776
H	-0.04028	-1.13483	2.32223
H	1.63342	-1.02250	0.71629
H	1.49059	-0.94946	-1.49729
H	-0.53930	0.72753	-2.18994
H	-1.39271	1.98459	-0.35472

Si	1.47904	1.98480	-1.39664
C	1.96424	1.60894	-3.16788
H	2.25222	0.56428	-3.32115
H	1.16578	1.85935	-3.87410
H	2.83373	2.23140	-3.41897
C	0.78863	3.71334	-1.19065
H	-0.08522	3.89347	-1.82674
H	0.52104	3.94806	-0.15516
H	1.56112	4.43038	-1.49818
C	2.79439	1.53958	-0.14164
H	3.62915	2.23913	-0.28708
H	2.46981	1.64848	0.89793
H	3.19720	0.53208	-0.28622
C	-0.40318	-1.91487	-1.73890
H	-0.50566	-1.67012	-2.80170
H	0.03741	-2.91092	-1.64929
H	-1.40482	-1.93668	-1.29691

19D

Filename: ts_minTMS_MeMe.out

B3LYP/6-31g*: -738.32887922 Hartree

ZPE: 801.533 kJ/mol

DeltaG (excl. ZPE): -111.759 kJ/mol

Low frequencies: 28.52 72.60 85.16

Cartesian coordinates:

C	-0.44580	0.94750	0.74122
C	-0.53968	-0.54330	1.13583
N	0.48398	-1.37348	0.50702
C	0.50714	-1.34724	-0.95183
C	0.11488	-0.01774	-1.52759
C	-0.27941	1.07421	-0.77583
H	0.38899	1.40986	1.28193
H	-1.34520	1.49535	1.04457
H	-1.52478	-0.93086	0.85168
H	-0.45787	-0.65540	2.22031
H	1.40558	-1.18794	0.89490
H	0.03730	0.03914	-2.61362
H	-0.92365	1.79235	-1.29402
Si	1.44395	2.32463	-1.26230
C	1.54721	2.42583	-3.12845
H	1.96155	1.52061	-3.58385
H	0.57588	2.63696	-3.59013
H	2.21307	3.25762	-3.39333
C	0.81070	3.90362	-0.47571
H	-0.10879	4.26560	-0.94715
H	0.63660	3.80360	0.59988
H	1.57979	4.67576	-0.61384
C	2.97780	1.65707	-0.42280
H	3.70830	2.47493	-0.36341
H	2.79514	1.32059	0.60294
H	3.44571	0.84328	-0.98363
C	1.87333	-1.84251	-1.46317
H	1.90118	-1.87969	-2.55621
H	2.69159	-1.20561	-1.11413
H	2.04137	-2.85312	-1.07915
C	-0.59733	-2.31589	-1.50680
H	-0.59044	-2.35417	-2.60027
H	-0.37063	-3.30971	-1.11211
H	-1.59939	-2.03278	-1.17365

19E

Filename: int_minMeTMS_f.out

B3LYP/6-31g*: -699.00656126 Hartree
 ZPE: 727.070 kJ/mol
 DeltaG (excl. ZPE): -107.707 kJ/mol
 Low frequencies: 32.36 91.30 95.26

Cartesian coordinates:

C	0.00000	0.00000	0.00000
C	0.00000	0.00000	1.58936
N	1.35059	0.00000	2.07952
C	2.14474	-1.13331	1.68335
C	1.87223	-1.65993	0.23159
C	0.72032	-1.21392	-0.41830
H	0.53015	0.91631	-0.29801
H	-1.00228	0.04531	-0.43521
H	-0.54152	-0.88155	1.94651
H	-0.52879	0.88731	1.94469
H	3.20002	-0.90962	1.85197
H	1.90826	-2.00147	2.31811
H	2.03640	-2.73955	0.10994
H	0.28994	-1.83720	-1.20187
C	1.98950	1.30997	2.14808
H	1.42006	1.95443	2.82379
H	2.99875	1.20666	2.55466
H	2.05717	1.81712	1.16933
Si	3.40847	-1.15023	-1.11309
C	4.87190	-2.03404	-0.33947
H	5.12889	-1.65849	0.65602
H	4.71217	-3.11546	-0.27206
H	5.74570	-1.87115	-0.98427
C	2.92016	-1.89134	-2.76343
H	2.63493	-2.94638	-2.68029
H	2.09869	-1.34775	-3.24239
H	3.78096	-1.84569	-3.44228
C	3.60673	0.71153	-1.16373
H	4.40838	0.94066	-1.87870
H	2.70905	1.23169	-1.51408
H	3.90495	1.13367	-0.19977

19F

Filename: ts_minMeTMS_eqMe.out

B3LYP/6-31g*: -738.31634764 Hartree
 ZPE: 802.604 kJ/mol
 DeltaG (excl. ZPE): -109.221 kJ/mol
 Low frequencies: 46.00 89.14 100.08

Cartesian coordinates:

C	0.04153	-0.13854	-0.05311
C	-0.00986	-0.01961	1.52774
N	1.32204	0.08576	2.06212
C	2.14192	-1.08238	1.82174
C	2.00054	-1.66395	0.35016
C	0.84042	-1.33985	-0.35599
H	0.52855	0.77985	-0.41117
H	-0.94744	-0.18593	-0.51775
H	-0.51586	-0.89994	1.93717
H	-0.59759	0.86047	1.79936
H	1.67395	-1.90231	2.39010
H	2.25000	-2.73206	0.28749
H	0.46328	-2.04275	-1.09827
C	1.89423	1.42665	1.99849
H	1.21690	2.11904	2.50600
H	2.85101	1.46098	2.52033
H	2.04677	1.79419	0.96876
Si	3.41092	-1.11491	-1.15401
C	4.93378	-2.09246	-0.65463

H	5.40034	-1.73670	0.26662
H	4.72417	-3.16250	-0.55150
H	5.66755	-1.98162	-1.46476
C	2.74290	-1.74809	-2.79145
H	2.45160	-2.80389	-2.74769
H	1.89136	-1.16851	-3.16332
H	3.54134	-1.66988	-3.54064
C	3.66501	0.74143	-1.16709
H	4.39505	0.96240	-1.95793
H	2.75438	1.29813	-1.41133
H	4.07329	1.12948	-0.23014
C	3.57045	-0.96523	2.34648
H	4.07050	-1.93549	2.27727
H	4.17231	-0.23177	1.80341
H	3.54838	-0.67768	3.40182

19G

Filename: ts_minMeTMS_axMe.out

B3LYP/6-31g*: -738.32238533 Hartree

ZPE: 801.148 kJ/mol

DeltaG (excl. ZPE): -111.518 kJ/mol

Low frequencies: 37.64 71.70 87.67

Cartesian coordinates:

C	-0.01017	0.02832	-0.03880
C	-0.03620	0.00226	1.54795
N	1.30584	-0.00212	2.06163
C	2.14084	-1.12827	1.67347
C	1.84525	-1.64856	0.22009
C	0.71005	-1.18685	-0.44764
H	0.53256	0.94399	-0.31526
H	-1.00285	0.08371	-0.49442
H	-0.58700	-0.88245	1.88025
H	-0.57062	0.88337	1.91062
H	3.17821	-0.79156	1.75031
H	1.99103	-2.72903	0.08897
H	0.29072	-1.80369	-1.24246
C	1.93195	1.31301	2.15252
H	1.33109	1.95494	2.80306
H	2.92450	1.21832	2.60097
H	2.03860	1.82168	1.17759
Si	3.40713	-1.16446	-1.10227
C	4.83730	-2.11250	-0.34274
H	5.09338	-1.77493	0.66652
H	4.64675	-3.19066	-0.31094
H	5.72246	-1.95527	-0.97357
C	2.91287	-1.84986	-2.77522
H	2.59776	-2.89832	-2.72258
H	2.11230	-1.27105	-3.24843
H	3.78183	-1.81108	-3.44453
C	3.66340	0.69080	-1.10797
H	4.48537	0.91138	-1.80241
H	2.78822	1.24463	-1.46367
H	3.95449	1.08370	-0.12960
C	1.97534	-2.32737	2.63409
H	2.63930	-3.15234	2.35499
H	2.22563	-2.01055	3.64942
H	0.94594	-2.70004	2.63061

19H

Filename: ts_minMeTMS_MeMe.out

B3LYP/6-31g*: -777.62733037 Hartree

ZPE: 876.364 kJ/mol

DeltaG (excl. ZPE): -112.912 kJ/mol

Low frequencies: 42.62 72.82 92.04

Cartesian coordinates:

C	0.08780	-0.13114	-0.05903
C	0.00430	-0.02478	1.51061
N	1.32549	0.03043	2.09230
C	2.16129	-1.15046	1.85447
C	2.01841	-1.68820	0.36960
C	0.89367	-1.33079	-0.36774
H	0.58131	0.78538	-0.41343
H	-0.89156	-0.17680	-0.54484
H	-0.55805	-0.87940	1.89477
H	-0.55225	0.87617	1.77887
H	2.29084	-2.74464	0.25580
H	0.54916	-1.99896	-1.15605
C	1.91167	1.36952	2.05946
H	1.19462	2.06852	2.49854
H	2.81670	1.41351	2.66472
H	2.15494	1.73035	1.04477
Si	3.40933	-1.09342	-1.18684
C	4.94786	-2.05424	-0.70360
H	5.43180	-1.68125	0.20130
H	4.75051	-3.12455	-0.58277
H	5.66046	-1.94618	-1.53297
C	2.73557	-1.74037	-2.81644
H	2.44666	-2.79648	-2.76713
H	1.88386	-1.16371	-3.19177
H	3.53504	-1.66482	-3.56510
C	3.64129	0.76479	-1.20846
H	4.34792	0.98886	-2.01974
H	2.71976	1.31238	-1.43068
H	4.07085	1.16037	-0.28451
C	1.62528	-2.32932	2.72305
H	2.23192	-3.22905	2.57955
H	1.67953	-2.03960	3.77564
H	0.58888	-2.58505	2.48693
C	3.61679	-0.91521	2.27967
H	4.18274	-1.84545	2.18381
H	4.12320	-0.14466	1.69385
H	3.64840	-0.61943	3.33259

20A

Filename: TS2_TMS_f.out

B3LYP/6-31g*: -659.68591593 Hartree

ZPE: 651.231 kJ/mol

DeltaG (excl. ZPE): -102.061 kJ/mol

Low frequencies: -244.78 37.24 90.73

Cartesian coordinates:

C	0.00000	0.00000	0.00000
C	0.00000	0.00000	2.10800
N	1.30422	0.00000	2.41075
C	2.10564	-1.13163	2.03587
C	2.08256	-1.35665	0.42468
C	0.70420	-1.18754	-0.04738
H	0.51263	0.95661	-0.02118
H	-1.03738	0.02211	-0.32597
H	-0.55163	-0.91728	2.27840
H	-0.55018	0.92621	2.24614
H	1.77412	0.90125	2.41161
H	3.13006	-0.99367	2.38318
H	1.69826	-2.03082	2.50460
H	2.37223	-2.40707	0.29747
H	0.13923	-2.08603	-0.30192

Si	3.48680	-0.31197	-0.46733
C	5.10511	-1.15809	-0.00804
H	5.30146	-1.15732	1.07079
H	5.13096	-2.19809	-0.35340
H	5.94397	-0.63725	-0.48553
C	3.16724	-0.37017	-2.31915
H	3.14055	-1.40061	-2.69233
H	2.22231	0.11166	-2.59477
H	3.96904	0.14936	-2.85730
C	3.48086	1.46994	0.17422
H	4.27844	2.02348	-0.33740
H	2.55180	2.01558	-0.02957
H	3.70614	1.54264	1.24644

20B

Filename: TS2_TMS_eqMe_f.out

B3LYP/6-31g*: -699.00124108 Hartree

ZPE: 725.280 kJ/mol

DeltaG (excl. ZPE): -104.300 kJ/mol

Low frequencies: -261.24 56.39 83.45

Cartesian coordinates:

C	0.00000	0.00000	0.00000
C	0.00000	0.00000	2.07213
N	1.29780	0.00000	2.41349
C	2.11877	-1.12035	2.03237
C	2.17785	-1.19548	0.38314
C	0.78485	-1.13678	-0.06987
H	0.45051	0.98687	-0.04917
H	-1.04353	-0.04806	-0.30325
H	-0.55451	-0.91607	2.24197
H	-0.55383	0.92408	2.21164
H	1.76762	0.90208	2.43914
H	1.58740	-2.02670	2.33886
H	2.56564	-2.20589	0.19964
H	0.27648	-2.07724	-0.29191
Si	3.41754	0.03132	-0.53056
C	5.15581	-0.68170	-0.38980
H	5.56951	-0.63861	0.62231
H	5.19393	-1.72431	-0.72720
H	5.82946	-0.11050	-1.04055
C	2.89323	0.06951	-2.33966
H	2.90090	-0.93341	-2.78282
H	1.89399	0.49349	-2.48756
H	3.59711	0.68220	-2.91579
C	3.34365	1.77542	0.20820
H	4.02880	2.41579	-0.36184
H	2.35567	2.24629	0.13420
H	3.67719	1.82759	1.25187
C	3.48990	-1.09944	2.69846
H	4.09713	-1.93067	2.33184
H	4.03128	-0.16997	2.50025
H	3.37799	-1.21077	3.78106

20C

Filename: TS2_TMS_axMe_f.out

B3LYP/6-31g*: -699.00193954 Hartree

ZPE: 725.016 kJ/mol

DeltaG (excl. ZPE): -106.284 kJ/mol

Low frequencies: -253.28 37.51 68.72

Cartesian coordinates:

C	0.00000	0.00000	0.00000
C	0.00000	0.00000	2.10159

N	1.30364	0.00000	2.40506
C	2.13985	-1.12862	2.05358
C	2.08590	-1.35251	0.42963
C	0.70951	-1.18447	-0.04621
H	0.50824	0.95900	-0.01701
H	-1.03553	0.01835	-0.33203
H	-0.56200	-0.90852	2.27619
H	-0.54313	0.93108	2.23462
H	1.76623	0.90476	2.39546
H	3.16220	-0.86223	2.32932
H	2.37422	-2.40118	0.29120
H	0.14963	-2.08186	-0.31430
Si	3.48143	-0.31034	-0.47529
C	5.10660	-1.14150	-0.00974
H	5.30553	-1.12616	1.06857
H	5.13654	-2.18580	-0.34185
H	5.94189	-0.62315	-0.49599
C	3.16362	-0.39428	-2.32666
H	3.14302	-1.42996	-2.68558
H	2.21557	0.07780	-2.60838
H	3.96233	0.12265	-2.87182
C	3.46670	1.47951	0.14319
H	4.26503	2.02951	-0.37098
H	2.53648	2.01845	-0.07236
H	3.68488	1.56686	1.21578
C	1.74398	-2.41469	2.78761
H	2.46036	-3.20544	2.54891
H	1.76101	-2.25492	3.87003
H	0.75049	-2.77329	2.50006

20D

Filename: TS2_TMS_MeMe_f.out

B3LYP/6-31g*: -738.31441480 Hartree

ZPE: 798.378 kJ/mol

DeltaG (excl. ZPE): -107.442 kJ/mol

Low frequencies: -269.38 52.25 77.59

Cartesian coordinates:

C	0.00000	0.00000	0.00000
C	0.00000	0.00000	2.06978
N	1.29771	0.00000	2.40894
C	2.16649	-1.10266	2.04212
C	2.19846	-1.16071	0.37290
C	0.80645	-1.12087	-0.08512
H	0.43262	0.99517	-0.03318
H	-1.04019	-0.06238	-0.31203
H	-0.56586	-0.90741	2.23698
H	-0.54412	0.92941	2.21154
H	1.75327	0.90891	2.43749
H	2.60294	-2.16065	0.17146
H	0.31919	-2.06187	-0.34569
Si	3.39486	0.07786	-0.58381
C	5.16458	-0.55171	-0.42307
H	5.59971	-0.40397	0.56969
H	5.24078	-1.61693	-0.67213
H	5.79725	-0.01146	-1.13825
C	2.87392	0.00265	-2.39366
H	2.92471	-1.02016	-2.78578
H	1.85796	0.37620	-2.56238
H	3.55280	0.61441	-2.99997
C	3.25089	1.85605	0.05654
H	3.92952	2.48277	-0.53625
H	2.25144	2.29020	-0.06651
H	3.55658	1.98134	1.10218

C	3.55954	-0.87274	2.63230
H	4.25546	-1.62633	2.25698
H	3.96135	0.11361	2.38406
H	3.51909	-0.96293	3.72264
C	1.60917	-2.44314	2.55645
H	2.31517	-3.24383	2.31983
H	1.49116	-2.40666	3.64432
H	0.64841	-2.71487	2.11018

20E

Filename: TS2_MeTMS_f.out

B3LYP/6-31g*: -698.99792305 Hartree

ZPE: 724.832 kJ/mol

DeltaG (excl. ZPE): -107.765 kJ/mol

Low frequencies: -294.13 30.82 69.61

Cartesian coordinates:

C	0.00000	0.00000	0.00000
C	0.00000	0.00000	2.06651
N	1.31523	0.00000	2.33582
C	2.05011	-1.20036	1.99699
C	1.77714	-1.72900	0.49835
C	0.49088	-1.29466	-0.03891
H	0.66668	0.85730	-0.01191
H	-0.99896	0.19490	-0.38317
H	-0.55108	-0.91121	2.26818
H	-0.54543	0.92528	2.22894
H	3.11096	-1.02465	2.17543
H	1.73008	-2.01028	2.65932
H	1.76543	-2.82396	0.56663
H	-0.20055	-2.07183	-0.36706
C	2.04169	1.27627	2.38713
H	1.39526	2.04425	2.81485
H	2.91751	1.16101	3.02897
H	2.37021	1.59037	1.38851
Si	3.29259	-1.42568	-0.74149
C	4.77162	-2.27603	0.05710
H	5.08427	-1.80933	0.99847
H	4.57862	-3.33721	0.25219
H	5.62983	-2.22330	-0.62427
C	2.80856	-2.25466	-2.35862
H	2.55477	-3.31203	-2.21905
H	1.95324	-1.76108	-2.83449
H	3.64455	-2.21355	-3.06714
C	3.61878	0.41515	-0.99008
H	4.39023	0.52791	-1.76249
H	2.73872	0.96411	-1.34405
H	4.00315	0.90724	-0.08996

20F

Filename: TS2_MeTMS_eqMe_f.out

B3LYP/6-31g*: -738.30962182 Hartree

ZPE: 800.190 kJ/mol

DeltaG (excl. ZPE): -108.484 kJ/mol

Low frequencies: -299.90 43.93 83.91

Cartesian coordinates:

C	0.00000	0.00000	0.00000
C	0.00000	0.00000	2.02046
N	1.31092	0.00000	2.33084
C	2.02653	-1.22486	2.01694
C	1.89624	-1.60460	0.41913
C	0.55768	-1.26847	-0.06294
H	0.62818	0.88537	-0.05207

H	-1.02134	0.14518	-0.34504
H	-0.55690	-0.90529	2.23580
H	-0.54888	0.92506	2.17366
H	1.46572	-2.03014	2.50181
H	1.99538	-2.69829	0.41027
H	-0.11144	-2.08705	-0.33292
C	2.02140	1.28446	2.40120
H	1.31895	2.05998	2.70979
H	2.81467	1.22327	3.14761
H	2.46154	1.55522	1.43525
Si	3.30386	-1.07628	-0.87588
C	4.85601	-2.07873	-0.50235
H	5.40074	-1.73555	0.38203
H	4.63784	-3.14575	-0.37650
H	5.53789	-1.99131	-1.35774
C	2.61500	-1.59443	-2.55242
H	2.35477	-2.65928	-2.57888
H	1.72433	-1.02208	-2.83607
H	3.37082	-1.42855	-3.32968
C	3.67903	0.77453	-0.87883
H	4.36006	0.97858	-1.71514
H	2.79272	1.39883	-1.04120
H	4.18669	1.11540	0.02996
C	3.45545	-1.26296	2.54236
H	3.89020	-2.24325	2.33246
H	4.09622	-0.50589	2.08402
H	3.46385	-1.12138	3.62808

20G

Filename: TS2_MeTMS_axMe_f.out

B3LYP/6-31g*: -738.31388921 Hartree

ZPE: 798.935 kJ/mol

DeltaG (excl. ZPE): -111.179 kJ/mol

Low frequencies: -310.49 42.19 47.79

Cartesian coordinates:

C	0.00000	0.00000	0.00000
C	0.00000	0.00000	2.04232
N	1.31681	0.00000	2.31220
C	2.09025	-1.20218	1.98337
C	1.66968	-1.82472	0.56519
C	0.43188	-1.31773	-0.01224
H	0.70233	0.82827	-0.01681
H	-0.97901	0.23014	-0.41396
H	-0.55682	-0.90348	2.25989
H	-0.54073	0.92756	2.20927
H	3.13290	-0.87769	1.95928
H	1.55374	-2.90606	0.70506
H	-0.28451	-2.06322	-0.35922
C	2.03769	1.27917	2.34241
H	1.38148	2.05931	2.73194
H	2.89966	1.18688	3.00731
H	2.39139	1.56704	1.34335
Si	3.16733	-1.74757	-0.73957
C	4.57324	-2.71595	0.05639
H	4.93441	-2.26618	0.98850
H	4.28580	-3.75237	0.26812
H	5.42585	-2.75162	-0.63311
C	2.56336	-2.58017	-2.31317
H	2.20551	-3.59967	-2.12750
H	1.75412	-2.01835	-2.79365
H	3.38440	-2.65294	-3.03660
C	3.64967	0.04892	-1.04463
H	4.44587	0.07697	-1.79916

H	2.82095	0.64901	-1.43733
H	4.04662	0.54253	-0.15034
C	1.95290	-2.28080	3.07044
H	2.57843	-3.14306	2.82191
H	2.27911	-1.88862	4.03799
H	0.91888	-2.62911	3.16404

20H

Filename: TS2_MeTMS_MeMe_f.out

B3LYP/6-31g*: -777.62043044 Hartree

ZPE: 873.766 kJ/mol

DeltaG (excl. ZPE): -110.951 kJ/mol

Low frequencies: -304.04 47.65 75.02

Cartesian coordinates:

C	0.00000	0.00000	0.00000
C	0.00000	0.00000	2.00702
N	1.31000	0.00000	2.32792
C	2.07350	-1.21514	2.02166
C	1.93900	-1.55679	0.39900
C	0.58895	-1.25412	-0.07332
H	0.60789	0.89935	-0.05416
H	-1.02554	0.12214	-0.34179
H	-0.57384	-0.89198	2.21892
H	-0.54023	0.93019	2.15900
H	2.07171	-2.64517	0.35627
H	-0.05937	-2.08661	-0.35093
C	1.98837	1.30365	2.41044
H	1.25260	2.06602	2.67008
H	2.74463	1.27916	3.19585
H	2.46672	1.57172	1.46237
Si	3.30620	-0.96333	-0.91023
C	4.90747	-1.90210	-0.57634
H	5.46897	-1.52591	0.28369
H	4.73538	-2.97498	-0.42996
H	5.55532	-1.80061	-1.45626
C	2.61201	-1.50721	-2.57742
H	2.39570	-2.58194	-2.60186
H	1.69403	-0.97218	-2.84652
H	3.34818	-1.30936	-3.36600
C	3.60968	0.90116	-0.92437
H	4.25959	1.12809	-1.77938
H	2.69685	1.49175	-1.06352
H	4.12879	1.26443	-0.03085
C	1.46163	-2.42503	2.76853
H	2.09209	-3.30458	2.61337
H	1.42202	-2.22165	3.84337
H	0.45695	-2.68498	2.42402
C	3.53666	-1.08170	2.45069
H	4.06540	-2.00594	2.20874
H	4.05820	-0.25955	1.95735
H	3.60331	-0.93849	3.53477

21A

Filename: int2_TMS_f.out

B3LYP/6-31g*: -659.69740404 Hartree

ZPE: 648.553 kJ/mol

DeltaG (excl. ZPE): -108.422 kJ/mol

Low frequencies: 32.62 78.31 87.90

Cartesian coordinates:

C	-1.76211	-2.40990	2.00941
C	1.65068	0.35878	3.22898
N	1.08426	-0.51017	2.48441

C	1.69347	-1.71130	1.84381
C	0.72170	-2.89210	1.98644
C	-0.60033	-2.53749	1.35360
H	-1.83841	-2.58336	3.08161
H	-2.68607	-2.17770	1.48732
H	2.71927	0.29305	3.41895
H	1.06376	1.16030	3.67011
H	0.06763	-0.45746	2.32061
H	1.84861	-1.44636	0.79125
H	2.66410	-1.87871	2.31626
H	0.57270	-3.08403	3.05904
H	-0.58735	-2.37571	0.27387
Si	1.47002	-4.55088	1.25942
C	3.15633	-4.81521	2.06818
H	3.89779	-4.06350	1.77064
H	3.09353	-4.81959	3.16310
H	3.55923	-5.78995	1.76758
C	0.26422	-5.91517	1.72628
H	0.16914	-6.01801	2.81369
H	-0.73535	-5.73247	1.31697
H	0.61087	-6.87911	1.33553
C	1.64068	-4.36610	-0.61050
H	2.06195	-5.28599	-1.03387
H	0.67478	-4.20154	-1.10166
H	2.31254	-3.54861	-0.90016

21B

Filename: int2_TMS_eqMe_f.out

B3LYP/6-31g*: -699.00542330 Hartree

ZPE: 723.631 kJ/mol

DeltaG (excl. ZPE): -108.304 kJ/mol

Low frequencies: 48.27 78.15 115.09

Cartesian coordinates:

C	0.03069	-0.37316	-0.50806
C	0.18575	0.39045	2.41609
N	1.44619	0.15603	2.34207
C	2.04369	-1.17099	2.07602
C	2.15498	-1.35115	0.51085
C	0.75535	-1.40919	-0.05477
H	0.43929	0.63041	-0.60396
H	-0.98476	-0.51242	-0.86894
H	-0.51112	-0.43763	2.47470
H	-0.17301	1.41410	2.47320
H	2.08545	0.95060	2.27546
H	1.31235	-1.89462	2.45329
H	2.58014	-2.36249	0.42586
H	0.27620	-2.38995	-0.03342
Si	3.44967	-0.24262	-0.46153
C	5.16975	-0.97295	-0.19846
H	5.52688	-0.91551	0.83494
H	5.20862	-2.02455	-0.50736
H	5.89276	-0.43057	-0.81991
C	3.02697	-0.30448	-2.29368
H	2.96211	-1.33775	-2.65410
H	2.08124	0.18944	-2.53568
H	3.81930	0.19146	-2.86727
C	3.42367	1.55654	0.15907
H	4.09769	2.15404	-0.46700
H	2.43772	2.03321	0.08634
H	3.80102	1.67209	1.18571
C	3.34726	-1.31789	2.86095
H	3.80520	-2.28072	2.61945
H	4.06974	-0.53439	2.61376

H 3.15819 -1.29179 3.93836

21C

Filename: int2_TMS_axMe_f.out

B3LYP/6-31g*: -699.01261427 Hartree

ZPE: 723.016 kJ/mol

DeltaG (excl. ZPE): -110.440 kJ/mol

Low frequencies: 42.41 57.86 106.31

Cartesian coordinates:

C	-1.61163	0.67551	0.58135
C	2.67954	0.91085	1.55879
N	1.65339	0.23192	1.21787
C	1.21798	-1.14347	1.65645
C	-0.30643	-1.03380	1.92586
C	-0.99195	-0.50829	0.68663
H	-1.68835	1.35993	1.42500
H	-2.11040	0.97610	-0.33584
H	3.42327	0.48501	2.22488
H	2.80418	1.92138	1.17809
H	0.94571	0.66839	0.60657
H	-0.45330	-0.31993	2.75028
H	-0.96886	-1.16368	-0.18716
Si	-1.17861	-2.70370	2.49535
C	-0.82490	-3.01972	4.32273
H	0.21600	-3.27681	4.54431
H	-1.09762	-2.15583	4.94076
H	-1.44083	-3.86186	4.66200
C	-3.02675	-2.43758	2.25883
H	-3.38402	-1.55894	2.80849
H	-3.30154	-2.30653	1.20716
H	-3.57605	-3.30724	2.63920
C	-0.54856	-4.11150	1.40418
H	-1.08101	-5.03632	1.65763
H	-0.73019	-3.92370	0.33898
H	0.52094	-4.31785	1.53258
H	1.37292	-1.76095	0.76152
C	2.09024	-1.65661	2.79318
H	1.79706	-2.68103	3.02724
H	3.15018	-1.69058	2.51822
H	1.96873	-1.05692	3.70198

21D

Filename: int2_TMS_MeMe_f.out

B3LYP/6-31g*: -738.32590672 Hartree

ZPE: 797.023 kJ/mol

DeltaG (excl. ZPE): -113.194 kJ/mol

Low frequencies: 31.59 53.67 101.01

Cartesian coordinates:

C	1.71391	-0.14624	5.42777
C	2.36606	1.38315	1.39580
N	1.74138	0.57227	2.15751
C	1.37871	-0.89454	1.94333
C	1.69359	-1.55997	3.32324
C	1.05036	-0.80559	4.46658
H	2.80202	-0.11059	5.45390
H	1.19159	0.33859	6.24809
H	2.70392	1.06622	0.41420
H	2.56155	2.39718	1.73602
H	1.46387	0.89303	3.09778
H	2.78507	-1.49975	3.44967
H	-0.03812	-0.82905	4.51792
Si	1.29764	-3.47496	3.60896

C	1.71255	-4.56720	2.12220
H	1.03978	-4.42419	1.26860
H	2.74524	-4.44947	1.77537
H	1.60051	-5.61290	2.43633
C	2.40777	-3.94724	5.05545
H	3.47052	-3.86905	4.79634
H	2.22741	-3.32123	5.93577
H	2.21990	-4.98746	5.34704
C	-0.52258	-3.69740	4.05961
H	-0.71028	-4.76001	4.25719
H	-0.79870	-3.15078	4.96788
H	-1.21012	-3.39625	3.26085
C	-0.11593	-0.90169	1.57114
H	-0.44104	-1.93656	1.43582
H	-0.74234	-0.44970	2.34498
H	-0.28575	-0.36663	0.63143
C	2.23205	-1.44625	0.80205
H	1.98880	-2.49774	0.65329
H	2.02629	-0.93877	-0.14713
H	3.30259	-1.37811	1.02505

21E

Filename: int2_MeTMS_f.out

B3LYP/6-31g*: -699.01605693 Hartree

ZPE: 722.949 kJ/mol

DeltaG (excl. ZPE): -112.647 kJ/mol

Low frequencies: 32.02 62.76 83.24

Cartesian coordinates:

C	4.00464	-3.94147	1.56084
C	3.86872	-1.47823	-0.70483
N	2.81830	-1.03645	-0.11046
C	2.87418	-0.59298	1.31406
C	2.81530	-1.82389	2.24797
C	4.01918	-2.69483	2.05554
H	3.07833	-4.42883	1.26225
H	4.91212	-4.53381	1.48265
H	4.83604	-1.38769	-0.22592
H	3.79117	-1.91688	-1.69490
H	1.90769	-2.39711	2.00717
H	4.97687	-2.26517	2.35801
Si	2.58637	-1.28507	4.12075
C	1.05425	-0.18401	4.20652
H	1.18378	0.77699	3.69408
H	0.16728	-0.67691	3.79026
H	0.82779	0.04704	5.25453
C	2.33895	-2.87196	5.09846
H	1.45233	-3.42206	4.76161
H	3.20167	-3.54154	5.01346
H	2.19830	-2.64511	6.16191
C	4.12628	-0.34640	4.67484
H	4.01366	-0.03983	5.72185
H	5.03153	-0.96190	4.61835
H	4.29999	0.56802	4.09429
H	2.03222	0.08455	1.46641
C	1.48035	-1.10776	-0.72988
H	1.54527	-1.59235	-1.70425
H	0.81704	-1.67513	-0.07305
H	1.09607	-0.09047	-0.84184
H	3.80374	-0.03299	1.44625

21F

Filename: int2_MeTMS_eqMe_f.out

B3LYP/6-31g*: -738.32672988 Hartree
 ZPE: 797.822 kJ/mol
 DeltaG (excl. ZPE): -114.855 kJ/mol
 Low frequencies: 38.12 50.26 75.12

Cartesian coordinates:

C	4.44737	2.02965	-0.31160
C	2.80534	-2.57959	-0.45497
N	2.44039	-1.39768	-0.12161
C	2.73432	-0.85864	1.27843
C	3.94530	0.10196	1.23723
C	3.69885	1.46187	0.64296
H	5.28306	1.50746	-0.77409
H	4.26594	3.04752	-0.64442
H	3.29522	-3.21826	0.27419
H	2.62943	-2.94449	-1.46271
H	4.73400	-0.39909	0.65631
H	2.89390	2.04844	1.08604
Si	4.79583	0.32369	3.00399
C	4.69690	-1.32215	3.93173
H	3.67380	-1.60281	4.21020
H	5.13816	-2.15113	3.36428
H	5.26560	-1.24283	4.86641
C	6.58636	0.76846	2.63390
H	7.11472	-0.04702	2.12594
H	6.65884	1.66273	2.00528
H	7.12506	0.97723	3.56583
C	3.95165	1.69578	3.98436
H	4.47717	1.83431	4.93719
H	3.98747	2.65394	3.45426
H	2.90401	1.48234	4.22589
H	3.02602	-1.75617	1.83010
C	1.76700	-0.50781	-1.09188
H	1.72830	-0.99498	-2.06653
H	0.75548	-0.30377	-0.73565
H	2.33149	0.42581	-1.14706
C	1.44585	-0.30904	1.89389
H	1.63581	-0.08116	2.94594
H	1.10559	0.61228	1.41526
H	0.63929	-1.04811	1.85543

21G

Filename: int2_MeTMS_axMe_f.out

B3LYP/6-31g*: -738.32789759 Hartree
 ZPE: 797.675 kJ/mol
 DeltaG (excl. ZPE): -113.978 kJ/mol
 Low frequencies: 46.66 58.03 94.81

Cartesian coordinates:

C	3.96136	-2.30560	-0.38940
C	3.07329	0.43259	1.05865
N	1.85106	0.07841	0.87551
C	1.30119	-1.12860	1.60505
C	1.71405	-2.38158	0.77401
C	3.21062	-2.48161	0.70819
H	3.51732	-2.08384	-1.35834
H	5.04064	-2.42907	-0.36723
H	3.64809	-0.00945	1.86345
H	3.52043	1.20158	0.43609
H	1.31174	-2.26903	-0.24396
H	3.71577	-2.72601	1.64595
Si	0.98689	-4.09751	1.41911
C	-0.83710	-4.23824	0.95281
H	-1.49572	-3.55812	1.50151
H	-0.99346	-4.07022	-0.11968

H	-1.17766	-5.25885	1.16751
C	1.95338	-5.44292	0.52422
H	1.89258	-5.33116	-0.56469
H	3.01313	-5.45248	0.79892
H	1.53615	-6.42550	0.77586
C	1.24953	-4.20930	3.28652
H	0.90958	-5.18919	3.64345
H	2.30776	-4.12239	3.56106
H	0.69135	-3.45471	3.85331
H	1.84217	-1.14433	2.55661
C	-0.18824	-0.94745	1.88810
H	-0.51013	-1.72450	2.58375
H	-0.38666	0.01772	2.36543
H	-0.80154	-1.03488	0.98689
C	1.03892	0.68574	-0.19781
H	0.18312	1.19745	0.24633
H	1.64755	1.39844	-0.75470
H	0.68380	-0.09977	-0.86799

21H

Filename: int2_MeTMS_MeMe_f.out

B3LYP/6-31g*: -777.63280940 Hartree

ZPE: 872.013 kJ/mol

DeltaG (excl. ZPE): -118.598 kJ/mol

Low frequencies: 13.49 48.39 66.89

Cartesian coordinates:

C	3.65852	-3.81239	1.00559
C	0.91523	-1.11681	-0.72897
N	2.10571	-0.83007	-0.35716
C	2.41973	-0.39902	1.12165
C	2.58105	-1.72291	1.93522
C	3.75003	-2.57168	1.49774
H	2.69768	-4.30131	0.85282
H	4.54267	-4.39783	0.76949
H	0.08657	-1.02097	-0.03755
H	0.72750	-1.46076	-1.74197
H	1.66042	-2.30256	1.76236
H	4.74446	-2.15197	1.65730
Si	2.62795	-1.61176	3.91223
C	0.94355	-1.08784	4.59656
H	0.71305	-0.02633	4.46370
H	0.12122	-1.67194	4.16571
H	0.93778	-1.28291	5.67626
C	2.97045	-3.37139	4.49187
H	2.25056	-4.08702	4.07755
H	3.97294	-3.71712	4.22288
H	2.88276	-3.41418	5.58438
C	3.98452	-0.44871	4.52662
H	4.10405	-0.59110	5.60790
H	4.95873	-0.65567	4.06869
H	3.75285	0.61168	4.37305
C	1.23769	0.45323	1.60909
H	1.52962	0.95176	2.53520
H	0.98472	1.23412	0.88412
H	0.34395	-0.13424	1.83713
C	3.22058	-0.98295	-1.31945
H	3.93892	-1.68788	-0.89910
H	2.82946	-1.36762	-2.26198
H	3.69167	-0.01284	-1.48052
C	3.68059	0.47674	1.09205
H	3.89055	0.80220	2.11223
H	4.56700	-0.04784	0.73183
H	3.52753	1.37537	0.48513

22E

Filename: TS3_MeTMS_f.out

B3LYP/6-31g*: -699.00587191 Hartree

ZPE: 726.564 kJ/mol

DeltaG (excl. ZPE): -103.477 kJ/mol

Low frequencies: -9.80 63.74 109.17

Cartesian coordinates:

C	0.00000	0.00000	0.00000
C	0.00000	0.00000	1.55145
N	1.34816	0.00000	2.10135
C	2.14073	-1.12958	1.67371
C	1.78632	-1.72542	0.34626
C	0.81811	-1.19205	-0.47971
H	0.40738	0.95402	-0.35356
H	-1.01589	-0.07020	-0.40276
H	-0.52888	-0.89384	1.90817
H	-0.53656	0.87284	1.93246
H	3.21191	-0.90165	1.73866
H	1.99727	-1.98576	2.36570
H	2.22601	-2.69488	0.11243
H	0.36979	-1.85790	-1.22186
C	2.01239	1.29899	2.14258
H	1.40026	1.99251	2.72634
H	2.97757	1.20063	2.64823
H	2.18804	1.75592	1.15153
Si	2.45694	-0.68607	-1.91814
C	3.88652	0.22138	-1.12407
H	3.56666	1.09159	-0.54219
H	4.50230	-0.42086	-0.48680
H	4.53200	0.59354	-1.93129
C	2.90741	-2.32992	-2.68998
H	3.52520	-2.95612	-2.03833
H	2.02788	-2.90648	-2.99694
H	3.49334	-2.13274	-3.59749
C	1.41925	0.40434	-3.03454
H	2.03450	0.64613	-3.91240
H	0.51479	-0.09677	-3.39278
H	1.13521	1.34929	-2.56280

22F

Filename: TS3_MeTMS_eqMe_f.out

B3LYP/6-31g*: -738.31529372 Hartree

ZPE: 802.830 kJ/mol

DeltaG (excl. ZPE): -106.798 kJ/mol

Low frequencies: -78.78 47.54 101.31

Cartesian coordinates:

C	0.00000	0.00000	0.00000
C	0.00000	0.00000	1.56244
N	1.34701	0.00000	2.09992
C	2.11744	-1.17041	1.72053
C	1.86155	-1.66161	0.27479
C	0.78879	-1.19161	-0.45211
H	0.43939	0.94319	-0.35123
H	-1.01113	-0.04430	-0.41864
H	-0.53523	-0.88998	1.91594
H	-0.53974	0.87462	1.93488
H	1.67339	-2.02186	2.27142
H	2.20731	-2.67583	0.06272
H	0.40767	-1.78488	-1.28144
C	1.96971	1.31835	2.17180
H	1.33294	1.96721	2.78068

H	2.93908	1.25799	2.66851
H	2.11185	1.81048	1.19489
Si	3.02880	-0.74271	-1.52012
C	4.46063	-1.94333	-1.36859
H	4.95712	-1.90234	-0.39599
H	4.15720	-2.97621	-1.56839
H	5.19798	-1.66482	-2.13426
C	2.15139	-0.92868	-3.16832
H	1.81817	-1.95441	-3.35842
H	1.29635	-0.25465	-3.27919
H	2.87548	-0.67355	-3.95416
C	3.45361	1.03446	-1.13220
H	4.13244	1.36721	-1.93059
H	2.58733	1.70219	-1.15292
H	3.97777	1.16276	-0.18251
C	3.58919	-1.13336	2.13652
H	4.04884	-2.11017	1.95578
H	4.16812	-0.37847	1.59718
H	3.66571	-0.92420	3.20703

22G

Filename: TS3_MeTMS_axMe_f.out

B3LYP/6-31g*: -738.32204264 Hartree

ZPE: 800.880 kJ/mol

DeltaG (excl. ZPE): -107.862 kJ/mol

Low frequencies: -21.57 55.81 85.74

Cartesian coordinates:

C	0.00000	0.00000	0.00000
C	0.00000	0.00000	1.56189
N	1.34549	0.00000	2.10099
C	2.16664	-1.13742	1.70525
C	1.93335	-1.58972	0.24275
C	0.83719	-1.13736	-0.46782
H	0.41267	0.95672	-0.35137
H	-1.00579	-0.07379	-0.42864
H	-0.54103	-0.88425	1.91545
H	-0.53731	0.87676	1.93208
H	3.21143	-0.84579	1.84046
H	2.26898	-2.60360	0.00146
H	0.53437	-1.67427	-1.36728
C	2.00431	1.30069	2.12418
H	1.36679	2.01851	2.64842
H	2.94444	1.22531	2.67888
H	2.22974	1.71911	1.12503
Si	3.30291	-0.76852	-1.28972
C	4.89066	-0.80717	-0.29400
H	4.93174	-0.02661	0.47121
H	5.07302	-1.77768	0.17794
H	5.71497	-0.62176	-0.99680
C	3.23615	-2.07174	-2.63178
H	3.41773	-3.08187	-2.24905
H	2.28967	-2.07294	-3.18230
H	4.03013	-1.85564	-3.35890
C	2.85593	0.94709	-1.88921
H	3.68063	1.29625	-2.52548
H	1.94680	0.96576	-2.49825
H	2.75185	1.67374	-1.07734
C	1.91711	-2.36407	2.61427
H	2.57421	-3.19866	2.34644
H	2.11804	-2.08198	3.65046
H	0.88105	-2.71066	2.54452

22H

Filename: TS3_MeTMS_MeMe_f.out

B3LYP/6-31g*: -777.62694822 Hartree

ZPE: 876.381 kJ/mol

DeltaG (excl. ZPE): -109.638 kJ/mol

Low frequencies: -42.27 51.06 92.62

Cartesian coordinates:

C	0.00000	0.00000	0.00000
C	0.00000	0.00000	1.56308
N	1.34829	0.00000	2.09850
C	2.16048	-1.16443	1.72406
C	1.92226	-1.60402	0.23961
C	0.80784	-1.16681	-0.45197
H	0.43839	0.94724	-0.34485
H	-1.00758	-0.04845	-0.42637
H	-0.55280	-0.87582	1.91528
H	-0.53157	0.88166	1.92949
H	2.25384	-2.61954	0.00326
H	0.44983	-1.74834	-1.29983
C	1.94301	1.33463	2.15520
H	1.26195	1.98826	2.70776
H	2.88534	1.31812	2.70265
H	2.12360	1.79757	1.16968
Si	3.16650	-0.75147	-1.45513
C	4.69407	-1.81038	-1.20709
H	5.20785	-1.62546	-0.26170
H	4.47414	-2.87978	-1.28913
H	5.38708	-1.55627	-2.02140
C	2.35470	-1.14652	-3.10130
H	2.06332	-2.19894	-3.18997
H	1.48079	-0.52223	-3.31278
H	3.09422	-0.95224	-3.88968
C	3.43833	1.08404	-1.22195
H	4.07641	1.41059	-2.05550
H	2.51573	1.66956	-1.28097
H	3.95733	1.33576	-0.29419
C	1.67254	-2.39676	2.54825
H	2.25167	-3.29275	2.30239
H	1.80748	-2.17568	3.61013
H	0.61701	-2.62104	2.37340
C	3.64622	-0.96783	2.05860
H	4.19480	-1.89101	1.85155
H	4.11463	-0.15727	1.49501
H	3.75998	-0.75152	3.12482

23A

Filename: prod_TMS_2.out

B3LYP/6-31g*: -250.67062876 Hartree

ZPE: 355.958 kJ/mol

DeltaG (excl. ZPE): -74.908 kJ/mol

Low frequencies: 169.38 295.04 402.09

Cartesian coordinates:

C	-0.53613	1.80275	-1.46131
C	-1.56583	2.15793	-0.68648
H	-2.35517	2.79347	-1.08569
H	-0.49421	2.11986	-2.50299
C	0.60308	0.94673	-0.95140
H	1.56688	1.37135	-1.26230
H	0.55437	-0.05020	-1.41931
C	-1.69442	1.70228	0.74857
H	-1.50803	2.54885	1.42964
H	-2.72647	1.38180	0.95258
C	-0.71391	0.55342	1.04905

H	-0.63189	0.38236	2.12890
H	-1.09517	-0.37591	0.60522
N	0.63140	0.77449	0.50641
H	1.00782	1.62666	0.92197

23B

Filename: prod_TMS_eqMe.out

B3LYP/6-31g*: -289.98753607 Hartree

ZPE: 429.651 kJ/mol

DeltaG (excl. ZPE): -79.724 kJ/mol

Low frequencies: 109.35 244.13 283.95

Cartesian coordinates:

C	0.14252	-0.51698	0.13900
C	-1.11271	-0.05743	0.11701
H	-1.93117	-0.72369	-0.15332
H	0.34617	-1.56438	-0.08450
C	1.33643	0.36058	0.47036
H	1.68611	0.09682	1.48308
C	-1.46184	1.36913	0.46844
H	-1.75842	1.91839	-0.44009
H	-2.34213	1.39170	1.12729
C	-0.27015	2.06781	1.14746
H	-0.18839	1.72075	2.18598
H	-0.42132	3.15315	1.18401
N	1.01522	1.79729	0.49488
H	0.96075	2.12355	-0.47180
C	2.50376	0.11992	-0.49375
H	3.34743	0.76691	-0.23253
H	2.83605	-0.92317	-0.45559
H	2.20594	0.33743	-1.52776

23C

Filename: prod_TMS_axMe.out

B3LYP/6-31g*: -289.98753743 Hartree

ZPE: 429.655 kJ/mol

DeltaG (excl. ZPE): -79.724 kJ/mol

Low frequencies: 109.16 244.51 284.00

Cartesian coordinates:

C	-0.55727	1.64751	-1.43061
C	-1.69300	1.99417	-0.81640
H	-2.44665	2.57074	-1.35159
H	-0.37054	1.96536	-2.45655
C	0.52130	0.81442	-0.76128
H	1.36801	1.47913	-0.51900
C	-1.98443	1.62832	0.61947
H	-2.76752	0.85353	0.65861
H	-2.40012	2.49512	1.15367
C	-0.70840	1.13116	1.32227
H	-0.06626	1.98942	1.56047
H	-0.95039	0.63956	2.27195
N	0.08531	0.20595	0.50663
H	-0.49442	-0.60506	0.28293
C	1.05232	-0.28185	-1.69205
H	1.48167	0.14998	-2.60259
H	1.82511	-0.86659	-1.18268
H	0.24464	-0.96131	-1.99398

23D

Filename: prod_TMS_MeMe.out

B3LYP/6-31g*: -329.30207771 Hartree

ZPE: 502.770 kJ/mol

DeltaG (excl. ZPE): -83.262 kJ/mol

Low frequencies: 107.78 224.49 235.03

Cartesian coordinates:

C	-0.21015	-0.40136	1.61737
C	-1.29054	0.38251	1.68926
H	-2.27935	-0.06541	1.78106
H	-0.31962	-1.48456	1.67799
C	1.20755	0.12626	1.44878
C	-1.20659	1.88913	1.65660
H	-1.55594	2.26511	0.68089
H	-1.88748	2.32380	2.40267
C	0.23689	2.35026	1.91813
H	0.46093	2.25012	2.98702
H	0.36253	3.41024	1.66757
N	1.23947	1.58218	1.17128
H	1.06057	1.71592	0.17537
C	1.88109	-0.58143	0.25884
H	1.30211	-0.43943	-0.66225
H	2.88759	-0.17654	0.10397
H	1.96411	-1.65865	0.43934
C	2.02792	-0.15474	2.72690
H	2.01848	-1.22414	2.96886
H	3.06523	0.16530	2.58249
H	1.61766	0.38282	3.58784

23E

Filename: prod_MeTMS.out

B3LYP/6-31g*: -289.98211726 Hartree

ZPE: 428.433 kJ/mol

DeltaG (excl. ZPE): -79.269 kJ/mol

Low frequencies: 156.14 204.45 262.52

Cartesian coordinates:

C	-0.86440	1.86894	-1.56424
C	-2.01669	1.70102	-0.91195
H	-2.96323	1.76199	-1.44672
H	-0.85178	2.04464	-2.63829
C	0.47495	1.82714	-0.87571
H	1.08717	2.67978	-1.20428
H	1.02331	0.91617	-1.20702
C	-2.05716	1.42463	0.56901
H	-2.38121	2.32583	1.11008
H	-2.79902	0.64517	0.79192
C	-0.67991	0.98301	1.07744
H	-0.65611	1.00511	2.17325
H	-0.49138	-0.06673	0.77049
N	0.35619	1.88579	0.57946
C	1.64045	1.67438	1.22588
H	1.53641	1.80870	2.30832
H	2.06470	0.66624	1.04332
H	2.36275	2.41323	0.85983

23F

Filename: prod_MeTMS_eqMe.out

B3LYP/6-31g*: -329.29624626 Hartree

ZPE: 502.557 kJ/mol

DeltaG (excl. ZPE): -84.338 kJ/mol

Low frequencies: 83.04 189.39 218.46

Cartesian coordinates:

C	1.46929	-0.34122	1.84062
C	0.36521	-0.35677	2.58899
H	0.24283	-1.10601	3.36956
H	2.26259	-1.06704	2.01283

C	1.70773	0.61690	0.69425
H	2.55081	1.28455	0.98137
C	-0.72656	0.66033	2.39447
H	-1.11265	1.00001	3.36541
H	-1.57633	0.21162	1.85924
C	-0.19029	1.85826	1.60876
H	0.46888	2.46178	2.26590
H	-1.01762	2.50888	1.30209
N	0.50771	1.41852	0.39849
C	2.15060	-0.18576	-0.54343
H	3.02460	-0.80128	-0.30167
H	1.33846	-0.84372	-0.86898
H	2.42878	0.46293	-1.37956
C	0.79753	2.55084	-0.47241
H	1.50984	3.27332	-0.02549
H	1.21446	2.21091	-1.42419
H	-0.13308	3.08525	-0.69214

23G

Filename: prod_MeTMS_axMe.out

B3LYP/6-31g*: -329.29625442 Hartree

ZPE: 502.532 kJ/mol

DeltaG (excl. ZPE): -84.339 kJ/mol

Low frequencies: 83.20 188.88 218.56

Cartesian coordinates:

C	0.24599	1.80262	1.26025
C	-0.94321	2.03674	1.81729
H	-1.11935	2.96125	2.36491
H	1.05388	2.52588	1.36035
C	0.57163	0.58087	0.42941
H	1.32637	-0.01671	0.98821
C	-2.06175	1.03445	1.72479
H	-2.80468	1.35804	0.98097
H	-2.59171	0.96053	2.68441
C	-1.50361	-0.33702	1.34069
H	-0.97502	-0.77443	2.21238
H	-2.32295	-1.02026	1.08835
N	-0.62738	-0.23516	0.17144
C	1.22198	1.03404	-0.89118
H	2.09348	1.66610	-0.68575
H	1.56627	0.18856	-1.49445
H	0.50210	1.61129	-1.48026
C	-0.29803	-1.55756	-0.34565
H	-1.22369	-2.10350	-0.55781
H	0.26005	-1.47934	-1.28251
H	0.30311	-2.16457	0.36094

23H

Filename: prod_MeTMS_MeMe.out

B3LYP/6-31g*: -368.60742804 Hartree

ZPE: 575.999 kJ/mol

DeltaG (excl. ZPE): -87.322 kJ/mol

Low frequencies: 94.59 176.25 215.85

Cartesian coordinates:

C	-1.06955	0.24075	0.33007
C	-1.50270	0.51463	1.56138
H	-2.25546	-0.12016	2.02669
H	-1.48191	-0.60496	-0.21907
C	0.00833	1.01380	-0.41010
C	-0.98020	1.68956	2.34063
H	-1.79848	2.19112	2.87569
H	-0.26793	1.34923	3.10681

C	-0.29626	2.68022	1.39764
H	0.27194	3.41776	1.97655
H	-1.06752	3.24531	0.83720
N	0.64371	1.99125	0.51341
C	-0.63137	1.67070	-1.66257
H	-1.35179	2.44517	-1.37827
H	0.12861	2.12423	-2.30841
H	-1.16718	0.92199	-2.25721
C	1.07613	-0.01041	-0.85739
H	0.61624	-0.80081	-1.46171
H	1.85618	0.45440	-1.46981
H	1.54624	-0.46618	0.01891
C	1.56224	2.93263	-0.11548
H	1.06829	3.70317	-0.73627
H	2.12611	3.45155	0.66826
H	2.28464	2.40543	-0.74429

24A

Filename: reac_minTMS_E.out

B3LYP/6-31g*: -659.70083622 Hartree

ZPE: 650.060 kJ/mol

DeltaG (excl. ZPE): -109.686 kJ/mol

Low frequencies: 27.75 50.74 89.12

Cartesian coordinates:

C	-0.98005	-0.24072	0.46558
H	-1.98603	-0.49823	0.12580
H	-0.95716	-0.24900	1.56162
C	-0.47561	1.11199	-0.08200
H	-1.14800	1.88227	0.31380
H	-0.57055	1.12099	-1.17376
C	0.95652	1.36120	0.33616
C	2.02361	1.23011	-0.47449
H	1.09839	1.63721	1.38280
N	-0.05145	-1.30654	0.02062
C	-0.33727	-2.49052	-0.36147
H	-1.37249	-2.82334	-0.37010
H	0.45777	-3.16157	-0.67617
H	0.93081	-0.98388	0.01360
Si	3.84711	1.51633	0.00259
C	4.74581	-0.13425	-0.22222
H	4.36735	-0.90566	0.46034
H	4.65819	-0.51311	-1.24766
H	5.81565	-0.01625	-0.01239
C	3.92597	2.08364	1.79893
H	3.51816	1.33774	2.49196
H	4.96747	2.25918	2.09303
H	3.38379	3.02360	1.95541
C	4.54073	2.81367	-1.17455
H	5.60130	2.99656	-0.96501
H	4.46317	2.49432	-2.22056
H	4.01391	3.76970	-1.07623
H	1.81215	0.98206	-1.52248

24B

Filename: reac_minTMS_E_eqMe_f.out

B3LYP/6-31g*: -699.03399833 Hartree

ZPE: 722.711 kJ/mol

DeltaG (excl. ZPE): -114.412 kJ/mol

Low frequencies: -193.12 24.66 38.88

Cartesian coordinates:

C	-0.95803	-0.25189	0.45637
H	-1.97039	-0.49470	0.12411

H	-0.93690	-0.23648	1.55201
C	-0.44271	1.08274	-0.11796
H	-1.11655	1.86682	0.24834
H	-0.52327	1.06489	-1.21099
C	0.98355	1.34484	0.31095
C	2.05912	1.23481	-0.48980
H	1.11270	1.61878	1.35999
N	-0.05514	-1.34489	0.02426
C	-0.38175	-2.53189	-0.34561
H	-1.44646	-2.76429	-0.32904
H	0.93505	-1.05828	0.01469
Si	3.86870	1.55932	0.00509
C	4.82143	-0.05686	-0.24723
H	4.46027	-0.85488	0.41353
H	4.75331	-0.41385	-1.28207
H	5.88549	0.08829	-0.02535
C	3.92459	2.09013	1.81423
H	3.53299	1.31918	2.48893
H	4.95973	2.28672	2.11749
H	3.35661	3.01165	1.98744
C	4.53806	2.90234	-1.13555
H	5.59157	3.10880	-0.91196
H	4.47815	2.60594	-2.18945
H	3.98489	3.84132	-1.02012
H	1.86191	0.98554	-1.54005
C	0.60450	-3.56240	-0.77656
H	0.09895	-4.48974	-1.04859
H	1.17966	-3.20771	-1.64118
H	1.31783	-3.77328	0.03030

24C

Filename: reac_minTMS_E_axMe_f.out

B3LYP/6-31g*: -699.03483790 Hartree

ZPE: 724.016 kJ/mol

DeltaG (excl. ZPE): -116.392 kJ/mol

Low frequencies: 26.21 36.95 64.24

Cartesian coordinates:

C	-0.41799	-0.95681	0.17364
H	-1.02556	-1.78231	0.56146
H	-0.23764	-0.24123	0.97734
C	-1.09613	-0.29442	-1.04591
H	-0.52451	0.59411	-1.33785
H	-2.08409	0.04547	-0.71348
C	-1.20512	-1.25974	-2.20355
C	-0.42059	-1.23095	-3.29732
H	-1.95612	-2.04447	-2.09337
N	0.87654	-1.53363	-0.26258
C	1.95872	-1.73323	0.40550
H	0.85133	-1.80547	-1.25707
Si	-0.47494	-2.44974	-4.75974
C	1.18351	-3.36312	-4.77536
H	2.02981	-2.67071	-4.86155
H	1.32759	-3.96720	-3.87069
H	1.23744	-4.04676	-5.63100
C	-0.68837	-1.44218	-6.33751
H	0.12459	-0.71807	-6.46778
H	-0.68841	-2.09730	-7.21683
H	-1.63361	-0.88771	-6.33750
C	-1.89979	-3.65733	-4.49930
H	-1.95006	-4.36724	-5.33330
H	-1.78518	-4.24737	-3.58186
H	-2.86676	-3.14311	-4.45251
H	0.29524	-0.40163	-3.36148

H	2.78477	-2.16515	-0.15948
C	2.17203	-1.43966	1.83989
H	2.48064	-2.36673	2.34250
H	3.01990	-0.74814	1.93873
H	1.29927	-1.02829	2.34652

24D

Filename: reac_minTMS_E_MeMe_f.out

B3LYP/6-31g*: -738.36572926 Hartree

ZPE: 796.868 kJ/mol

DeltaG (excl. ZPE): -122.114 kJ/mol

Low frequencies: 24.92 32.49 53.01

Cartesian coordinates:

C	-0.83410	-0.43279	0.80596
H	-1.90920	-0.62301	0.83047
H	-0.48508	-0.26436	1.83173
C	-0.49102	0.76990	-0.09999
H	-0.94509	1.65581	0.35968
H	-0.96452	0.62880	-1.07851
C	1.00277	0.93648	-0.25652
C	1.69388	0.61046	-1.36438
H	1.52905	1.31459	0.62220
N	-0.14340	-1.63416	0.29000
C	-0.47375	-2.87990	0.41834
H	0.71895	-1.39861	-0.21895
Si	3.57685	0.73804	-1.60216
C	4.21754	-1.02742	-1.85281
H	4.05382	-1.65191	-0.96510
H	3.73730	-1.51735	-2.70879
H	5.29665	-1.02246	-2.04789
C	4.34342	1.51199	-0.06223
H	4.16205	0.91425	0.83932
H	5.43039	1.59370	-0.18083
H	3.96076	2.52289	0.12030
C	3.89875	1.77641	-3.14154
H	4.97403	1.84545	-3.34464
H	3.42425	1.34076	-4.02888
H	3.51709	2.79713	-3.02546
H	1.10285	0.26002	-2.21990
C	0.38625	-3.93295	-0.19599
H	0.74056	-4.61280	0.58926
H	-0.21788	-4.53985	-0.88238
H	1.24476	-3.52425	-0.73456
C	-1.70662	-3.27469	1.16994
H	-1.76770	-4.35898	1.27352
H	-1.72483	-2.81800	2.16580
H	-2.60129	-2.92930	0.63492

24E

Filename: reac_minMeTMS_E.out

B3LYP/6-31g*: -699.01941621 Hartree

ZPE: 724.359 kJ/mol

DeltaG (excl. ZPE): -114.618 kJ/mol

Low frequencies: 25.17 41.70 66.56

Cartesian coordinates:

C	0.21528	0.25815	1.32412
H	-0.01218	0.64973	2.31838
H	1.29141	0.33085	1.15507
C	-0.58556	1.02028	0.22830
H	-0.34378	0.60047	-0.75508
H	-0.20242	2.04826	0.24382
C	-2.06827	0.99024	0.47657

C	-2.94329	0.20383	-0.18121
H	-2.42585	1.65800	1.26316
N	-0.14828	-1.17812	1.30142
C	-1.22445	-1.58487	1.87603
H	-1.78535	-0.90882	2.50928
H	-1.54965	-2.61387	1.75705
C	0.67259	-2.06351	0.45096
H	0.22089	-3.05446	0.40237
H	0.73689	-1.63142	-0.55083
H	1.67446	-2.12902	0.88292
Si	-4.83092	0.15596	0.06998
C	-5.28026	-1.57853	0.68145
H	-4.94509	-2.35786	-0.01365
H	-4.85154	-1.79308	1.66859
H	-6.36823	-1.67775	0.77659
C	-5.62907	0.48856	-1.60442
H	-5.32893	-0.25637	-2.35097
H	-6.72203	0.45072	-1.52440
H	-5.35948	1.47784	-1.99104
C	-5.31279	1.45800	1.34650
H	-6.39916	1.45591	1.49457
H	-4.85597	1.27654	2.32710
H	-5.03236	2.46763	1.02448
H	-2.52842	-0.42445	-0.97859

24F

Filename: reac_minMeTMS_E_eqMe_f.out

B3LYP/6-31g*: -738.34606385 Hartree

ZPE: 797.433 kJ/mol

DeltaG (excl. ZPE): -122.877 kJ/mol

Low frequencies: 22.05 29.15 56.05

Cartesian coordinates:

C	-0.82329	-0.36011	0.61186
H	-1.88114	-0.48890	0.37015
H	-0.73274	-0.23759	1.69442
C	-0.23780	0.85240	-0.14271
H	-0.93292	1.67825	0.06707
H	-0.29039	0.66298	-1.22226
C	1.16135	1.25245	0.25899
C	2.22567	1.26368	-0.55927
H	1.26638	1.58577	1.29420
N	-0.13771	-1.64594	0.26969
C	-0.57973	-2.38903	-0.68852
H	-1.47939	-2.02331	-1.18112
Si	3.97874	1.84587	-0.11434
C	5.14830	0.37255	-0.32315
H	4.91102	-0.44295	0.37118
H	5.11554	-0.03167	-1.34207
H	6.18410	0.67475	-0.12691
C	3.99279	2.45497	1.67270
H	3.72459	1.66574	2.38571
H	4.99568	2.80534	1.94405
H	3.30456	3.29487	1.82370
C	4.44621	3.22509	-1.31294
H	5.46563	3.57892	-1.11770
H	4.41114	2.88412	-2.35450
H	3.77326	4.08511	-1.21996
H	2.05146	0.93979	-1.59219
C	0.02429	-3.66838	-1.15660
H	-0.57303	-4.08573	-1.96846
H	1.04702	-3.51322	-1.52227
H	0.07021	-4.40520	-0.34493
C	1.06617	-1.96731	1.06169

H	1.52590	-2.88809	0.70915
H	1.76296	-1.13142	0.96048
H	0.76956	-2.07479	2.10860

24G

Filename: reac_minMeTMS_E_axMe_f.out

B3LYP/6-31g*: -738.34690263 Hartree

ZPE: 798.437 kJ/mol

DeltaG (excl. ZPE): -120.646 kJ/mol

Low frequencies: 25.16 27.64 54.96

Cartesian coordinates:

C	-1.24298	-0.13841	1.10290
H	-1.94111	-0.12777	1.94173
H	-1.46383	0.72732	0.47432
C	-1.35554	-1.44911	0.29436
H	-2.41822	-1.53053	0.02484
H	-1.12721	-2.30180	0.94509
C	-0.49777	-1.49570	-0.94716
C	0.50194	-2.36638	-1.15688
H	-0.75955	-0.76883	-1.71978
N	0.13270	0.08768	1.64487
C	0.56364	-0.42869	2.74656
C	1.01181	0.93477	0.80840
H	1.07592	0.47731	-0.18102
H	0.56802	1.93064	0.73254
H	2.00333	0.99889	1.25786
Si	1.57169	-2.50253	-2.72029
C	1.05708	-1.15777	-3.94208
H	0.00702	-1.25547	-4.24172
H	1.20069	-0.14809	-3.53794
H	1.66087	-1.22671	-4.85470
C	1.31801	-4.22255	-3.45128
H	0.27702	-4.38173	-3.75475
H	1.94735	-4.36209	-4.33852
H	1.58167	-5.00970	-2.73501
C	3.37582	-2.27239	-2.19803
H	4.04276	-2.38724	-3.06096
H	3.55923	-1.27685	-1.77561
H	3.68002	-3.01593	-1.45148
H	0.69840	-3.08637	-0.35355
C	-0.18543	-1.29941	3.68370
H	-1.19554	-1.55244	3.36501
H	0.38759	-2.22403	3.83367
H	-0.22308	-0.80592	4.66471
H	1.59228	-0.18604	3.00959

24H

Filename: reac_minMeTMS_E_MeMe_f.out

B3LYP/6-31g*: -777.67086009 Hartree

ZPE: 872.188 kJ/mol

DeltaG (excl. ZPE): -125.827 kJ/mol

Low frequencies: 20.67 31.89 48.25

Cartesian coordinates:

C	-0.49616	0.05436	1.28625
H	-0.76316	0.27795	2.32330
H	0.22143	0.80409	0.95704
C	-1.75178	0.05161	0.38339
H	-2.22259	1.03342	0.52399
H	-2.46681	-0.69477	0.74926
C	-1.44313	-0.19067	-1.07431
C	-1.68665	-1.33683	-1.72943
H	-0.99363	0.65249	-1.60387

N	0.17096	-1.27722	1.30025
C	1.26467	-1.53449	0.64159
C	-0.55353	-2.32531	2.06579
H	0.10143	-2.75391	2.82638
H	-1.40718	-1.86179	2.55677
H	-0.91127	-3.10609	1.39163
Si	-1.32472	-1.69323	-3.55770
C	-0.68223	-0.12308	-4.38563
H	-1.41483	0.69089	-4.33580
H	0.25200	0.23675	-3.93715
H	-0.47741	-0.31076	-5.44630
C	-2.91993	-2.29390	-4.36244
H	-3.70263	-1.52770	-4.32374
H	-2.75408	-2.54558	-5.41668
H	-3.30808	-3.19231	-3.86774
C	-0.00882	-3.05639	-3.62265
H	0.19528	-3.34726	-4.66017
H	0.94326	-2.72559	-3.18762
H	-0.33118	-3.96009	-3.09095
H	-2.16938	-2.13545	-1.15265
C	1.86650	-2.90222	0.60939
H	1.86758	-3.24645	-0.43400
H	2.91907	-2.83526	0.91091
H	1.36378	-3.64680	1.22294
C	1.99951	-0.46590	-0.11883
H	2.85595	-0.89955	-0.63753
H	1.35100	0.01201	-0.85810
H	2.37184	0.30928	0.56241

25A

Filename: TS_TMS_E_f.out

B3LYP/6-31g*: -659.69077574 Hartree

ZPE: 651.675 kJ/mol

DeltaG (excl. ZPE): -102.615 kJ/mol

Low frequencies: -223.44 32.12 94.33

Cartesian coordinates:

C	0.00000	0.00000	0.00000
C	0.00000	0.00000	1.95891
N	1.29366	0.00000	2.38280
C	2.13798	-1.08474	1.97006
C	2.22778	-1.04513	0.33889
C	0.83571	-1.11324	-0.06028
H	0.42573	0.98844	-0.16458
H	-1.05009	-0.09788	-0.27112
H	-0.56147	-0.90709	2.16408
H	-0.55597	0.91893	2.13080
H	1.74809	0.90804	2.42716
H	3.14159	-0.96609	2.37945
H	1.72126	-2.03921	2.29822
H	2.65161	-0.05979	0.10509
H	0.36225	-2.09614	-0.10220
Si	3.43610	-2.43633	-0.34692
C	3.61816	-2.11026	-2.19001
H	2.66358	-2.19915	-2.72157
H	4.02558	-1.11274	-2.39142
H	4.30808	-2.83843	-2.63341
C	5.07330	-2.22630	0.55915
H	5.47409	-1.21043	0.46051
H	5.00902	-2.46796	1.62641
H	5.81703	-2.90582	0.12506
C	2.65353	-4.11542	0.00079
H	3.32543	-4.90587	-0.35594
H	2.49068	-4.29914	1.06950

H 1.69893 -4.25605 -0.52001

25B

Filename: TS_TMS_E_eqMe_f.out

B3LYP/6-31g*: -699.00670504 Hartree

ZPE: 725.200 kJ/mol

DeltaG (excl. ZPE): -105.698 kJ/mol

Low frequencies: -234.96 44.52 82.44

Cartesian coordinates:

C	0.00000	0.00000	0.00000
C	0.00000	0.00000	1.95817
N	1.28954	0.00000	2.38820
C	2.15740	-1.09171	2.01217
C	2.21765	-1.06839	0.36318
C	0.82362	-1.12121	-0.03362
H	0.43734	0.98279	-0.16718
H	-1.04968	-0.08933	-0.27522
H	-0.56777	-0.90184	2.16867
H	-0.55307	0.92300	2.11779
H	1.74717	0.90773	2.43005
H	1.68658	-2.03102	2.31401
H	2.65066	-0.08912	0.12039
H	0.33566	-2.09754	-0.06909
Si	3.32060	-2.48890	-0.45067
C	2.73671	-2.65130	-2.23481
H	1.69736	-2.99168	-2.31118
H	2.82329	-1.70472	-2.78112
H	3.35612	-3.38666	-2.76258
C	5.12034	-1.93787	-0.41716
H	5.25294	-0.96529	-0.90577
H	5.54807	-1.87235	0.58787
H	5.72252	-2.66294	-0.97890
C	3.02330	-4.08825	0.50326
H	3.57774	-4.90267	0.02088
H	3.36537	-4.04214	1.54342
H	1.96749	-4.38582	0.50697
C	3.53231	-0.94799	2.65685
H	4.15894	-1.81043	2.42607
H	4.04914	-0.04830	2.30405
H	3.42724	-0.88994	3.74438

25C

Filename: TS_TMS_E_axMe_f.out

B3LYP/6-31g*: -699.00473873 Hartree

ZPE: 725.957 kJ/mol

DeltaG (excl. ZPE): -104.907 kJ/mol

Low frequencies: -245.62 52.43 93.79

Cartesian coordinates:

C	0.00000	0.00000	0.00000
C	0.00000	0.00000	1.96312
N	1.29342	0.00000	2.38481
C	2.16768	-1.08535	1.99900
C	2.24008	-1.00024	0.34693
C	0.85740	-1.09597	-0.07411
H	0.40927	0.99814	-0.14749
H	-1.04623	-0.11116	-0.28079
H	-0.57174	-0.89898	2.16745
H	-0.54824	0.92425	2.13024
H	1.74114	0.91181	2.41812
H	3.17300	-0.84261	2.34923
H	2.61802	0.01418	0.16227
H	0.40785	-2.08521	-0.16583

Si	3.52732	-2.23662	-0.47944
C	3.95797	-1.44878	-2.13370
H	3.08078	-1.34899	-2.78351
H	4.40369	-0.45454	-2.01256
H	4.68919	-2.06963	-2.66544
C	5.04126	-2.31781	0.63956
H	5.47226	-1.32604	0.82212
H	4.84501	-2.78859	1.60954
H	5.81853	-2.91574	0.14782
C	2.72967	-3.92658	-0.72390
H	3.46414	-4.60279	-1.17890
H	2.39766	-4.39794	0.20739
H	1.87397	-3.88421	-1.40829
C	1.74024	-2.44066	2.55915
H	2.47903	-3.20195	2.29958
H	1.68550	-2.38270	3.65045
H	0.77062	-2.78007	2.18434

25D

Filename: TS_TMS_E_MeMe_f.out

B3LYP/6-31g*: -738.31835009 Hartree

ZPE: 799.073 kJ/mol

DeltaG (excl. ZPE): -108.124 kJ/mol

Low frequencies: -253.67 31.88 83.78

Cartesian coordinates:

C	0.00000	0.00000	0.00000
C	0.00000	0.00000	1.96414
N	1.29058	0.00000	2.38413
C	2.19465	-1.08887	2.04574
C	2.20759	-1.08926	0.36988
C	0.81180	-1.12883	-0.02788
H	0.44625	0.98024	-0.15788
H	-1.04953	-0.07844	-0.27918
H	-0.58055	-0.89113	2.17737
H	-0.54215	0.93076	2.11532
H	1.73885	0.91247	2.41126
H	2.63351	-0.10651	0.12911
H	0.31570	-2.09789	-0.08586
Si	3.27106	-2.44240	-0.60652
C	3.49677	-1.67430	-2.31225
H	2.53945	-1.47336	-2.80724
H	4.05598	-0.73215	-2.26692
H	4.06243	-2.35592	-2.95886
C	4.95555	-2.76304	0.17480
H	5.54119	-1.84939	0.32263
H	4.90494	-3.30279	1.12661
H	5.52321	-3.39732	-0.51847
C	2.28610	-4.04844	-0.71656
H	2.89470	-4.79538	-1.24129
H	2.03393	-4.47551	0.26043
H	1.35877	-3.93994	-1.29102
C	1.71773	-2.42744	2.61911
H	2.42933	-3.21542	2.36048
H	1.66677	-2.36279	3.71053
H	0.73615	-2.73565	2.24834
C	3.58392	-0.72421	2.57800
H	4.30812	-1.50256	2.34304
H	3.94654	0.21701	2.14807
H	3.54350	-0.61743	3.66694

25E

Filename: TS_MeTMS_E_f.out

B3LYP/6-31g*: -699.00364256 Hartree
 ZPE: 724.652 kJ/mol
 DeltaG (excl. ZPE): -107.907 kJ/mol
 Low frequencies: -254.17 28.50 83.44

Cartesian coordinates:

C	0.00000	0.00000	0.00000
C	0.00000	0.00000	1.91296
N	1.30256	0.00000	2.32731
C	2.06352	-1.14874	1.94229
C	2.17498	-1.15801	0.29251
C	0.78661	-1.15055	-0.11707
H	0.46901	0.96901	-0.16850
H	-1.05140	-0.04490	-0.28071
H	-0.55787	-0.90577	2.13492
H	-0.55619	0.91460	2.10641
H	3.07528	-1.10045	2.34444
H	1.57900	-2.06904	2.27367
H	2.65631	-0.20024	0.05556
H	0.26936	-2.10754	-0.20778
C	2.01985	1.27907	2.44534
H	1.34012	2.03991	2.83136
H	2.84477	1.15975	3.15053
H	2.42241	1.61161	1.47897
Si	3.31022	-2.62737	-0.33570
C	3.66920	-2.27764	-2.14882
H	2.75566	-2.25286	-2.75415
H	4.19052	-1.32296	-2.28535
H	4.31469	-3.06207	-2.56222
C	4.88945	-2.59276	0.69174
H	5.38307	-1.61388	0.66217
H	4.72670	-2.86372	1.74141
H	5.60217	-3.32033	0.28441
C	2.36622	-4.24199	-0.09988
H	3.00298	-5.08106	-0.40618
H	2.08475	-4.42451	0.94428
H	1.45861	-4.29570	-0.71275

25F

Filename: TS_MeTMS_E_eqMe_f.out

B3LYP/6-31g*: -738.31690995 Hartree
 ZPE: 799.198 kJ/mol
 DeltaG (excl. ZPE): -109.781 kJ/mol
 Low frequencies: -277.12 45.28 71.06

Cartesian coordinates:

C	0.00000	0.00000	0.00000
C	0.00000	0.00000	1.91538
N	1.29974	0.00000	2.33086
C	2.05394	-1.18547	1.99216
C	2.15276	-1.20347	0.32114
C	0.76545	-1.16410	-0.09310
H	0.48797	0.95993	-0.16527
H	-1.05011	-0.02747	-0.28731
H	-0.56356	-0.90026	2.14482
H	-0.55371	0.91915	2.09247
H	1.46154	-2.05750	2.27889
H	2.65637	-0.25722	0.08337
H	0.22685	-2.10966	-0.18440
C	2.00808	1.28499	2.43508
H	2.71043	1.25122	3.26976
H	2.56159	1.52089	1.51681
H	1.28268	2.07645	2.62727
Si	3.16732	-2.70044	-0.45146
C	2.69585	-2.75451	-2.27560

H	1.63169	-2.96609	-2.43253
H	2.93038	-1.81207	-2.78448
H	3.26127	-3.54533	-2.78340
C	5.01127	-2.34972	-0.29139
H	5.27474	-1.37002	-0.70763
H	5.38658	-2.39353	0.73532
H	5.56348	-3.10079	-0.87004
C	2.64816	-4.28842	0.42495
H	3.15696	-5.14121	-0.04102
H	2.91200	-4.30248	1.48869
H	1.57143	-4.48098	0.34184
C	3.42601	-1.25588	2.65435
H	3.86077	-2.24439	2.49904
H	4.12285	-0.51268	2.25795
H	3.32412	-1.10650	3.73424

25G

Filename: TS_MeTMS_E_axMe_f.out

B3LYP/6-31g*: -738.31716589 Hartree

ZPE: 798.839 kJ/mol

DeltaG (excl. ZPE): -109.981 kJ/mol

Low frequencies: -278.87 50.70 82.36

Cartesian coordinates:

C	0.00000	0.00000	0.00000
C	0.00000	0.00000	1.92226
N	1.30151	0.00000	2.33411
C	2.09572	-1.14773	1.97059
C	2.19392	-1.10444	0.30062
C	0.81333	-1.12982	-0.13144
H	0.45004	0.98118	-0.14878
H	-1.04828	-0.06113	-0.28901
H	-0.56780	-0.89881	2.13713
H	-0.54993	0.91857	2.11243
H	3.11646	-0.97569	2.31675
H	2.62620	-0.11254	0.11334
H	0.32523	-2.09389	-0.27766
C	2.00372	1.28624	2.46417
H	1.30550	2.04676	2.81643
H	2.80467	1.18273	3.19903
H	2.43765	1.61157	1.50886
Si	3.42669	-2.41997	-0.47060
C	3.97385	-1.67337	-2.11044
H	3.13094	-1.51192	-2.79242
H	4.48614	-0.71369	-1.97390
H	4.67725	-2.34767	-2.61387
C	4.89876	-2.59904	0.69437
H	5.38881	-1.63743	0.88957
H	4.64487	-3.05418	1.65841
H	5.64940	-3.24729	0.22563
C	2.53313	-4.05800	-0.73853
H	3.23968	-4.78597	-1.15610
H	2.13128	-4.49585	0.18175
H	1.71153	-3.96679	-1.45902
C	1.58104	-2.47394	2.52914
H	2.29372	-3.27097	2.30616
H	1.48792	-2.40168	3.61726
H	0.61327	-2.77475	2.11923

25H

Filename: TS_MeTMS_E_MeMe_f.out

B3LYP/6-31g*: -777.62578300 Hartree

ZPE: 873.665 kJ/mol

DeltaG (excl. ZPE): -112.559 kJ/mol

Low frequencies: -299.74 22.13 73.34

Cartesian coordinates:

C	0.00000	0.00000	0.00000
C	0.00000	0.00000	1.93029
N	1.30155	0.00000	2.33287
C	2.09474	-1.18798	2.02690
C	2.14591	-1.21447	0.33040
C	0.75800	-1.16692	-0.08812
H	0.49291	0.95977	-0.15009
H	-1.04927	-0.01999	-0.29089
H	-0.58029	-0.88653	2.15633
H	-0.54227	0.92720	2.09693
H	2.63770	-0.25969	0.10168
H	0.21743	-2.10572	-0.20934
C	1.97689	1.30671	2.42222
H	1.22677	2.08180	2.58264
H	2.66418	1.31442	3.26898
H	2.53860	1.53814	1.50814
Si	3.14515	-2.62943	-0.61423
C	3.43749	-1.88630	-2.32229
H	2.50048	-1.63211	-2.83145
H	4.05014	-0.97796	-2.27384
H	3.97158	-2.60307	-2.95767
C	4.80606	-3.04751	0.17473
H	5.42520	-2.16615	0.37287
H	4.72029	-3.62654	1.10055
H	5.35840	-3.67278	-0.53870
C	2.07843	-4.18234	-0.73221
H	2.65159	-4.95994	-1.25233
H	1.79772	-4.59466	0.24346
H	1.16179	-4.02772	-1.31317
C	1.45231	-2.46961	2.57890
H	2.10065	-3.32210	2.36296
H	1.34990	-2.39197	3.66631
H	0.47080	-2.69562	2.15609
C	3.51815	-1.05223	2.57709
H	4.06244	-1.98252	2.42472
H	4.08637	-0.25032	2.09961
H	3.48221	-0.86370	3.65562

26A

Filename: int_TMS_E_f.out

B3LYP/6-31g*: -659.69739959 Hartree

ZPE: 648.482 kJ/mol

DeltaG (excl. ZPE): -108.148 kJ/mol

Low frequencies: 34.45 78.79 89.80

Cartesian coordinates:

C	-0.64572	-3.01369	4.42434
C	0.54818	0.66100	2.02840
N	0.75955	-0.47358	2.57420
C	1.53869	-1.62491	2.03305
C	0.77248	-2.92416	2.33037
C	0.54890	-3.04923	3.81707
H	-1.57353	-2.91716	3.86121
H	-0.74009	-3.13557	5.49973
H	1.00415	0.89181	1.06783
H	-0.08588	1.39159	2.52467
H	0.31156	-0.69761	3.47625
H	1.69927	-1.44043	0.96858
H	2.50565	-1.60540	2.55003
H	-0.20001	-2.87214	1.81894
H	1.44498	-3.17485	4.42784

Si	1.67496	-4.49262	1.58162
C	0.51582	-5.94710	1.86249
H	0.31198	-6.10884	2.92729
H	-0.44542	-5.80257	1.35539
H	0.95986	-6.86761	1.46752
C	1.94108	-4.16726	-0.25948
H	1.00183	-3.94133	-0.77896
H	2.64438	-3.34792	-0.45300
H	2.36285	-5.06150	-0.73536
C	3.32421	-4.71671	2.47066
H	3.83490	-5.60491	2.07809
H	4.00588	-3.87023	2.32405
H	3.20142	-4.87104	3.54896

26B

Filename: int_TMS_E_eqMe_f.out

B3LYP/6-31g*: -699.01263830 Hartree

ZPE: 723.016 kJ/mol

DeltaG (excl. ZPE): -110.426 kJ/mol

Low frequencies: 42.60 58.32 106.06

Cartesian coordinates:

C	-0.91195	-3.05557	4.08892
C	0.52118	0.69298	2.26707
N	0.74127	-0.49035	2.69287
C	1.61627	-1.57501	2.11693
C	0.77995	-2.87893	2.20727
C	0.35018	-3.09397	3.63952
H	-1.75393	-2.88230	3.42031
H	-1.15016	-3.25017	5.13089
H	1.04216	1.06714	1.39149
H	-0.19280	1.32578	2.78795
H	0.21323	-0.83388	3.51025
H	2.44855	-1.64117	2.83047
H	-0.11329	-2.75150	1.57746
H	1.15142	-3.29683	4.35399
Si	1.68059	-4.49981	1.54692
C	0.70495	-5.95842	2.22747
H	0.75319	-6.02313	3.31938
H	-0.35256	-5.90930	1.94301
H	1.11009	-6.89334	1.82181
C	1.62410	-4.53962	-0.33966
H	0.59854	-4.43408	-0.71341
H	2.24008	-3.77722	-0.82733
H	1.99055	-5.51465	-0.68419
C	3.45438	-4.50770	2.19777
H	3.94767	-5.44158	1.90191
H	4.06795	-3.68825	1.80418
H	3.49385	-4.46238	3.29293
C	2.14397	-1.18067	0.74504
H	2.83322	-1.95188	0.39808
H	1.33771	-1.09529	0.00811
H	2.71204	-0.24432	0.77361

26C

Filename: int_TMS_E_axMe_f.out

B3LYP/6-31g*: -699.01328886 Hartree

ZPE: 722.849 kJ/mol

DeltaG (excl. ZPE): -111.265 kJ/mol

Low frequencies: 43.64 62.30 86.91

Cartesian coordinates:

C	5.08785	-1.08810	2.58759
C	0.91671	0.08034	3.84002

N	1.77666	-0.26164	2.96095
C	1.61873	-1.26223	1.84863
C	2.90017	-2.12947	1.87275
C	4.13937	-1.29473	1.66294
H	5.03243	-1.53827	3.57781
H	5.97794	-0.50478	2.36876
H	-0.08195	-0.34949	3.81194
H	1.18292	0.79536	4.61447
H	2.72838	0.13132	3.00021
H	2.95301	-2.57701	2.87705
H	4.26933	-0.84646	0.67801
Si	2.86071	-3.69686	0.69139
C	4.08047	-4.90970	1.45439
H	5.07933	-4.46990	1.55343
H	3.75830	-5.24282	2.44808
H	4.17564	-5.80231	0.82488
C	1.10623	-4.40018	0.70652
H	0.76361	-4.63840	1.72103
H	0.36866	-3.73250	0.24479
H	1.08401	-5.33682	0.13621
C	3.39045	-3.22513	-1.05653
H	3.39944	-4.12415	-1.68498
H	2.72156	-2.50446	-1.54049
H	4.40468	-2.81033	-1.07701
C	1.33524	-0.48693	0.55614
H	1.20063	-1.19745	-0.26313
H	0.41882	0.10436	0.64648
H	2.15710	0.18407	0.29064
H	0.74752	-1.86574	2.12005

26D

Filename: int_TMS_E_MeMe_f.out

B3LYP/6-31g*: -738.32491929 Hartree

ZPE: 796.751 kJ/mol

DeltaG (excl. ZPE): -113.778 kJ/mol

Low frequencies: 17.54 72.60 107.96

Cartesian coordinates:

C	4.05138	0.22033	3.73591
C	1.14406	0.64154	2.86684
N	0.94110	-0.62794	2.92426
C	1.60275	-1.68894	2.07638
C	3.01250	-1.86348	2.76477
C	3.81008	-0.59674	2.69606
H	3.70211	-0.01286	4.74051
H	4.66495	1.11109	3.63059
H	1.63736	1.07512	2.00754
H	0.75502	1.28515	3.65019
H	0.45699	-0.98957	3.74725
H	2.80878	-2.08546	3.82446
H	4.22149	-0.32320	1.72382
Si	4.16953	-3.37843	2.23449
C	5.72538	-3.15194	3.27302
H	6.27691	-2.24316	3.01136
H	5.49751	-3.10688	4.34472
H	6.39732	-4.00483	3.11879
C	3.36946	-5.02779	2.69020
H	2.96475	-5.02977	3.70911
H	2.57319	-5.34093	2.00745
H	4.14347	-5.80469	2.65387
C	4.58349	-3.31698	0.39364
H	5.38356	-4.03991	0.19078
H	3.73932	-3.59220	-0.24874
H	4.95206	-2.33624	0.07151

C	0.70825	-2.92751	2.20532
H	1.09304	-3.73096	1.57635
H	0.67584	-3.30128	3.23555
H	-0.31208	-2.70623	1.87438
C	1.66011	-1.21652	0.61945
H	2.08302	-2.01465	0.00633
H	0.65456	-1.00049	0.24427
H	2.28802	-0.33420	0.47147

26E

Filename: int_MeTMS_E_f.out

B3LYP/6-31g*: -699.01606534 Hartree

ZPE: 722.928 kJ/mol

DeltaG (excl. ZPE): -112.681 kJ/mol

Low frequencies: 31.64 62.50 83.05

Cartesian coordinates:

C	0.00000	0.00000	0.00000
C	0.00000	0.00000	3.34733
N	1.28491	0.00000	3.31292
C	2.03330	-1.12242	2.67391
C	2.04951	-0.93472	1.13910
C	0.66160	-1.01257	0.57986
H	0.44927	0.98419	-0.11982
H	-0.99354	-0.13446	-0.41878
H	-0.54620	-0.88821	3.05380
H	-0.53623	0.87620	3.69887
H	3.03670	-1.11703	3.10326
H	1.53466	-2.05272	2.95881
H	2.47796	0.05372	0.91602
H	0.16723	-1.98393	0.65300
C	2.07888	1.17169	3.73235
H	1.41620	1.98453	4.03012
H	2.71273	0.87746	4.57307
H	2.70851	1.48864	2.89776
Si	3.26393	-2.21410	0.27992
C	3.32785	-1.73871	-1.53795
H	2.34051	-1.79590	-2.00890
H	3.70816	-0.71989	-1.67771
H	3.99592	-2.41487	-2.08443
C	4.95536	-2.02060	1.09733
H	5.31876	-0.98659	1.05578
H	4.96801	-2.34592	2.14466
H	5.69085	-2.63827	0.56771
C	2.58632	-3.95656	0.53181
H	3.25616	-4.68426	0.05781
H	2.51312	-4.23626	1.59002
H	1.59812	-4.08854	0.07626

26F

Filename: int_MeTMS_E_eqMe_f.out

B3LYP/6-31g*: -738.32655655 Hartree

ZPE: 796.759 kJ/mol

DeltaG (excl. ZPE): -115.914 kJ/mol

Low frequencies: 28.00 54.17 79.40

Cartesian coordinates:

C	4.22233	0.24114	3.75134
C	0.89117	-0.03138	4.04765
N	0.71314	-0.55445	2.89349
C	1.49941	-1.77922	2.42182
C	2.94154	-1.79333	2.96035
C	3.61326	-0.45782	2.78648
H	4.27973	-0.12162	4.77672

H	4.72560	1.18042	3.54190
H	1.60251	-0.47119	4.73482
H	0.31906	0.84323	4.34342
H	1.51697	-1.64521	1.33527
H	2.93214	-2.06506	4.02708
H	3.60934	-0.05094	1.77245
Si	4.05958	-3.18996	2.11521
C	5.85510	-2.72244	2.42594
H	6.14029	-1.79263	1.92414
H	6.06396	-2.59991	3.49505
H	6.51018	-3.51899	2.05274
C	3.71635	-4.86246	2.92331
H	3.82843	-4.81499	4.01320
H	2.72752	-5.27847	2.70521
H	4.45494	-5.58683	2.55785
C	3.67698	-3.22042	0.26479
H	4.34765	-3.92967	-0.23515
H	2.65292	-3.54194	0.03879
H	3.83907	-2.24392	-0.20787
C	0.66072	-3.01503	2.77105
H	1.07304	-3.89007	2.26583
H	0.67264	-3.20507	3.84917
H	-0.37931	-2.90833	2.44682
C	-0.22708	0.02707	1.91587
H	0.34999	0.44461	1.08615
H	-0.87891	-0.76427	1.53920
H	-0.82445	0.80766	2.38796

26G

Filename: int_MeTMS_E_axMe_f.out

B3LYP/6-31g*: -738.33000711 Hartree

ZPE: 797.496 kJ/mol

DeltaG (excl. ZPE): -114.816 kJ/mol

Low frequencies: 42.79 61.00 77.45

Cartesian coordinates:

C	0.83652	1.64331	-0.17931
C	0.25483	0.13403	2.70233
N	1.49865	-0.17817	2.78015
C	2.17243	-1.04733	1.74130
C	2.47929	-0.13454	0.51630
C	1.23732	0.36264	-0.15915
H	1.41220	2.43178	0.30247
H	-0.05256	1.95390	-0.72132
H	-0.38038	-0.34158	1.96745
H	-0.16820	0.85474	3.39562
H	3.03152	0.73564	0.90300
H	0.63400	-0.37526	-0.68875
Si	3.74665	-0.91190	-0.76766
C	4.50936	0.56350	-1.65325
H	3.74529	1.18304	-2.13621
H	5.07803	1.20295	-0.96765
H	5.20087	0.22532	-2.43394
C	5.05510	-1.86411	0.20899
H	5.55062	-1.23725	0.96065
H	4.65628	-2.75191	0.71460
H	5.83674	-2.21562	-0.47548
C	2.85475	-2.03893	-1.98908
H	3.58069	-2.43624	-2.70908
H	2.36856	-2.90045	-1.51760
H	2.09635	-1.49677	-2.56533
C	1.35709	-2.31030	1.46208
H	1.96004	-2.98864	0.85342
H	1.10689	-2.83023	2.39220

H	0.43446	-2.11380	0.90920
H	3.11509	-1.33619	2.21207
C	2.38287	0.42576	3.79576
H	2.77136	-0.37125	4.43539
H	3.21544	0.92141	3.29100
H	1.82747	1.14808	4.39478

26H

Filename: int_MeTMS_E_MeMe_f.out

B3LYP/6-31g*: -777.63322162 Hartree

ZPE: 872.029 kJ/mol

DeltaG (excl. ZPE): -116.334 kJ/mol

Low frequencies: 38.76 53.15 66.31

Cartesian coordinates:

C	5.09025	-1.60324	2.70887
C	1.71125	-0.22720	4.10347
N	1.91130	-0.03072	2.85541
C	1.59405	-1.15191	1.79730
C	2.76968	-2.17064	1.88622
C	4.13533	-1.53845	1.77397
H	4.93314	-2.11568	3.65652
H	6.07562	-1.17545	2.54667
H	1.26547	-1.15306	4.44713
H	1.98801	0.53280	4.82822
H	2.69797	-2.63368	2.88212
H	4.36763	-1.04119	0.83149
Si	2.78409	-3.72489	0.66090
C	3.83487	-4.99935	1.56695
H	4.82625	-4.60980	1.82042
H	3.35557	-5.33873	2.49317
H	3.97886	-5.88243	0.93302
C	1.07495	-4.46442	0.32592
H	0.53361	-4.73486	1.23913
H	0.42697	-3.82521	-0.28504
H	1.22326	-5.39174	-0.24233
C	3.57960	-3.23954	-0.98126
H	3.61103	-4.11976	-1.63506
H	3.02562	-2.46210	-1.52014
H	4.61169	-2.89498	-0.85624
C	0.24571	-1.77296	2.19805
H	-0.11056	-2.40008	1.38110
H	0.31495	-2.41673	3.08036
H	-0.50863	-0.99942	2.37564
C	1.45223	-0.48785	0.42145
H	1.18328	-1.26516	-0.29740
H	0.64803	0.25508	0.40877
H	2.37378	-0.02274	0.06535
C	2.54551	1.23022	2.41362
H	3.49084	0.98674	1.92723
H	1.88425	1.74233	1.71437
H	2.73078	1.86293	3.28225

27A

Filename: reac_TMS_eqMeeqMe.out

B3LYP/6-31g*: -738.34950610 Hartree

ZPE: 798.094 kJ/mol

DeltaG (excl. ZPE): -118.561 kJ/mol

Low frequencies: 24.19 47.83 61.16

Cartesian coordinates:

C	0.06239	0.01048	0.01148
H	0.07209	0.10419	1.10208
C	1.51751	-0.05958	-0.51675

H	1.93315	-1.00962	-0.15722
H	2.10245	0.74125	-0.05385
C	1.60103	0.01528	-2.02357
C	2.14384	1.01973	-2.73801
H	2.10095	0.87736	-3.82189
H	1.17621	-0.84137	-2.55111
N	-0.53795	1.27583	-0.50794
C	-1.33213	2.07196	0.11303
H	-1.59331	1.79631	1.13540
Si	3.10966	2.57827	-2.19717
C	3.59280	3.47493	-3.78143
H	4.22952	2.84920	-4.41781
H	2.71434	3.76247	-4.37177
H	4.15270	4.39040	-3.55759
C	2.00796	3.72067	-1.14880
H	1.10227	4.02353	-1.69051
H	1.71311	3.27396	-0.19112
H	2.55675	4.64047	-0.91284
C	4.63739	2.08142	-1.20613
H	5.23007	2.96859	-0.95207
H	4.39034	1.57263	-0.26708
H	5.28095	1.41007	-1.78588
H	-0.24260	1.50083	-1.46770
C	-1.89809	3.31023	-0.46942
H	-2.99397	3.26185	-0.42236
H	-1.59990	4.16753	0.14850
H	-1.58135	3.47771	-1.50143
C	-0.82135	-1.17253	-0.40249
H	-0.91993	-1.24756	-1.48936
H	-0.36901	-2.09929	-0.03658
H	-1.82272	-1.08765	0.03129

27B

Filename: reac_TMS_eqMeaxMe.out

B3LYP/6-31g*: -738.34951830 Hartree

ZPE: 798.073 kJ/mol

DeltaG (excl. ZPE): -118.700 kJ/mol

Low frequencies: 23.66 47.39 60.72

Cartesian coordinates:

C	0.05944	-0.01152	0.01182
H	0.06707	-0.10671	1.10229
C	1.51548	0.05829	-0.51448
H	2.09939	-0.74307	-0.05122
H	1.93120	1.00793	-0.15386
C	1.60139	-0.01592	-2.02133
C	2.14700	-1.01868	-2.73590
H	2.10502	-0.87465	-3.81956
H	1.17729	0.84101	-2.54884
N	-0.54116	-1.27567	-0.51014
C	-1.33629	-2.07224	0.10868
H	-1.59887	-1.79764	1.13092
Si	3.11258	-2.57789	-2.19606
C	3.58813	-3.47806	-3.78031
H	2.70722	-3.76706	-4.36624
H	4.22234	-2.85410	-4.42094
H	4.14892	-4.39308	-3.55660
C	4.64529	-2.08133	-1.21260
H	5.28814	-1.41341	-1.79707
H	4.40281	-1.56862	-0.27449
H	5.23713	-2.96887	-0.95768
C	2.01369	-3.71679	-1.14117
H	2.56163	-4.63732	-0.90609
H	1.72380	-3.26793	-0.18300

H	1.10510	-4.01858	-1.67854
H	-0.24512	-1.49961	-1.46980
C	-1.90175	-3.30961	-0.47557
H	-1.60485	-4.16754	0.14217
H	-2.99771	-3.26083	-0.42988
H	-1.58372	-3.47640	-1.50724
C	-0.82381	1.17218	-0.40097
H	-0.92161	1.24894	-1.48769
H	-1.82539	1.08651	0.03209
H	-0.37153	2.09829	-0.03322

27C

Filename: reac_TMS_axMeeqMe_f.out

B3LYP/6-31g*: -738.34742804 Hartree

ZPE: 798.968 kJ/mol

DeltaG (excl. ZPE): -118.600 kJ/mol

Low frequencies: 24.64 43.45 58.47

Cartesian coordinates:

C	0.00000	0.00000	0.00000
H	0.00000	0.00000	1.09274
C	1.46706	0.00000	-0.50848
H	1.88656	-0.98119	-0.25435
H	2.03548	0.74802	0.05274
C	1.56992	0.25106	-1.99456
C	2.04280	1.37056	-2.57723
H	2.01998	1.35112	-3.67092
H	1.21059	-0.56446	-2.62557
N	-0.60213	1.29395	-0.43800
C	-1.49396	2.02449	0.13315
Si	2.89969	2.92120	-1.85461
C	4.55337	2.41586	-1.10025
H	4.43427	1.72288	-0.25907
H	5.19266	1.92587	-1.84316
H	5.09182	3.29634	-0.72933
C	3.13274	4.11186	-3.29465
H	3.73971	3.66672	-4.09157
H	2.17484	4.41287	-3.73589
H	3.64344	5.02446	-2.96555
C	1.82359	3.76613	-0.53267
H	2.32867	4.67810	-0.19173
H	0.84970	4.07984	-0.93162
H	1.65652	3.14722	0.35709
H	-0.19976	1.61947	-1.32825
C	-2.18039	1.73401	1.41255
H	-3.26492	1.74274	1.23991
H	-1.89383	0.78612	1.86769
H	-1.97978	2.55532	2.11407
H	-1.75335	2.94479	-0.38960
C	-0.85134	-1.16369	-0.52407
H	-0.91569	-1.15950	-1.61584
H	-0.39296	-2.10708	-0.21185
H	-1.86711	-1.12840	-0.11803

27D

Filename: reac_TMS_axMeaxMe_f.out

B3LYP/6-31g*: -738.34743508 Hartree

ZPE: 798.956 kJ/mol

DeltaG (excl. ZPE): -118.517 kJ/mol

Low frequencies: 25.08 43.69 58.69

Cartesian coordinates:

C	0.00000	0.00000	0.00000
H	0.00000	0.00000	1.09277

C	1.46758	0.00000	-0.50751
H	2.03629	-0.74672	0.05517
H	1.88630	0.98181	-0.25421
C	1.57224	-0.25337	-1.99311
C	2.04612	-1.37362	-2.57378
H	2.02354	-1.35653	-3.66748
H	1.21367	0.56110	-2.62585
N	-0.60245	-1.29394	-0.43764
C	-1.49588	-2.02272	0.13346
Si	2.90302	-2.92267	-1.84740
C	3.13835	-4.11550	-3.28532
H	2.18104	-4.41463	-3.72919
H	3.74861	-3.67215	-4.08078
H	3.64603	-5.02898	-2.95411
C	4.55570	-2.41755	-1.09042
H	5.19668	-1.92980	-1.83342
H	4.43656	-1.72285	-0.25067
H	5.09256	-3.29793	-0.71699
C	1.82421	-3.76569	-0.52605
H	2.32694	-4.67923	-0.18579
H	1.65896	-3.14716	0.36430
H	0.84953	-4.07663	-0.92540
H	-0.19892	-1.62156	-1.32653
C	-2.18487	-1.72883	1.41079
H	-1.99323	-2.55271	2.11179
H	-1.89358	-0.78357	1.86826
H	-3.26885	-1.72986	1.23382
H	-1.75525	-2.94399	-0.38772
C	-0.85060	1.16423	-0.52420
H	-0.91464	1.15998	-1.61597
H	-1.86665	1.12975	-0.11875
H	-0.39199	2.10741	-0.21174

27E

Filename: reac_MeTMS_eqMeeqMe_f.out

B3LYP/6-31g*: -777.65968429 Hartree

ZPE: 872.556 kJ/mol

DeltaG (excl. ZPE): -124.616 kJ/mol

Low frequencies: 18.52 38.99 56.75

Cartesian coordinates:

C	0.10503	0.38455	0.64621
H	-0.28137	1.09988	1.37897
C	-0.95992	0.18972	-0.46334
H	-0.65769	-0.61324	-1.14110
H	-0.94720	1.11858	-1.05033
C	-2.33943	-0.03881	0.09624
C	-3.12542	-1.11865	-0.06055
H	-4.09390	-1.03776	0.44533
H	-2.71520	0.80249	0.68719
N	0.25651	-0.90720	1.41534
C	-0.47439	-1.10741	2.46211
H	-1.11548	-0.27490	2.74246
Si	-2.99555	-2.74158	-1.04343
C	-4.62834	-2.91919	-1.96751
H	-5.48554	-2.89759	-1.28457
H	-4.76569	-2.11437	-2.69880
H	-4.66405	-3.87075	-2.51136
C	-1.55998	-2.80454	-2.27722
H	-1.56593	-1.95411	-2.96856
H	-0.57271	-2.85420	-1.80137
H	-1.65819	-3.71197	-2.88606
C	-2.79952	-4.14760	0.21287
H	-2.84248	-5.12114	-0.29025

H	-1.83836	-4.10045	0.74148
H	-3.59816	-4.13481	0.96419
C	1.16915	-1.92168	0.84844
H	0.92606	-2.91128	1.22685
H	1.05664	-1.92112	-0.23587
H	2.19963	-1.66430	1.10434
C	-0.53571	-2.31518	3.32258
H	-0.48291	-1.99971	4.37141
H	-1.52102	-2.78367	3.19009
H	0.23931	-3.05690	3.13392
C	1.45090	0.89390	0.13094
H	1.85531	0.27426	-0.67478
H	1.29987	1.89857	-0.27443
H	2.19266	0.96766	0.93261

27F

Filename: reac_MeTMS_eqMeaxMe_f.out

B3LYP/6-31g*: -777.65830279 Hartree

ZPE: 872.439 kJ/mol

DeltaG (excl. ZPE): -124.392 kJ/mol

Low frequencies: 17.04 47.93 60.17

Cartesian coordinates:

C	0.18180	0.23506	0.75066
H	1.20412	0.22097	0.36420
C	-0.78370	0.02848	-0.44963
H	-0.51287	-0.89697	-0.96857
H	-0.56354	0.85163	-1.14407
C	-2.24867	0.03613	-0.09961
C	-3.13293	-0.95101	-0.33635
H	-4.15745	-0.72153	-0.02814
H	-2.60625	0.96510	0.35125
N	0.12192	-0.97244	1.66038
C	-0.87475	-1.14235	2.46449
H	-1.61040	-0.34453	2.46357
Si	-2.95232	-2.62523	-1.23589
C	-4.66892	-3.40139	-1.25149
H	-5.05446	-3.56151	-0.23728
H	-5.38959	-2.76975	-1.78412
H	-4.65354	-4.37540	-1.75438
C	-2.32457	-2.35627	-2.99671
H	-2.99003	-1.68721	-3.55402
H	-1.31783	-1.92351	-3.03076
H	-2.28907	-3.31023	-3.53689
C	-1.75854	-3.76797	-0.29826
H	-1.72364	-4.74920	-0.78696
H	-0.73053	-3.38557	-0.28025
H	-2.08361	-3.93689	0.73577
C	1.23721	-1.92344	1.49046
H	1.05337	-2.85280	2.02258
H	1.34948	-2.13414	0.42460
H	2.15253	-1.45485	1.86289
C	-1.13013	-2.27247	3.39177
H	-1.20539	-1.87189	4.41168
H	-2.11585	-2.69351	3.15633
H	-0.38799	-3.06896	3.37586
C	-0.01419	1.54140	1.52254
H	-1.02596	1.66405	1.91830
H	0.69788	1.62044	2.34999
H	0.16930	2.37657	0.83993

27G

Filename: reac_MeTMS_axMeeqMe_f.out

B3LYP/6-31g*: -777.65395986 Hartree
 ZPE: 873.276 kJ/mol
 DeltaG (excl. ZPE): -122.061 kJ/mol
 Low frequencies: 27.23 36.44 57.52

Cartesian coordinates:

C	-0.18101	0.29127	1.14280
H	-0.81500	1.16076	1.33655
C	-0.12021	0.09621	-0.39060
H	0.40833	-0.82542	-0.64454
H	0.49829	0.92621	-0.76152
C	-1.48014	0.14944	-1.04244
C	-2.06465	-0.79261	-1.80067
H	-3.05824	-0.51502	-2.16662
H	-2.01164	1.08970	-0.86504
N	-0.95405	-0.83719	1.80512
C	-0.54757	-2.05007	1.97511
Si	-1.51012	-2.49516	-2.44269
C	-2.17081	-3.82699	-1.26321
H	-1.73769	-3.74589	-0.25717
H	-3.26036	-3.76791	-1.15862
H	-1.93149	-4.82872	-1.64022
C	-2.30427	-2.69401	-4.13938
H	-3.39603	-2.60744	-4.08812
H	-1.94368	-1.93506	-4.84335
H	-2.07141	-3.67688	-4.56601
C	0.37038	-2.66644	-2.60207
H	0.60085	-3.56763	-3.18358
H	0.81333	-1.81703	-3.13468
H	0.89036	-2.77132	-1.64212
C	-2.31514	-0.45265	2.24661
H	-2.81712	-1.30492	2.70543
H	-2.23505	0.36637	2.96554
H	-2.87152	-0.12171	1.36659
C	0.74680	-2.66640	1.59143
H	0.53874	-3.63946	1.13130
H	1.35747	-2.07116	0.91854
H	1.31729	-2.87646	2.50779
H	-1.25554	-2.70666	2.47908
C	1.16864	0.55356	1.81979
H	1.93672	-0.17741	1.55945
H	1.52550	1.53290	1.48700
H	1.07002	0.58957	2.90945

27H

Filename: reac_MeTMS_axMeaxMe_f.out

B3LYP/6-31g*: -777.65626284 Hartree
 ZPE: 873.950 kJ/mol
 DeltaG (excl. ZPE): -124.343 kJ/mol
 Low frequencies: 11.48 34.84 46.81

Cartesian coordinates:

C	-0.25399	0.35090	1.03886
H	0.81558	0.48791	1.19960
C	-0.47620	0.16567	-0.48748
H	0.10466	-0.69646	-0.82531
H	-0.01317	1.05377	-0.94280
C	-1.90516	0.06703	-0.96068
C	-2.45684	-0.93885	-1.66271
H	-3.50138	-0.76243	-1.94077
H	-2.51459	0.94683	-0.74196
N	-0.60298	-0.92077	1.78041
C	0.25970	-1.84270	2.05638
Si	-1.81570	-2.58467	-2.36862
C	-3.22336	-3.82510	-2.15795

H	-3.46436	-3.99978	-1.10226
H	-4.13932	-3.48212	-2.65318
H	-2.95663	-4.79306	-2.59881
C	-1.41623	-2.32447	-4.19372
H	-2.28872	-1.95397	-4.74386
H	-0.60460	-1.60119	-4.33325
H	-1.10781	-3.26778	-4.66058
C	-0.28213	-3.26278	-1.47158
H	-0.07742	-4.27682	-1.83635
H	0.62289	-2.67145	-1.65411
H	-0.44084	-3.34046	-0.38798
C	-2.02528	-1.11473	2.15083
H	-2.15950	-2.11630	2.56019
H	-2.30838	-0.36940	2.89567
H	-2.63084	-0.99379	1.25050
C	1.71104	-1.87599	1.74818
H	1.90378	-2.76475	1.13205
H	2.10131	-1.00015	1.23302
H	2.26423	-2.02744	2.68442
H	-0.13788	-2.71146	2.57936
C	-0.96849	1.55951	1.64823
H	-2.05054	1.53809	1.50136
H	-0.75588	1.65483	2.71782
H	-0.58676	2.45808	1.15402

28A

Filename: TS1_TMS_eqMeeqMe_f.out

B3LYP/6-31g*: -738.32659577 Hartree

ZPE: 799.717 kJ/mol

DeltaG (excl. ZPE): -107.618 kJ/mol

Low frequencies: -103.74 57.30 79.76

Cartesian coordinates:

C	0.00000	0.00000	0.00000
C	0.00000	0.00000	1.66261
N	1.35195	0.00000	2.11034
C	2.18881	-1.03971	1.70895
C	2.22741	-1.13109	-0.08426
C	0.85164	-1.10531	-0.39428
H	0.39480	0.98414	-0.26163
H	-1.03326	-0.09581	-0.33845
H	-0.48048	-0.93394	1.96575
H	1.72574	-2.00238	1.93136
H	2.66995	-2.10912	-0.30512
H	0.35984	-2.01773	-0.73833
H	1.78849	0.91795	2.14851
Si	3.38036	0.25143	-0.91066
C	5.13836	-0.41768	-0.87837
H	5.57755	-0.45230	0.12297
H	5.19620	-1.42325	-1.31097
H	5.77461	0.23269	-1.49169
C	2.77393	0.40916	-2.68655
H	2.79755	-0.55325	-3.21049
H	1.75239	0.80167	-2.74953
H	3.42277	1.09792	-3.24116
C	3.25276	1.92465	-0.03902
H	3.87093	2.63456	-0.60414
H	2.23925	2.34256	-0.03168
H	3.64023	1.92885	0.98574
C	3.60053	-0.99275	2.26832
H	4.21796	-1.77818	1.82701
H	4.08603	-0.02873	2.09806
H	3.55089	-1.16664	3.34857
C	-0.79455	1.20011	2.16791

H	-0.85944	1.17017	3.25970
H	-0.32246	2.14374	1.87084
H	-1.81008	1.18622	1.76406

28B

Filename: TS1_TMS_eqMeaxMe_f.out

B3LYP/6-31g*: -738.32312486 Hartree

ZPE: 800.207 kJ/mol

DeltaG (excl. ZPE): -107.589 kJ/mol

Low frequencies: -175.54 60.74 81.31

Cartesian coordinates:

C	0.00000	0.00000	0.00000
C	0.00000	0.00000	1.65237
N	1.36188	0.00000	2.09637
C	2.20785	-1.02771	1.70191
C	2.22666	-1.12423	-0.12293
C	0.85054	-1.10712	-0.41112
H	0.40044	0.97817	-0.27474
H	-1.03267	-0.08878	-0.34215
H	-0.44976	0.95394	1.93860
H	1.76954	-2.00203	1.91203
H	2.67830	-2.09680	-0.34910
H	0.36080	-2.01666	-0.76409
H	1.79735	0.91690	2.13622
Si	3.35968	0.28200	-0.93703
C	5.12445	-0.36933	-0.92758
H	5.57502	-0.40536	0.06866
H	5.18854	-1.37121	-1.36771
H	5.74699	0.29206	-1.54323
C	2.73530	0.45495	-2.70522
H	2.76856	-0.49992	-3.24220
H	1.70736	0.83243	-2.75339
H	3.36865	1.16100	-3.25598
C	3.22259	1.94455	-0.04605
H	3.81744	2.66919	-0.61747
H	2.20330	2.34705	-0.01390
H	3.63175	1.94665	0.97016
C	3.62552	-0.95715	2.23830
H	4.25045	-1.72815	1.78245
H	4.09115	0.01695	2.07099
H	3.59443	-1.14184	3.31779
C	-0.84256	-1.15126	2.20455
H	-0.85151	-1.10955	3.29781
H	-1.87379	-1.06334	1.85052
H	-0.46893	-2.13412	1.90040

28C

Filename: TS1_TMS_axMeeqMe_f.out

B3LYP/6-31g*: -738.32641067 Hartree

ZPE: 799.872 kJ/mol

DeltaG (excl. ZPE): -109.489 kJ/mol

Low frequencies: -256.55 35.76 67.56

Cartesian coordinates:

C	0.00000	0.00000	0.00000
C	0.00000	0.00000	1.63670
N	1.37319	0.00000	2.05475
C	2.20990	-1.04048	1.71963
C	2.16485	-1.25320	-0.19039
C	0.79059	-1.15719	-0.40904
H	0.43671	0.95997	-0.28735
H	-1.03823	-0.04951	-0.33579
H	-0.48239	-0.92336	1.96302

H	3.25329	-0.76845	1.87276
H	2.53586	-2.26606	-0.37819
H	0.23358	-2.05345	-0.68897
H	1.80578	0.91870	2.00598
Si	3.51163	-0.00303	-0.87135
C	5.15222	-0.87231	-0.56508
H	5.35948	-1.04053	0.49854
H	5.19189	-1.84356	-1.07195
H	5.97609	-0.26651	-0.96101
C	3.15217	0.19563	-2.70644
H	3.13921	-0.77092	-3.22264
H	2.18828	0.68576	-2.88571
H	3.92821	0.80995	-3.17891
C	3.46296	1.66741	0.01126
H	4.20341	2.32144	-0.46671
H	2.49958	2.18420	-0.07020
H	3.74925	1.61094	1.06907
C	1.89288	-2.42695	2.25425
H	2.57278	-3.16880	1.82898
H	2.04232	-2.41666	3.34048
H	0.86772	-2.74236	2.04867
C	-0.76663	1.20793	2.16687
H	-0.80587	1.17888	3.25966
H	-0.29341	2.14739	1.85826
H	-1.79150	1.20388	1.78669

28D

Filename: TS1_TMS_axMexaMe_f.out

B3LYP/6-31g*: -738.31932387 Hartree

ZPE: 800.654 kJ/mol

DeltaG (excl. ZPE): -109.245 kJ/mol

Low frequencies: -267.85 38.48 74.18

Cartesian coordinates:

C	0.00000	0.00000	0.00000
C	0.00000	0.00000	1.63063
N	1.38330	0.00000	2.04924
C	2.29232	-0.96612	1.68231
C	2.19568	-1.18226	-0.25029
C	0.81644	-1.13584	-0.43005
H	0.41926	0.96426	-0.29690
H	-1.03752	-0.06742	-0.33536
H	-0.40984	0.96994	1.92458
H	3.30684	-0.58603	1.79510
H	2.60325	-2.17772	-0.45389
H	0.28649	-2.04616	-0.71522
H	1.78025	0.93440	2.03553
Si	3.47700	0.13524	-0.93334
C	5.16235	-0.65061	-0.64440
H	5.39070	-0.80726	0.41665
H	5.24615	-1.61865	-1.15198
H	5.94951	-0.00352	-1.04974
C	3.09293	0.31943	-2.76489
H	3.12705	-0.64517	-3.28371
H	2.10311	0.75838	-2.93488
H	3.83202	0.97515	-3.24099
C	3.35113	1.79778	-0.04388
H	4.05148	2.49118	-0.52675
H	2.36165	2.26445	-0.11199
H	3.65127	1.75288	1.01065
C	2.18512	-2.39136	2.19684
H	2.99386	-2.99738	1.78080
H	2.31179	-2.36794	3.28597
H	1.23676	-2.87623	1.96915

C	-0.89550	-1.09775	2.20988
H	-0.79540	-1.13033	3.29854
H	-1.93904	-0.86880	1.97294
H	-0.67745	-2.09061	1.81026

28E

Filename: TS1_MeTMS_eqMeeqMe_f.out

B3LYP/6-31g*: -777.62918325 Hartree

ZPE: 874.987 kJ/mol

DeltaG (excl. ZPE): -112.149 kJ/mol

Low frequencies: -248.24 34.72 78.44

Cartesian coordinates:

C	0.00000	0.00000	0.00000
C	0.00000	0.00000	1.66265
N	1.37312	0.00000	2.07527
C	2.07943	-1.15753	1.75700
C	1.99873	-1.49819	-0.06537
C	0.64088	-1.25329	-0.33967
H	0.55935	0.89799	-0.27444
H	-1.03514	0.07544	-0.33710
H	-0.45799	-0.94159	1.97548
H	1.51150	-2.03451	2.06839
H	2.22398	-2.56957	-0.14158
H	-0.02057	-2.09171	-0.56859
C	2.03656	1.29771	2.23390
H	1.51299	1.87711	2.99657
H	3.06126	1.15213	2.56927
H	2.04808	1.87519	1.30117
Si	3.35827	-0.63166	-1.21446
C	4.98199	-1.54952	-0.95437
H	5.48258	-1.30878	-0.01201
H	4.85297	-2.63689	-1.00449
H	5.66679	-1.27113	-1.76559
C	2.71719	-0.95226	-2.95763
H	2.54915	-2.01916	-3.14429
H	1.77661	-0.42396	-3.15341
H	3.45009	-0.60402	-3.69566
C	3.57417	1.22289	-0.94943
H	4.27019	1.58169	-1.71912
H	2.64666	1.79189	-1.07884
H	4.01142	1.48229	0.01945
C	3.52257	-1.27397	2.20747
H	3.91933	-2.24875	1.91501
H	4.17233	-0.50442	1.78830
H	3.56420	-1.21005	3.30115
C	-0.85204	1.16327	2.16413
H	-0.82313	1.20787	3.25777
H	-0.52625	2.12619	1.76168
H	-1.89088	1.00500	1.86300

28F

Filename: TS1_MeTMS_eqMeaxMe_f.out

B3LYP/6-31g*: -777.62829173 Hartree

ZPE: 874.456 kJ/mol

DeltaG (excl. ZPE): -112.327 kJ/mol

Low frequencies: -268.80 42.10 85.25

Cartesian coordinates:

C	0.00000	0.00000	0.00000
C	0.00000	0.00000	1.64590
N	1.37520	0.00000	2.06502
C	2.13722	-1.11026	1.72457
C	2.03212	-1.44566	-0.10867

C	0.67169	-1.23333	-0.37886
H	0.54323	0.90694	-0.27952
H	-1.03470	0.06230	-0.34252
H	-0.43756	0.96064	1.92800
H	1.63181	-2.02821	2.01843
H	2.29439	-2.50645	-0.21134
H	0.04045	-2.07617	-0.66560
C	1.96745	1.32512	2.27952
H	1.35973	1.86318	3.01091
H	2.97490	1.23252	2.68170
H	2.00629	1.91298	1.35355
Si	3.36037	-0.50588	-1.24524
C	5.00389	-1.39908	-1.03183
H	5.50345	-1.18921	-0.08171
H	4.89752	-2.48559	-1.13005
H	5.67826	-1.06996	-1.83280
C	2.70948	-0.77623	-2.99272
H	2.56570	-1.83914	-3.21806
H	1.75483	-0.26384	-3.16021
H	3.42707	-0.38260	-3.72303
C	3.53325	1.34106	-0.90924
H	4.21982	1.74487	-1.66507
H	2.59248	1.89236	-1.01695
H	3.96525	1.57391	0.06866
C	3.58974	-1.14704	2.15499
H	4.04197	-2.08902	1.83686
H	4.18501	-0.32801	1.74856
H	3.64081	-1.10595	3.24955
C	-0.86073	-1.12829	2.21714
H	-0.85965	-1.07770	3.31041
H	-1.89305	-1.01571	1.87232
H	-0.51922	-2.12393	1.91848

28G

Filename: TS1_MeTMS_axMeeqMe_f.out

B3LYP/6-31g*: -777.63159446 Hartree

ZPE: 874.121 kJ/mol

DeltaG (excl. ZPE): -113.001 kJ/mol

Low frequencies: -276.53 30.94 80.19

Cartesian coordinates:

C	0.00000	0.00000	0.00000
C	0.00000	0.00000	1.64820
N	1.38269	0.00000	2.05028
C	2.12851	-1.12049	1.74130
C	2.05521	-1.42659	-0.14800
C	0.69098	-1.22272	-0.38171
H	0.51430	0.92079	-0.28611
H	-1.04001	0.03158	-0.33120
H	-0.46238	-0.93542	1.96409
H	3.19038	-0.93679	1.88572
H	2.32248	-2.48304	-0.26054
H	0.05849	-2.08013	-0.62062
C	2.05613	1.29967	2.16167
H	1.64524	1.85379	3.00892
H	3.11967	1.13992	2.34103
H	1.93350	1.90676	1.25663
Si	3.48107	-0.44259	-1.07484
C	5.03826	-0.46889	-0.01322
H	4.99784	0.20960	0.84651
H	5.27298	-1.47511	0.35417
H	5.88931	-0.14861	-0.62706
C	3.72177	-1.48335	-2.62591
H	4.00304	-2.51656	-2.39216

H	2.81522	-1.51151	-3.24135
H	4.52416	-1.05703	-3.24038
C	2.99311	1.31407	-1.55270
H	3.78115	1.71521	-2.20302
H	2.06203	1.34637	-2.12957
H	2.90379	2.00339	-0.70746
C	1.71027	-2.46366	2.32713
H	2.37000	-3.25590	1.96523
H	1.81681	-2.41082	3.41706
H	0.68205	-2.74579	2.09240
C	-0.83691	1.16459	2.17152
H	-0.80856	1.18931	3.26574
H	-0.50033	2.13123	1.78741
H	-1.87762	1.02479	1.86691

28H

Filename: TS1_MeTMS_axMeaxMe_f.out

B3LYP/6-31g*: -777.62584267 Hartree

ZPE: 873.854 kJ/mol

DeltaG (excl. ZPE): -114.603 kJ/mol

Low frequencies: -290.76 22.71 82.12

Cartesian coordinates:

C	0.00000	0.00000	0.00000
C	0.00000	0.00000	1.63014
N	1.38921	0.00000	2.03696
C	2.24368	-1.01925	1.67507
C	2.10797	-1.33183	-0.23635
C	0.73326	-1.19240	-0.41938
H	0.48696	0.93315	-0.29395
H	-1.04071	0.00387	-0.33216
H	-0.40736	0.97268	1.91704
H	3.27763	-0.69654	1.77119
H	2.42543	-2.37161	-0.37272
H	0.13850	-2.07133	-0.67353
C	1.94412	1.34400	2.26925
H	1.51210	1.75575	3.18590
H	3.02596	1.28693	2.39530
H	1.71273	2.02294	1.43928
Si	3.47593	-0.26315	-1.15546
C	5.09884	-0.44308	-0.21410
H	5.14127	0.14593	0.70934
H	5.31971	-1.48763	0.03578
H	5.91847	-0.08805	-0.85109
C	3.58365	-1.11827	-2.82953
H	3.84688	-2.17815	-2.73729
H	2.63914	-1.05171	-3.38145
H	4.35882	-0.64104	-3.44165
C	2.99897	1.54570	-1.37383
H	3.76902	2.02280	-1.99376
H	2.04785	1.67002	-1.90334
H	2.95457	2.11004	-0.43743
C	2.07990	-2.42948	2.22989
H	2.88114	-3.06805	1.84918
H	2.18492	-2.37905	3.32021
H	1.12590	-2.89875	1.99534
C	-0.91770	-1.07989	2.21210
H	-0.81360	-1.12011	3.30037
H	-1.95617	-0.82043	1.98301
H	-0.73160	-2.07666	1.80817

29A

Filename: int1_TMS_eqMeeqMe.out

B3LYP/6-31g*: -738.33157016 Hartree
 ZPE: 801.161 kJ/mol
 DeltaG (excl. ZPE): -113.152 kJ/mol
 Low frequencies: 21.19 62.94 86.94

Cartesian coordinates:

C	0.23983	-0.43323	-0.10101
C	0.10697	-0.02863	1.39190
N	1.39503	-0.02165	2.08959
C	2.11986	-1.27441	2.05976
C	1.99893	-2.03047	0.76496
C	1.17501	-1.62881	-0.26241
H	0.57592	0.43441	-0.68323
H	-0.73691	-0.70894	-0.51691
H	-0.50374	-0.79834	1.88483
H	1.60341	-1.97800	2.74822
H	2.48549	-3.00461	0.71173
H	0.90927	-2.38186	-1.00748
H	1.97776	0.76425	1.80806
Si	3.02224	-1.01326	-1.42785
C	4.34916	-2.32924	-1.32527
H	4.87234	-2.33618	-0.36412
H	3.95706	-3.33363	-1.51970
H	5.09442	-2.11961	-2.10431
C	2.14067	-0.98925	-3.08089
H	1.82361	-1.98785	-3.39815
H	1.27180	-0.32428	-3.08965
H	2.85204	-0.61442	-3.82977
C	3.55986	0.68547	-0.85788
H	4.28122	1.05349	-1.60112
H	2.74032	1.40943	-0.82589
H	4.06983	0.68082	0.10883
C	3.54949	-1.13049	2.60124
H	4.04227	-2.10418	2.68197
H	4.16369	-0.48573	1.96422
H	3.50552	-0.68076	3.59636
C	-0.58240	1.32390	1.55258
H	-0.71353	1.55890	2.61211
H	0.01399	2.12440	1.09529
H	-1.56516	1.32298	1.07053

29B

Filename: intl_TMS_eqMeaxMe.out

B3LYP/6-31g*: -738.32795274 Hartree
 ZPE: 802.140 kJ/mol
 DeltaG (excl. ZPE): -112.871 kJ/mol
 Low frequencies: 21.58 67.01 85.12

Cartesian coordinates:

C	0.25068	-0.39926	-0.19022
C	0.13167	0.03241	1.30159
N	1.43457	0.04813	1.98204
C	2.18060	-1.19438	1.95045
C	2.06707	-1.95096	0.65163
C	1.20303	-1.57757	-0.35140
H	0.56600	0.45727	-0.79819
H	-0.72450	-0.69934	-0.59184
H	-0.23643	1.06286	1.32843
H	1.68825	-1.90723	2.64334
H	2.57441	-2.91395	0.58976
H	0.95995	-2.32511	-1.10839
H	2.00842	0.83314	1.68560
Si	3.09051	-0.89704	-1.47186
C	4.49225	-2.12912	-1.32837
H	4.99043	-2.10388	-0.35459

H	4.16693	-3.15529	-1.53147
H	5.24171	-1.87286	-2.08949
C	2.24260	-0.95206	-3.14186
H	1.98885	-1.97231	-3.44674
H	1.33828	-0.33725	-3.18060
H	2.94755	-0.55105	-3.88319
C	3.51257	0.84039	-0.92109
H	4.20623	1.24659	-1.67079
H	2.64760	1.50974	-0.89653
H	4.02420	0.88131	0.04383
C	3.60949	-1.01894	2.48304
H	4.12375	-1.98211	2.55814
H	4.20752	-0.35947	1.84556
H	3.56196	-0.57374	3.48004
C	-0.86862	-0.84498	2.06500
H	-0.88718	-0.55372	3.11880
H	-1.87498	-0.72285	1.65234
H	-0.61965	-1.91161	2.00799

29C

Filename: int1_TMS_axMeeqMe_f.out

B3LYP/6-31g*: -738.33321702 Hartree

ZPE: 801.085 kJ/mol

DeltaG (excl. ZPE): -112.211 kJ/mol

Low frequencies: 32.00 57.57 92.36

Cartesian coordinates:

C	0.00000	0.00000	0.00000
C	0.00000	0.00000	1.56411
N	1.35681	0.00000	2.08972
C	2.24943	-1.06457	1.66342
C	2.07143	-1.43925	0.16577
C	0.93272	-1.03876	-0.51076
H	0.31430	0.99785	-0.34492
H	-0.99675	-0.16073	-0.42869
H	-0.48365	-0.92977	1.88732
H	3.27136	-0.71671	1.84616
H	2.47466	-2.40891	-0.14505
H	0.67969	-1.54091	-1.44465
H	1.78287	0.91984	2.02320
Si	3.45223	-0.29353	-1.04426
C	5.01618	-1.23926	-0.62672
H	5.23147	-1.26052	0.44609
H	4.98327	-2.26911	-0.99740
H	5.85792	-0.73708	-1.12238
C	2.98686	-0.43911	-2.85260
H	2.84097	-1.47972	-3.16346
H	2.08850	0.13121	-3.11091
H	3.81233	-0.03808	-3.45517
C	3.43651	1.46212	-0.39515
H	4.20437	2.01970	-0.94896
H	2.48822	1.98378	-0.55805
H	3.70143	1.52717	0.66494
C	2.05183	-2.34790	2.49913
H	2.76442	-3.12660	2.20712
H	2.20691	-2.10905	3.55402
H	1.04061	-2.75001	2.37914
C	-0.78789	1.18172	2.12415
H	-0.81730	1.13068	3.21583
H	-0.32477	2.13444	1.83616
H	-1.81557	1.18071	1.74796

29D

Filename: int1_TMS_axMeaxMe_f.out

B3LYP/6-31g*: -738.32844631 Hartree
 ZPE: 801.751 kJ/mol
 DeltaG (excl. ZPE): -112.148 kJ/mol
 Low frequencies: 31.68 60.33 84.11

Cartesian coordinates:

C	0.00000	0.00000	0.00000
C	0.00000	0.00000	1.57284
N	1.36128	0.00000	2.09149
C	2.33592	-0.97262	1.61700
C	2.08781	-1.41178	0.14711
C	0.90831	-1.06410	-0.49170
H	0.35537	0.98418	-0.33776
H	-0.99968	-0.12828	-0.42840
H	-0.44886	0.94228	1.90097
H	3.31470	-0.48936	1.70344
H	2.48054	-2.39580	-0.13099
H	0.61584	-1.62684	-1.37817
H	1.74662	0.93697	2.12122
Si	3.41101	-0.31729	-1.14890
C	5.02048	-1.16848	-0.70011
H	5.26517	-1.09461	0.36401
H	5.01813	-2.22573	-0.98542
H	5.82909	-0.67853	-1.25909
C	2.92005	-0.61175	-2.93208
H	2.80517	-1.67691	-3.16269
H	1.99681	-0.09353	-3.21169
H	3.71878	-0.22861	-3.58047
C	3.33622	1.47906	-0.62622
H	4.11882	2.01473	-1.18066
H	2.38713	1.96683	-0.86962
H	3.54612	1.62556	0.43810
C	2.40897	-2.24589	2.49067
H	3.23785	-2.88750	2.17129
H	2.57781	-1.95101	3.52915
H	1.48538	-2.82850	2.44327
C	-0.85903	-1.14889	2.11719
H	-0.80270	-1.17117	3.20858
H	-1.90555	-1.01107	1.82582
H	-0.53530	-2.12453	1.73742

29E

Filename: int1_MeTMS_eqMeeqMe.out

B3LYP/6-31g*: -777.63199571 Hartree
 ZPE: 876.627 kJ/mol
 DeltaG (excl. ZPE): -112.617 kJ/mol
 Low frequencies: 47.91 76.01 99.91

Cartesian coordinates:

C	0.05900	-0.09480	-0.06985
C	-0.01286	0.01348	1.53434
N	1.33897	0.12667	2.03511
C	2.13656	-1.05819	1.80733
C	1.99937	-1.64238	0.32539
C	0.82144	-1.31260	-0.35899
H	0.57669	0.82103	-0.38754
H	-0.92502	-0.10570	-0.54541
H	-0.42410	-0.93119	1.90658
H	1.64157	-1.86411	2.37071
H	2.20783	-2.72084	0.28626
H	0.40144	-2.03549	-1.05824
C	1.94767	1.44985	1.95677
H	1.36621	2.15578	2.55332
H	2.95477	1.42527	2.37116

H	2.00682	1.84425	0.92704
Si	3.42265	-1.13274	-1.13472
C	4.93595	-2.12952	-0.64053
H	5.41284	-1.77843	0.27746
H	4.70939	-3.19563	-0.53090
H	5.66825	-2.03508	-1.45377
C	2.75257	-1.75400	-2.77741
H	2.45515	-2.80830	-2.73829
H	1.90177	-1.16879	-3.14287
H	3.54787	-1.67536	-3.52960
C	3.70926	0.72076	-1.16199
H	4.45301	0.92408	-1.94450
H	2.80984	1.28762	-1.42445
H	4.10947	1.11394	-0.22364
C	3.56340	-0.98097	2.34355
H	4.02766	-1.97000	2.29267
H	4.19843	-0.28091	1.79493
H	3.54317	-0.67725	3.39453
C	-0.95752	1.14088	1.94877
H	-0.95035	1.25459	3.03736
H	-0.69156	2.09876	1.49231
H	-1.97797	0.89455	1.64123

29F

Filename: intl_MeTMS_eqMeaxMe.out

B3LYP/6-31g*: -777.63205772 Hartree

ZPE: 876.322 kJ/mol

DeltaG (excl. ZPE): -112.701 kJ/mol

Low frequencies: 48.15 82.88 94.54

Cartesian coordinates:

C	0.05444	-0.16990	-0.05580
C	-0.02549	-0.04484	1.53733
N	1.32254	0.05279	2.05703
C	2.16487	-1.09628	1.80707
C	2.03029	-1.67315	0.32935
C	0.84658	-1.37142	-0.35376
H	0.56046	0.74599	-0.39341
H	-0.92831	-0.20047	-0.53346
H	-0.52990	0.90153	1.75105
H	1.72250	-1.93161	2.37039
H	2.28307	-2.74125	0.27177
H	0.45978	-2.08902	-1.07658
C	1.88279	1.39959	2.01030
H	1.20844	2.07945	2.53804
H	2.84740	1.43438	2.51684
H	2.01588	1.78307	0.98320
Si	3.42564	-1.10519	-1.15291
C	4.97108	-2.05810	-0.67311
H	5.44171	-1.69812	0.24453
H	4.77968	-3.13172	-0.57076
H	5.69504	-1.93376	-1.48993
C	2.76188	-1.74001	-2.79234
H	2.49359	-2.80215	-2.75473
H	1.89421	-1.17681	-3.15235
H	3.55164	-1.63822	-3.54770
C	3.65353	0.75575	-1.16595
H	4.37870	0.98879	-1.95766
H	2.73419	1.29885	-1.40842
H	4.05704	1.15005	-0.22949
C	3.59353	-0.95575	2.32770
H	4.10759	-1.91818	2.25254
H	4.18329	-0.21150	1.78656
H	3.57095	-0.67427	3.38471

C	-0.84761	-1.18374	2.14814
H	-0.86288	-1.08911	3.23794
H	-1.87898	-1.14081	1.78418
H	-0.45037	-2.17357	1.89499

29G

Filename: int1_MeTMS_axMeeqMe.out

B3LYP/6-31g*: -777.63788742 Hartree

ZPE: 875.372 kJ/mol

DeltaG (excl. ZPE): -114.874 kJ/mol

Low frequencies: 37.77 63.86 86.91

Cartesian coordinates:

C	0.02106	0.08329	-0.04523
C	-0.03002	0.03054	1.56106
N	1.32985	0.03233	2.04925
C	2.13993	-1.11374	1.66451
C	1.84210	-1.62822	0.20359
C	0.70477	-1.14534	-0.45253
H	0.59348	0.99251	-0.27727
H	-0.96290	0.17800	-0.51194
H	-0.48812	-0.92401	1.83726
H	3.18431	-0.80280	1.74662
H	1.94850	-2.71488	0.08491
H	0.24966	-1.76830	-1.22276
C	1.99757	1.32854	2.12063
H	1.48093	1.97906	2.82979
H	3.01805	1.18776	2.48477
H	2.04673	1.85602	1.15091
Si	3.41139	-1.18473	-1.09600
C	4.82989	-2.14180	-0.32411
H	5.08935	-1.79543	0.68144
H	4.62385	-3.21667	-0.27827
H	5.71843	-2.00579	-0.95489
C	2.92217	-1.87763	-2.76832
H	2.59997	-2.92365	-2.70985
H	2.12598	-1.29739	-3.24733
H	3.79297	-1.84820	-3.43552
C	3.69625	0.66739	-1.12496
H	4.52627	0.86853	-1.81548
H	2.83075	1.22739	-1.49471
H	3.98429	1.07021	-0.14966
C	1.94540	-2.31034	2.62235
H	2.59684	-3.14540	2.34410
H	2.19728	-2.00009	3.63948
H	0.91059	-2.66743	2.61390
C	-0.91007	1.15478	2.10653
H	-0.89371	1.14646	3.20084
H	-0.59208	2.14151	1.75751
H	-1.94319	1.00037	1.78206

29H

Filename: int1_MeTMS_axMeaxMe_f.out

B3LYP/6-31g*: -777.63660415 Hartree

ZPE: 874.920 kJ/mol

DeltaG (excl. ZPE): -115.340 kJ/mol

Low frequencies: 39.50 65.27 78.19

Cartesian coordinates:

C	0.04564	0.04531	-0.07056
C	-0.06915	0.00612	1.52323
N	1.26327	-0.05308	2.08525
C	2.17006	-1.11307	1.64782
C	1.85269	-1.66294	0.21985

C	0.73047	-1.19219	-0.46151
H	0.64640	0.93737	-0.29736
H	-0.92007	0.15588	-0.57055
H	-0.49964	0.96621	1.82156
H	3.17267	-0.67415	1.65667
H	1.99248	-2.74581	0.10870
H	0.30398	-1.81183	-1.24978
C	1.87499	1.25515	2.31327
H	1.22972	1.85129	2.96408
H	2.83485	1.13067	2.82195
H	2.04646	1.82809	1.38346
Si	3.40490	-1.18051	-1.11692
C	4.84998	-2.10204	-0.35237
H	5.10176	-1.75325	0.65415
H	4.67422	-3.18243	-0.31238
H	5.73188	-1.93725	-0.98581
C	2.91998	-1.88817	-2.78334
H	2.61856	-2.94005	-2.71926
H	2.11164	-1.32514	-3.26219
H	3.78828	-1.84518	-3.45321
C	3.63212	0.67907	-1.13329
H	4.48252	0.90765	-1.78967
H	2.76554	1.21287	-1.53729
H	3.86894	1.08968	-0.14713
C	2.21384	-2.31078	2.62428
H	2.98235	-3.02950	2.31898
H	2.46070	-1.94753	3.62507
H	1.25325	-2.83013	2.67482
C	-1.01203	-1.10809	1.99091
H	-1.06465	-1.11639	3.08319
H	-2.01988	-0.93847	1.59773
H	-0.68607	-2.09941	1.65910

30A

Filename: TS2_TMS_eqMeeqMe_f.out

B3LYP/6-31g*: -738.32488563 Hartree

ZPE: 799.165 kJ/mol

DeltaG (excl. ZPE): -108.863 kJ/mol

Low frequencies: -320.76 49.70 64.35

Cartesian coordinates:

C	0.00000	0.00000	0.00000
C	0.00000	0.00000	1.92994
N	1.32185	0.00000	2.28777
C	2.15819	-1.08369	1.87965
C	2.19657	-1.17793	0.21125
C	0.80662	-1.12416	-0.20151
H	0.43935	0.98870	-0.09990
H	-1.04251	-0.05609	-0.30721
H	-0.49068	-0.95184	2.12194
H	1.66856	-2.01384	2.18245
H	2.59684	-2.18109	0.01910
H	0.30665	-2.05536	-0.47556
H	1.77266	0.91180	2.32074
Si	3.39527	0.08357	-0.71645
C	5.14729	-0.59921	-0.61052
H	5.57898	-0.54621	0.39346
H	5.19629	-1.64178	-0.94625
H	5.79708	-0.01735	-1.27598
C	2.82709	0.11621	-2.51244
H	2.84950	-0.88421	-2.96060
H	1.81255	0.51345	-2.62970
H	3.49718	0.75114	-3.10442
C	3.29749	1.82245	0.02849

H	3.96136	2.47572	-0.55220
H	2.29946	2.27323	-0.03046
H	3.64398	1.87919	1.06715
C	3.54713	-1.02955	2.50693
H	4.16856	-1.84196	2.12279
H	4.05620	-0.08343	2.30232
H	3.46274	-1.14811	3.59144
C	-0.82178	1.20978	2.31432
H	-0.98082	1.19661	3.39916
H	-0.32009	2.14550	2.04737
H	-1.80104	1.18754	1.83134

30B

Filename: TS2_TMS_eqMeaxMe_f.out

B3LYP/6-31g*: -738.32031009 Hartree

ZPE: 799.608 kJ/mol

DeltaG (excl. ZPE): -108.464 kJ/mol

Low frequencies: -313.17 53.30 68.36

Cartesian coordinates:

C	0.00000	0.00000	0.00000
C	0.00000	0.00000	1.96942
N	1.32746	0.00000	2.30161
C	2.17412	-1.08494	1.90673
C	2.18567	-1.19697	0.24249
C	0.79401	-1.13309	-0.17534
H	0.45129	0.98389	-0.08485
H	-1.04218	-0.04256	-0.30920
H	-0.45805	0.97906	2.10704
H	1.71236	-2.01908	2.23239
H	2.57669	-2.20465	0.05389
H	0.29059	-2.06045	-0.45400
H	1.77993	0.91027	2.28086
Si	3.37907	0.04737	-0.71593
C	5.13712	-0.61821	-0.60244
H	5.57708	-0.52961	0.39531
H	5.19320	-1.67012	-0.90634
H	5.77548	-0.05128	-1.29149
C	2.80561	0.03361	-2.51047
H	2.83942	-0.97656	-2.93563
H	1.78573	0.41495	-2.63344
H	3.46599	0.66298	-3.11896
C	3.27058	1.80146	-0.00793
H	3.92898	2.44731	-0.60282
H	2.26999	2.24547	-0.07440
H	3.61853	1.88248	1.02871
C	3.56790	-0.99417	2.51834
H	4.20041	-1.80028	2.13880
H	4.05738	-0.04170	2.29625
H	3.49740	-1.09962	3.60521
C	-0.88803	-1.14283	2.41513
H	-1.03072	-1.05918	3.49967
H	-1.86959	-1.07023	1.94070
H	-0.47245	-2.12862	2.19868

30C

Filename: TS2_TMS_axMeeqMe_f.out

B3LYP/6-31g*: -738.32579283 Hartree

ZPE: 799.039 kJ/mol

DeltaG (excl. ZPE): -111.100 kJ/mol

Low frequencies: -334.92 33.47 49.24

Cartesian coordinates:

C	0.00000	0.00000	0.00000
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C	0.00000	0.00000	1.96097
N	1.32711	0.00000	2.27911
C	2.17819	-1.09982	1.90504
C	2.07085	-1.39378	0.28866
C	0.70744	-1.19115	-0.16480
H	0.52064	0.95042	-0.06492
H	-1.03313	0.03321	-0.33976
H	-0.49910	-0.94438	2.15664
H	3.20294	-0.79712	2.12928
H	2.33673	-2.44897	0.16092
H	0.13981	-2.06300	-0.49403
H	1.77138	0.91407	2.26645
Si	3.46570	-0.39239	-0.67683
C	5.08870	-1.21157	-0.18640
H	5.30060	-1.13850	0.88683
H	5.10622	-2.27243	-0.46166
H	5.92077	-0.72632	-0.71096
C	3.12149	-0.56404	-2.51697
H	3.09137	-1.61542	-2.82593
H	2.17013	-0.10137	-2.80384
H	3.91234	-0.07631	-3.09917
C	3.44907	1.42057	-0.13859
H	4.25694	1.94403	-0.66557
H	2.52308	1.94891	-0.39325
H	3.64776	1.55489	0.93231
C	1.86358	-2.38832	2.67735
H	2.58370	-3.16715	2.41187
H	1.93888	-2.20571	3.75358
H	0.86259	-2.77220	2.45582
C	-0.80783	1.22004	2.33619
H	-0.96264	1.21709	3.42205
H	-0.29857	2.14914	2.06063
H	-1.78946	1.20245	1.85787

30D

Filename: TS2_TMS_axMexaMe_f.out

B3LYP/6-31g*: -738.31908126 Hartree

ZPE: 799.985 kJ/mol

DeltaG (excl. ZPE): -110.507 kJ/mol

Low frequencies: -310.33 41.30 49.95

Cartesian coordinates:

C	0.00000	0.00000	0.00000
C	0.00000	0.00000	2.03411
N	1.33725	0.00000	2.28395
C	2.24532	-1.07183	1.86833
C	1.80900	-1.71228	0.46760
C	0.52577	-1.28461	-0.05839
H	0.64419	0.87165	-0.02478
H	-0.99914	0.16592	-0.39695
H	-0.44146	0.98979	2.14549
H	3.21590	-0.57918	1.77292
H	1.79267	-2.80278	0.57773
H	-0.14283	-2.07232	-0.40672
H	1.75843	0.92116	2.22053
Si	3.24075	-1.41231	-0.88429
C	4.78851	-2.21312	-0.17192
H	5.12429	-1.74842	0.76209
H	4.64623	-3.28421	0.01212
H	5.60997	-2.11486	-0.89247
C	2.69229	-2.25573	-2.47136
H	2.49305	-3.32299	-2.31895
H	1.78967	-1.79813	-2.89224
H	3.48124	-2.17926	-3.22922

C	3.45316	0.44748	-1.10460
H	4.29441	0.63350	-1.78365
H	2.57245	0.91975	-1.55351
H	3.68685	0.96870	-0.16816
C	2.40580	-2.18535	2.91660
H	3.17056	-2.89332	2.58284
H	2.72799	-1.75935	3.87073
H	1.47743	-2.73951	3.07849
C	-0.89587	-1.11566	2.51632
H	-0.98999	-1.02287	3.60594
H	-1.89356	-1.01701	2.08152
H	-0.51048	-2.11136	2.29345

30E

Filename: TS2_MeTMS_eqMeeqMe_f.out

B3LYP/6-31g*: -777.62925485 Hartree

ZPE: 874.766 kJ/mol

DeltaG (excl. ZPE): -112.290 kJ/mol

Low frequencies: -329.55 46.83 68.11

Cartesian coordinates:

C	0.00000	0.00000	0.00000
C	0.00000	0.00000	1.91189
N	1.33936	0.00000	2.23024
C	2.04010	-1.22204	1.89690
C	1.88528	-1.62266	0.30165
C	0.55872	-1.27193	-0.16422
H	0.63483	0.87853	-0.09441
H	-1.01788	0.15579	-0.35167
H	-0.47171	-0.95335	2.13932
H	1.48044	-2.02766	2.38328
H	1.98881	-2.71565	0.28100
H	-0.10879	-2.07211	-0.48785
C	2.04471	1.28223	2.31264
H	1.50374	1.95163	2.98298
H	3.03911	1.12650	2.72625
H	2.14349	1.76607	1.33106
Si	3.27175	-1.05992	-1.00832
C	4.82362	-2.07870	-0.68495
H	5.38055	-1.76448	0.20238
H	4.59972	-3.14738	-0.58682
H	5.49427	-1.97006	-1.54677
C	2.55615	-1.52534	-2.68895
H	2.29613	-2.58917	-2.74347
H	1.65992	-0.94554	-2.93846
H	3.29759	-1.33444	-3.47424
C	3.63140	0.79142	-0.94377
H	4.34826	1.02462	-1.74161
H	2.74474	1.40796	-1.13122
H	4.08731	1.11367	-0.00200
C	3.47751	-1.29779	2.39698
H	3.87157	-2.29828	2.20071
H	4.14091	-0.57782	1.91285
H	3.50954	-1.13432	3.47913
C	-0.87348	1.17945	2.28519
H	-0.88645	1.28075	3.37778
H	-0.53315	2.12178	1.85045
H	-1.89906	0.99684	1.95638

30F

Filename: TS2_MeTMS_eqMeaxMe_f.out

B3LYP/6-31g*: -777.62712720 Hartree

ZPE: 874.498 kJ/mol

DeltaG (excl. ZPE): -112.007 kJ/mol

Low frequencies: -329.86 45.63 74.27

Cartesian coordinates:

C	0.00000	0.00000	0.00000
C	0.00000	0.00000	1.96354
N	1.33823	0.00000	2.24859
C	2.08359	-1.19767	1.91687
C	1.88806	-1.62201	0.33736
C	0.55904	-1.26958	-0.13477
H	0.63146	0.88184	-0.06964
H	-1.01825	0.15374	-0.35144
H	-0.45324	0.98076	2.10161
H	1.59378	-2.02426	2.43764
H	1.98159	-2.71642	0.33109
H	-0.10069	-2.07359	-0.46265
C	2.02506	1.29813	2.26698
H	1.33113	2.06045	2.62423
H	2.86933	1.25940	2.95634
H	2.39274	1.58237	1.27321
Si	3.24379	-1.11342	-1.02876
C	4.84465	-2.03793	-0.66426
H	5.41414	-1.62016	0.17065
H	4.67152	-3.10152	-0.46300
H	5.48272	-1.98068	-1.55534
C	2.51510	-1.74273	-2.64959
H	2.29377	-2.81606	-2.61072
H	1.59351	-1.21791	-2.92691
H	3.23425	-1.59188	-3.46371
C	3.53005	0.74922	-1.12365
H	4.17895	0.94925	-1.98592
H	2.60894	1.31974	-1.28851
H	4.04008	1.15401	-0.24309
C	3.53687	-1.17220	2.37496
H	3.99524	-2.14268	2.16972
H	4.13112	-0.40575	1.87224
H	3.58799	-1.00349	3.45569
C	-0.89776	-1.12359	2.44139
H	-0.99742	-1.04270	3.53112
H	-1.89390	-1.01646	2.00429
H	-0.52677	-2.12174	2.20318

30G

Filename: TS2_MeTMS_axMeeqMe_f.out

B3LYP/6-31g*: -777.63384521 Hartree

ZPE: 873.552 kJ/mol

DeltaG (excl. ZPE): -114.894 kJ/mol

Low frequencies: -351.19 39.83 46.80

Cartesian coordinates:

C	0.00000	0.00000	0.00000
C	0.00000	0.00000	1.93466
N	1.34111	0.00000	2.22453
C	2.10202	-1.19923	1.87649
C	1.69489	-1.80906	0.44557
C	0.45558	-1.31622	-0.11073
H	0.69899	0.82993	-0.06829
H	-0.98538	0.22672	-0.40204
H	-0.47390	-0.95181	2.15736
H	3.14982	-0.89414	1.86284
H	1.62143	-2.89847	0.54620
H	-0.24696	-2.05595	-0.49632
C	2.06147	1.27533	2.27649
H	1.55818	1.96224	2.95881
H	3.06804	1.09685	2.65773

H	2.14030	1.75358	1.28800
Si	3.18219	-1.63250	-0.86907
C	4.63393	-2.55194	-0.09942
H	4.98557	-2.09928	0.83466
H	4.39128	-3.60177	0.10145
H	5.47927	-2.54277	-0.79874
C	2.60052	-2.46182	-2.45250
H	2.28941	-3.49909	-2.28145
H	1.76187	-1.92760	-2.91377
H	3.41568	-2.48562	-3.18572
C	3.57009	0.19176	-1.13448
H	4.38290	0.27691	-1.86665
H	2.71823	0.74889	-1.54043
H	3.91188	0.69303	-0.22222
C	1.94803	-2.30196	2.93985
H	2.56848	-3.16518	2.68136
H	2.27026	-1.92857	3.91605
H	0.91094	-2.64398	3.02158
C	-0.86268	1.18335	2.31601
H	-0.87198	1.27989	3.40926
H	-0.51411	2.12475	1.88587
H	-1.89041	1.01204	1.98783

30H

Filename: TS2_MeTMS_axMeaxMe_f.out

B3LYP/6-31g*: -777.63020836 Hartree

ZPE: 873.201 kJ/mol

DeltaG (excl. ZPE): -113.823 kJ/mol

Low frequencies: -336.48 43.86 56.60

Cartesian coordinates:

C	0.00000	0.00000	0.00000
C	0.00000	0.00000	1.98465
N	1.34030	0.00000	2.24553
C	2.18976	-1.12748	1.81456
C	1.66170	-1.83477	0.49708
C	0.43615	-1.31983	-0.07594
H	0.70759	0.82321	-0.04399
H	-0.97899	0.23663	-0.41170
H	-0.44670	0.98488	2.11808
H	3.16418	-0.67013	1.62411
H	1.53210	-2.90747	0.68903
H	-0.26991	-2.05805	-0.45635
C	2.01340	1.30547	2.28491
H	1.37184	2.03575	2.78093
H	2.93588	1.21364	2.86310
H	2.26551	1.67095	1.27792
Si	3.07634	-1.85483	-0.91709
C	4.58109	-2.67110	-0.13375
H	4.98707	-2.10520	0.71218
H	4.36469	-3.68971	0.20794
H	5.37848	-2.74398	-0.88399
C	2.39917	-2.88425	-2.33627
H	2.10777	-3.88980	-2.01048
H	1.53048	-2.41586	-2.81283
H	3.16823	-3.00605	-3.10862
C	3.42893	-0.07802	-1.43036
H	4.20927	-0.07514	-2.20137
H	2.54987	0.41251	-1.86280
H	3.79906	0.53942	-0.60372
C	2.39650	-2.17620	2.92155
H	3.10768	-2.93605	2.58340
H	2.80611	-1.70141	3.81773
H	1.46292	-2.67652	3.19249

C	-0.89731	-1.11376	2.48098
H	-0.98719	-1.01658	3.57007
H	-1.89660	-1.01504	2.04882
H	-0.51777	-2.11290	2.26264

31A

Filename: int2_TMS_eqMeeqMe.out

B3LYP/6-31g*: -738.34817605 Hartree

ZPE: 796.349 kJ/mol

DeltaG (excl. ZPE): -117.331 kJ/mol

Low frequencies: 41.52 47.04 76.01

Cartesian coordinates:

C	0.01550	-0.01880	0.04101
C	-0.02156	0.13108	4.60828
N	0.55406	-0.02002	3.47065
C	1.55314	-1.07195	3.07744
C	1.12386	-1.58690	1.68296
C	1.11238	-0.48135	0.65670
H	-0.97200	-0.43297	0.23971
H	0.07318	0.75617	-0.71838
H	0.26294	-0.57109	5.39257
H	0.09392	-1.95939	1.79520
H	2.07687	-0.04930	0.38964
Si	2.09595	-3.16482	1.04749
C	2.41532	-4.29250	2.53153
H	3.10835	-3.85723	3.26184
H	1.48892	-4.55706	3.05628
H	2.86600	-5.23198	2.18923
C	0.93927	-3.99142	-0.18637
H	0.01555	-4.34065	0.29020
H	0.66224	-3.31026	-0.99895
H	1.42381	-4.86420	-0.63980
C	3.71318	-2.66754	0.21209
H	4.20739	-3.56445	-0.18109
H	3.54317	-1.99707	-0.63811
H	4.42561	-2.18083	0.88771
H	1.44398	-1.86983	3.81820
H	0.30526	0.60483	2.69277
C	2.95444	-0.45876	3.18124
H	3.70087	-1.21427	2.92401
H	3.08202	0.38855	2.50126
H	3.15662	-0.11657	4.20116
C	-1.02529	1.18019	4.90434
H	-1.23044	1.82524	4.04632
H	-1.95758	0.70657	5.23921
H	-0.67141	1.79076	5.74556

31B

Filename: int2_TMS_eqMeaxMe.out

B3LYP/6-31g*: -738.34570329 Hartree

ZPE: 797.094 kJ/mol

DeltaG (excl. ZPE): -117.143 kJ/mol

Low frequencies: 39.54 52.00 74.54

Cartesian coordinates:

C	-0.01539	-0.02749	0.09458
C	-0.03214	0.04410	4.63209
N	0.54700	-0.01646	3.48462
C	1.81284	-0.71730	3.07026
C	1.55313	-1.26058	1.64353
C	1.18164	-0.15776	0.68457
H	-0.81758	-0.74528	0.26053
H	-0.21707	0.77127	-0.61378

H	-0.97311	0.59415	4.65973
H	0.69368	-1.94365	1.72668
H	1.95556	0.57414	0.45271
Si	2.96400	-2.40990	0.91759
C	3.65561	-3.46428	2.32707
H	4.19390	-2.87718	3.08110
H	2.87280	-4.03933	2.83685
H	4.37109	-4.19067	1.92266
C	2.10579	-3.48684	-0.36581
H	1.35852	-4.14746	0.08966
H	1.60060	-2.88115	-1.12673
H	2.83398	-4.12302	-0.88250
C	4.32334	-1.37577	0.11592
H	5.07917	-2.04384	-0.31497
H	3.93548	-0.76022	-0.70381
H	4.84396	-0.71359	0.81684
H	1.93989	-1.55703	3.75677
H	0.09565	0.44868	2.68601
C	2.98097	0.26406	3.22792
H	3.91331	-0.23611	2.95455
H	2.86492	1.14234	2.58669
H	3.07238	0.60505	4.26411
C	0.45974	-0.55411	5.89517
H	1.41538	-1.06960	5.80144
H	0.54834	0.24141	6.64732
H	-0.29873	-1.24959	6.27883

31C

Filename: int2_TMS_axMeeqMe.out

B3LYP/6-31g*: -738.34690724 Hartree

ZPE: 796.747 kJ/mol

DeltaG (excl. ZPE): -116.074 kJ/mol

Low frequencies: 40.61 49.07 92.40

Cartesian coordinates:

C	-0.16578	0.16183	0.03244
C	0.55304	-0.49659	4.37643
N	0.49750	0.27178	3.34890
C	1.39030	1.41956	2.95221
C	1.64215	1.26337	1.42987
C	0.31672	1.21391	0.70743
H	0.39774	-0.76507	-0.06346
H	-1.11618	0.21014	-0.49194
H	1.32761	-0.28878	5.11126
H	2.17295	0.31244	1.27125
H	-0.28452	2.12531	0.74925
Si	2.77240	2.65360	0.62283
C	4.58959	2.28998	0.98729
H	4.87154	2.40414	2.03900
H	4.86579	1.27606	0.67342
H	5.21403	2.98413	0.41132
C	2.48833	2.56458	-1.23619
H	2.69573	1.56314	-1.63102
H	1.46293	2.82618	-1.51704
H	3.16107	3.26425	-1.74664
C	2.24317	4.33504	1.30492
H	2.81706	5.12801	0.81023
H	1.18357	4.54331	1.11277
H	2.41702	4.44350	2.38232
H	0.76695	2.30858	3.11494
C	2.62127	1.49174	3.84610
H	3.20340	2.37394	3.57654
H	2.35854	1.60352	4.90377
H	3.26531	0.61391	3.72322

H	-0.20989	0.07705	2.62624
C	-0.37043	-1.63390	4.60566
H	-1.10955	-1.74899	3.80883
H	0.21219	-2.55949	4.70202
H	-0.88492	-1.49330	5.56527

31D

Filename: int2_TMS_axMeaxMe.out

B3LYP/6-31g*: -738.34192867 Hartree

ZPE: 796.445 kJ/mol

DeltaG (excl. ZPE): -118.786 kJ/mol

Low frequencies: 19.29 43.60 61.90

Cartesian coordinates:

C	-0.05745	0.18556	-0.04385
C	-0.03053	0.15602	4.42013
N	0.60894	0.16784	3.30325
C	1.82299	0.97849	2.89752
C	1.90130	0.96771	1.35159
C	0.52853	1.10161	0.73865
H	0.44384	-0.74236	-0.31487
H	-1.03860	0.35319	-0.47919
H	-0.88998	-0.51319	4.46671
H	2.32294	-0.00290	1.04774
H	-0.01285	2.02420	0.95886
Si	3.07205	2.33631	0.56730
C	4.87671	2.07196	1.06536
H	5.09711	2.38432	2.09238
H	5.19806	1.03052	0.94709
H	5.51276	2.67889	0.40896
C	2.90607	2.15000	-1.29805
H	3.20107	1.14748	-1.63084
H	1.88387	2.32872	-1.64604
H	3.56213	2.86750	-1.80509
C	2.47220	4.02991	1.15321
H	3.07439	4.81580	0.68123
H	1.42759	4.22210	0.88189
H	2.57221	4.16583	2.23747
H	1.62653	1.99162	3.26400
C	3.05653	0.38399	3.58714
H	3.93702	0.97365	3.32687
H	2.96071	0.38516	4.67698
H	3.22846	-0.64491	3.25507
H	0.22464	-0.39038	2.53419
C	0.28773	0.96318	5.62060
H	1.08723	1.68793	5.46890
H	-0.62346	1.47814	5.95061
H	0.56517	0.28464	6.43968

31E

Filename: int2_MeTMS_eqMeeqMe_f.out

B3LYP/6-31g*: -777.65541078 Hartree

ZPE: 871.138 kJ/mol

DeltaG (excl. ZPE): -122.582 kJ/mol

Low frequencies: 25.64 47.75 54.28

Cartesian coordinates:

C	4.44570	2.14423	-0.24407
C	2.73900	-2.56993	-0.42837
N	2.42430	-1.34808	-0.15621
C	2.70741	-0.79115	1.23914
C	3.93285	0.15151	1.22162
C	3.69992	1.54054	0.68983
H	5.26968	1.63445	-0.74035

H	4.27180	3.17801	-0.52850
H	3.19590	-3.12316	0.39143
H	4.70710	-0.33567	0.60959
H	2.90596	2.11518	1.16720
Si	4.80999	0.28457	2.97941
C	4.75505	-1.41663	3.80774
H	3.74262	-1.72513	4.09596
H	5.18708	-2.20341	3.17630
H	5.34937	-1.39029	4.72928
C	6.58904	0.77970	2.61485
H	7.12012	0.00723	2.04584
H	6.63945	1.71393	2.04508
H	7.13977	0.93403	3.55032
C	3.96292	1.57713	4.06117
H	4.51544	1.67901	5.00330
H	3.95364	2.56361	3.58449
H	2.93044	1.31880	4.32359
H	2.97110	-1.68390	1.81170
C	1.80373	-0.42672	-1.13252
H	1.96472	-0.77940	-2.14859
H	0.73284	-0.35907	-0.92646
H	2.26772	0.55280	-1.01108
C	1.41534	-0.21526	1.82306
H	1.59481	0.06078	2.86550
H	1.07634	0.68210	1.30007
H	0.61020	-0.95685	1.80808
C	2.55607	-3.30921	-1.70260
H	2.01496	-2.76920	-2.47808
H	3.54337	-3.60238	-2.08560
H	2.02639	-4.24541	-1.48337

31F

Filename: int2_MeTMS_eqMeaxMe_f.out

B3LYP/6-31g*: -777.65447471 Hartree

ZPE: 871.753 kJ/mol

DeltaG (excl. ZPE): -121.487 kJ/mol

Low frequencies: 28.82 46.92 53.57

Cartesian coordinates:

C	4.52322	1.88770	-0.38624
C	2.83084	-2.55750	-0.47162
N	2.40992	-1.40610	-0.06378
C	2.70571	-0.84598	1.32366
C	3.95124	0.07376	1.27421
C	3.75603	1.40508	0.59898
H	5.34025	1.30970	-0.81448
H	4.37670	2.88863	-0.78192
H	2.56004	-2.81892	-1.49387
H	4.73416	-0.47783	0.73181
H	2.97068	2.04446	1.00302
Si	4.77407	0.36043	3.03744
C	4.64580	-1.24656	4.03057
H	3.61463	-1.51859	4.28696
H	5.10631	-2.09644	3.51039
H	5.18491	-1.13086	4.97888
C	6.57757	0.76983	2.68504
H	7.10552	-0.06999	2.21768
H	6.67106	1.63780	2.02318
H	7.10291	1.00863	3.61736
C	3.93773	1.78049	3.95501
H	4.45843	1.95423	4.90470
H	3.98741	2.71500	3.38502
H	2.88620	1.58890	4.19731
H	2.95058	-1.72363	1.91982

C	1.64303	-0.54020	-0.99008
H	1.60129	-1.00753	-1.97435
H	0.63221	-0.40514	-0.60244
H	2.15004	0.42455	-1.05354
C	1.43456	-0.23318	1.91846
H	1.62651	0.00072	2.96873
H	1.13211	0.69359	1.42590
H	0.59954	-0.94049	1.88654
C	3.63516	-3.56408	0.26776
H	3.99380	-3.24900	1.24594
H	3.03397	-4.47708	0.38051
H	4.49361	-3.84300	-0.35652

31G

Filename: int2_MeTMS_axMeeqMe_f.out

B3LYP/6-31g*: -777.65583551 Hartree

ZPE: 870.607 kJ/mol

DeltaG (excl. ZPE): -122.761 kJ/mol

Low frequencies: 37.55 45.97 54.25

Cartesian coordinates:

C	3.89104	-2.45553	-0.54365
C	3.01475	0.54932	1.10837
N	1.84628	0.08716	0.81118
C	1.31772	-1.13923	1.54129
C	1.69664	-2.39977	0.72360
C	3.19368	-2.50771	0.59691
H	3.40490	-2.32047	-1.50840
H	4.96907	-2.59080	-0.55875
H	3.50745	0.05681	1.94373
H	1.25431	-2.31772	-0.28074
H	3.73871	-2.66894	1.53067
Si	1.00098	-4.09632	1.43959
C	-0.83904	-4.25889	1.04363
H	-1.47940	-3.55545	1.58466
H	-1.03070	-4.13423	-0.02917
H	-1.17257	-5.26924	1.31104
C	1.93653	-5.47228	0.55808
H	1.83791	-5.39627	-0.53117
H	3.00526	-5.47073	0.79461
H	1.52978	-6.44592	0.85712
C	1.32721	-4.15353	3.30072
H	1.00529	-5.12309	3.69974
H	2.39438	-4.05361	3.53359
H	0.78631	-3.38347	3.86379
H	1.87730	-1.15297	2.48214
C	-0.16347	-0.94071	1.86603
H	-0.47060	-1.70014	2.58756
H	-0.33895	0.03699	2.32684
H	-0.80716	-1.04119	0.98782
C	1.02781	0.60200	-0.30541
H	0.26036	1.27398	0.08632
H	1.64795	1.12618	-1.02864
H	0.54754	-0.24216	-0.79983
C	3.74666	1.67738	0.47963
H	3.20179	2.20637	-0.30083
H	4.02349	2.39098	1.26649
H	4.68971	1.29351	0.06853

31H

Filename: int2_MeTMS_axMeaxMe_f.out

B3LYP/6-31g*: -777.65413084 Hartree

ZPE: 871.042 kJ/mol

DeltaG (excl. ZPE): -122.036 kJ/mol

Low frequencies: 30.96 40.92 60.86

Cartesian coordinates:

C	3.81556	-2.51199	-0.63510
C	3.05433	0.59182	1.33408
N	1.94586	0.04977	0.95271
C	1.33376	-1.19011	1.58553
C	1.67382	-2.42443	0.71148
C	3.16324	-2.56543	0.53058
H	3.29612	-2.34782	-1.57771
H	4.88879	-2.66986	-0.69563
H	3.39656	1.42811	0.72557
H	1.20310	-2.30225	-0.27495
H	3.73844	-2.75840	1.43931
Si	0.95382	-4.12423	1.39655
C	-0.89211	-4.25153	1.01457
H	-1.51920	-3.55953	1.58526
H	-1.09436	-4.08926	-0.05118
H	-1.23411	-5.26642	1.25254
C	1.85810	-5.49950	0.48260
H	1.75364	-5.39912	-0.60408
H	2.92829	-5.52295	0.71089
H	1.43415	-6.47078	0.76502
C	1.28821	-4.22164	3.25526
H	0.95101	-5.19254	3.63806
H	2.35788	-4.14491	3.48598
H	0.76117	-3.45332	3.83405
H	1.83403	-1.29374	2.54829
C	-0.15410	-0.93810	1.84534
H	-0.52793	-1.71030	2.52032
H	-0.31434	0.02839	2.33469
H	-0.75303	-0.98008	0.93130
C	1.24994	0.58710	-0.23867
H	0.29927	1.02683	0.06786
H	1.87038	1.34652	-0.71429
H	1.06523	-0.22595	-0.94165
C	3.91062	0.25074	2.49767
H	3.54558	-0.55737	3.12804
H	4.90883	-0.01090	2.12350
H	4.03808	1.15645	3.10522

32A

Filename: prod_TMS_eqMeeqMe.out

B3LYP/6-31g*: -329.30505165 Hartree

ZPE: 502.800 kJ/mol

DeltaG (excl. ZPE): -84.269 kJ/mol

Low frequencies: 110.09 159.21 245.25

Cartesian coordinates:

C	-0.18777	-0.01685	-0.77190
C	-1.39321	0.52325	-0.56857
H	-2.28586	0.01418	-0.93035
H	-0.09527	-0.97956	-1.27472
C	1.09654	0.65527	-0.32327
H	1.47820	0.11475	0.55948
C	-1.58696	1.82787	0.16688
H	-1.88821	2.61927	-0.54035
H	-2.42058	1.73742	0.87889
C	-0.30134	2.25174	0.90739
H	-0.18496	1.59264	1.78008
N	0.90520	2.05510	0.08877
H	0.80934	2.62279	-0.75683
C	2.18245	0.59140	-1.40372
H	3.09268	1.08782	-1.05203

H	2.42398	-0.44642	-1.65784
H	1.84752	1.09070	-2.32220
C	-0.35937	3.69931	1.39417
H	0.54847	3.95299	1.95012
H	-0.44102	4.39168	0.54533
H	-1.22857	3.86470	2.04134

32B

Filename: prod_TMS_eqMeaxMe.out

B3LYP/6-31g*: -329.30363227 Hartree
 ZPE: 503.218 kJ/mol
 DeltaG (excl. ZPE): -84.158 kJ/mol
 Low frequencies: 116.19 151.37 234.47
 Cartesian coordinates:

C	1.07516	-0.76786	0.68521
C	-0.08508	-0.17656	0.98578
H	-1.02408	-0.62781	0.66766
H	1.08627	-1.68717	0.09983
C	2.41852	-0.21656	1.11948
H	2.96537	-1.01904	1.63614
C	-0.16074	1.11898	1.75762
H	-0.91446	1.78195	1.30820
H	-0.51171	0.92656	2.78596
C	1.20857	1.82584	1.79744
H	1.40156	2.23236	0.79537
N	2.31020	0.89274	2.08832
H	2.14167	0.49447	3.01320
C	3.27904	0.20516	-0.08606
H	4.26466	0.53562	0.25633
H	3.40826	-0.62902	-0.78582
H	2.81022	1.02893	-0.63541
C	1.24394	2.97949	2.79934
H	0.45472	3.71046	2.58839
H	1.09086	2.61162	3.82303
H	2.21311	3.48675	2.76488

32C

Filename: prod_TMS_axMeeqMe.out

B3LYP/6-31g*: -329.30363575 Hartree
 ZPE: 503.159 kJ/mol
 DeltaG (excl. ZPE): -84.156 kJ/mol
 Low frequencies: 116.82 151.62 234.18
 Cartesian coordinates:

C	-2.77689	2.90060	1.78326
C	-2.49550	2.43147	0.56388
H	-3.03754	2.80855	-0.30245
H	-3.52931	3.67873	1.91093
C	-2.08721	2.40283	3.03773
H	-2.86329	2.10147	3.75665
C	-1.43502	1.38447	0.32089
H	-0.84639	1.64424	-0.57109
H	-1.90734	0.41400	0.09115
C	-0.50643	1.23656	1.54237
H	0.13526	2.12727	1.58132
N	-1.25366	1.20500	2.81105
H	-1.86624	0.38852	2.78856
C	-1.26034	3.51275	3.71301
H	-1.88421	4.38727	3.93259
H	-0.83027	3.14115	4.64834
H	-0.44201	3.84397	3.06429
C	0.38982	0.00189	1.45140
H	1.06717	-0.04345	2.30984

H	-0.21192	-0.91713	1.44634
H	0.98560	0.01297	0.53129

32D

Filename: prod_TMS_axMeaxMe.out

B3LYP/6-31g*: -329.30505415 Hartree

ZPE: 502.871 kJ/mol

DeltaG (excl. ZPE): -84.272 kJ/mol

Low frequencies: 109.30 158.84 245.27

Cartesian coordinates:

C	-0.54827	1.65494	-1.43831
C	-1.68472	2.00654	-0.82919
H	-2.43085	2.59228	-1.36496
H	-0.35196	1.97542	-2.46152
C	0.51677	0.81263	-0.76103
H	1.36322	1.47082	-0.50141
C	-1.98887	1.63613	0.60287
H	-2.77911	0.86687	0.63464
H	-2.40307	2.50483	1.13565
C	-0.72913	1.12030	1.32939
H	-0.07701	1.98446	1.52304
N	0.05834	0.19877	0.49552
H	-0.53609	-0.59935	0.25854
C	1.05614	-0.28148	-1.68981
H	1.50212	0.15249	-2.59134
H	1.81743	-0.87334	-1.17140
H	0.24957	-0.95503	-2.00742
C	-1.05845	0.44977	2.66266
H	-0.14118	0.13445	3.16942
H	-1.61118	1.12941	3.32165
H	-1.68193	-0.44092	2.50610

32E

Filename: prod_MeTMS_eqMeeqMe.out

B3LYP/6-31g*: -368.60867840 Hartree

ZPE: 576.626 kJ/mol

DeltaG (excl. ZPE): -88.712 kJ/mol

Low frequencies: 67.04 134.46 203.43

Cartesian coordinates:

C	1.37102	-0.73628	1.72942
C	0.15648	-1.20064	2.01951
H	0.03829	-2.12006	2.59065
H	2.26235	-1.26471	2.06423
C	1.62793	0.48825	0.88607
H	2.16405	1.22679	1.52077
C	-1.07552	-0.45710	1.59361
H	-1.83420	-0.49195	2.38772
H	-1.52993	-0.93345	0.71108
C	-0.76285	1.01298	1.27512
H	-0.51677	1.51833	2.23255
N	0.38701	1.09205	0.35119
C	2.57065	0.08801	-0.26753
H	3.48912	-0.35871	0.13051
H	2.07405	-0.64590	-0.91007
H	2.86326	0.94356	-0.88357
C	0.64134	2.46245	-0.09060
H	1.52822	2.49085	-0.72720
H	-0.19317	2.83674	-0.68779
H	0.80827	3.16278	0.75214
C	-2.01240	1.68334	0.68972
H	-2.88158	1.44366	1.31254
H	-1.93214	2.77329	0.64903

H -2.20438 1.31052 -0.32352

32F

Filename: prod_MeTMS_eqMeaxMe_f.out

B3LYP/6-31g*: -368.60799039 Hartree

ZPE: 576.923 kJ/mol

DeltaG (excl. ZPE): -87.955 kJ/mol

Low frequencies: 108.22 136.27 210.20

Cartesian coordinates:

C	-1.40030	0.65744	-0.78875
C	-1.84427	1.85482	-1.18412
H	-2.84768	1.95531	-1.59617
H	-2.03039	-0.22463	-0.90134
C	-0.02460	0.44342	-0.18333
H	-0.15248	-0.13797	0.74071
C	-0.99799	3.10020	-1.08823
H	-1.37735	3.75826	-0.28988
H	-1.08085	3.68553	-2.01532
C	0.48058	2.73796	-0.83449
H	0.85562	2.27278	-1.75515
N	0.63540	1.70547	0.21208
C	0.88233	-0.39542	-1.10436
H	1.07449	0.11592	-2.05349
H	1.84197	-0.58369	-0.61254
H	0.41129	-1.35759	-1.33850
C	0.22629	2.13706	1.54856
H	-0.85196	2.35429	1.65296
H	0.47750	1.34790	2.26591
H	0.78475	3.03067	1.84100
C	1.35351	3.96692	-0.56906
H	2.38048	3.66127	-0.34269
H	1.37131	4.61346	-1.45391
H	0.98144	4.56995	0.26688

32G

Filename: prod_MeTMS_axMeeqMe_f.out

B3LYP/6-31g*: -368.60798981 Hartree

ZPE: 576.932 kJ/mol

DeltaG (excl. ZPE): -87.948 kJ/mol

Low frequencies: 108.36 136.56 209.71

Cartesian coordinates:

C	1.52197	1.55848	-0.91780
C	1.07356	1.11010	0.25906
H	0.72819	1.81437	1.01500
H	1.51908	2.62669	-1.13384
C	2.04139	0.64046	-2.00974
H	3.01193	1.03365	-2.34389
C	1.01807	-0.36011	0.59343
H	0.05927	-0.60228	1.07409
H	1.79167	-0.61135	1.33689
C	1.19099	-1.21666	-0.67866
H	0.28206	-1.08047	-1.27863
N	2.29597	-0.73591	-1.53489
C	1.12101	0.64260	-3.24560
H	1.55502	0.02126	-4.03542
H	0.12590	0.25300	-3.00643
H	0.99181	1.66163	-3.62948
C	3.62346	-0.86695	-0.93453
H	3.80956	-1.90923	-0.66076
H	4.37635	-0.58757	-1.67989
H	3.78873	-0.24023	-0.03976
C	1.30332	-2.71244	-0.37389

H	0.37488	-3.07358	0.08312
H	1.47706	-3.27580	-1.29680
H	2.11780	-2.93567	0.32442

32H

Filename: prod_MeTMS_axMeaxMe.out

B3LYP/6-31g*: -368.60867815 Hartree

ZPE: 576.702 kJ/mol

DeltaG (excl. ZPE): -88.726 kJ/mol

Low frequencies: 66.12 134.47 202.95

Cartesian coordinates:

C	-1.40634	1.15057	3.46705
C	-1.98228	1.81226	2.46439
H	-2.50669	2.74839	2.64923
H	-1.45744	1.53149	4.48584
C	-0.60116	-0.11357	3.29243
H	-1.11363	-0.91958	3.86123
C	-1.94737	1.27351	1.06400
H	-1.19170	1.80339	0.46368
H	-2.91209	1.44469	0.56656
C	-1.64554	-0.23283	1.04863
H	-2.53076	-0.75606	1.46712
N	-0.45401	-0.51328	1.87549
C	0.78380	0.10670	3.93534
H	0.67205	0.40469	4.98425
H	1.40158	-0.79615	3.91586
H	1.31528	0.90007	3.40044
C	-0.04034	-1.91255	1.78505
H	-0.84545	-2.61949	2.06924
H	0.28597	-2.15387	0.77098
H	0.80977	-2.09390	2.44616
C	-1.45777	-0.69886	-0.40087
H	-0.51284	-0.31559	-0.80426
H	-1.46235	-1.78778	-0.50262
H	-2.27540	-0.31048	-1.01845

Me₃Si⁺

Filename: silylcation_f.out

B3LYP/6-31g*: -408.98270655 Hartree

ZPE: 288.240 kJ/mol

DeltaG (excl. ZPE): -84.821 kJ/mol

Low frequencies: -56.55 23.34 30.30

Cartesian coordinates:

Si	3.36259	-0.66932	-1.69297
C	4.65374	-1.84446	-1.09824
H	5.11497	-1.51724	-0.16162
H	4.25012	-2.85696	-0.97636
H	5.44882	-1.91634	-1.85790
C	2.19064	-1.21121	-3.00975
H	1.79600	-2.21344	-2.79950
H	1.36084	-0.51176	-3.14587
H	2.73308	-1.28839	-3.96552
C	3.31576	1.05166	-1.03350
H	4.10283	1.64195	-1.53136
H	2.35929	1.54763	-1.22429
H	3.54048	1.07665	0.03940

**Experimental and quantum-mechanical investigation
of the vinylsilane-iminium ion cyclization**

Lisbet Kværnø, Per-Ola Norrby and David Tanner*

Electronic Supplementary Information

Experimental

General Methods. Reactions were conducted under atmospheres of argon or nitrogen when anhydrous solvents were used. Anhydrous solvents were either distilled from appropriate drying agents immediately before use or dried by storage over activated molecular sieves. All reagents were obtained from commercial suppliers and were used without further purification unless otherwise stated. After column chromatography which was performed using dry column vacuum chromatography,^{S1} fractions containing product were pooled, the solvents were evaporated under reduced pressure and the residue was dried under high vacuum to give the product. Silica gel 60 (15-40 μm) was purchased from Merck Eurolab. ^1H NMR spectra were recorded at 300 MHz and ^{13}C NMR spectra were recorded at 75.5 MHz unless otherwise stated. Chemical shifts are reported in ppm relative to the deuterated solvent as the internal standard for ^1H and ^{13}C and NMR assignments are all based on 2D spectra except for compounds **11A** and **11B**. Coupling constants J are given in Hz. Electron impact ionization mass spectra by direct inlet (EI) was recorded in positive ion mode. Microanalyses were performed by The Microanalytical Laboratory, Department of Physical Chemistry, University of Vienna, Austria. Column chromatographic purification of cyclization products **11A**, **11B**, **12**, **13** and **14** proved troublesome, which is both ascribed to the tendency of the reacting aldehydes to undergo aldol condensation and polymerizations and to slight instability of the cyclized products.

6-Benzyloxy-4-hydroxy-1-C-trimethylsilyl-1-hexyne **4**^{S2,S3}

HC≡CSiMe₃ (7.812 g, 79.5 mmol) was dissolved in anhydrous THF (80 cm³) at -78°C, *n*-BuLi (1.6M, 49 cm³, 78 mmol) was slowly added and the solution was stirred for 35 min. BF₃·Et₂O (10.5 cm³, 83 mmol) was added dropwise and after 10 min, **3**^{S4} (4.700 g, 26.4 mmol) was added dropwise and the solution was stirred at -78°C for 1 h. Sat. aq. NH₄Cl (300 cm³) was added and the mixture was extracted with EtOAc (4 x 100 cm³). The combined organic phase was washed successively with sat. aq. NaHCO₃ (100 cm³) and H₂O (100 cm³), dried (MgSO₄), celite was added and the solvents were evaporated under reduced pressure. The solid residue was applied to dry column vacuum chromatography (5.2 x 5.5 cm) on silica gel eluting with a gradient of 0-25% EtOAc in hexane (v/v) to give alkyne **4** (8.079 g, quant.) as a colourless oil. R_f (1:1 EtOAc/hexane (v/v)) 0.61; *m/z* (EI) 275 [M-H]⁺, 91 [C₅H₆CH₂]⁺; δ_H (CDCl₃) 7.31-7.19 (5 H, m, Bn), 4.46 (2 H, s, Bn), 3.90 (1 H, bs, 4-H), 3.71-3.55 (2 H, m, 6-H), 2.92 (1 H, bs, OH), 2.39 (1 H, d, *J* 2.4, 3'-H), 2.37 (1 H, d, *J* 2.8, 3''-H), 1.91-1.70 (2 H, m, 5-H), 0.09 (9 H, s, Si(CH₃)₃). δ_C (CDCl₃) 137.88, 128.40, 127.70, 127.60 (Bn), 103.31 (2-C), 87.11 (1-C), 73.26 (Bn), 69.37 (4-C), 68.48 (6-C), 35.37 (5-C), 28.60 (3-C), 0.08 (Si(CH₃)₃).

6-Benzyloxy-4-methanesulfonyloxy-1-C-trimethylsilyl-1-hexyne **4A**

4 (301 mg, 1.09 mmol) was dissolved in anhydrous pyridine (5 cm³) at 0°C, MsCl (0.20 cm³, 2.6 mmol) was added and the solution was stirred at 0°C for 2.5 h. H₂O (50 cm³) was added, the solution was extracted with EtOAc (4 x 30 cm³) and the combined organic phase was washed successively with sat. aq. NaHCO₃ (20 cm³) and H₂O (20 cm³), dried (MgSO₄) and evaporated to dryness under reduced pressure. The residue was purified by dry column vacuum chromatography (5.1 x 3.3 cm) on silica gel eluting with a gradient of 0-25% EtOAc in hexane (v/v) to give mesylate **4A** (343 mg, 89%) as a colourless oil. R_f (1:9 EtOAc/CH₂Cl₂ (v/v)) 0.82; IR (neat) ν 2180 cm⁻¹

(medium, sharp); δ_{H} (CDCl_3) 7.28-7.18 (5 H, m, Bn), 4.89-4.81 (1 H, m, 4-H), 4.45 (1 H, d, J 11.9, Bn), 4.41 (1 H, d, J 11.7, Bn), 3.54 (2 H, t, J 4.9, 6-H), 2.95 (3 H, s, Ms), 2.64 (2 H, d, J 5.9, 3-H), 2.11-1.91 (2 H, m, 5-H), 0.08 (9 H, s, $\text{Si}(\underline{\text{C}}\text{H}_3)_3$). δ_{C} (CDCl_3) 137.93, 128.39, 127.73, 127.69 (Bn), 101.03 (2-C), 88.11 (1-C), 78.12 (4-C), 73.04 (Bn), 65.49 (6-C), 38.36 (Ms), 34.18 (5-C), 26.68 (3-C), -0.08 ($\text{Si}(\underline{\text{C}}\text{H}_3)_3$).

4-Azido-6-benzyloxy-1-C-trimethylsilyl-1-hexyne 4B

4 (1177 mg, 4.26 mmol) was converted into mesylate **4A** as described above and crude **4A** (1418 mg, 94%) was dissolved in anhydrous DMSO (20 cm^3), NaN_3 (2.512 g, 38.6 mmol) was added and the suspension was stirred at 60°C for 15 h. The reaction mixture was cooled and, after addition of H_2O (100 cm^3), extracted with 1:1 hexane/EtOAc ((v/v), 4 x 70 cm^3). The combined organic phase was washed successively with sat. aq. NaHCO_3 (70 cm^3) and H_2O (70 cm^3), dried (MgSO_4) and evaporated to dryness under reduced pressure. The residue was purified by dry column vacuum chromatography (5.5 x 5.5 cm) on silica gel eluting with a gradient of 0-20% EtOAc in hexane (v/v) to give a 86:14 mixture of azide **4B** and conjugated enynes **4C** (923 mg, 70% **4B**) as a colourless oil. R_f (1:3 EtOAc/hexane (v/v)) 0.54; IR (neat) ν 2179 cm^{-1} (medium, sharp), 2102 cm^{-1} (strong); m/z (EI) 300 $[\text{M}-\text{H}]^+$, 162 $[\text{M}-\text{Me}_3\text{SiC}\equiv\text{CCH}_2]^+$, 91 $[\text{C}_5\text{H}_6\text{CH}_2]^+$; δ_{H} (CDCl_3 , selected signals) 7.39-7.26 (5 H, m, Bn), 4.53 (2 H, s, Bn), 3.78-3.70 (1 H, m, 4-H), 3.66-3.55 (2 H, m, 6-H), 2.52 (1 H, d, J 1.6, 3'-H), 2.50 (1 H, d, J 2.2, 3''-H), 2.02-1.91 (1 H, m, 5'-H), 1.82-1.71 (1 H, m, 5''-H), 0.17 (9 H, s, $\text{Si}(\underline{\text{C}}\text{H}_3)_3$). δ_{C} (CDCl_3 , selected signals) 138.13, 128.39, 127.63 (Bn), 102.07 (2-C), 87.96 (1-C), 73.09 (Bn), 66.47 (6-C), 58.03 (4-C), 33.85 (5-C), 26.48 (3-C), -0.10 ($\text{Si}(\underline{\text{C}}\text{H}_3)_3$).

cis-4-Azido-6-benzyloxy-1-C-trimethylsilyl-1-hexene 5

BH₃·THF (1M, 49 cm³, 49 mmol) was added to anhydrous THF (50 cm³) at 0°C, cyclohexene (10.0 cm³, 98.6 mmol) was added dropwise and the resulting slurry was stirred at 0°C for 75 min. Then **4B/4C** (84:16 **4B:4C**, 5.02 g, 17.0 mmol **4B**) dissolved in anhydrous THF (30 cm³) was added dropwise and the mixture was slowly heated to room temperature. After 14.5 h, the solution was cooled to 0°C, cyclohexene (5 cm³, 49.3 mmol) followed by AcOH (5 cm³, 70 mmol) were added dropwise and stirring was continued at room temperature for 2.5 h. The reaction mixture was poured into sat. aq. NaHCO₃ (300 cm³) and extracted with ether (4 x 100 cm³). The combined organic phase was washed successively with sat. aq. NaHCO₃ (100 cm³) and H₂O (100 cm³), dried (MgSO₄), celite was added and the solvents were evaporated under reduced pressure. The solid residue was applied to dry column vacuum chromatography (5.4 x 5.5 cm) on silica gel eluting with a gradient of 0-10% EtOAc in hexane (v/v) to give *cis*-olefin **5** (3.719 g, 84%) as a light yellow oil. R_f (1:3 EtOAc/hexane (v/v)) 0.65; IR (neat) ν 2100 cm⁻¹ (strong, broad); *m/z* (EI) 275 [M-N₂]⁺, 162 [M-Me₃SiCH=CHCH₂]⁺, 91 [C₅H₆CH₂]⁺; δ_H (CDCl₃) 7.39-7.29 (5 H, m, Bn), 6.32 (1 H, dt, *J* 7.1 and 14.1, 2-H), 5.69 (1 H, dt, *J* 1.4 and 14.1, 1-H), 4.53 (2 H, s, Bn), 3.70-3.58 (3 H, m, 4-H, 6-H), 2.41 (2 H, tt, *J* 1.3 and 7.1, 3-H), 1.94-1.84 (1 H, m, 5'-H), 1.71 (1 H, ddd, *J* 4.7, 9.5 and 19.2, 5''-H), 0.15 (9 H, s, Si(CH₃)₃). δ_C (CDCl₃) 143.04 (2-C), 138.17 (Bn), 132.89 (1-C), 128.36, 127.66, 127.62, 73.15 (Bn), 66.69 (6-C), 59.77 (4-C), 38.39 (3-C), 34.43 (5-C), 0.14 (Si(CH₃)₃).

***cis*-4-Amino-6-benzyloxy-1-C-trimethylsilyl-1-hexene 6**

5 (158 mg, 0.521 mmol) was dissolved in anhydrous THF (10 cm³) at 0°C, LiAlH₄ (59 mg, 1.5 mmol) was added and the suspension was stirred at 0°C for 4.5 h and at room temperature for 19 h. Additional LiAlH₄ (29 mg, 0.76 mmol) was added and after stirring for 5 h, the suspension was cooled to 0°C and sat. aq. NHCO₃ (1 cm³) was carefully added. Celite was added and the solvents were evaporated under reduced pressure. The solid residue was applied to dry column vacuum chromatography (5.0 x 2.0 cm) on silica gel eluting with a gradient of 0-10% MeOH in CH₂Cl₂

(v/v) to give amine **6** (116 mg, 81%) as a colourless oil (Found: C, 69.0; H, 9.6; N, 4.8. Calc. for C₁₆H₂₇NOSi: C, 69.3; H, 9.8; N, 5.1%); R_f (1:9 MeOH/CH₂Cl₂ (v/v)) 0.24; *m/z* (EI) 278 [M+H]⁺, 276 [M-H]⁺, 262 [M-CH₃]⁺, 164 [M-N₂-Me₃SiCH=CHCH₂]⁺, 91 [C₅H₆CH₂]⁺; δ_H (CDCl₃) 7.37-7.25 (5 H, m, Bn), 6.31 (1 H, dt, *J* 7.3 and 14.3, 2-H), 5.63 (1 H, dt, *J* 1.4 and 14.3, 1-H), 4.51 (2 H, s, Bn), 3.67-3.55 (2 H, m, 6-H), 3.07-2.99 (1 H, m, 4-H), 2.34-2.25 (1 H, m, 3'-H), 2.22-2.12 (1 H, m, 3''-H), 1.86-1.75 (3 H, m, 5'-H, NH₂), 1.65-1.53 (1 H, m, 5''-H), 0.13 (9 H, s, Si(CH₃)₃). δ_C (CDCl₃) 145.26 (2-C), 138.36 (Bn), 131.84 (1-C), 128.31, 127.57, 127.50, 73.00 (Bn), 68.04 (6-C), 49.39 (4-C), 41.80 (3-C), 37.11 (5-C), 0.28 (Si(CH₃)₃).

cis*-4-Cyclopentylidenamino-6-benzyloxy-1-*C*-trimethylsilyl-1-hexene **8*

6 (260 mg, 0.937 mmol) was dissolved in anhydrous ether (10 cm³), cyclopentanone (0.17 cm³, 1.9 mmol) and 4A mol sieves (1.22 g) were added and the mixture was stirred for 18 h. After filtration through celite and washing of the mol sieves with several ether portions, the filtrate was evaporated to dryness under reduced pressure. The residue was coevaporated with anhydrous toluene (3 x 10 cm³) and dried under high vacuum to give imine **8** (296 mg, 92%) as a colourless oil. R_f (1:9 MeOH/CH₂Cl₂ (v/v)) 0.47; δ_H (CDCl₃) 7.36-7.26 (5 H, m, Bn), 6.24 (1 H, dt, *J* 1.3, 6.8 and 14.1, 2-H), 5.52 (1 H, dd, *J* 1.3 and 14.3, 1-H), 4.48 (1 H, d, *J* 11.9, Bn), 4.40 (1 H, d, *J* 12.1, Bn), 3.52-3.43 (2 H, m, 4-H, 6_a-H), 3.39-3.31 (1 H, m, 6_b-H), 2.41-2.06 (6 H, m, 3-H, 2'-H, 5'-H), 1.97-1.89 (1 H, m, 5_a-H), 1.81-1.64 (5 H, m, 5_b-H, 3'-H, 4'-H), 0.11 (9 H, s, Si(CH₃)₃). ¹³C NMR (CDCl₃): δ 178.99 (1'-C), 145.69 (2-C), 138.46 (Bn), 130.60 (1-C), 128.23, 127.62, 127.41, 72.92 (Bn), 67.42 (6-C), 59.47 (4-C), 40.06 (3-C), 36.27, 35.83 (5-C, 2'-C/5'-C), 29.18 (2'-C/5'-C), 24.99, 24.08 (3'-C, 4'-C), 0.22 (Si(CH₃)₃).

cis/trans*-(2'-Benzyloxyethyl)-2-phenyl-3,4-didehydropiperidine **11A** and **11B*

6 (109 mg, 0.39 mmol) was dissolved in anhydrous ether (5 cm³), 4A molsieves (0.92 g) and benzaldehyde (0.042 cm³, 0.41 mmol) were added and the mixture was stirred for 18 h. After filtration and washing of the mol sieves with several ether portions, the filtrate was evaporated to dryness under reduced pressure. The residue was coevaporated with anhydrous acetonitrile (3 x 10 cm³) and dried under high vacuum to give crude imine **10**. This was dissolved in anhydrous acetonitrile (7 cm³), TFA (0.15 cm³, 2.0 mmol) was added and the solution was stirred at 80°C for 70 h. The solution was cooled and evaporated to dryness under reduced pressure. The residue was dissolved in EtOAc (20 cm³) and the organic phase was washed successively with sat. aq. NaHCO₃ (5 cm³) and H₂O (5 cm³). The combined aqueous phase was extracted with EtOAc (10 cm³) and the combined organic phase was dried (MgSO₄), celite was added and the solvents were evaporated under reduced pressure. The solid residue was applied to dry column vacuum chromatography (5.0 x 2.0 cm) on silica gel eluting with a gradient of 0-100% EtOAc in hexane followed by 5-10% MeOH in CH₂Cl₂ (v/v) to give amines **11A** and **11B** (43 mg, 37% from **6**) as light brown oils. **11A** (assignments from 1D-spectra based on assignments of **14**): R_f (1:4 MeOH/CH₂Cl₂ (v/v)) 0.71; *m/z* (EI) 292 [M-H]⁺, 216 [M-Ph]⁺, 158 [M-BnOCH₂CH₂]⁺, 91 [C₅H₆CH₂]⁺; δ_H (CDCl₃, selected signals) 7.37-7.25 (10 H, m, Ph, Bn), 5.91-5.83 (1 H, m, 3-H), 5.72-5.67 (1 H, m, 4'-H), 4.53 (1 H, bs, 2-H), 4.50 (2 H, s, OBn), 3.64-3.59 (2 H, m, 2'-H), 3.20-3.11 (1 H, m, 6-H), 2.19-1.59 (5 H, m, NH, 5-H, 1'-H). δ_C (CDCl₃) 143.83 (Ph), 138.37 (Bn), 130.30 (4-C), 128.45, 128.34, 127.66, 127.59, 127.52, 127.24 (Ph, Bn), 125.78 (3-C), 72.95 (OBn), 68.00 (2'-C), 60.15 (2-C), 52.24 (6-C), 36.36, 32.25 (5-C, 1'-C). **11B** (assignments from 1D ¹³C-spectrum based on assignments of **14**): R_f (1:4 MeOH/CH₂Cl₂ (v/v)) 0.63; *m/z* (EI) 292 [M-H]⁺, 216 [M-Ph]⁺, 158 [M-BnOCH₂CH₂]⁺, 91 [C₅H₆CH₂]⁺; δ_C (CDCl₃) 141.10, 139.86, 137.89, 137.67, 128.78, 128.67, 128.56, 128.50, 128.36, 128.10, 127.99, 127.85, 127.76, 127.66, 127.63, 126.64, 125.45 (Ph, Bn, 3-C, 4-C), 73.20 (OBn), 68.13 (2'-C), 55.75 (2-C), 46.93 (6-C), 33.83, 30.42 (5-C, 1'-C).

***cis*-4-Benzylidenamino-6-benzyloxy-1-*C*-trimethylsilyl-1-hexene 10**

6 (926 mg, 3.34 mmol) was dissolved in anhydrous ether (50 cm³), 4A molsieves (1.945 g) and benzaldehyde (0.40 cm³, 3.9 mmol) were added and the mixture was stirred for 14 h. After filtration and washing of the mol sieves with several ether portions, the filtrate was evaporated to dryness under reduced pressure. The residue was coevaporated with anhydrous acetonitrile (10 cm³) and dried under high vacuum to give a mixture of imine **10** and PhCHO (5:1, 1510 mg) as a colourless oil. R_f (1:9 MeOH/CH₂Cl₂ (v/v)) 0.87; δ_H (CDCl₃) 8.21 (1 H, s, RN=CHPh), 7.91-7.26 (10 H, m, Ph, Bn), 6.28 (1 H, dt, J 7.2 and 14.3, 2-H), 5.57 (1 H, d, J 14.1, 1-H), 4.51 (1 H, d, J 12.1, Bn), 4.41 (1 H, d, J 12.1, Bn), 3.56-3.38 (3 H, m, 4-H, 6-H), 2.50 (2 H, t, J 7.1, 3-H), 2.11-1.90 (2 H, m, 5-H), 0.13 (9 H, s, Si(CH₃)₃). δ_C (CDCl₃) 160.32 (PhHC=NR), 145.30 (2-C), 138.48, 136.38, 136.08, 134.33, 131.06, 130.41, 129.64, 128.90, 128.40, 128.23, 128.18, 127.57, 127.40 (Ph, Bn, 1-C), 72.85 (Bn), 68.05 (4-C), 67.17 (6-C), 40.12 (3-C), 35.63 (5-C), 0.17 (Si(CH₃)₃).

cis*-4-(*N*-Benzyl)amino-6-benzyloxy-1-*C*-trimethylsilyl-1-hexene **7*

Crude **10** (3.34 mmol) was dissolved in anhydrous THF/MeOH (3:1 (v/v), 40 cm³) at 0°C, NaBH₄ (259 mg, 6.85 mmol) was added and the solution was stirred at 0°C for 2 h. AcOH (1.5 cm³, 26 mmol) followed by NaHCO₃(s) (2003 mg, 23.8 mmol) was carefully added. Celite was added and the solvents were evaporated under reduced pressure. The solid residue was applied to dry column vacuum chromatography (4.8 x 5.5 cm) on silica gel eluting with a gradient of 0-35% EtOAc in hexane (v/v) followed by 2.5:30:67.5 Et₃N/EtOAc/hexane (v/v/v) and then 35-50% EtOAc in hexane (v/v) to give benzylamine **7** (886 mg, 72% from **6**) as a colourless oil (Found: C, 75.4; H, 8.9; N, 3.8. Calcd. for C₂₃H₃₃NOSi: C, 75.2; H, 9.1; N, 3.8) after coevaporation with anhydrous acetonitrile (2 x 20 cm³). R_f (1:1 EtOAc/hexane (v/v)) 0.53; m/z (EI) 352 [M-CH₃]⁺, 254 [M-Me₃SiCH=CHCH₂]⁺, 91 [C₅H₆CH₂]⁺; δ_H (CDCl₃) 7.37-7.21 (10 H, m, Bn), 6.32 (1 H, dt, J 7.1 and 14.3, 2-H), 5.62 (1 H, dt, J 1.5 and 14.3, 1-H), 4.50 (2 H, s, OBn), 3.83 (1 H, d, J 13.0, NBn), 3.76

(1 H, d, J 13.2, NBn), 3.67-3.54 (2 H, m, 6-H), 2.84 (1 H, p, J 6.2, 4-H), 2.43-2.24 (2 H, m, 3-H), 1.82-1.75 (2 H, m, 5-H), 1.60 (1 H, bs, NH), 0.14 (9 H, s, Si(CH₃)₃). δ_C (CDCl₃) 145.50 (2-C), 140.78, 138.43 (Bn), 131.36 (1-C), 128.25, 128.05, 127.57, 127.44, 126.71 (Bn), 73.02 (OBn), 68.24 (6-C), 55.24 (4-C), 51.40 (NBn), 38.28 (3-C), 34.17 (5-C), 0.23 (Si(CH₃)₃).

***N*-Benzyl-(2'-benzyloxyethyl)-3,4-didehydropiperidine 12**

7 (85 mg, 0.23 mmol) was dissolved in anhydrous acetonitrile (7 cm³), paraformaldehyde (218 mg, 7.3 mmol) and (1S)-(+)-camphor-10-sulfonic acid monohydrate (CSA, 54.1 mg, 0.23 mmol) were added and the solution was stirred at reflux for 19 h, cooled and evaporated to dryness under reduced pressure. The residue was dissolved in EtOAc (20 cm³), washed successively with sat. aq. NaHCO₃ (5 cm³) and H₂O (5 cm³), dried (MgSO₄), celite was added and the solvents were evaporated under reduced pressure. The solid residue was applied to dry column vacuum chromatography (5.0 x 2.0 cm) on silica gel eluting with a gradient of 0-50% EtOAc in hexane (v/v) to give amine **12** (51 mg, 72%) as a colourless oil. R_f (1:1 EtOAc/hexane) 0.40; m/z (EI) 307 [M]⁺, 306 [M-H]⁺, 216 [M-PhCH₂]⁺, 172 [M-BnOCH₂CH₂]⁺, 91 [C₅H₆CH₂]⁺; δ_H (CDCl₃) 7.32-7.19 (10 H, m, Bn), 5.74-5.69 (1 H, m, 3-H), 5.60-5.56 (1 H, m, 4-H), 4.48 (2 H, s, OBn), 3.64 (2 H, s, NBn), 3.56 (2 H, dd, J 6.6 and 13.4, 2'-H), 3.03-2.97 (3 H, m, 2-H, 6-H), 2.28 (1 H, dp, J 2.7 and 17.6, 5_a-H), 2.03-1.91 (1 H, m, 1'_a-H), 1.94-1.84 (1 H, m, 5_b-H), 1.74-1.62 (1 H, m, 1'_b-H). δ_C (CDCl₃) 139.69, 138.55, 128.72, 128.27, 128.10, 127.54, 127.41, 126.69 (Bn), 125.01 (4-C), 124.14 (3-C), 72.93 (BnO), 68.20 (2'-C), 56.38 (BnN), 52.80 (6-C), 47.80 (2-C), 29.07 (1'-C), 27.94 (5-C).

***trans*-N-Benzyl-(2'-benzyloxyethyl)-2-(*n*-hexyl)-3,4-didehydropiperidine 13**

7 (103 mg, 0.28 mmol) was dissolved in anhydrous acetonitrile (2.5 cm³), heptanal (0.20 cm³, 1.43 mmol) and CSA (65 mg, 0.28 mmol) were added and the mixture was stirred at 120°C in a pressure

bottle for 70 h. After cooling, sat. aq. NaHCO₃ (0.25 cm³) and celite were added and the solvents were evaporated under reduced pressure. The solid residue was applied twice to dry column vacuum chromatography (5.2 x 2.0 cm) on silica gel eluting with CH₂Cl₂ followed by a gradient of 0-10% EtOAc in hexane (v/v) to give amine **13** (32 mg, 29%) as a light yellow oil after coevaporation with hexane (10 cm³). R_f (1:9 EtOAc/hexane (v/v)) 0.24; *m/z* (EI) 391 [M]⁺, 390 [M-H]⁺, 306 [M-C₆H₁₃]⁺, 300 [M-PhCH₂]⁺, 256 [M-BnOCH₂CH₂]⁺, 91 [C₅H₆CH₂]⁺; δ_H (CDCl₃, selected signals) 7.37-7.22 (10 H, m, Bn), 5.81 (1 H, dt, *J* 2.2 and 10.0, 3-H), 5.60 (1 H, dt, *J* 1.6 and 10.2, 4-H), 4.58 (1 H, d, *J* 11.9, OBn), 4.52 (1 H, d, *J* 11.9, OBn), 3.77 (1 H, d, *J* 13.7, NBn), 3.72-3.66 (2 H, m, 2'-H), 3.38 (1 H, d, *J* 13.7, NBn), 3.25 (1 H, septet, *J* 4.8, 6-H), 2.87 (1 H, bs, 2-H), 2.06-1.87 (2 H, m, 1'_a-H, 5_a-H), 1.84-1.72 (2 H, m, 1'_b-H, 5_b-H), 1.58-1.44 (2 H, m, 1''-H), 1.39-1.04 (8 H, m, 2''-H, 3''-H, 4''-H, 5''-H), 0.86 (3 H, t, *J* 6.8, 6''-H). δ_C (CDCl₃, selected signals) 140.92, 138.62 (Bn), 129.78 (4-C), 128.72, 128.40, 128.27, 127.90, 127.63, 127.57, 127.41, 126.38 (Bn), 124.99 (3-C), 73.06 (OBn), 68.07 (2'-C), 56.86 (2-C), 49.63 (NBn), 48.32 (6-C), 34.02 (1''-C), 32.25 (1'-C), 31.89 (2''-C), 29.22 (3''-C), 26.91 (5-C), 26.29 (4''-C), 22.65 (5''-C), 14.11 (6''-C).

4-(*N*-Benzyl)amino-6-benzyloxy-1-hexene **15B**

7 (51.1 mg, 0.14 mmol) was dissolved in anhydrous acetonitrile (2.5 cm³), cyclopentanone (0.075 cm³, 0.85 mmol) and triflic acid (21.8 mg, 0.145 mmol) were added and the mixture was stirred at 120°C in a pressure bottle for 40 h. After cooling, sat. aq. NaHCO₃ (0.25 cm³) and celite were added and the solvents were evaporated under reduced pressure. The solid residue was applied to dry column vacuum chromatography (5.7 x 2.0 cm) on silica gel eluting with a gradient of 0-100% EtOAc in hexane (v/v) to give alkene **15B** (31 mg, 75%) as a colourless oil. R_f (1:1 EtOAc/hexane (v/v)) 0.12; *m/z* (EI) 296 [M+H]⁺, 294 [M-H]⁺, 254 [M-CH₂=CHCH₂]⁺, 160 [M-BnOCH₂CH₂]⁺, 91 [C₅H₆CH₂]⁺; δ_H (CDCl₃) 7.34-7.22 (10 H, m, Bn), 5.87-5.73 (1 H, m, 2-H), 5.13-5.09 (1 H, m, 1'-

H), 5.07 (1 H, t, J 1.1, 1''-H), 4.50 (2 H, s, OBn), 3.82 (1 H, d, J 13.0, NBn), 3.75 (1 H, d, J 12.8, NBn), 3.67-3.54 (2 H, m, 6-H), 2.83 (1 H, p, J 6.0, 4-H), 2.29-2.24 (2 H, m, 3-H), 1.78 (2 H, q, J 6.2, 5-H), 1.66 (1 H, bs, NH). δ_C (CDCl₃) 140.70, 138.46 (Bn), 135.44 (2-C), 128.27, 128.10, 127.57, 127.44, 126.74 (Bn), 117.28 (1-C), 72.99 (OBn), 68.08 (6-C), 54.36 (4-C), 51.17 (NBn), 38.64 (3-C), 33.99 (5-C).

cis*-4-[(*N*-Benzyl)-{*N*-(*R,S*)-(2-phenyl)-acetonitrile}]amino-6-benzyloxy-1-*C*-trimethylsilyl-1-hexene **16*

7 (124 mg, 0.34 mmol), benzaldehyde (0.050 cm³, 0.49 mmol) and KCN (33 mg, 0.51 mmol) were dissolved in anhydrous MeOH (5 cm³), AcOH (0.07 cm³, 1.2 mmol) was added and the solution was stirred at 60°C for 27 h. After cooling, celite was added and the solvents were evaporated under reduced pressure. The solid residue was coevaporated with anhydrous acetonitrile (20 cm³) and applied to dry column vacuum chromatography (3.9 x 3.3 cm) on silica gel eluting with a gradient of 0-20% EtOAc in hexane (v/v) to give diastereomeric nitriles **16** (137 mg, 84%) as a colourless oil. R_f (1:3 EtOAc/hexane (v/v)) 0.60; m/z (EI) 482 [M]⁺, 467 [M-CH₃]⁺, 369 [M-Me₃SiCH=CHCH₂]⁺, 91 [C₅H₆CH₂]⁺; δ_H (CDCl₃) 7.49-7.17 (30 H, m, Ph, Bn), 6.13-5.98 (2 H, m, 2-H, 2'-H), 5.55 (1 H, dd, J 1.1 and 14.1, 1-H), 5.47 (1 H, dt, J 1.6 and 14.3, 1'-H), 4.86 (2 H, 2s, α -H, α' -H), 4.50 (1 H, d, J 11.9, OBn), 4.42 (1 H, d, J 11.9, OBn), 4.28 (1 H, d, J 11.9, OBn'), 4.20 (1 H, d, J 12.1, OBn'), 3.89 (1 H, d, J 13.6, NBn), 3.85 (1 H, d, J 13.7, NBn'), 3.71 (1 H, d, J 13.6, NBn), 3.70 (1 H, d, J 13.7, NBn'), 3.59-3.52 (1 H, m), 3.49-3.41 (2 H, m) (2 x 6-H, 6'-H), 3.14-3.06 (1 H, m, 6'-H), 3.05-2.95 (2 H, m), 2.88 (1 H, tt, J 3.5 and 10.1) (3'-H, 4-H, 4'-H), 2.53-2.42 (1 H, m, 5'-H), 2.33-2.22 (3 H, m, 2 x 3-H, 3'-H), 1.82-1.54 (3 H, m, 2 x 5-H, 5'-H), 0.13 (9 H, s, Si(CH₃)₃), 0.00 (9 H, s, Si(CH₃)₃'). δ_C (CDCl₃) 146.39, 145.32 (2-C, 2'-C), 138.36, 137.96, 137.82 (Bn), 134.28, 134.19 (Ph), 131.32, 129.81 (1-C, 1'-C), 129.06, 128.98, 128.60, 128.57, 128.43, 128.36, 128.27, 128.20, 128.03, 127.55, 127.44, 127.39, 127.36 (Bn, Ph), 118.15, 117.97 (CN,

CN'), 72.73 (OBn, OBn'), 67.96, 67.63 (6-C, 6'-C), 54.99, 54.52 (4-C, 4'-C), 54.30, 53.88 (α -C, α' -C), 50.93, 50.62 (NBn, NBn'), 35.63 (3-C), 32.95 (3'-C), 31.79 (5-C), 29.44 (5'-C), 0.22, 0.041 ((Si(CH₃)₃), (Si(CH₃)₃)).

***trans*-N-Benzyl-(2'-benzyloxyethyl)-2-phenyl-3,4-didehydropiperidine 14**

16 (137 mg, 0.28 mmol) was dissolved in anhydrous acetonitrile (2.5 cm³), AgBF₄ (57 mg, 0.29 mmol) was added and the mixture was stirred at 120°C in a pressure bottle for 20 h. After cooling, sat. aq. NaHCO₃ (0.25 cm³) and celite were added and the solvents were evaporated under reduced pressure. The solid residue was applied to dry column vacuum chromatography (5.3 x 2.0 cm) on silica gel eluting with a gradient of 0-40% EtOAc in hexane (v/v) to give piperidine **16** (50.4 mg, 46%) and amine **7** (14.6 mg, 14%) as colourless oils. **16**: R_f (1:9 EtOAc/hexane (v/v)) 0.25; *m/z* (EI) 383 [M]⁺, 382 [M-H]⁺, 292 [M-PhCH₂]⁺, 248 [M-BnOCH₂CH₂]⁺, 91 [C₅H₆CH₂]⁺; δ_{H} (CDCl₃) 7.44-7.23 (15 H, m, Ph, Bn), 5.92 (1 H, ddt, *J* 1.6, 3.7 and 10.1, 4-H), 5.77 (1 H, ddt, *J* 1.8, 3.0 and 9.9, 3-H), 4.46 (1 H, d, *J* 11.7, OBn), 4.40 (1 H, d, *J* 11.7, OBn), 4.15 (1 H, bs, 2-H), 3.69 (1 H, d, *J* 13.7, NBn), 3.59 (1 H, d, *J* 13.2, NBn), 3.54 (2 H, dt, *J* 1.3 and 6.8, 2'-H), 3.14-3.06 (1 H, m, 6-H), 2.22 (1 H, d(sextet), *J* 2.6 and 17.6, 5_a-H), 2.11-2.00 (2 H, m, 1'_a-H, 5_b-H), 1.83-1.72 (1 H, m, 1'_b-H). δ_{C} (CDCl₃) 143.54 (Ph), 140.31, 138.51 (Bn), 128.73, 128.60, 128.39, 128.23, 128.09, 128.05, 127.57, 127.36, 126.73, 126.60 (Bn, Ph, 4-C), 124.76 (3-C), 72.89 (OBn), 68.41 (2'-C), 60.90 (2-C), 51.32 (NBn), 48.51 (6-C), 28.44, 28.23 (5-C, 1'-C).

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