Modification of Silica-supported Tungsten Neosilyl Oxo Precatalysts: Impact of Substituted Phenol on Activity and Stability in Olefin Metathesis.

Y. Bouhoute,[a] I. Del Rosal,[b] K. C. Szeto,[a] N. Merle,[a] D. Grekov,[c] A. De Mallmann,[a] E. Le Roux,[d] L. Delevoye,[c] R. M. Gauvin,[c,*] L. Maron,[b,*] M. Taoufik[a,*]

[a] Laboratoire de Chimie, Catalyse, Polymères et Procédés, UMR 5265 CNRS/ESCPE-Lyon/UCBL, ESCPE Lyon, F-308-43, Boulevard du 11 Novembre 1918, F-69616 Villeurbanne Cedex, France. E-mail : mostafa.taoufik@univ-lyon1.fr

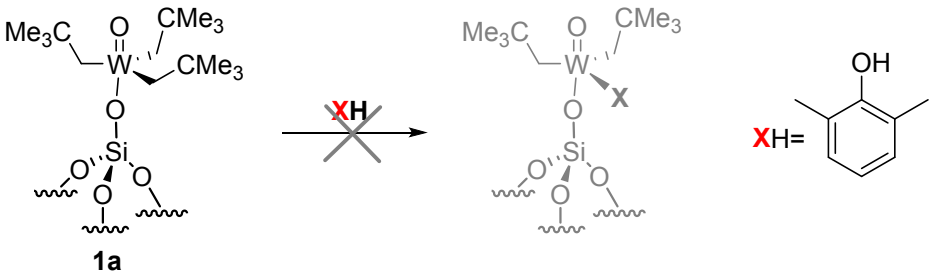
[b] Laboratoire de Physico-Chimie des Nano-Objets, CNRS UMR 5215, Université de Toulouse, INSA, UPS, 135 avenue de Rangueil, F-31077 Toulouse, France. E-mail : laurent.maron@irsamc.ups-tlse.fr

[c] Univ. Lille, CNRS, Centrale Lille, ENSCL, Univ. Artois, UMR 8181, UCCS – Unité de Catalyse et Chimie du Solide, F-59000 Lille, France. E-mail : regis.gauvin@ensc-lille.fr

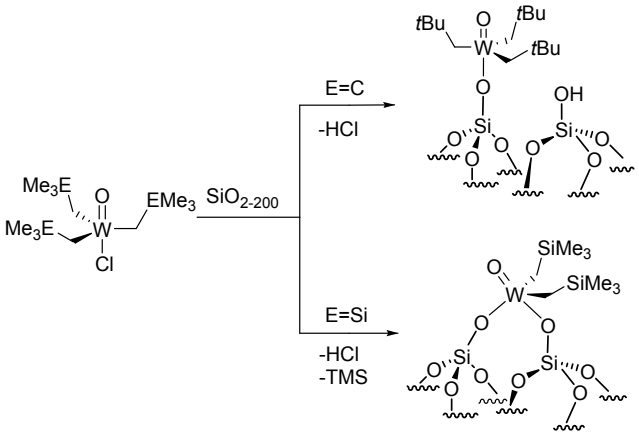
[d] Kjemisk Institutt, Universitetet i Bergen, Allégaten 41, N-5007, Bergen, Norway.

SUPPORTING INFORMATION

Table of contents



Scheme S1. Reaction of $[(\equiv SiO)W(=O)(CH_2CMe_3)_3]$ with 2,6-dimethylphenol



Scheme S2. Reaction of $[(\equiv SiO)W(=O)(CH_2EMe_3)_3]$ (E = Si, C) with $SiO_{2\text{-}200}$

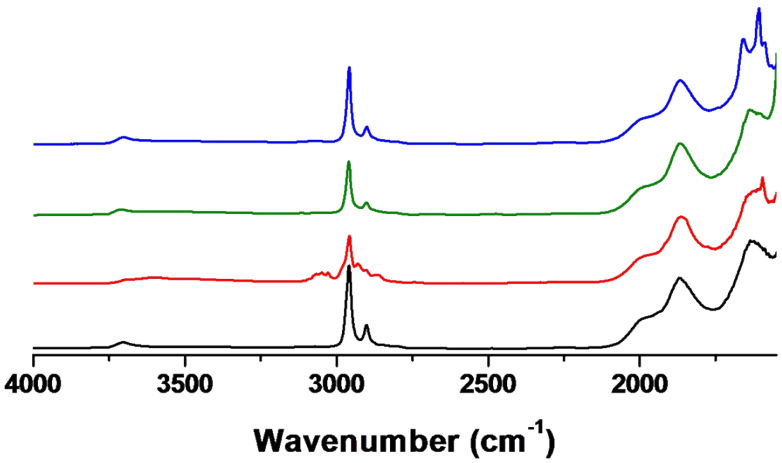


Figure S1. DRIFT spectra of **1b** (black), **2a** (red), **2b** (green) and **2c** (blue).

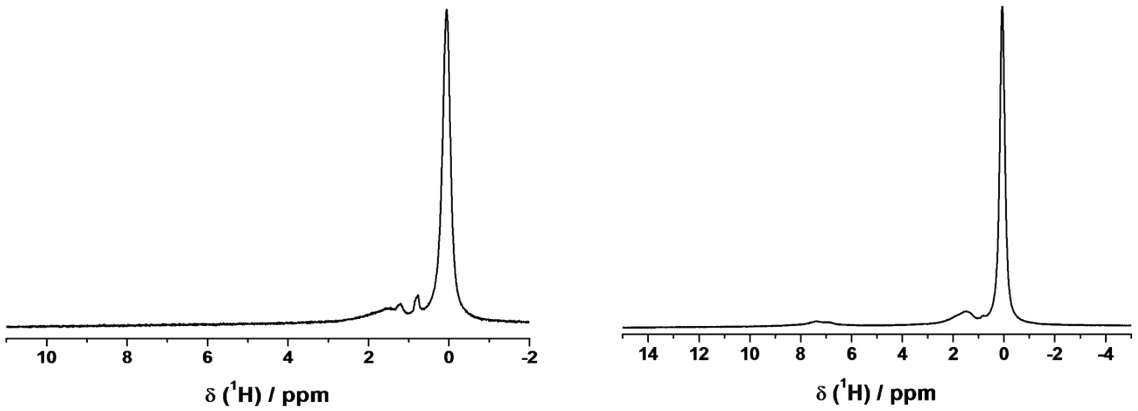


Figure S2. ^{1}H MAS NMR spectra of **2b** (left) and **2c** (right) (11.75 T, spinning rate 10 kHz).

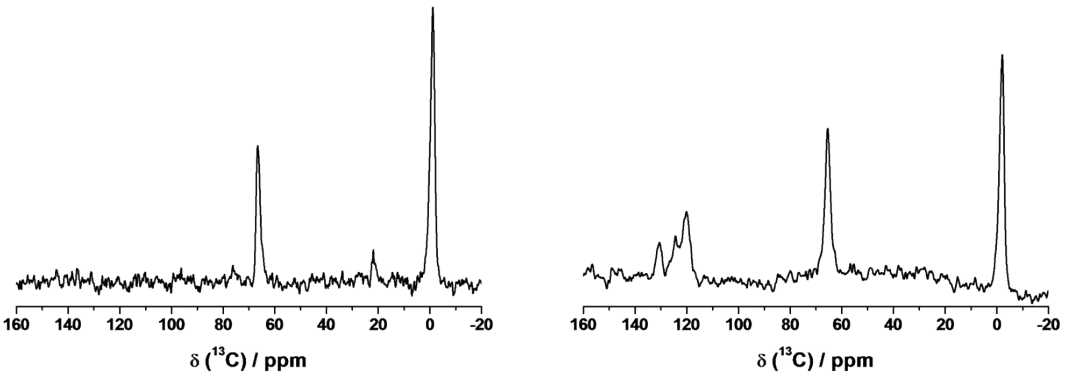


Figure S3 ^{13}C CPMAS NMR spectra of **2b** (left) and **2c** (right) (11.75 T, spinning rate 10 kHz).

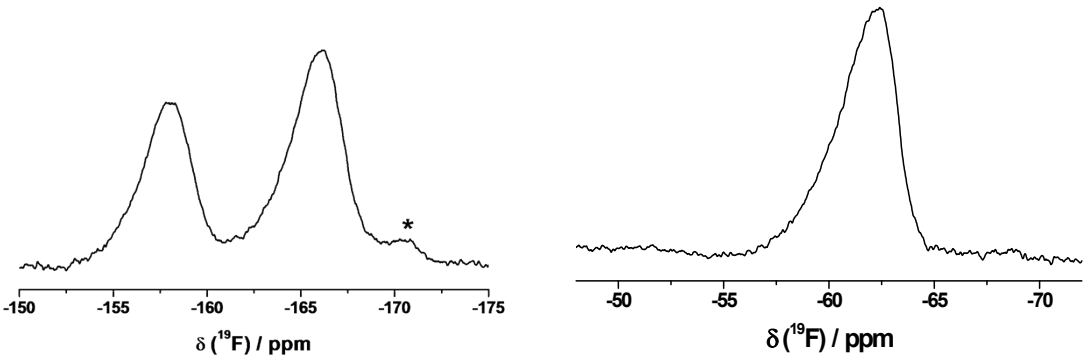


Figure S4 ^{19}F MAS NMR spectra of **2b** (left) and **2c** (right) (11.75 T, spinning rate 12 kHz).

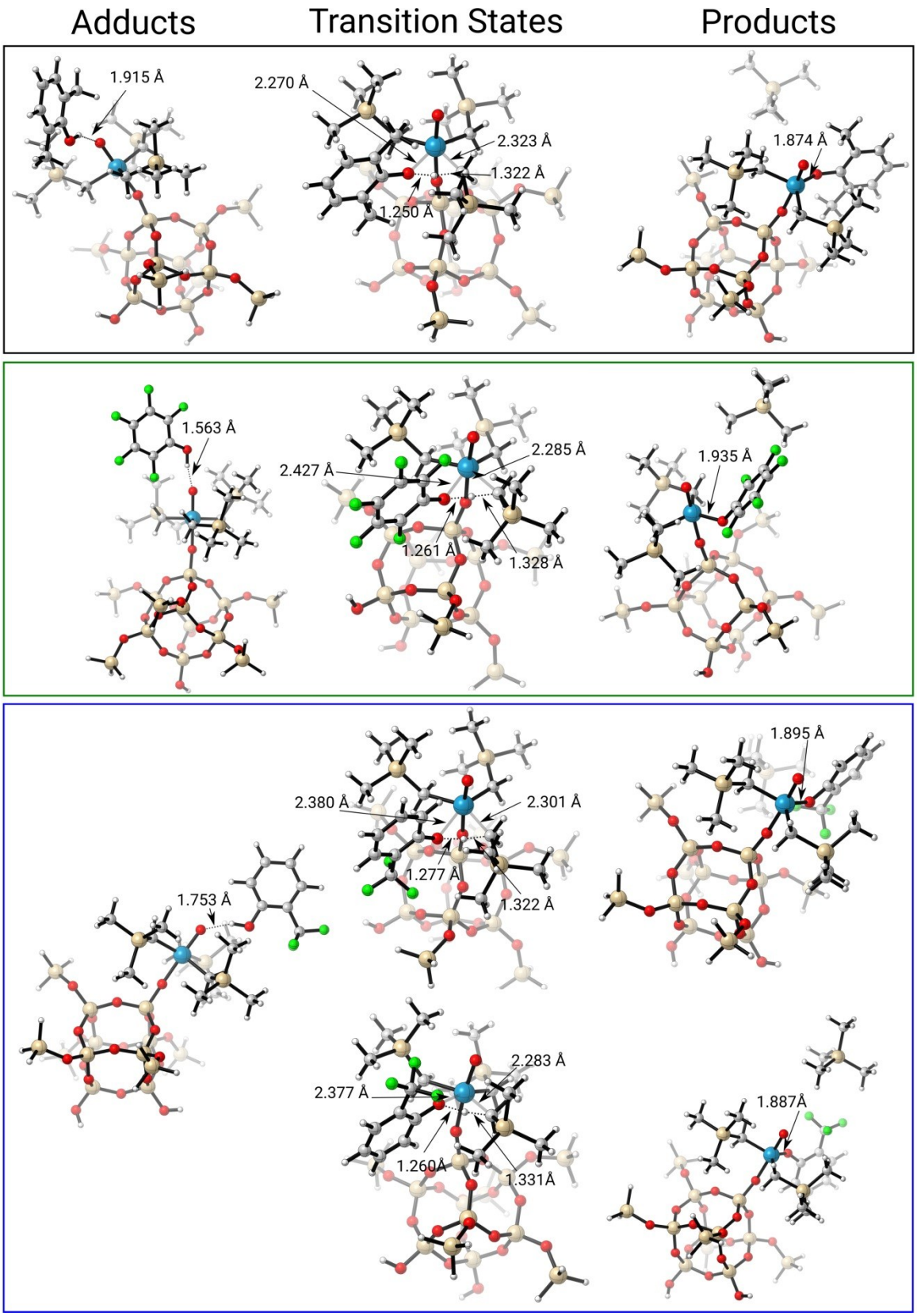


Figure S5. Optimized geometries and relevant distances (in Å) of the extrema for the modification of **1b** by XH (XH = 2,6-dimethylphenol (black), pentafluorophenol (green) or trifluoromethylphenol (blue)).

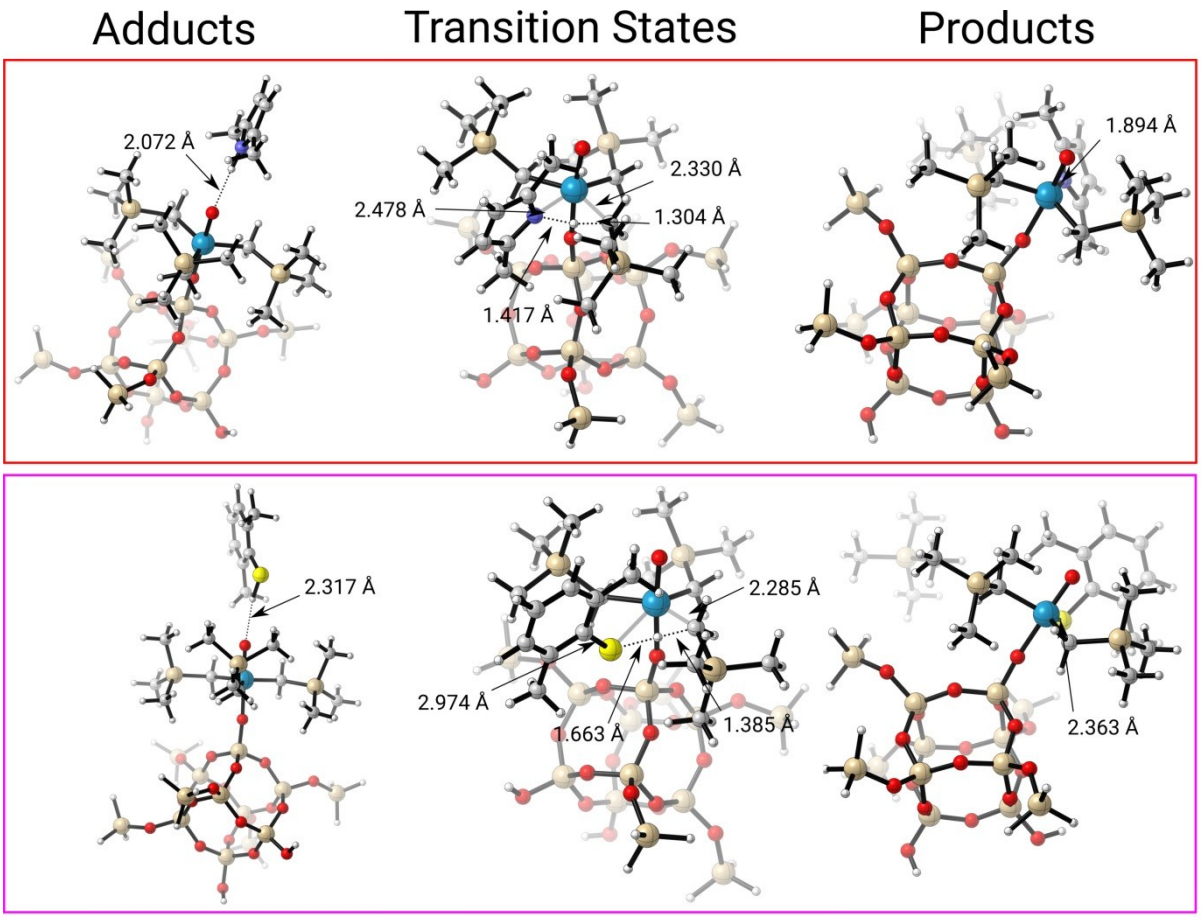
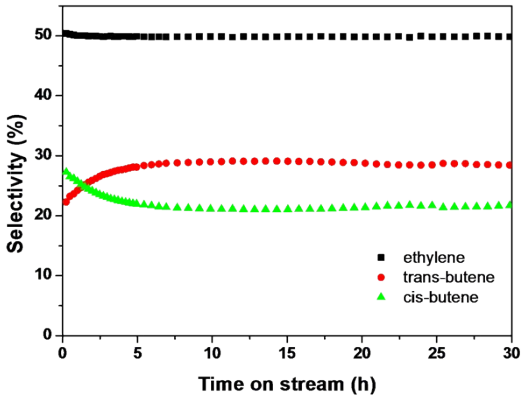
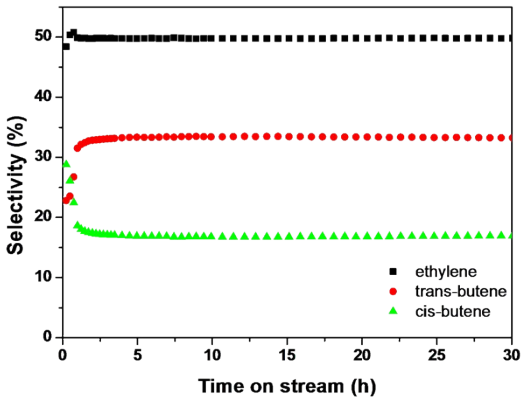


Figure S6. Optimized geometries and relevant distances (in Å) of the extrema for the modification of **1b** by XH (XH = 2,5-dimethyl-1H-pyrrole (red) or 2,6-dimethylbenzenethiol (pink)).





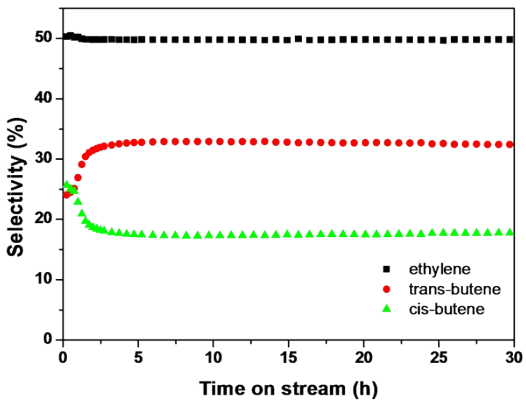


Figure S7. Product distribution of propylene self-metathesis (20 mL_{C3H6} min^{-1}; 80 °C; 60 mol_{C3H6} mol_W^{-1} min^{-1}, 1 bar) over **2a** (top), **2b** (middle) and **2c** (bottom).

Table S1. Functional and solvation effect on the Gibbs free energy data (in kcal mol^{-1}) for the modification of **1b** by XH (XH = pentafluorophenol, trifluoromethylphenol or 2,5-dimethyl-1H-pyrrole). All the Gibbs free energies are calculated with respect to the separated reactants, **1b** + XH. In black using the B3PW91 functional, in blue a single point calculation using the B3PW91 functional + the SMD solvation model, in green by using the B3PW91 functional + the SMD solvation (with geometry optimization) and in red using the M06L functional + the SMD solvation model.

	Adduct	Transition State	Activation Barrier	Δ(Activation Barrier)
pentafluorophenol	-0.1	32.5	32.6	
	0.9	38.9	38.9	+6.3
	0.9	33.8	33.8	+1.2
	-2.1	21.1	23.2	-9.4
trifluoromethylphenol	1.6	34.0	34.0	
	8.7	42.9	42.9	+8.9
	1.9	36.0	36.0	+2.0
	-1.7	25.1	26.8	-7.2
2,5-dimethyl-1H-pyrrole	4.1	58.9	58.9	
	12.0	64.7	64.7	+6.2
	9.3	60.5	60.5	+1.6
	6.4	45.5	45.5	-13.4

Cartesian Coordinates:

17
TMS
C -5.32626 0.58465 12.82872
Si -7.04569 0.10837 12.18134
C -7.49709 -1.62855 12.79820
C -8.32864 1.35723 12.81069
C -7.03222 0.12302 10.28369
H -4.56497 -0.12192 12.48164
H -9.33237 1.10792 12.45028
H -8.36196 1.37405 13.90518
H -8.09417 2.37082 12.46842
H -6.77753 1.11627 9.89888
H -8.01284 -0.14983 9.87949
H -6.29857 -0.58659 9.88660
H -8.48518 -1.93123 12.43575
H -6.77212 -2.37226 12.45066
H -7.51640 -1.66749 13.89249
H -5.30269 0.59027 13.92353
H -5.03831 1.58288 12.48265
100
Grafted neosylil complex **1b**
O -1.05881 1.09470 12.99887
W -0.98806 0.13404 14.41730
O -0.87964 -0.99205 16.06742
Si -0.85975 -1.95742 17.36513
O -1.23895 -1.08554 18.72977
Si -2.00964 -1.24368 20.17567
O -0.91242 -1.61591 21.35997
Si 0.54227 -2.38941 21.53476
O 0.30153 -3.97906 21.91759
Si -0.82019 -5.18194 21.72830
O -0.88057 -6.14305 23.06089
C -2.31817 -1.30259 13.65939
Si -1.82508 -2.67265 12.41276
C -0.17392 -3.49181 12.85460
C 1.11376 -0.11278 14.34856
Si 2.21663 0.71911 13.03823
C 2.04577 2.60303 13.10193
O 0.64369 -2.63311 17.56292
Si 1.68768 -3.12280 18.73856
O 1.50964 -4.74639 19.00897
Si 0.33756 -5.91406 18.94230
O -0.41978 -6.08193 20.39851
O -1.97921 -3.17430 17.18139
Si -2.20974 -4.75410 17.58557
O -3.05217 -5.47337 16.37555
Si -4.25022 -6.66517 16.34581
O 3.22167 -2.84675 18.23175
Si 4.56293 -2.08316 18.91632
O 1.42862 -2.28095 20.14344
C -3.19154 -3.98473 12.51093
C -1.75394 -1.93944 10.67106
C 1.77497 0.11535 11.29977
C 4.01368 0.23982 13.43423

O	-0.75358	-5.52058	17.76034
O	-3.07722	-4.88194	18.99355
Si	-3.36556	-4.03552	20.38411
O	-2.33213	-4.53629	21.57651
O	1.02228	-7.37871	18.63546
O	-3.17754	-2.41702	20.10412
O	-2.72371	0.18552	20.54745
Si	-4.24352	0.59318	21.16432
O	-4.90882	-4.29485	20.86206
Si	-5.63553	-5.18674	22.09994
O	1.39037	-1.67380	22.73880
Si	1.05586	-0.45744	23.86124
H	4.85212	-2.64875	20.26602
H	-3.94746	-7.73654	17.33909
H	-4.24781	-7.23009	14.96731
H	-5.57748	-6.05447	16.64538
H	-4.55086	-0.22488	22.37373
H	-5.29191	0.37814	20.12573
H	0.86235	0.84718	23.16401
H	-0.16510	-0.79729	24.64829
H	1.55181	-7.41628	17.83348
H	2.24134	-0.38506	24.76057
H	5.70471	-2.34507	17.99559
H	4.32068	-0.61494	19.02342
H	-0.10556	-6.69671	23.19465
H	-5.36420	-4.54611	23.41903
H	-5.12637	-6.58855	22.09854
H	-7.09803	-5.17133	21.81553
H	-4.17110	2.03574	21.52855
H	0.75592	0.42106	11.04695
H	1.84549	-0.97389	11.21443
H	2.45440	0.55113	10.55921
H	4.15170	-0.84613	13.40139
H	4.70633	0.68708	12.71271
H	4.30411	0.58341	14.43283
H	1.02172	2.89363	12.85060
H	2.72040	3.07294	12.37803
H	2.29118	3.00258	14.09130
H	1.25189	-1.20564	14.30327
H	1.46204	0.16383	15.35567
H	-3.00843	-4.78919	11.79006
H	-3.22812	-4.42769	13.51121
H	-4.17411	-3.55403	12.29218
H	-2.72447	-1.51989	10.38635
H	-1.49043	-2.70628	9.93475
H	-1.01211	-1.13866	10.60946
H	-0.02046	-4.38095	12.23329
H	0.67221	-2.81985	12.68343
H	-0.15474	-3.80905	13.90211
H	-2.73472	-1.80816	14.53958
H	-3.11904	-0.73475	13.16419
C	-1.93545	1.58150	15.60781
H	-2.68087	2.07561	14.97049
H	-2.45889	0.99984	16.37866
Si	-1.02422	2.98891	16.54108

C -2.16358 3.49060 17.97269
C 0.63464 2.42447 17.25955
C -0.77689 4.45656 15.37260
H -0.28914 5.28844 15.89214
H -0.15581 4.18300 14.51528
H -1.73784 4.81694 14.99079
H -1.74713 4.34351 18.51979
H -3.15600 3.77645 17.60892
H -2.28276 2.66248 18.67872
H 1.03911 3.19621 17.92342
H 0.51460 1.50675 17.84356
H 1.37471 2.24147 16.47475
13
Pentafluoro
F -0.90065 2.97498 15.23558
C -1.34625 3.30172 16.44833
C -1.67320 2.29840 17.36306
C -2.13647 2.68332 18.62167
C -2.27628 4.01848 18.97695
C -1.94627 5.00740 18.05469
C -1.48218 4.64351 16.79281
O -1.53571 1.00187 17.01386
F -2.44891 1.70881 19.49648
F -2.72134 4.34965 20.18785
F -2.07320 6.29468 18.37665
F -1.16577 5.58805 15.90872
H -1.80433 0.45959 17.76746
113
Adduct
C 1.06274 -6.24346 16.26465
C 1.23828 -5.42132 17.38252
C 1.09373 -6.02424 18.64077
C 0.79049 -7.37453 18.76826
C 0.62077 -8.16993 17.63758
C 0.75923 -7.59559 16.37977
O 1.53003 -4.11810 17.32777
F 1.25119 -5.28593 19.74145
F 0.66068 -7.91442 19.98113
F 0.32901 -9.46708 17.76179
F 0.60161 -8.33752 15.28122
F 1.19278 -5.71215 15.03334
O 1.85372 -2.84615 15.00845
W 2.02102 -2.28819 13.38162
C 0.10986 -2.96501 12.85047
Si -1.50111 -1.94767 13.09574
C -2.11662 -2.16279 14.87097
C 2.41338 -0.28388 13.91517
Si 2.47389 0.34433 15.71573
C 2.86718 2.20182 15.63019
O 2.19908 -1.65930 11.51961
Si 2.33980 -1.27455 9.94684
O 3.62736 -2.09483 9.29501
Si 4.11279 -2.80242 7.88691
O 5.04273 -4.10149 8.25244
Si 5.08793 -5.69672 7.69183

C	3.54668	-3.66159	12.95470
Si	5.40854	-3.36745	13.32295
C	5.77106	-3.75998	15.13685
C	3.83092	-0.53373	16.69818
C	0.80893	0.09552	16.57759
O	2.58895	0.35501	9.78199
Si	3.39310	1.43052	8.82409
O	4.73116	0.72441	8.14710
Si	5.17027	-0.09493	6.77968
O	4.22987	0.39413	5.51110
Si	2.85383	-0.05048	4.70435
O	1.57434	0.79949	5.32072
Si	1.08635	1.48570	6.73934
O	0.19957	0.40958	7.63323
Si	0.03530	-1.22044	7.86331
O	-1.53075	-1.56550	8.20315
Si	-2.85623	-2.00969	7.25056
O	0.94973	-1.70589	9.14781
O	2.38315	1.98914	7.63803
O	3.86761	2.69430	9.75151
Si	5.29424	3.59005	9.88036
O	0.16599	2.77817	6.30520
C	6.34580	-4.58104	12.20726
C	5.95115	-1.60505	12.88955
C	-1.26641	-0.11252	12.68687
C	-2.75779	-2.68204	11.88130
O	0.48179	-2.02541	6.48498
Si	1.80442	-2.75200	5.80878
O	2.61158	-1.67759	4.84269
O	1.31367	-4.02907	4.91307
Si	1.26838	-4.37732	3.25915
O	2.80701	-3.30734	7.00176
O	5.01219	-1.72903	7.00426
O	6.73560	0.26056	6.46161
Si	8.09060	-0.63572	5.99893
O	2.99678	0.24126	3.09306
H	0.17322	-3.17990	11.77569
H	5.74057	4.05508	8.53497
H	-2.84987	-1.25346	5.96443
H	-4.07336	-1.67021	8.03910
H	-2.81051	-3.47533	6.98097
H	5.09555	-5.72178	6.20028
H	3.90992	-6.45097	8.20853
H	8.57733	-1.45175	7.14876
H	7.75804	-1.52647	4.84921
H	-0.15756	3.31023	7.03813
H	9.12852	0.35473	5.59836
H	4.97344	4.75876	10.74675
H	6.36211	2.76223	10.51191
H	2.97863	1.17061	2.84598
H	2.65429	-4.45351	2.71435
H	0.49002	-3.33313	2.53260
H	0.59425	-5.70000	3.13622
H	6.34893	-6.28671	8.22076
H	1.61927	-3.77516	16.40484

H	0.58524	-0.97005	16.67737
H	-0.00918	0.57611	16.03142
H	0.83412	0.52742	17.58390
H	2.10111	2.74701	15.06878
H	2.91617	2.63421	16.63562
H	3.83083	2.38183	15.14195
H	3.60183	-1.59764	16.80327
H	3.90667	-0.10692	17.70413
H	4.81063	-0.43098	16.22020
H	1.66684	0.29824	13.35151
H	3.37086	-0.05432	13.42033
H	-3.73536	-2.20222	12.00093
H	-2.42794	-2.52748	10.84923
H	-2.88747	-3.75696	12.04323
H	-2.28734	-3.22055	15.09705
H	-3.06340	-1.63219	15.01855
H	-1.39718	-1.77566	15.59763
H	-2.24135	0.38290	12.62395
H	-0.68202	0.40649	13.45247
H	-0.76384	0.01579	11.72316
H	-0.04238	-3.90792	13.39167
H	3.27597	-4.58908	13.47677
H	3.47860	-3.83376	11.87261
H	6.84014	-3.64878	15.34769
H	5.22375	-3.09979	15.81489
H	5.49025	-4.79177	15.37258
H	7.42588	-4.50294	12.37310
H	6.04894	-5.61523	12.41033
H	6.14942	-4.37092	11.15113
H	7.04303	-1.52800	12.93105
H	5.63508	-1.33757	11.87639
H	5.54182	-0.86685	13.58568

113
TS

C	-0.59376	2.10305	11.73591
C	-0.58420	0.97980	12.58051
C	-1.24067	1.11790	13.81180
C	-1.86739	2.30033	14.19089
C	-1.85546	3.39663	13.33415
C	-1.21310	3.29193	12.10295
O	0.00318	-0.14523	12.18385
W	1.64815	-1.79303	12.86747
C	2.86027	-3.51251	12.89842
Si	4.69150	-3.53817	13.47364
C	4.81950	-2.94919	15.26797
F	-1.26643	0.07415	14.65679
F	0.01804	2.03692	10.54900
O	1.23462	-1.97979	14.51415
O	2.05733	-1.72656	10.91592
Si	2.36891	-1.14194	9.43688
O	0.98523	-1.07955	8.52213
Si	0.28963	-0.14454	7.35930
O	0.59880	-0.78238	5.86088
Si	1.74906	-1.68037	5.08836
O	1.03182	-2.62056	3.95668

Si	0.97422	-2.60796	2.26844
C	-0.37729	-2.64657	12.24161
Si	-2.31461	-2.67957	11.99214
C	-3.13504	-2.60836	13.68963
C	2.76539	-0.05608	13.12482
Si	2.90519	1.17207	14.59130
C	2.19192	2.85170	14.08587
O	3.46131	-2.13061	8.66559
Si	3.84509	-2.66916	7.15704
O	4.42202	-4.20007	7.26941
Si	3.93446	-5.68650	6.63599
O	3.02526	0.37901	9.55990
Si	4.11878	1.37373	8.83800
O	5.29742	0.50353	8.06288
Si	5.59759	-0.16111	6.57892
O	7.21889	-0.16446	6.34913
Si	8.34155	-1.31052	5.82358
O	5.03079	-1.71509	6.50493
O	2.51464	-2.67197	6.16902
O	4.88558	0.75929	5.40522
Si	3.49328	0.82692	4.51144
O	2.84801	-0.68355	4.35259
O	3.80234	1.34410	2.98118
O	2.43492	1.86564	5.24752
Si	2.03177	2.37648	6.76471
O	1.46906	3.91084	6.57532
C	-2.90095	-1.27697	10.87735
C	-2.64752	-4.34773	11.16161
C	4.76665	1.40827	14.89918
C	2.08500	0.54850	16.17252
O	3.35656	2.37173	7.75943
O	4.82019	2.28479	10.00915
Si	6.32491	3.04145	10.13912
O	0.85792	1.40892	7.41591
O	-1.33111	-0.14147	7.61218
Si	-2.59445	0.83755	7.06592
C	5.25642	-5.34632	13.37062
C	5.78556	-2.50270	12.32566
H	6.73328	3.62984	8.83030
H	-2.28181	1.39244	5.71654
H	-2.81739	1.95107	8.03226
H	-3.80796	-0.02452	6.99565
H	3.97133	-5.65587	5.14502
H	2.55758	-6.02395	7.10193
H	8.51839	-2.36793	6.86092
H	7.89629	-1.92818	4.54061
H	1.15576	4.32623	7.38459
H	9.62205	-0.57615	5.62110
H	6.16882	4.11781	11.15795
H	7.34735	2.05548	10.59406
H	4.00948	2.28049	2.90800
H	2.31705	-2.93352	1.70714
H	0.52354	-1.27557	1.77230
H	-0.00928	-3.65838	1.88132
H	4.90576	-6.69350	7.14923

H	-0.43269	-1.32120	12.31286
H	2.51631	-0.40208	16.49810
H	1.01387	0.38874	16.03031
H	2.22581	1.28228	16.97408
H	1.10429	2.82489	13.98649
H	2.43877	3.60268	14.84437
H	2.61405	3.18640	13.13291
H	5.24892	0.47939	15.22072
H	4.92925	2.15487	15.68436
H	5.27604	1.75815	13.99524
H	2.81726	0.48055	12.17110
H	3.68978	-0.68231	13.16814
H	-3.72564	-4.49292	11.03136
H	-2.18052	-4.39703	10.17288
H	-2.26704	-5.17991	11.76228
H	-2.82742	-3.45340	14.31410
H	-4.22477	-2.64698	13.58532
H	-2.87380	-1.68784	14.21672
H	-3.94186	-1.45722	10.58594
H	-2.85904	-0.30949	11.38537
H	-2.29778	-1.21015	9.96721
H	-0.01478	-3.06031	11.29525
H	-0.31217	-3.37985	13.05357
H	2.37067	-4.23865	13.56238
H	2.87378	-3.91284	11.87675
H	5.85424	-3.00920	15.62223
H	4.48240	-1.91536	15.38478
H	4.20202	-3.57266	15.92270
H	6.29951	-5.44250	13.69126
H	4.64724	-5.99037	14.01310
H	5.18407	-5.72439	12.34570
H	6.83846	-2.63390	12.59875
H	5.66446	-2.82388	11.28630
H	5.56768	-1.43152	12.37056
F	-2.48205	2.38367	15.37220
F	-2.45591	4.53511	13.68651
F	-1.19683	4.33823	11.27318

113

Product

C	-2.54777	0.69515	14.35187
C	-1.33043	0.93266	13.72247
C	-0.51673	-0.12311	13.29899
C	-0.96613	-1.42721	13.53074
C	-2.17756	-1.67613	14.16200
C	-2.97532	-0.61139	14.57212
F	-0.93367	2.19199	13.52430
O	0.62804	0.11716	12.63961
W	2.43741	-0.28854	13.21452
C	3.81535	1.20815	13.68353
Si	3.19826	3.02614	13.84539
C	2.04095	3.17217	15.33203
F	-0.20515	-2.45672	13.13569
F	-2.58310	-2.93058	14.37059
F	-4.13982	-0.84173	15.17575
F	-3.30636	1.71651	14.74737

C	3.24135	-2.20125	13.04662
Si	4.97715	-2.58954	13.79475
C	6.33088	-1.57943	12.94238
O	1.97910	-0.51116	14.84937
O	2.89285	0.03714	11.32141
Si	3.17124	0.15679	9.72409
O	4.36970	1.27423	9.45355
Si	5.62609	1.54609	8.42242
O	6.81509	2.29865	9.26416
Si	8.50140	2.28921	9.17053
C	4.97614	-2.28271	15.66014
C	5.25552	-4.43114	13.43783
O	1.80055	0.61950	8.92033
Si	1.32696	1.49912	7.61072
O	-0.10322	2.20708	7.97257
Si	-1.02694	3.46194	7.32647
O	3.67150	-1.31987	9.15190
Si	3.54753	-2.27034	7.81000
O	2.18018	-1.90641	6.95029
Si	1.69237	-0.93203	5.70595
O	2.95457	-0.66401	4.66678
Si	4.14680	0.44729	4.41167
O	3.69478	1.94832	4.94430
Si	3.78355	2.88498	6.29902
O	2.44461	2.67199	7.25122
O	1.14119	0.50799	6.29746
O	0.48668	-1.69589	4.90658
Si	0.07652	-1.88104	3.27764
C	2.33139	3.55614	12.25240
C	4.75292	4.07752	14.12075
O	3.48238	-3.83841	8.28002
Si	2.43286	-5.11975	7.94403
O	4.88872	-2.05708	6.86044
Si	6.00790	-0.88483	6.51788
O	5.52954	-0.00465	5.20355
O	6.21463	0.12233	7.81334
O	5.13892	2.53035	7.18337
O	7.44878	-1.59298	6.19481
Si	7.94376	-3.18427	5.92003
O	4.38697	0.48185	2.78544
O	3.86004	4.43605	5.75322
C	-1.84454	-6.28151	16.05534
Si	-0.64043	-6.71034	14.65435
C	-0.27046	-8.57233	14.67856
C	0.97699	-5.74572	14.89986
C	-1.41212	-6.23594	12.98823
H	8.94862	2.36246	7.74897
H	-0.92483	3.47612	5.83755
H	-0.55098	4.76532	7.87530
H	-2.43588	3.21813	7.74349
H	2.36859	-5.36431	6.47373
H	1.07058	-4.82317	8.47241
H	7.80149	-3.98796	7.16858
H	7.13777	-3.79990	4.82595
H	3.94671	5.10193	6.44169

H 9.37711 -3.10943 5.52068
H 8.96836 3.49211 9.91613
H 9.03862 1.05340 9.80949
H 4.93669 1.20710 2.47419
H 1.02145 -2.82870 2.61971
H 0.10852 -0.56278 2.58043
H -1.30455 -2.43941 3.25846
H 3.00348 -6.31037 8.63474
H 0.78378 -4.66792 14.90049
H 2.49656 2.75221 16.23416
H 1.10068 2.64557 15.14913
H 1.80339 4.22304 15.52990
H 1.42158 2.97253 12.08495
H 2.04890 4.61317 12.30462
H 2.98811 3.42111 11.38756
H 5.28307 3.77281 15.02889
H 4.48679 5.13499 14.22618
H 5.44402 3.98694 13.27659
H 4.57044 1.21103 12.88759
H 4.27951 0.96104 14.64715
H -1.18573 -9.15750 14.53884
H 0.42610 -8.84784 13.87948
H 0.17712 -8.87540 15.63107
H -1.41222 -6.50871 17.03554
H -2.77653 -6.84942 15.96177
H -2.10021 -5.21736 16.03686
H -2.35483 -6.76880 12.82451
H -1.62189 -5.16279 12.95159
H -0.74272 -6.47839 12.15591
H 1.69083 -5.96386 14.09887
H 1.45142 -6.00321 15.85289
H 2.55710 -2.88804 13.56278
H 3.28401 -2.46538 11.98324
H 5.93330 -2.58670 16.09746
H 4.81427 -1.22732 15.89693
H 4.18247 -2.85570 16.14949
H 6.22801 -4.75801 13.82192
H 4.48260 -5.04515 13.90913
H 5.23467 -4.62678 12.36094
H 7.31852 -1.90494 13.28658
H 6.29406 -1.71040 11.85629
H 6.23781 -0.51150 13.15958
96
Product without TMS
C -2.67163 1.91371 13.76210
C -1.62419 1.00467 13.86676
C -1.83057 -0.27730 14.38559
C -3.12290 -0.61666 14.79815
C -4.17558 0.28472 14.70434
C -3.95036 1.55470 14.17956
F -0.40303 1.36746 13.46634
O -0.82667 -1.16931 14.42892
W -0.01277 -1.98618 15.98265
C 1.96669 -1.57528 16.51059
Si 2.86669 -0.08346 15.68766

C	2.02364	1.53189	16.19142
F	-3.34212	-1.83782	15.30081
F	-5.39648	-0.06235	15.10899
F	-4.95397	2.42481	14.08203
F	-2.45310	3.13022	13.26444
C	-0.89945	-3.57691	16.99536
Si	-0.05145	-4.31781	18.56124
C	1.65376	-5.03042	18.15905
O	-0.61961	-0.82303	17.08281
O	0.71800	-3.29338	14.69183
Si	1.50020	-4.34104	13.72728
O	3.13649	-4.18041	13.97107
Si	4.51963	-5.07408	13.99695
O	5.51400	-4.42670	15.13057
Si	6.70827	-5.08182	16.13121
C	0.06081	-3.00632	19.91901
C	-1.19589	-5.72359	19.12018
O	1.15371	-4.04988	12.13573
Si	1.86665	-4.10580	10.65207
O	1.24923	-2.88845	9.75065
Si	1.70933	-2.05306	8.35948
O	1.04739	-5.89248	14.10894
Si	0.82074	-7.35907	13.38709
O	0.43364	-7.17776	11.78753
Si	1.17481	-7.11837	10.30987
O	2.55718	-8.03120	10.33052
Si	4.17567	-7.84423	10.58739
O	4.67284	-6.31122	10.20607
Si	4.88030	-4.83840	10.91845
O	3.51004	-3.91738	10.78354
O	1.54538	-5.55661	9.92260
O	0.13718	-7.72811	9.20240
Si	0.27939	-8.76358	7.87495
C	2.87998	-0.28394	13.80902
C	4.64161	-0.13123	16.35473
O	-0.40245	-8.13909	14.14848
Si	-1.91222	-8.71718	13.65632
O	2.19487	-8.27092	13.54049
Si	3.83546	-8.08864	13.66840
O	4.53990	-8.14466	12.17515
O	4.20368	-6.64947	14.39700
O	5.26809	-4.99898	12.52217
O	4.44251	-9.29605	14.59241
Si	3.79367	-10.69161	15.28870
O	4.91498	-8.93162	9.60056
O	6.12880	-4.13460	10.10905
H	7.49154	-6.12121	15.40203
H	2.27284	-2.99287	7.34609
H	2.72838	-1.02032	8.70797
H	0.48130	-1.39929	7.82796
H	-1.74686	-9.77959	12.62246
H	-2.74300	-7.60303	13.11524
H	2.77742	-10.32690	16.31795
H	3.17058	-11.55373	14.24290
H	6.38481	-3.26733	10.43638

H 4.93540 -11.40447 15.92722
H 7.59676 -3.95087 16.52141
H 6.07808 -5.67660 17.34481
H 5.86786 -8.82576 9.52426
H 0.49064 -10.16365 8.34314
H 1.41377 -8.34046 7.00386
H -1.00673 -8.66206 7.12985
H -2.55113 -9.28702 14.87591
H 1.90158 1.59621 17.27714
H 1.03540 1.62058 15.73285
H 2.62191 2.38983 15.86578
H 1.86689 -0.24830 13.39858
H 3.45894 0.52225 13.34538
H 3.33333 -1.23769 13.52349
H 4.65899 -0.03080 17.44485
H 5.23384 0.68843 15.93319
H 5.13253 -1.07339 16.09105
H 2.56695 -2.46220 16.27556
H 1.99473 -1.37248 17.58921
H -1.88625 -3.25015 17.34786
H -1.02441 -4.40356 16.28546
H 0.46288 -3.44155 20.84019
H 0.70867 -2.17513 19.62601
H -0.92672 -2.59117 20.14375
H -0.80381 -6.19894 20.02609
H -2.20149 -5.35270 19.34249
H -1.28017 -6.49295 18.34614
H 2.03435 -5.59981 19.01399
H 1.60384 -5.70631 17.29977
H 2.38041 -4.24479 17.93339
16
Pyrrole
N -0.86994 1.42286 8.69283
C -2.14123 1.95157 8.67716
C -3.01936 1.93639 9.88235
C -0.26623 1.55990 7.46296
C 1.11839 1.07113 7.20290
C -1.17604 2.19176 6.64297
C -2.35282 2.43745 7.40494
H -0.43943 0.99423 9.49591
H -3.25984 2.91819 7.06316
H -1.00852 2.44782 5.60518
H -3.98101 2.39672 9.64385
H -3.22218 0.91779 10.23805
H -2.58652 2.49629 10.72169
H 1.39546 1.28073 6.16710
H 1.86129 1.55977 7.84681
H 1.21430 -0.01178 7.35578
116
Adduct
C -0.88828 0.81116 13.63164
Si 0.02130 2.25857 14.50913
C 1.49976 1.67227 15.53763
W 0.08678 -0.80459 12.71085
C 2.15233 -1.15370 12.97652

Si	3.48867	-0.65414	11.71505
C	3.23784	-1.56349	10.07483
N	-0.86529	1.41606	8.70016
C	-2.13546	1.94504	8.67887
C	-3.02075	1.94128	9.87922
C	-0.26674	1.55878	7.46965
C	1.11611	1.07080	7.19744
C	-1.17443	2.19196	6.64666
C	-2.35126	2.43477	7.40784
O	0.25922	0.03571	11.21731
O	-0.12802	-1.75938	14.44098
Si	-0.23390	-2.55818	15.84808
O	1.17994	-3.37328	16.14484
Si	2.15874	-3.82586	17.39078
O	3.71053	-3.78972	16.86661
Si	5.17524	-3.30393	17.55300
C	-1.21491	-2.23647	11.90011
Si	-0.65321	-3.90148	11.11987
C	-2.14877	-5.05991	11.25140
C	0.57437	3.52910	13.22187
C	-1.25542	3.03264	15.67874
O	-1.48434	-3.65001	15.78300
Si	-1.90007	-5.13097	16.37776
O	-2.81526	-5.90215	15.25735
Si	-4.31584	-6.67938	15.31492
O	-0.51193	-1.48284	17.08365
Si	-1.29971	-1.36840	18.52585
O	-2.59601	-2.39804	18.57855
Si	-2.97039	-3.93878	19.04858
O	-1.99903	-4.39972	20.30657
Si	-0.57539	-5.19475	20.56458
O	-0.28225	-6.29777	19.36603
Si	0.49099	-6.39745	17.91161
O	-0.54045	-6.02711	16.66919
O	-2.78116	-4.97411	17.77356
O	-4.53339	-3.96649	19.52957
Si	-5.34564	-4.48796	20.91730
C	-0.21193	-3.63252	9.30047
C	0.80483	-4.68912	12.03883
C	5.16415	-1.15816	12.45835
C	3.47780	1.21451	11.42160
O	-1.83737	0.17133	18.69406
Si	-3.18718	0.86089	19.44235
O	-0.25589	-1.71646	19.76508
Si	1.10188	-2.62226	20.05310
O	0.67914	-4.11577	20.62050
O	1.99609	-2.78690	18.67226
O	1.78836	-5.36913	17.86072
O	2.03082	-1.86630	21.16868
Si	1.81534	-0.56273	22.21975
O	-0.75211	-5.96544	22.00582
O	0.99864	-7.95793	17.79480
H	5.31059	-3.85148	18.93413
H	-4.34692	-7.66780	16.43159
H	-4.47092	-7.37681	14.00797

H	-5.40433	-5.67529	15.49246
H	-3.47477	0.17199	20.73440
H	-4.36973	0.76285	18.53943
H	1.73280	0.70994	21.44585
H	0.57445	-0.74524	23.02781
H	1.45286	-8.17635	16.97571
H	3.00937	-0.54357	23.11009
H	6.24861	-3.85103	16.67652
H	5.25272	-1.81478	17.58709
H	-0.05910	-6.59913	22.21373
H	-4.93861	-3.66177	22.09037
H	-5.05267	-5.92648	21.17874
H	-6.79707	-4.30080	20.63841
H	-2.84760	2.29008	19.68898
H	-0.43277	0.98130	9.50904
H	2.28920	-1.26961	9.61707
H	3.23717	-2.64972	10.21204
H	4.04211	-1.31856	9.37289
H	5.20786	-2.23567	12.64930
H	5.98524	-0.90515	11.77852
H	5.34620	-0.64253	13.40731
H	2.51525	1.53040	11.01014
H	4.26186	1.49564	10.71027
H	3.65887	1.76786	12.34901
H	2.23042	-2.23032	13.19270
H	2.37101	-0.66507	13.94024
H	-1.93745	-6.01724	10.76239
H	-2.39381	-5.26201	12.29897
H	-3.03149	-4.62533	10.77110
H	-1.04645	-3.17673	8.75781
H	0.01884	-4.58853	8.81796
H	0.65896	-2.98099	9.18793
H	0.95613	-5.71345	11.68088
H	1.73705	-4.14109	11.87245
H	0.62280	-4.73513	13.11675
H	-1.87584	-2.50651	12.73517
H	-1.81036	-1.73263	11.12757
H	-1.52047	1.27929	12.86548
H	-1.53656	0.35443	14.39068
H	1.05810	4.38341	13.70773
H	1.28640	3.09684	12.51332
H	-0.27875	3.90913	12.65052
H	-0.84373	3.92674	16.15964
H	-2.16395	3.32598	15.14308
H	-1.53283	2.32406	16.46550
H	1.83080	2.47487	16.20567
H	1.23041	0.81044	16.15578
H	2.35086	1.39747	14.90730
H	-3.25885	2.91691	7.06859
H	-1.00496	2.44937	5.60926
H	-3.99288	2.36971	9.62240
H	-3.19985	0.92898	10.26465
H	-2.60850	2.53722	10.70442
H	1.39738	1.31286	6.16942
H	1.85876	1.53252	7.86038

H 1.20581 -0.01674 7.31562
116
Transition state
C -0.86974 1.25031 14.55497
Si 0.23534 2.44992 15.56365
C 1.69697 1.54485 16.36367
W -0.24589 0.31069 12.75665
C 1.82565 0.27977 12.64641
Si 3.12011 1.00358 11.43288
C 2.46273 2.45351 10.41629
N -0.00088 -1.05868 10.70625
C -0.12160 -0.49758 9.42547
C -0.80648 0.79854 9.12842
C 0.64428 -2.28948 10.55239
C 0.98168 -3.22138 11.67007
C 0.91299 -2.49166 9.21715
C 0.43088 -1.36016 8.50537
O -0.46803 1.77943 11.91939
O -0.20262 -1.36796 13.85265
Si -0.06277 -2.35903 15.12664
O 1.52703 -2.77965 15.35217
Si 2.61245 -3.10257 16.54768
O 4.07757 -2.54578 16.06867
Si 5.44720 -1.99843 16.89265
C -2.29524 -0.53335 12.03755
Si -3.43679 -1.82877 11.13214
C -5.09200 -1.68506 12.04692
C 0.85033 3.86777 14.46911
C -0.85302 3.15335 16.95016
O -0.96362 -3.73599 14.89264
Si -0.92443 -5.34223 15.26361
O -1.59890 -6.16583 14.01923
Si -2.58447 -7.53154 13.89612
O -0.61324 -1.60620 16.50580
Si -1.38202 -1.91850 17.92865
O -2.34430 -3.26151 17.80279
Si -2.24812 -4.89560 18.04594
O -1.16181 -5.22699 19.24967
Si 0.43035 -5.62245 19.43499
O 1.01009 -6.41759 18.10458
Si 1.75395 -6.08549 16.66909
O 0.63836 -5.84415 15.47006
O -1.79277 -5.64480 16.64481
O -3.72886 -5.43543 18.48468
Si -4.32357 -6.39755 19.74054
C -3.66484 -1.37758 9.31453
C -2.74313 -3.57155 11.29104
C 3.76703 -0.36711 10.31024
C 4.53911 1.62157 12.53994
O -2.32043 -0.62752 18.30563
Si -3.93155 -0.45014 18.78297
O -0.26553 -2.13465 19.13152
Si 1.30108 -2.63879 19.32644
O 1.32973 -4.25396 19.67910
O 2.18262 -2.34713 17.95989

O	2.70781	-4.73740	16.79612
O	1.99345	-1.80292	20.55175
Si	1.42076	-0.98639	21.91425
O	0.49534	-6.61020	20.74783
O	2.67718	-7.40773	16.34320
H	5.65964	-2.79274	18.13777
H	-2.11793	-8.59731	14.83045
H	-2.48013	-8.00235	12.48685
H	-3.99618	-7.16581	14.21000
H	-4.23539	-1.34683	19.93585
H	-4.84118	-0.76273	17.64266
H	0.81888	0.31687	21.50951
H	0.40499	-1.81355	22.62890
H	3.14852	-7.37580	15.50540
H	2.60231	-0.75402	22.79120
H	6.59913	-2.18078	15.96524
H	5.28691	-0.55534	17.23097
H	1.33132	-7.07138	20.86429
H	-4.11368	-5.71912	21.05186
H	-3.64820	-7.72727	19.73890
H	-5.78070	-6.56217	19.47680
H	-4.09053	0.97471	19.18693
H	-1.24453	-0.92876	11.37375
H	1.86976	3.14628	11.01982
H	1.83432	2.09524	9.59722
H	3.30131	3.00843	9.98103
H	2.95996	-0.79806	9.71048
H	4.53012	0.03180	9.63263
H	4.22547	-1.17109	10.89552
H	4.21886	2.44327	13.18946
H	5.36972	1.98772	11.92626
H	4.92434	0.81771	13.17628
H	2.17025	-0.70544	12.97886
H	1.85197	0.94151	13.54725
H	-5.83152	-2.35555	11.59520
H	-4.99119	-1.96078	13.10173
H	-5.49014	-0.66637	11.99766
H	-4.07738	-0.37189	9.18730
H	-4.36405	-2.08501	8.85446
H	-2.71593	-1.43818	8.77330
H	-3.47523	-4.29073	10.90638
H	-1.82550	-3.67680	10.70469
H	-2.52324	-3.83490	12.32925
H	-2.49571	-0.79439	13.08256
H	-2.73417	0.43752	11.78981
H	-1.72048	1.89158	14.27799
H	-1.21084	0.50159	15.27838
H	1.42313	4.59136	15.05933
H	1.49256	3.50964	13.65916
H	0.00832	4.39505	14.00939
H	-0.28351	3.84488	17.58089
H	-1.70977	3.69957	16.54165
H	-1.23637	2.35093	17.58851
H	2.21961	2.22447	17.04608
H	1.34917	0.68645	16.94585

H 2.43360 1.18217 15.64032
H 0.46754 -1.19513 7.43541
H 1.40516 -3.36343 8.80327
H -0.85103 0.93004 8.04348
H -1.83718 0.83049 9.50054
H -0.29826 1.66618 9.55693
H 1.43415 -4.12318 11.24743
H 1.69923 -2.79858 12.38178
H 0.10435 -3.53101 12.24506
116
Product
C 0.18291 1.41881 14.14600
Si 1.14669 2.47971 15.42738
C 2.36779 1.45016 16.44412
W 1.19337 0.38143 12.61685
C 3.26702 0.04912 12.77862
Si 4.39420 0.44179 11.27615
C 4.75447 2.29801 11.25548
N 0.08516 -0.45988 11.18534
C -0.90233 0.19702 10.42219
C -1.35183 1.59834 10.67029
C 0.24040 -1.75924 10.66116
C 1.19324 -2.77880 11.19403
C -0.62830 -1.89781 9.61232
C -1.35117 -0.67643 9.46829
O 1.46822 1.88456 11.83949
O 0.99469 -1.18620 13.82584
Si 0.82277 -2.15763 15.11648
O 2.30788 -2.52714 15.76085
Si 3.00995 -2.83751 17.21947
O 4.54776 -2.27330 17.16930
Si 5.62981 -1.69947 18.33189
C -4.79414 -0.91887 12.03527
Si -5.63891 -2.49851 11.41256
C -7.26450 -2.76727 12.35638
C 2.04733 3.89649 14.55552
C -0.17626 3.18056 16.59261
O 0.06293 -3.56071 14.66411
Si 0.00766 -5.16446 15.04202
O -0.28320 -6.00465 13.66825
Si -1.22667 -7.34409 13.25859
O -0.09101 -1.39898 16.27931
Si -1.22660 -1.71282 17.43165
O -2.08782 -3.07723 17.06026
Si -2.04508 -4.70687 17.34067
O -1.33892 -5.01384 18.80620
Si 0.14759 -5.37331 19.42744
O 1.08342 -6.17178 18.32046
Si 2.19365 -5.84278 17.14447
O 1.45921 -5.64893 15.67384
O -1.19967 -5.46370 16.13864
O -3.58471 -5.25925 17.35274
Si -4.45205 -6.34179 18.31863
C -6.00747 -2.33154 9.55774
C -4.48704 -3.97829 11.69634

C	3.60402	-0.07537	9.63418
C	6.00505	-0.53183	11.52669
O	-2.25139	-0.43595	17.50886
Si	-3.93304	-0.28914	17.60458
O	-0.48675	-1.89463	18.90223
Si	0.97330	-2.37444	19.52223
O	0.92802	-3.98634	19.88535
O	2.18849	-2.07612	18.44239
O	3.04435	-4.46813	17.50444
O	1.29196	-1.52154	20.88293
Si	0.35986	-0.62377	21.96783
O	-0.13518	-6.34319	20.72468
O	3.19931	-7.14491	17.12103
H	5.46522	-2.44494	19.61381
H	-0.83133	-8.52187	14.08635
H	-0.95599	-7.61905	11.81986
H	-2.67163	-7.04326	13.46469
H	-4.45899	-1.09553	18.74457
H	-4.56071	-0.73991	16.32995
H	-0.06185	0.65982	21.33594
H	-0.84255	-1.40054	22.38854
H	3.87653	-7.12123	16.43857
H	1.23325	-0.35259	23.14376
H	6.99769	-1.91966	17.78296
H	5.40027	-0.24360	18.55767
H	0.64628	-6.77243	21.08546
H	-4.67438	-5.75391	19.67079
H	-3.71708	-7.63429	18.43824
H	-5.75634	-6.55465	17.63098
H	-4.20933	1.15693	17.83114
H	-3.85174	-0.75252	11.50249
H	5.28217	2.61018	12.16306
H	3.82196	2.86496	11.18434
H	5.38238	2.56043	10.39722
H	2.64686	0.43060	9.47790
H	4.26651	0.19481	8.80420
H	3.43166	-1.15473	9.58038
H	6.49371	-0.25514	12.46664
H	6.70854	-0.33347	10.71061
H	5.81605	-1.61023	11.55083
H	3.43265	-0.95887	13.17227
H	3.56940	0.75725	13.57040
H	-7.77497	-3.67514	12.01759
H	-7.08153	-2.86904	13.43139
H	-7.95001	-1.92537	12.21213
H	-6.66466	-1.47843	9.35810
H	-6.49922	-3.22978	9.16922
H	-5.08412	-2.18308	8.98808
H	-4.92539	-4.90477	11.31009
H	-3.52599	-3.82221	11.19502
H	-4.28743	-4.12085	12.76373
H	-4.56698	-0.99205	13.10435
H	-5.42980	-0.03936	11.88625
H	-0.46904	2.14433	13.64008
H	-0.42860	0.70370	14.70622

H 2.53620 4.54714 15.28880
H 2.80862 3.52594 13.86347
H 1.34631 4.50512 13.97567
H 0.28584 3.80243 17.36719
H -0.89553 3.80128 16.04843
H -0.72806 2.37497 17.08676
H 2.83642 2.08063 17.20793
H 1.85987 0.62704 16.95419
H 3.16873 1.02379 15.83252
H -2.11956 -0.45619 8.73849
H -0.73338 -2.79123 9.01017
H -2.13204 1.84923 9.94733
H -1.78144 1.72897 11.67156
H -0.53836 2.32309 10.56328
H 1.24493 -3.60954 10.48540
H 2.21189 -2.39179 11.31368
H 0.87661 -3.17930 12.16076
99
Prodcut without TMS
C 0.09005 1.33944 14.27964
C 0.79598 2.11319 15.15988
N 1.70961 1.27963 15.83807
C 1.55516 -0.02770 15.33435
C 0.57265 0.00108 14.38177
W 3.09807 1.89160 17.13184
O 2.70664 0.41657 18.40716
Si 2.41998 -0.50719 19.71221
O 1.70028 0.39871 20.90579
Si 0.58461 0.27038 22.11319
O 1.35030 -0.04677 23.54652
Si 2.72727 -0.77740 24.10853
O 3.24050 -0.00181 25.45581
Si 2.58630 1.17494 26.47476
C 0.65780 3.57681 15.41681
C 2.33933 -1.21079 15.80037
C 2.46713 3.13191 18.71370
Si 3.75687 3.92349 19.89908
C 2.74859 4.95409 21.13233
C 4.74022 2.62028 20.85575
C 4.92728 5.05240 18.93161
C 5.06460 1.13711 17.10857
Si 6.08128 1.25572 15.48416
C 7.43756 -0.06950 15.58718
O 3.60527 3.29824 16.29304
C 6.85995 2.97644 15.38773
C 5.03114 0.94393 13.93851
O 3.84170 -1.13530 20.29452
Si 4.54979 -1.57031 21.71751
O 4.32214 -3.18558 22.00106
Si 3.23012 -4.38885 21.68037
O 3.99005 -5.84583 21.60160
O 1.40614 -1.75451 19.30219
Si 1.09896 -3.33188 19.67889
O -0.10783 -3.41784 20.81235
Si -0.74070 -2.53797 22.06026

O	-2.34862	-2.82617	22.15024
Si	-3.35661	-3.56639	23.28758
O	6.15585	-1.27195	21.58836
Si	7.40573	-1.01707	22.69437
O	3.93059	-0.69017	22.97901
O	0.63020	-4.13220	18.33012
Si	-0.86080	-4.56263	17.66211
O	2.47151	-4.05580	20.24729
O	-0.51624	-0.92209	21.78217
O	-0.20275	1.70189	22.24634
Si	-1.83430	2.14367	22.23846
O	-0.02454	-2.97196	23.48781
Si	1.39893	-3.58834	24.05238
O	1.00177	-4.50286	25.35966
O	2.14116	-4.53107	22.91239
O	2.42126	-2.35818	24.47965
H	7.20615	-1.85479	23.91314
H	-1.45191	-5.69534	18.43179
H	-0.58270	-4.98798	16.26168
H	-1.79400	-3.39910	17.67139
H	-2.57503	1.40778	23.30406
H	-2.43969	1.85731	20.90608
H	2.51684	2.48501	25.76468
H	1.22376	0.77170	26.92911
H	4.55902	-5.96456	20.83538
H	3.50778	1.27442	27.64107
H	8.66857	-1.40717	22.00602
H	7.45573	0.42437	23.07256
H	1.70756	-5.06966	25.68476
H	-3.33332	-2.80220	24.56805
H	-2.92420	-4.97369	23.52467
H	-4.72576	-3.54131	22.70067
H	-1.86584	3.60769	22.51245
H	7.54021	3.15219	16.22797
H	6.08242	3.74547	15.40507
H	7.43497	3.09078	14.46254
H	4.24243	1.69434	13.83122
H	5.66804	0.99664	13.04822
H	4.56108	-0.04404	13.94924
H	8.07258	0.07941	16.46664
H	8.07886	-0.03607	14.69956
H	7.00657	-1.07429	15.65038
H	5.05815	0.12581	17.52730
H	5.59173	1.78293	17.83258
H	1.96530	3.99081	18.24781
H	1.75172	2.57572	19.32973
H	5.63047	5.54714	19.61053
H	5.50355	4.49409	18.18856
H	4.37022	5.82831	18.39715
H	3.41091	5.43664	21.85947
H	2.18136	5.73958	20.62258
H	2.04126	4.32572	21.68265
H	5.43185	3.11164	21.54907
H	4.07487	1.98236	21.44401
H	5.33208	1.97451	20.20019

H -0.69581 1.69989 13.62846
H 0.23269 -0.85796 13.81750
H -0.11867 3.97675 14.75988
H 0.35571 3.79532 16.44919
H 1.58653 4.12350 15.22331
H 2.17447 -2.03526 15.10163
H 3.41911 -1.02471 15.83150
H 2.03555 -1.54594 16.79574
16
Trifluoride
C -0.28857 -1.24514 6.27042
C -0.07821 -0.24296 7.23311
C -0.00584 1.09330 6.83229
C -0.14024 1.43222 5.48906
C -0.34831 0.44371 4.53034
C -0.42077 -0.88815 4.92964
O 0.04757 -0.62062 8.52745
H 0.15679 1.86748 7.57960
C -0.36776 -2.68713 6.68944
H 0.18728 0.16040 9.07465
H -0.08122 2.47644 5.19526
H -0.45346 0.70481 3.48238
H -0.58224 -1.67162 4.19752
F -0.57665 -3.49646 5.63009
F 0.76626 -3.10255 7.28394
F -1.37409 -2.90622 7.55618
116
Adduct
C 0.07373 0.18851 7.61721
C -0.56272 0.64724 8.78564
C -1.42838 1.74414 8.70881
C -1.65658 2.37081 7.48780
C -1.03062 1.91756 6.32770
C -0.16761 0.82785 6.40222
O -0.30471 0.00170 9.93787
W -1.17083 -0.15579 13.87119
C -1.49449 1.59501 14.99849
Si -0.27401 2.75163 15.91392
C 0.90382 3.60365 14.70258
H -1.91610 2.09671 9.61365
C 1.01456 -0.97895 7.69366
O -1.28003 0.67350 12.35913
O -0.93728 -1.09514 15.59239
Si -0.81857 -1.94649 16.97359
O -1.74970 -3.31689 16.86848
Si -1.75664 -4.87704 17.40340
O -2.63320 -5.00481 18.80154
Si -3.08840 -4.10222 20.10844
O -4.58849 -4.54624 20.58443
Si -5.21647 -5.49166 21.83667
C -2.94396 -1.22999 13.57270
Si -3.06640 -2.78255 12.44093
C -3.00696 -2.26339 10.62618
C 0.62371 -1.08442 13.26544
Si 2.36715 -0.33868 12.96661

C	3.35480	-1.71584	12.11376
O	-1.36115	-1.03151	18.24750
Si	-2.14569	-1.17425	19.69082
O	-3.05053	0.17089	19.92732
Si	-4.67590	0.45195	20.29225
O	0.75999	-2.37961	17.23668
Si	1.82784	-2.60323	18.47290
O	1.40569	-1.69269	19.79075
Si	0.51023	-1.81766	21.17573
O	1.21644	-0.88864	22.32298
Si	0.68529	0.32060	23.37540
O	-1.03837	-1.28903	20.91635
O	-3.13657	-2.50108	19.69482
O	0.49682	-3.39007	21.68444
Si	-0.44151	-4.75085	21.58756
O	-2.02148	-4.33673	21.35257
O	-0.40693	-5.59321	22.99879
O	0.12229	-5.69779	20.35162
Si	0.89213	-5.53868	18.90153
O	1.79320	-6.90466	18.73018
C	-1.71757	-4.05177	12.82420
C	-4.75710	-3.55048	12.83372
C	3.20617	0.07815	14.61348
C	2.31700	1.16833	11.82803
O	1.87533	-4.20610	18.88599
O	3.31423	-2.14445	17.95728
Si	4.63302	-1.40584	18.71479
O	-0.21077	-5.41097	17.67094
O	-2.45460	-5.79161	16.23716
Si	-2.57833	-7.44787	15.92898
C	-1.35683	4.08073	16.73093
C	0.67094	1.82135	17.26031
H	4.86995	-2.01977	20.05390
H	-2.68721	-8.20932	17.20753
H	-1.37783	-7.90243	15.16970
H	-3.80589	-7.64027	15.10791
H	-5.06624	-0.28376	21.52966
H	-5.53959	0.02619	19.15286
H	0.25974	1.52329	22.60256
H	-0.44945	-0.17588	24.20706
H	2.36834	-6.91634	17.95940
H	1.84883	0.65504	24.24339
H	5.80811	-1.63817	17.82929
H	4.38137	0.05590	18.86304
H	0.42894	-6.02911	23.18958
H	-5.04540	-4.78915	23.14081
H	-4.53586	-6.81829	21.87768
H	-6.66491	-5.66673	21.53525
H	-4.80247	1.92071	20.50764
H	-0.74552	0.42056	10.70885
H	1.63559	1.94238	12.19097
H	1.98976	0.87021	10.82866
H	3.31729	1.60749	11.74425
H	2.92818	-1.94587	11.13248
H	4.39364	-1.40238	11.96136

H 3.36594 -2.63392 12.71029
H 2.74251 0.93617 15.10780
H 4.25981 0.32585 14.44214
H 3.16640 -0.77165 15.30223
H 0.34315 -1.47333 12.27245
H 0.76652 -1.93615 13.94179
H -4.93434 -4.42871 12.20319
H -4.80958 -3.87131 13.87911
H -5.57054 -2.83993 12.65398
H -3.79567 -1.53747 10.40120
H -3.16305 -3.13435 9.98024
H -2.04717 -1.81464 10.35567
H -1.87339 -4.94865 12.21436
H -0.71768 -3.66932 12.60018
H -1.74869 -4.34941 13.87638
H -3.28284 -1.54126 14.56914
H -3.67220 -0.51530 13.16269
H -2.08289 2.24726 14.33902
H -2.16376 1.22120 15.79104
H 1.47097 4.38791 15.21576
H 1.62267 2.90504 14.26745
H 0.35138 4.07361 13.88212
H -0.73772 4.79177 17.28913
H -1.92404 4.64639 15.98440
H -2.06963 3.63597 17.43291
H 1.34917 2.49827 17.79103
H -0.02644 1.39949 17.98952
H 1.26523 0.99860 16.85427
H -2.33157 3.22150 7.44605
H -1.20998 2.40701 5.37582
H 0.33197 0.46223 5.51175
F 1.53239 -1.28148 6.48441
F 2.06217 -0.73684 8.51304
F 0.41357 -2.09525 8.15100
116
Transition state down
C 0.35056 -2.65854 10.87198
C -0.30422 -1.44292 11.16848
C -0.44345 -0.48990 10.14724
C 0.03457 -0.74879 8.86566
C 0.66922 -1.95614 8.57451
C 0.82711 -2.90218 9.58353
O -0.78666 -1.24695 12.40519
W -0.92150 0.66705 13.81324
C -1.48088 2.01633 15.33299
Si -0.28833 3.20543 16.25375
C 0.55156 4.37523 15.02532
H -0.91975 0.45665 10.38414
C 0.54923 -3.68018 11.95358
O -1.07265 1.85977 12.59540
O -0.95510 -0.73096 15.22446
Si -0.78611 -1.79465 16.43471
O -1.66976 -3.16736 16.14454
Si -1.58651 -4.79246 16.40782
O -2.43333 -5.17174 17.78115

Si	-2.90279	-4.49780	19.21281
O	-4.38137	-5.05988	19.63310
Si	-4.95597	-6.39197	20.49690
C	-2.97217	-0.18381	13.20733
Si	-4.23131	-1.28679	12.20810
C	-4.13848	-0.84840	10.37447
C	1.14433	0.44962	13.70296
Si	2.45938	1.12165	12.47992
C	3.16953	-0.28823	11.43827
O	-1.33193	-1.10189	17.84710
Si	-2.08579	-1.50467	19.25412
O	-3.04488	-0.25300	19.70688
Si	-4.64149	-0.14085	20.24393
O	0.81284	-2.19497	16.62366
Si	1.91356	-2.56123	17.78982
O	1.48607	-1.89098	19.24501
Si	0.61373	-2.26086	20.59841
O	1.30386	-1.47974	21.86203
Si	0.71808	-0.69730	23.23789
O	-0.95851	-1.76399	20.43994
O	-3.02686	-2.85475	19.06630
O	0.66624	-3.89050	20.87026
Si	-0.21091	-5.25935	20.55404
O	-1.80911	-4.88285	20.39541
O	-0.12003	-6.31542	21.81190
O	0.38351	-5.97474	19.18460
Si	1.11182	-5.56016	17.76267
O	2.05701	-6.84835	17.36684
C	-3.90231	-3.11413	12.50741
C	-5.92312	-0.79363	12.90548
C	3.85597	1.80693	13.57507
C	1.81676	2.49857	11.35621
O	2.04545	-4.20473	17.94920
O	3.36548	-1.95013	17.33315
Si	4.73277	-1.44083	18.18218
O	-0.01383	-5.28563	16.58061
O	-2.26728	-5.56797	15.13896
Si	-1.94595	-6.97504	14.26492
C	-1.36184	4.21685	17.44711
C	0.99458	2.25059	17.26737
H	4.95255	-2.29457	19.38602
H	-2.36623	-8.16285	15.06725
H	-0.49583	-7.08081	13.93978
H	-2.75471	-6.89852	13.01725
H	-4.87281	-1.05708	21.39831
H	-5.58301	-0.47328	19.13538
H	0.11994	0.61656	22.86187
H	-0.30363	-1.54029	23.92503
H	2.53260	-6.75609	16.53577
H	1.89172	-0.48595	24.13116
H	5.88590	-1.56898	17.24661
H	4.56908	-0.01663	18.59342
H	0.72070	-6.77642	21.88743
H	-4.84550	-6.12973	21.96074
H	-4.18792	-7.62042	20.14022

H -6.38716 -6.55447 20.11473
H -4.83699 1.27426 20.66864
H -1.96444 -0.79636 12.60961
H 1.39874 3.33588 11.92141
H 1.03462 2.12296 10.69236
H 2.63904 2.87892 10.73949
H 2.45894 -0.63242 10.68282
H 4.07250 0.05563 10.92141
H 3.44411 -1.14403 12.06250
H 3.51473 2.64009 14.19830
H 4.68275 2.17184 12.95560
H 4.25209 1.02978 14.23716
H 1.40312 -0.57040 14.00615
H 1.23994 1.07187 14.62661
H -6.71523 -1.35888 12.40186
H -5.98986 -1.00791 13.97692
H -6.12534 0.27195 12.75713
H -4.29172 0.22341 10.21127
H -4.91845 -1.38554 9.82369
H -3.17158 -1.12361 9.94379
H -4.67007 -3.71786 12.01093
H -2.92530 -3.41269 12.12212
H -3.92064 -3.35248 13.57479
H -3.22658 -0.45711 14.23632
H -3.34360 0.81463 12.95516
H -2.22805 2.69351 14.89499
H -1.95694 1.43235 16.13101
H 1.17528 5.10662 15.55053
H 1.18918 3.83301 14.32137
H -0.19351 4.92440 14.44063
H -0.74701 4.92352 18.01532
H -2.12227 4.79113 16.90783
H -1.87419 3.56557 18.16268
H 1.58533 2.95072 17.86860
H 0.50419 1.55127 17.95147
H 1.69538 1.67887 16.65171
H -0.08622 0.00343 8.09042
H 1.04423 -2.15687 7.57593
H 1.32878 -3.84168 9.37843
F 1.21380 -4.76537 11.50130
F 1.26046 -3.20009 12.99530
F -0.62024 -4.13360 12.46101
116
Product down
C -0.96308 -1.23051 10.61839
C -0.25076 -0.10828 11.07664
C 0.00613 0.95873 10.21529
C -0.44248 0.90192 8.89788
C -1.14350 -0.20825 8.43199
C -1.40092 -1.26940 9.29552
O 0.18002 -0.12759 12.36572
W 0.76807 1.05832 13.72157
C -0.61789 2.10900 14.89080
Si 0.01071 3.41128 16.16570
C 0.69723 4.91527 15.24610

H	0.54499	1.82242	10.58984
C	-1.24757	-2.37376	11.55254
O	1.03730	2.44691	12.75132
O	0.54605	-0.40954	15.03162
Si	0.32656	-1.45794	16.25201
O	-0.52535	-2.78017	15.74391
Si	-0.66751	-4.40563	15.96844
O	-1.85949	-4.71087	17.07384
Si	-2.65195	-3.98547	18.32701
O	-4.22842	-4.42224	18.32752
Si	-5.08888	-5.77396	18.86306
C	-5.55734	-0.95629	13.07656
Si	-6.13574	-2.72077	12.68457
C	-5.78162	-3.11449	10.86183
C	2.79003	1.02739	14.30038
Si	3.96849	-0.03952	13.21597
C	3.44263	-1.85323	13.27509
O	-0.51818	-0.71455	17.47774
Si	-1.65157	-1.05965	18.62370
O	-2.60512	0.26151	18.81728
Si	-4.26032	0.45627	19.10412
O	1.80531	-1.94083	16.83889
Si	2.50276	-2.41969	18.25278
O	1.75056	-1.71560	19.55008
Si	0.52855	-2.01600	20.62253
O	0.91675	-1.29208	22.03944
Si	0.07291	-0.35703	23.16348
O	-0.90169	-1.39503	20.06367
O	-2.59731	-2.33978	18.17117
O	0.38990	-3.64430	20.86470
Si	-0.47969	-4.94255	20.31337
O	-1.94991	-4.44504	19.75604
O	-0.79400	-5.99725	21.53536
O	0.39393	-5.70423	19.13076
Si	1.50741	-5.36370	17.96244
O	2.44103	-6.71410	17.84162
C	-5.20986	-3.95129	13.78911
C	-8.00327	-2.85446	13.00471
C	5.70270	0.15491	13.95923
C	3.95287	0.60432	11.43567
O	2.44579	-4.06770	18.39297
O	4.07301	-1.94485	18.22674
Si	5.14293	-1.40799	19.41832
O	0.76700	-5.03962	16.51651
O	-1.06667	-5.12125	14.55375
Si	-0.40403	-6.34554	13.60140
C	-1.52082	3.89956	17.17171
C	1.31014	2.69703	17.34094
H	4.98645	-2.21181	20.66522
H	-0.39010	-7.63053	14.36204
H	0.98758	-5.99608	13.19311
H	-1.27629	-6.47331	12.40252
H	-4.72874	-0.51229	20.13753
H	-5.02244	0.26090	17.83769
H	-0.23207	0.98459	22.58693

H -1.19413 -1.03691 23.56150
H 3.16293 -6.65042 17.20942
H 0.97039 -0.21343 24.34397
H 6.51392 -1.58757 18.86200
H 4.89725 0.03431 19.70813
H -0.03576 -6.51228 21.82660
H -5.43129 -5.60565 20.30469
H -4.28381 -7.01538 18.67239
H -6.33378 -5.83695 18.04722
H -4.43529 1.85201 19.59551
H -4.48131 -0.85639 12.90269
H 4.18976 1.67234 11.39808
H 2.97145 0.46025 10.97334
H 4.69076 0.07108 10.82664
H 2.44900 -1.99659 12.84109
H 4.15039 -2.47407 12.71491
H 3.41511 -2.21315 14.30792
H 6.02557 1.20092 13.94942
H 6.43280 -0.42820 13.38721
H 5.72555 -0.19989 14.99451
H 2.85310 0.62333 15.31730
H 3.18383 2.05043 14.27348
H -8.37092 -3.86312 12.78767
H -8.24018 -2.63134 14.05054
H -8.56435 -2.15266 12.37831
H -6.27186 -2.39621 10.19598
H -6.14198 -4.11466 10.59797
H -4.70637 -3.08432 10.66147
H -5.50824 -4.98253 13.57150
H -4.12878 -3.87501 13.63611
H -5.41179 -3.76178 14.84876
H -5.75253 -0.70392 14.12434
H -6.07245 -0.21836 12.45227
H -1.25372 2.69114 14.20912
H -1.23331 1.39091 15.44335
H 1.01288 5.68775 15.95576
H 1.55721 4.64888 14.62474
H -0.06238 5.35166 14.58946
H -1.27135 4.68110 17.89789
H -2.31861 4.28055 16.52619
H -1.90701 3.03638 17.72259
H 1.52514 3.41246 18.14216
H 0.95025 1.77202 17.80105
H 2.25042 2.48107 16.82545
H -0.23878 1.73684 8.23335
H -1.49075 -0.24901 7.40449
H -1.94821 -2.13921 8.94984
F -1.96295 -3.34436 10.94551
F -0.11576 -2.95186 12.00517
F -1.95537 -1.98360 12.63120
116
Transition state up
C 0.71807 -2.36795 12.45000
C 0.00393 -1.54706 11.56478
C 0.11245 -1.80494 10.17862

C	0.90463	-2.85975	9.72063
C	1.60466	-3.66698	10.61062
C	1.50654	-3.41181	11.97731
O	-0.75853	-0.52520	11.99694
W	-0.92896	0.88070	13.90604
C	-1.41839	1.82780	15.72547
Si	-0.25706	3.05731	16.63370
C	0.16636	4.52279	15.51201
C	-0.63655	-0.96599	9.18541
H	0.64291	-2.16625	13.51147
O	-1.50203	2.23251	13.03915
O	-0.44675	-0.69755	15.06470
Si	-0.46355	-1.77171	16.27520
O	-1.53809	-2.99480	15.93139
Si	-1.71698	-4.61962	16.13933
O	-2.65303	-4.90901	17.47484
Si	-3.04235	-4.20684	18.92230
O	-4.60057	-4.53384	19.29686
Si	-5.59054	-5.90091	19.23342
C	-2.83504	-0.29018	13.44838
Si	-4.16010	-1.19530	12.33850
C	-4.63358	-0.05009	10.91824
C	1.08784	1.12088	13.44557
Si	1.95135	2.10342	12.04067
C	2.72816	0.90122	10.80543
O	-0.93499	-1.05044	17.69871
Si	-1.76958	-1.37765	19.08275
O	-2.53997	-0.00993	19.55724
Si	-4.10975	0.30079	20.10546
O	1.04858	-2.42712	16.47189
Si	2.05729	-2.99470	17.64507
O	1.70108	-2.30553	19.10934
Si	0.75665	-2.58222	20.43797
O	1.53273	-1.96536	21.74010
Si	1.05302	-1.11929	23.12124
O	-0.71485	-1.83955	20.27227
O	-2.89966	-2.56189	18.82951
O	0.54834	-4.20889	20.63908
Si	-0.53113	-5.41294	20.27987
O	-2.04800	-4.79100	20.10719
O	-0.62800	-6.49993	21.50905
O	-0.02965	-6.17027	18.89451
Si	0.80149	-5.83456	17.51048
O	1.55938	-7.23510	17.09443
C	-3.53551	-2.87945	11.76906
C	-5.63330	-1.42893	13.50760
C	3.36331	3.06520	12.87970
C	0.79916	3.31767	11.17084
O	1.92856	-4.64373	17.74229
O	3.60051	-2.62275	17.23990
Si	4.89198	-1.91112	18.06463
O	-0.24671	-5.36369	16.31521
O	-2.46895	-5.23137	14.81677
Si	-2.33362	-6.69140	13.97467
C	-1.22509	3.68336	18.14035

C	1.31187	2.19281	17.25305
H	5.14946	-2.63194	19.34502
H	-2.33218	-7.83986	14.92749
H	-1.08011	-6.70089	13.16762
H	-3.52169	-6.76939	13.08019
H	-4.47400	-0.64138	21.20272
H	-5.07772	0.17081	18.97827
H	0.67618	0.27704	22.75691
H	-0.10075	-1.80239	23.77566
H	2.24276	-7.13840	16.42475
H	2.22987	-1.11054	24.03445
H	6.07273	-2.02937	17.16368
H	4.59904	-0.47504	18.33947
H	0.15616	-7.04316	21.63141
H	-6.59985	-5.75201	20.31879
H	-4.78619	-7.14012	19.44045
H	-6.27116	-5.95317	17.90710
H	-4.10050	1.70111	20.61310
H	-1.88127	-0.58001	12.56642
H	0.36495	4.03441	11.87332
H	-0.02311	2.79117	10.68088
H	1.35779	3.87597	10.41123
H	1.96716	0.37649	10.22559
H	3.36688	1.45093	10.10511
H	3.34925	0.15559	11.31194
H	2.98707	3.80238	13.59660
H	3.95330	3.60358	12.12958
H	4.04057	2.38976	13.41322
H	1.60388	0.16740	13.60312
H	1.24277	1.71283	14.37782
H	-6.46461	-1.90259	12.97339
H	-5.36900	-2.07212	14.35277
H	-5.99055	-0.47238	13.90253
H	-5.01553	0.90299	11.29822
H	-5.42026	-0.50826	10.30892
H	-3.77854	0.15247	10.27044
H	-4.35343	-3.43354	11.29514
H	-2.72644	-2.78562	11.04190
H	-3.17974	-3.46594	12.62157
H	-2.84163	-0.88834	14.36377
H	-3.39701	0.64279	13.58114
H	-2.32040	2.42983	15.54712
H	-1.64248	1.06394	16.47957
H	0.76844	5.26062	16.05326
H	0.72858	4.21463	14.62596
H	-0.74681	5.01868	15.16755
H	-0.62661	4.39400	18.72093
H	-2.14638	4.19094	17.83578
H	-1.49587	2.85148	18.79798
H	1.91096	2.88971	17.84946
H	1.04823	1.34287	17.89005
H	1.94872	1.82061	16.44506
H	0.97159	-3.03790	8.65298
H	2.21988	-4.48104	10.24032
H	2.04997	-4.02867	12.68839

F -0.31587 -1.28397 7.91424
F -1.97868 -1.13192 9.28902
F -0.40292 0.35413 9.32313
116
Product up
C -1.68122 -3.41539 13.21770
C -2.22846 -2.23835 12.70396
C -2.94412 -2.26056 11.49371
C -3.09545 -3.46668 10.81121
C -2.54569 -4.64128 11.31849
C -1.84349 -4.61072 12.52187
O -2.13498 -1.06967 13.37903
W -1.05680 0.17654 14.30083
C -2.02736 0.99894 15.95552
Si -1.20890 2.46011 16.91121
C -1.02395 3.95372 15.76825
C -3.55445 -0.99628 10.95749
H -1.14619 -3.38272 14.15970
O -1.37424 1.55849 13.34699
O -0.44206 -1.30373 15.51758
Si 0.23675 -2.18108 16.69562
O 0.09593 -3.79651 16.32384
Si 0.89412 -5.22377 16.52301
O 0.32513 -6.01020 17.86229
Si -0.38754 -5.68531 19.32178
O -1.45543 -6.86539 19.69529
Si -1.44654 -8.55410 19.69769
C -7.10863 1.86022 10.42372
Si -5.88599 2.97527 9.49509
C -4.46371 3.46235 10.64935
C 1.00423 0.57086 14.13114
Si 1.92543 -0.09405 12.58008
C 1.94371 -1.98638 12.60998
O -0.52178 -1.88694 18.14310
Si -1.00525 -2.64899 19.52320
O -2.41630 -1.98751 20.02615
Si -3.94230 -2.61282 20.39924
O 1.85116 -1.81178 16.85642
Si 3.01071 -1.71073 18.02381
O 2.34037 -1.38146 19.50144
Si 1.76454 -2.16720 20.83814
O 2.06248 -1.22533 22.14298
Si 1.15790 -0.71251 23.47422
O 0.13418 -2.42334 20.70395
O -1.23202 -4.26698 19.25118
O 2.55484 -3.60782 21.01479
Si 2.37409 -5.21217 20.64474
O 0.77739 -5.59219 20.49191
O 2.94752 -6.16259 21.85698
O 3.20361 -5.52213 19.24374
Si 3.66087 -4.75208 17.86004
O 5.09252 -5.43705 17.42415
C -5.19624 2.04068 7.99420
C -6.78414 4.54151 8.90304
C 3.70408 0.55614 12.69296

C	1.10724	0.54516	11.00040
O	3.86801	-3.12707	18.09979
O	4.03387	-0.49885	17.60881
Si	5.03230	0.54465	18.48618
O	2.52614	-4.97795	16.67159
O	0.62083	-6.14829	15.19384
Si	1.54586	-7.31847	14.39919
C	-2.41526	2.86237	18.31857
C	0.46348	1.97392	17.64929
H	5.71225	-0.19176	19.59172
H	2.12450	-8.28227	15.37981
H	2.63899	-6.66499	13.62292
H	0.61602	-8.02427	13.47305
H	-3.83488	-3.61937	21.49465
H	-4.55278	-3.23639	19.19004
H	0.11422	0.25995	23.03845
H	0.51680	-1.87854	24.14852
H	5.54877	-4.99363	16.70298
H	2.11991	-0.04987	24.39876
H	6.04192	1.06696	17.52271
H	4.22711	1.66846	19.04349
H	3.89984	-6.12421	21.98583
H	-2.38245	-8.98881	20.77181
H	-0.07277	-9.06939	19.96769
H	-1.92301	-9.04874	18.37358
H	-4.76215	-1.45270	20.84815
H	-6.60665	0.96107	10.79389
H	1.06394	1.63887	11.00013
H	0.08290	0.17754	10.89321
H	1.67550	0.22737	10.11932
H	0.93435	-2.40270	12.53232
H	2.53071	-2.37835	11.77229
H	2.38973	-2.35498	13.53919
H	3.72614	1.65053	12.67023
H	4.30259	0.19099	11.85103
H	4.18625	0.22701	13.61905
H	1.53316	0.16343	14.99953
H	1.13041	1.66054	14.08494
H	-6.10162	5.20839	8.36527
H	-7.61116	4.29512	8.22850
H	-7.19858	5.10109	9.74852
H	-4.83425	3.99246	11.53351
H	-3.75024	4.11995	10.14112
H	-3.91775	2.57837	10.99249
H	-4.46874	2.65115	7.44864
H	-4.69520	1.11887	8.30544
H	-5.99532	1.76947	7.29574
H	-7.93197	1.54572	9.77349
H	-7.54229	2.38024	11.28467
H	-2.97885	1.41255	15.59364
H	-2.22672	0.19339	16.67145
H	-0.62589	4.81201	16.32038
H	-0.34928	3.73649	14.93551
H	-1.98881	4.24283	15.34002
H	-2.03958	3.70155	18.91424

H -3.40000 3.14005 17.92940
H -2.54252 2.00446 18.98633
H 0.82764 2.77360 18.30350
H 0.38343 1.06146 18.24739
H 1.21648 1.80938 16.87329
H -3.65070 -3.47630 9.87983
H -2.67147 -5.57438 10.77826
H -1.41900 -5.52029 12.93595
F -4.18626 -1.20808 9.78457
F -4.46540 -0.47358 11.80342
F -2.62968 -0.03936 10.73581
99
Product up without TMS
C -1.20403 -2.41966 12.41337
C -1.29894 -1.14227 11.86693
C -1.65249 -0.99136 10.52513
C -1.91220 -2.12058 9.72946
C -1.81039 -3.39097 10.29393
C -1.45598 -3.54569 11.63188
O -1.80985 0.23729 9.97868
W -1.09824 1.95724 9.67003
C 0.90817 2.58287 9.55681
Si 2.29115 1.25040 9.45278
C 2.03292 0.14009 7.94435
C -2.31101 -1.95028 8.29008
F -1.36641 -1.29614 7.58170
C -2.54178 3.45720 9.84284
Si -2.10838 5.27076 9.35390
C -0.64975 5.95023 10.34806
O -1.18342 1.98569 7.96367
O -0.79937 2.16038 11.65161
Si -0.41976 2.71674 13.12247
O 1.09982 3.39473 13.12627
Si 1.94016 4.61805 13.84320
O 3.01215 5.20016 12.74747
Si 3.73434 6.70974 12.50926
C -1.75767 5.36419 7.49944
C -3.66158 6.27574 9.77532
F -2.50195 -3.13906 7.68446
F -3.45501 -1.25286 8.16100
O -0.43961 1.45903 14.21145
Si 0.31268 0.95749 15.58868
O 0.39415 -0.68196 15.55723
Si 1.52828 -1.78733 16.14733
O -1.51493 3.86924 13.60244
Si -2.30383 4.41709 14.94216
O -2.43140 3.21950 16.07940
Si -1.60283 2.62952 17.38186
O -0.75608 3.85006 18.10762
Si 0.74692 4.52515 18.09354
O 1.90098 3.41520 17.66561
Si 2.66391 2.86451 16.31246
O 1.85229 1.56318 15.68135
O -0.55631 1.43294 16.91443
O -2.70537 2.02392 18.42621

Si	-2.68000	0.91929	19.70333
C	2.33385	0.22188	11.04057
C	3.92248	2.20364	9.28115
O	-3.80565	4.90358	14.50591
Si	-5.35881	4.59318	15.09780
O	-1.48631	5.71311	15.57104
Si	0.05546	6.31229	15.64284
O	0.80553	5.78304	17.01734
O	0.92709	5.83831	14.31890
O	2.77725	4.03961	15.15162
O	0.00698	7.94810	15.64669
Si	-1.17889	9.10733	15.96735
O	1.01911	5.05125	19.62682
O	4.17046	2.41861	16.80255
H	-1.11141	-0.25902	12.46625
H	4.03875	7.35499	13.81965
H	1.91018	-1.44793	17.54886
H	2.73922	-1.79123	15.27668
H	0.86736	-3.12226	16.10482
H	-5.43475	4.92270	16.55052
H	-5.71449	3.16166	14.87898
H	-2.15059	9.16611	14.83726
H	-1.89380	8.78451	17.23629
H	4.77904	2.20277	16.08987
H	-0.46531	10.40869	16.09621
H	4.99587	6.45862	11.75691
H	2.82706	7.58143	11.70995
H	1.91423	5.35950	19.79629
H	-3.77980	1.30824	20.62943
H	-1.36709	0.96637	20.41047
H	-2.92033	-0.45369	19.17211
H	-6.27736	5.47418	14.32344
H	1.96397	0.73481	7.02796
H	1.11537	-0.44970	8.02352
H	2.87271	-0.55492	7.83495
H	1.42831	-0.38054	11.16206
H	3.18864	-0.46324	11.02616
H	2.43110	0.86857	11.91798
H	3.93399	2.80674	8.36742
H	4.77126	1.51219	9.23763
H	4.07479	2.87450	10.13265
H	1.14777	3.18328	10.44164
H	1.02672	3.18175	8.64510
H	-3.36510	3.18487	9.16797
H	-2.90330	3.46406	10.87742
H	-1.54423	6.39585	7.19965
H	-0.90343	4.73962	7.22395
H	-2.61902	5.01484	6.92126
H	-3.51940	7.32883	9.50879
H	-4.53461	5.90517	9.22858
H	-3.88398	6.22545	10.84597
H	-0.52747	7.01983	10.14517
H	-0.81330	5.82914	11.42290
H	0.28762	5.45177	10.08562
H	-2.01463	-4.25730	9.67452

H -1.38216 -4.54038 12.06034
H -0.93584 -2.52368 13.46039
19
phenol
O 0.04248 -0.66352 8.50959
H 0.18211 0.11052 9.06586
C -0.08204 -0.26251 7.20957
C -0.00391 1.08997 6.84327
C -0.14144 1.41679 5.49151
C -0.35006 0.43166 4.53164
C -0.42336 -0.90390 4.92391
C -0.29188 -1.27638 6.26190
C 0.22205 2.14702 7.89254
H -0.08282 2.46188 5.19605
H -0.45510 0.70151 3.48500
H -0.58617 -1.67995 4.17956
C -0.36755 -2.70949 6.70721
H 0.25820 3.14114 7.44075
H -0.58156 2.16645 8.64205
H 1.17169 2.00519 8.42734
H -0.53369 -3.37488 5.85596
H 0.55469 -3.01865 7.21152
H -1.18031 -2.86032 7.42633
119
Adduct
C 0.96433 -5.00879 12.39354
C 1.88335 -6.05998 12.46577
C 2.90950 -6.19275 11.53604
C 3.02339 -5.25896 10.50823
C 2.13131 -4.19258 10.39679
C 1.10555 -4.07654 11.35151
C 2.24069 -3.17891 9.29268
O 0.26293 -3.01677 11.19527
W -2.15105 -0.20393 12.70993
C -3.30058 -0.44825 10.96109
Si -4.29314 -1.95426 10.32683
C -6.06914 -1.89389 10.98867
C -0.15153 -4.88309 13.39621
O -1.70502 -1.86529 12.79899
C -2.82393 -0.16638 14.70524
Si -4.62809 -0.59265 15.17896
C -4.93729 -2.44332 14.91844
C -0.18190 0.39060 12.31353
Si 1.01715 0.78924 13.75880
C 1.25595 -0.72588 14.86853
O -2.64825 1.71468 12.66060
Si -3.01766 3.24798 12.27917
O -4.19365 3.26134 11.10559
Si -5.49642 4.14155 10.61462
O -5.04594 5.19841 9.42172
Si -3.71476 6.05588 8.93584
O -2.34946 5.23113 9.37610
Si -1.24216 5.17635 10.60586
O 0.22302 4.78059 9.98992
Si 1.60364 5.65356 9.55914

C	-4.81917	-0.19013	17.02356
C	-5.84691	0.46613	14.19141
C	2.67285	1.23227	12.94472
C	0.40082	2.26833	14.76466
O	-1.66560	4.01893	11.69996
O	-3.58205	4.05333	13.61487
Si	-3.58144	5.55994	14.28262
O	-3.54581	5.39337	15.91102
Si	-4.26910	6.19082	17.21069
O	-1.14977	6.66331	11.33182
Si	-1.79228	7.47733	12.62050
O	-0.65138	8.47780	13.23090
Si	-0.51688	10.14829	13.44387
O	-2.24684	6.40513	13.79108
O	-3.09741	8.37106	12.12639
Si	-4.25103	8.35902	10.94634
O	-3.72600	7.57337	9.58750
O	-4.95168	6.38877	13.84870
Si	-6.05344	6.45393	12.61803
O	-5.61662	7.61573	11.52108
O	-7.52534	6.82098	13.23423
Si	-8.47407	8.21678	13.29172
O	-6.16220	4.97902	11.88006
C	-3.48490	-3.60693	10.75637
C	-4.35984	-1.77076	8.43701
O	-6.61579	3.10530	10.01387
Si	-8.30514	3.08364	10.01662
O	-3.75085	6.28993	7.30764
O	-4.56772	9.92894	10.57153
H	-0.39381	-2.94126	11.91024
H	-8.71169	2.08659	8.98678
H	1.23647	6.82059	8.70458
H	2.46998	4.71250	8.79563
H	2.31166	6.12407	10.78434
H	-5.70181	5.78956	17.31946
H	-4.17056	7.66989	17.03777
H	-9.60324	7.91471	14.21525
H	-7.67858	9.36707	13.81094
H	-3.69644	5.48739	6.78043
H	-8.99721	8.53537	11.93145
H	-8.80786	2.66942	11.35775
H	-8.84443	4.43031	9.66602
H	-4.85975	10.06774	9.66566
H	-1.61619	10.64756	14.31967
H	-0.56260	10.84137	12.12398
H	0.80251	10.37615	14.09698
H	-3.52653	5.76703	18.43054
H	-3.45534	-3.76955	11.83707
H	-2.45703	-3.65137	10.38403
H	-4.04813	-4.42799	10.29904
H	-3.35715	-1.82903	8.00034
H	-4.96485	-2.56776	7.99092
H	-4.80032	-0.81148	8.14574
H	-6.11273	-2.02215	12.07364
H	-6.66674	-2.69269	10.53592

H -6.54685 -0.94025 10.74055
H -2.44529 -0.35861 10.25781
H -3.90446 0.45575 10.81519
H 3.42130 1.48137 13.70498
H 3.05749 0.39417 12.35494
H 2.56698 2.09529 12.27963
H 0.23787 3.13698 14.11946
H 1.13847 2.54619 15.52524
H -0.54032 2.04897 15.27720
H 2.00889 -0.52041 15.63703
H 0.32817 -1.00859 15.37516
H 1.59817 -1.58576 14.28416
H 0.29367 -0.41086 11.73327
H -0.24045 1.29981 11.70035
H -2.18909 -0.85586 15.27737
H -2.65228 0.85787 15.06201
H -6.87777 0.25778 14.49748
H -5.65214 1.52965 14.36265
H -5.77190 0.28031 13.11620
H -5.96866 -2.70881 15.17423
H -4.75483 -2.74605 13.88352
H -4.27149 -3.03454 15.55622
H -5.83126 -0.43144 17.36687
H -4.11274 -0.76457 17.63158
H -4.64418 0.87347 17.21520
H 3.81948 -5.35360 9.77302
H 3.61271 -7.01724 11.60949
H 1.78159 -6.78555 13.26984
H 3.07829 -3.41309 8.63000
H 1.32529 -3.14355 8.69140
H 2.38980 -2.16835 9.68982
H -0.10329 -3.94323 13.95919
H -1.13794 -4.91427 12.91749
H -0.11092 -5.70183 14.11933
119
Transition state
O -1.01070 2.13658 12.80944
W -0.87540 0.68866 13.70475
O -0.82546 -0.91009 14.92729
Si -0.68341 -1.91106 16.18542
O -1.24769 -1.18522 17.57570
Si -2.02422 -1.52395 18.98579
O -0.91593 -1.74315 20.19701
Si 0.65424 -2.23398 20.39404
O 0.69820 -3.85294 20.72800
Si -0.18398 -5.22797 20.45994
O -0.11608 -6.23163 21.76090
O -0.81698 -0.83146 12.01984
C -2.97237 -0.05742 13.03892
Si -4.20538 -1.31407 12.21234
C -3.60925 -3.08201 12.47738
C 1.19744 0.56336 13.58587
Si 2.52547 1.37828 12.46890
C 3.87394 1.99389 13.66233
O 0.90886 -2.32700 16.41887

Si	1.98803	-2.64977	17.61763
O	2.10428	-4.28683	17.84677
Si	1.16386	-5.64190	17.69788
O	0.41397	-6.00010	19.12403
O	-1.56779	-3.29808	15.93488
Si	-1.51140	-4.90645	16.28310
O	-2.16851	-5.72405	15.02415
Si	-3.11851	-7.11174	14.88196
O	3.45261	-2.07159	17.15940
Si	4.79614	-1.49900	18.00765
O	1.54284	-1.91782	19.03777
C	-5.85810	-1.02223	13.09261
C	-4.39134	-0.95350	10.36710
C	1.87428	2.84865	11.47716
C	3.29254	0.08477	11.32492
O	0.05425	-5.39959	16.49390
O	-2.38601	-5.23962	17.65423
Si	-2.85919	-4.51183	19.06058
O	-1.77948	-4.84978	20.26885
O	2.10431	-6.95052	17.36338
O	-2.97186	-2.87616	18.84004
O	-2.98228	-0.24964	19.37248
Si	-4.58521	-0.10620	19.88464
O	-4.33799	-5.07210	19.48214
Si	-4.92510	-6.08328	20.70180
O	1.33024	-1.40715	21.63518
Si	0.73514	-0.58758	22.98571
H	5.01216	-2.29940	19.24831
H	-2.61530	-8.18564	15.78769
H	-3.01662	-7.55019	13.46174
H	-4.53689	-6.79240	15.21630
H	-4.84593	-1.00574	21.04605
H	-5.51383	-0.44073	18.76592
H	0.13054	0.71058	22.56853
H	-0.28431	-1.41705	23.69256
H	2.59642	-6.89331	16.53903
H	1.90412	-0.34399	23.87658
H	5.96504	-1.64494	17.09474
H	4.59884	-0.06306	18.35721
H	0.72666	-6.67970	21.87970
H	-4.74095	-5.44168	22.03536
H	-4.22505	-7.39988	20.66720
H	-6.37652	-6.26789	20.41954
H	-4.76703	1.31599	20.28929
H	-2.00826	-0.56686	12.29126
H	1.29807	3.53774	12.10033
H	1.22781	2.52199	10.65892
H	2.71700	3.39895	11.04364
H	2.57182	-0.29798	10.59796
H	4.12916	0.52856	10.77346
H	3.68308	-0.76336	11.89668
H	3.49590	2.77057	14.33552
H	4.71352	2.42025	13.10208
H	4.26402	1.17490	14.27597
H	1.50815	-0.45082	13.85782

H 1.21726 1.14751 14.54275
H -6.63014 -1.68007 12.67832
H -5.77920 -1.23152 14.16423
H -6.19787 0.01142 12.97182
H -4.62110 0.09967 10.17695
H -5.21157 -1.55291 9.95669
H -3.48258 -1.21547 9.81733
H -4.38696 -3.78908 12.16816
H -2.71506 -3.28298 11.88061
H -3.36577 -3.27793 13.52520
H -3.15442 -0.32581 14.08710
H -3.39606 0.92451 12.80918
C -1.53707 1.71544 15.44043
H -2.34711 2.38647 15.11851
H -1.93866 1.00138 16.16836
Si -0.41448 2.88460 16.46514
C -1.51918 3.64135 17.81084
C 0.99550 1.94632 17.31712
C 0.28393 4.26754 15.37570
H 0.84554 4.98886 15.97936
H 0.95707 3.87479 14.60816
H -0.51990 4.80573 14.86346
H -0.94739 4.32961 18.44310
H -2.35056 4.20149 17.37024
H -1.93855 2.86133 18.45432
H 1.51520 2.61721 18.01038
H 0.60826 1.10124 17.89348
H 1.74399 1.56196 16.61731
C -0.14994 -1.25637 10.91266
C -0.20607 -0.51602 9.71475
C 0.46987 -1.01312 8.59590
C 1.17711 -2.21082 8.65029
C 1.21637 -2.92970 9.84239
C 0.56257 -2.46981 10.98786
C -0.98543 0.76785 9.63627
H 0.43513 -0.44491 7.66889
H 1.69472 -2.58121 7.76989
H 1.76560 -3.86735 9.89316
C 0.62150 -3.23945 12.27796
H -0.72985 1.32109 8.72790
H -2.06564 0.58366 9.61037
H -0.80061 1.41235 10.49977
H 1.00744 -4.24893 12.11009
H 1.27644 -2.74986 13.00810
H -0.36186 -3.31369 12.74937
119
Product
O 0.62013 2.07935 12.91529
W 0.38764 0.55777 13.66926
O 0.34480 -1.04679 14.86870
Si 0.41177 -1.97806 16.19138
O -0.69090 -1.44879 17.31929
Si -1.72416 -2.00806 18.47285
O -0.99500 -1.92940 19.95819
Si 0.52789 -1.98108 20.60871

O	0.90640	-3.53175	21.03825
Si	0.53191	-5.09286	20.63359
O	0.49238	-6.05206	21.96855
O	-0.44412	-0.40455	12.29338
C	-5.32660	0.58450	12.82856
Si	-7.04578	0.10812	12.18092
C	-7.49680	-1.62844	12.79841
C	2.44384	0.56550	14.16514
Si	3.72804	-0.01635	12.86402
C	5.43687	0.33037	13.61397
O	1.93102	-1.91768	16.86803
Si	2.65855	-1.97675	18.34499
O	3.11851	-3.52785	18.69725
Si	2.67073	-5.09187	18.38782
O	1.66583	-5.65762	19.56830
O	0.06067	-3.55322	15.80253
Si	0.42497	-5.09747	16.24367
O	0.39310	-6.05438	14.91380
Si	-0.43387	-7.47168	14.51519
O	3.99303	-1.02651	18.28331
Si	4.88532	-0.17684	19.43842
O	1.64250	-1.41420	19.52799
C	-8.32832	1.35737	12.81096
C	-7.03181	0.12317	10.28367
C	3.53046	0.94987	11.24819
C	3.55438	-1.87234	12.53443
O	1.94138	-5.15894	16.90342
O	-0.68624	-5.66581	17.33711
Si	-1.71944	-5.11425	18.50314
O	-0.98519	-5.16502	19.98616
O	3.98614	-6.07993	18.42663
O	-2.18801	-3.56655	18.15438
O	-3.05572	-1.05159	18.49337
Si	-4.71627	-1.35794	18.43466
O	-3.05171	-6.06412	18.52736
Si	-3.71155	-7.14812	19.64377
O	0.58263	-1.02516	21.93677
Si	-0.57272	-0.28833	22.92316
H	4.91326	-0.92223	20.73077
H	-0.16902	-8.53186	15.53075
H	0.08884	-7.89588	13.18580
H	-1.89928	-7.20765	14.42701
H	-5.11354	-2.27558	19.54207
H	-5.08424	-1.95869	17.12031
H	-1.26759	0.79866	22.17466
H	-1.56828	-1.29281	23.39882
H	4.62863	-5.92470	17.72802
H	0.17168	0.28244	24.08054
H	6.26646	-0.04478	18.89432
H	4.28724	1.17335	19.64323
H	1.35265	-6.23927	22.35580
H	-4.13033	-6.42333	20.87812
H	-2.71943	-8.20764	19.98542
H	-4.89956	-7.75196	18.97750
H	-5.38658	-0.03789	18.60054

H	-4.56663	-0.12343	12.48071
H	3.51189	2.02824	11.43332
H	2.60245	0.68108	10.73392
H	4.36204	0.73381	10.56861
H	2.62617	-2.10020	12.00161
H	4.38477	-2.22718	11.91414
H	3.56270	-2.44395	13.46787
H	5.57667	1.39979	13.80275
H	6.23132	0.00202	12.93469
H	5.56294	-0.19962	14.56353
H	2.61141	-0.03635	15.06468
H	2.71509	1.61150	14.36196
H	-9.33212	1.10816	12.45064
H	-8.36154	1.37421	13.90548
H	-8.09377	2.37093	12.46867
H	-6.77725	1.11651	9.89903
H	-8.01235	-0.14995	9.87934
H	-6.29757	-0.58607	9.88719
H	-8.48486	-1.93126	12.43589
H	-6.77144	-2.37171	12.45099
H	-7.51606	-1.66738	13.89272
H	-5.30414	0.58983	13.92367
H	-5.03996	1.58306	12.48136
C	-0.98906	1.40500	15.01136
H	-1.72162	1.94492	14.39421
H	-1.49562	0.59159	15.54164
Si	-0.41391	2.70644	16.30516
C	-1.92005	3.00587	17.41981
C	1.02093	2.08214	17.36994
C	0.06851	4.30705	15.42130
H	0.39523	5.06397	16.14255
H	0.87780	4.13459	14.70642
H	-0.78112	4.71637	14.86498
H	-1.68693	3.74746	18.19185
H	-2.77227	3.37868	16.84219
H	-2.22697	2.08111	17.91845
H	1.25771	2.81971	18.14473
H	0.76398	1.14344	17.86920
H	1.92636	1.91725	16.77860
C	-0.33360	-0.93338	11.03159
C	-0.41551	-0.09000	9.91051
C	-0.30495	-0.68395	8.64962
C	-0.13950	-2.05831	8.50760
C	-0.10677	-2.87076	9.63727
C	-0.21384	-2.32958	10.92088
C	-0.65011	1.38711	10.05427
H	-0.35852	-0.04850	7.76907
H	-0.05238	-2.49708	7.51769
H	-0.00462	-3.94798	9.53160
C	-0.25150	-3.20588	12.14005
H	-0.77265	1.85047	9.07187
H	-1.55465	1.58592	10.63948
H	0.16955	1.89063	10.57470
H	-0.03010	-4.24323	11.87774
H	0.45568	-2.88612	12.90847

H -1.24140 -3.17765 12.60928
102
Product without TMS
O 0.61457 2.06908 12.91665
W 0.39340 0.54864 13.67648
O 0.36292 -1.05092 14.88150
Si 0.42570 -1.98258 16.20430
O -0.67918 -1.45131 17.32895
Si -1.71880 -2.00784 18.47889
O -0.99547 -1.92887 19.96661
Si 0.52570 -1.98360 20.62108
O 0.89977 -3.53494 21.05211
Si 0.52397 -5.09545 20.64637
O 0.47761 -6.05431 21.98133
O -0.44748 -0.41985 12.31077
C 2.45343 0.56419 14.15610
Si 3.73278 0.00137 12.84174
C 5.44407 0.34959 13.58545
O 1.94332 -1.92389 16.88441
Si 2.66454 -1.98401 18.36453
O 3.12041 -3.53580 18.71897
Si 2.67117 -5.09920 18.40862
O 1.66082 -5.66268 19.58552
O 0.07339 -3.55697 15.81372
Si 0.43342 -5.10194 16.25622
O 0.40522 -6.05895 14.92637
Si -0.42966 -7.46975 14.52103
O 4.00094 -1.03619 18.30848
Si 4.88941 -0.18660 19.46653
O 1.64423 -1.41954 19.54291
C 3.52240 0.98092 11.23562
C 3.56632 -1.85238 12.49618
O 1.94725 -5.16575 16.92153
O -0.68302 -5.66834 17.34532
Si -1.71926 -5.11392 18.50728
O -0.99077 -5.16457 19.99312
O 3.98475 -6.08944 18.45293
O -2.18284 -3.56530 18.15551
O -3.04929 -1.05012 18.49849
Si -4.70219 -1.33801 18.29714
O -3.05298 -6.06181 18.52674
Si -3.72955 -7.12915 19.64919
O 0.57886 -1.02714 21.94875
Si -0.57821 -0.29101 22.93385
H 4.91651 -0.93405 20.75772
H -0.17193 -8.53549 15.53258
H 0.09225 -7.89151 13.19055
H -1.89342 -7.19699 14.43232
H -5.18535 -2.31374 19.31696
H -4.97222 -1.85936 16.92602
H -1.27072 0.79743 22.18535
H -1.57519 -1.29559 23.40621
H 4.63077 -5.93478 17.75745
H 0.16436 0.27772 24.09343
H 6.27122 -0.05109 18.92499

H	4.28850	1.16215	19.67261
H	1.33626	-6.24499	22.37048
H	-4.15387	-6.38836	20.87211
H	-2.74751	-8.19150	20.01050
H	-4.91595	-7.73219	18.97931
H	-5.37673	-0.02356	18.48774
H	3.49821	2.05748	11.43037
H	2.59404	0.71155	10.72234
H	4.35277	0.77578	10.55118
H	2.63645	-2.07960	11.96594
H	4.39512	-2.19768	11.86845
H	3.58214	-2.43258	13.42423
H	5.57937	1.41777	13.78432
H	6.23625	0.03242	12.89824
H	5.57871	-0.18933	14.52879
H	2.63107	-0.04241	15.05050
H	2.71885	1.61074	14.35852
C	-0.97771	1.39617	15.02522
H	-1.71420	1.93481	14.41142
H	-1.47971	0.58283	15.55999
Si	-0.39772	2.69962	16.31512
C	-1.89801	2.99734	17.43801
C	1.04413	2.07792	17.37181
C	0.07688	4.30055	15.42757
H	0.40623	5.05829	16.14676
H	0.88255	4.12957	14.70826
H	-0.77658	4.70821	14.87592
H	-1.66108	3.73880	18.20900
H	-2.75375	3.36996	16.86546
H	-2.20160	2.07234	17.93823
H	1.28429	2.81650	18.14459
H	0.79125	1.13937	17.87341
H	1.94643	1.91371	16.77547
C	-0.34843	-0.94568	11.04668
C	-0.46070	-0.10207	9.92857
C	-0.35978	-0.69229	8.66516
C	-0.17499	-2.06371	8.51847
C	-0.11320	-2.87729	9.64611
C	-0.20965	-2.33975	10.93210
C	-0.71791	1.37067	10.07875
H	-0.43665	-0.05652	7.78657
H	-0.09586	-2.49966	7.52664
H	0.00338	-3.95269	9.53703
C	-0.21735	-3.21827	12.15023
H	-0.85710	1.83470	9.09891
H	-1.62094	1.55248	10.67214
H	0.09782	1.88617	10.59348
H	0.00881	-4.25309	11.88209
H	0.50077	-2.89367	12.90647
H	-1.19881	-3.19967	12.63712

19

thiol

C	2.49073	3.36788	-4.15540
C	1.78582	2.57943	-3.24415
C	2.48714	1.59331	-2.52145

C 3.87032 1.40014 -2.70759
C 4.53113 2.21553 -3.63213
C 3.85606 3.19293 -4.35396
C 0.30953 2.78325 -3.04264
S 1.51632 0.62912 -1.37712
C 4.65052 0.35746 -1.95368
H 2.50329 -0.16122 -0.92989
H 5.59857 2.07270 -3.78166
H 4.39085 3.81428 -5.06640
H 1.95213 4.12934 -4.71418
H 5.70311 0.37751 -2.24677
H 4.61175 0.51952 -0.86881
H 4.27785 -0.65615 -2.14997
H -0.06530 3.58494 -3.68389
H -0.25765 1.87329 -3.27437
H 0.07781 3.04727 -2.00336
119
Adduct
O 2.665545 -4.130029 6.151808
H -0.664039 -8.798520 6.143091
C -0.473922 -7.721343 6.204051
Si 0.849320 -7.375597 7.514423
C 2.525973 -8.047468 6.954558
W 0.989762 -3.966158 6.499503
O -0.954755 -3.772266 6.895155
Si -2.548000 -3.737622 7.184028
O -2.960119 -2.308675 7.924737
Si -4.214332 -1.243039 8.005357
O -5.091880 -1.286840 6.603160
Si -6.435192 -2.017282 5.967238
O -7.511054 -2.398579 7.159013
Si -7.877236 -3.660517 8.165515
O -7.466558 -5.078660 7.416613
Si -6.228909 -6.170801 7.339180
O -5.265392 -5.824927 6.041094
Si -4.777118 -4.516296 5.147723
O -4.484587 -4.998958 3.609704
Si -4.985908 -6.304029 2.662936
C 0.358733 -4.292411 4.509532
Si 1.554514 -4.542303 3.048607
C 0.485035 -4.781219 1.495028
C 2.661339 -3.025766 2.811059
C 2.624475 -6.080548 3.308453
C 1.217528 -2.053027 7.331094
Si 1.076698 -0.413743 6.337368
C 2.764820 0.018764 5.601923
C 1.009008 -5.506759 7.926930
C -0.236828 -0.490993 4.975623
C 0.563657 0.908479 7.597029
C 0.325673 -8.211666 9.135129
O -2.964087 -5.001107 8.181703
Si -4.021844 -5.383963 9.384794
O -3.278476 -6.415107 10.420899
Si -3.197304 -6.514426 12.106209
O -3.390437 -3.873294 5.760892

O	-5.350314	-6.137270	8.743611
O	-4.489319	-4.031905	10.220546
Si	-5.679850	-2.883620	10.207993
O	-7.083589	-3.523313	9.606857
O	-6.849418	-7.670727	7.126884
Si	-6.943105	-9.063158	8.077615
O	-5.970614	-3.368778	5.130223
O	-7.238862	-0.984375	4.969900
O	-5.202499	-1.594609	9.290050
O	-3.592963	0.260677	8.205678
Si	-4.071096	1.612180	9.100653
O	-5.928911	-2.382767	11.745458
Si	-7.289727	-2.223978	12.735570
O	-9.478330	-3.635250	8.538172
C	9.009678	-4.520855	4.880689
C	8.580120	-4.705894	6.310376
C	9.491751	-5.164139	7.263795
C	9.117020	-5.346500	8.590628
C	7.813722	-5.055688	8.977248
C	6.867523	-4.584175	8.061711
C	7.259745	-4.423000	6.717569
S	6.154895	-3.819876	5.455778
C	5.479513	-4.252192	8.534483
H	-6.449209	-6.541683	2.831856
H	-5.549367	1.795897	9.018532
H	-3.374548	2.783503	8.498855
H	-3.657379	1.447016	10.523983
H	-4.563061	-6.423615	12.700067
H	-2.336075	-5.420788	12.641376
H	-5.582352	-9.641455	8.275906
H	-7.558201	-8.750040	9.400287
H	-6.734951	-0.683964	4.207800
H	-7.801531	-10.021690	7.326995
H	-4.686504	-5.936734	1.250365
H	-4.225619	-7.529537	3.043617
H	-10.068092	-3.561267	7.782001
H	-7.895309	-3.561935	12.994267
H	-8.292724	-1.323742	12.097109
H	-6.802295	-1.626857	14.010565
H	-2.593240	-7.840385	12.415779
H	4.980195	-4.033103	6.077516
H	3.291487	-2.870745	3.691223
H	2.074772	-2.117523	2.637575
H	3.319975	-3.165234	1.947184
H	-0.151620	-3.909092	1.312297
H	1.112280	-4.929197	0.609003
H	-0.166665	-5.655967	1.592785
H	3.275609	-5.950576	4.177112
H	3.260184	-6.255258	2.433808
H	2.013659	-6.976989	3.458656
H	-0.329813	-3.462268	4.289904
H	-0.296705	-5.175333	4.591373
H	0.535633	1.898331	7.128402
H	-0.433672	0.694753	7.994561
H	1.265227	0.953032	8.436338

H 3.523466 0.104734 6.386700
H 2.720629 0.977022 5.073081
H 3.102528 -0.741576 4.892301
H -0.401039 0.509080 4.559764
H 0.067461 -1.145507 4.153538
H -1.192026 -0.851480 5.368945
H 0.439697 -2.002435 8.105404
H 2.201751 -2.026874 7.816095
H 1.955183 -5.408668 8.476846
H 0.181038 -5.273593 8.608854
H 2.463129 -9.122258 6.752948
H 2.871990 -7.552691 6.042883
H 3.286270 -7.897352 7.728062
H 0.256108 -9.297385 9.006375
H 1.047152 -8.013660 9.934638
H -0.653500 -7.846217 9.460548
H -1.417752 -7.229293 6.458310
H -0.164066 -7.385652 5.209817
H 7.514575 -5.185882 10.014680
H 9.836705 -5.708489 9.319360
H 10.509589 -5.384076 6.950658
H 5.394790 -4.399677 9.614519
H 5.220950 -3.209083 8.315070
H 4.716351 -4.875909 8.052969
H 10.053092 -4.817509 4.745660
H 8.392188 -5.116734 4.198332
H 8.915190 -3.475748 4.560931
119
Transition state
C 0.70296 0.32916 -0.66472
C 0.25253 0.26970 0.65647
C 1.20526 0.18480 1.70346
C 2.58588 0.17688 1.40432
C 2.98485 0.23667 0.06417
C 2.05929 0.30915 -0.96906
C -1.22814 0.30853 0.92769
S 0.52010 0.10716 3.35253
W 1.68389 -1.27110 5.71670
C 0.70605 -2.82116 4.73678
Si 1.16508 -3.91914 3.23552
C 2.98205 -3.79883 2.73233
C 3.63955 0.12098 2.47149
C 2.04248 -1.82120 7.72441
Si 2.21491 -3.62622 8.34785
C 0.54002 -4.51228 8.34218
O 3.26003 -1.71009 5.22340
O -0.08347 -0.54283 6.32615
Si -1.63214 -0.57661 6.80459
O -2.44102 -1.81691 6.04696
Si -3.64811 -2.90241 6.32092
O -3.27089 -4.27913 5.51171
Si -4.17336 -5.61938 5.02025
C 2.27479 0.93548 5.68260
Si 1.91737 2.83204 5.40148
C 2.93437 3.67948 6.76156

C	3.48577	-4.56952	7.31101
C	2.82478	-3.51150	10.14182
O	-2.39509	0.85493	6.46241
Si	-3.86038	1.45025	6.00715
O	-3.63963	2.72154	4.99904
Si	-4.19092	4.31630	4.96801
O	-1.70202	-0.82440	8.44975
Si	-2.60313	-0.39788	9.76085
O	-3.36480	1.05365	9.51305
Si	-4.80953	1.63848	8.95907
O	-6.01667	0.54188	9.24289
Si	-6.79486	-0.69615	8.47693
O	-6.78038	-0.48628	6.83494
Si	-5.86389	-0.87497	5.51917
O	-4.72921	0.28866	5.21057
O	-4.70587	1.96208	7.34120
O	-5.13996	3.02635	9.76147
Si	-6.49272	3.63731	10.56886
C	2.52343	3.43307	3.71731
C	0.08835	3.20511	5.63541
C	0.04497	-3.48256	1.77740
C	0.79284	-5.70385	3.77812
O	-1.61045	-0.25837	11.05899
Si	-1.33904	0.95726	12.19859
O	-3.72465	-1.57365	10.08183
Si	-4.59179	-2.73493	9.27844
O	-6.07082	-2.13945	8.84105
O	-3.77234	-3.23946	7.93658
O	-5.09693	-2.32538	5.75742
O	-4.81125	-4.02387	10.26396
Si	-4.48515	-4.34964	11.88772
O	-8.34206	-0.65889	9.03248
O	-6.92064	-0.98748	4.26267
H	-5.31714	-5.85241	5.94946
H	-5.68291	4.34898	4.95393
H	-3.65685	4.91769	3.71401
H	-3.68175	5.06631	6.15262
H	-2.61448	1.33523	12.87370
H	-0.73837	2.15539	11.54289
H	-3.01192	-4.38005	12.12095
H	-5.11463	-3.31776	12.76231
H	-6.51093	-0.99776	3.39255
H	-5.07437	-5.68856	12.16991
H	-4.68338	-5.39119	3.63677
H	-3.25263	-6.79056	5.03364
H	-8.95113	-1.24254	8.57051
H	-6.77702	2.82209	11.78478
H	-7.67995	3.63936	9.66610
H	-6.14350	5.03246	10.95876
H	-0.38443	0.38864	13.19143
H	1.55443	0.65236	4.53465
H	3.64786	-3.85219	3.59791
H	3.18177	-2.85920	2.21062
H	3.23055	-4.62160	2.05260
H	0.25913	-2.47691	1.40593

H 0.20098 -4.18846 0.95420
H -1.01018 -3.52822 2.06595
H 1.45268 -6.02526 4.59118
H 0.93572 -6.39707 2.94177
H -0.24107 -5.80364 4.12425
H -0.36306 -2.59003 4.69068
H 0.85130 -3.46507 5.63820
H 2.81761 4.76687 6.69386
H 2.60770 3.37094 7.76005
H 4.00126 3.45240 6.66732
H 3.60549 3.31223 3.60624
H 2.30018 4.50222 3.62475
H 2.02756 2.91447 2.89249
H -0.07491 4.28621 5.55916
H -0.51687 2.70810 4.87386
H -0.26766 2.87555 6.61516
H 1.98187 0.89818 6.74528
H 3.35906 0.82684 5.59479
H 3.02242 -1.37766 7.96065
H 1.28093 -1.34176 8.35131
H 3.65773 -5.56762 7.72820
H 3.15741 -4.68803 6.27443
H 4.44289 -4.03878 7.29358
H 2.94136 -4.50953 10.57831
H 3.79429 -3.00562 10.20010
H 2.11537 -2.95439 10.76250
H 0.64251 -5.49960 8.80610
H -0.19881 -3.94613 8.91810
H 0.13430 -4.66523 7.33770
H 4.04871 0.22779 -0.16115
H 2.39177 0.35368 -2.00241
H -0.03190 0.39406 -1.46367
H 4.63784 0.07736 2.02710
H 3.60311 1.00798 3.11185
H 3.52340 -0.74679 3.12572
H -1.78602 0.38980 -0.00949
H -1.56826 -0.59157 1.45131
H -1.49779 1.15799 1.56470
119
Product
C 1.52621 0.06778 -0.65458
C 0.73043 -0.21222 0.45947
C 1.32792 -0.16812 1.73971
C 2.67499 0.21804 1.90248
C 3.42733 0.48866 0.75449
C 2.86852 0.40276 -0.51452
C -0.73277 -0.50911 0.26319
S 0.25868 -0.46356 3.14634
W 0.90276 -2.37451 4.37984
C 0.08841 -4.30115 4.15679
Si 0.20734 -5.31142 2.53731
C 1.99985 -5.83270 2.23862
C 3.33099 0.35981 3.24792
C 2.02781 -2.01741 6.10875
Si 2.44829 -3.46017 7.30903

C	0.88010	-4.26256	7.99721
O	2.27030	-2.71886	3.41186
O	-0.71523	-1.88498	5.42230
Si	-2.11714	-1.58668	6.18759
O	-3.16469	-2.84999	5.93019
Si	-4.36942	-3.66954	6.69904
O	-4.29627	-5.22871	6.19870
Si	-5.33147	-6.55822	6.28975
C	2.42154	3.55382	6.94113
Si	2.37970	5.32409	7.62410
C	2.58324	5.28151	9.51070
C	3.54182	-4.73619	6.43593
C	3.42049	-2.67212	8.73508
O	-2.80403	-0.18404	5.63443
Si	-4.28187	0.48778	5.34371
O	-4.21853	1.44185	4.01589
Si	-3.79461	3.04920	3.71926
O	-1.83223	-1.43900	7.81823
Si	-2.37913	-0.61277	9.13372
O	-3.05533	0.83414	8.69411
Si	-4.52734	1.46926	8.28844
O	-5.73730	0.64384	9.05994
Si	-6.76246	-0.62357	8.79977
O	-7.10049	-0.79782	7.18834
Si	-6.52953	-1.59326	5.85976
O	-5.40017	-0.69491	5.05011
O	-4.74648	1.39476	6.65212
O	-4.55179	3.03509	8.76478
Si	-5.68803	4.01148	9.54718
C	3.79615	6.32880	6.85852
C	0.72008	6.13239	7.18709
C	-0.43515	-4.30838	1.06803
C	-0.87991	-6.85166	2.76786
O	-1.10542	-0.32335	10.12549
Si	-0.64432	0.99405	11.07580
O	-3.49315	-1.52712	9.95078
Si	-4.61558	-2.70749	9.64491
O	-6.09617	-2.03079	9.36242
O	-4.15512	-3.60829	8.33913
O	-5.85027	-3.03738	6.30719
O	-4.73424	-3.69134	10.94833
Si	-3.90891	-3.83671	12.41303
O	-8.13644	-0.25596	9.62490
O	-7.83722	-1.85035	4.89428
H	-6.22770	-6.44930	7.47777
H	-4.97334	3.92816	3.97199
H	-3.40172	3.12845	2.28443
H	-2.65713	3.46391	4.59041
H	-1.78784	1.46142	11.91272
H	-0.16313	2.10734	10.20846
H	-2.45690	-4.07867	12.16929
H	-4.08524	-2.60184	13.23142
H	-7.62621	-2.00513	3.96881
H	-4.51045	-5.00499	13.11509
H	-6.14925	-6.63037	5.04383

H	-4.47344	-7.77119	6.40276
H	-8.86797	-0.86394	9.48264
H	-5.77867	3.63374	10.98705
H	-7.02415	3.87741	8.89870
H	-5.19068	5.41001	9.41673
H	0.46321	0.51106	11.94776
H	2.31104	3.55218	5.85152
H	2.36162	-6.48634	3.03959
H	2.65159	-4.95602	2.18962
H	2.08802	-6.38272	1.29539
H	0.21912	-3.45393	0.87069
H	-0.46552	-4.92502	0.16327
H	-1.44814	-3.93688	1.25507
H	-0.54308	-7.44966	3.62116
H	-0.84414	-7.48893	1.87739
H	-1.92503	-6.57576	2.94298
H	-0.94093	-4.29056	4.53203
H	0.69766	-4.86210	4.89172
H	2.55780	6.29154	9.93338
H	1.78019	4.70344	9.98016
H	3.53606	4.82365	9.79693
H	4.76905	5.88425	7.09376
H	3.80005	7.35746	7.23444
H	3.70443	6.37277	5.76806
H	0.66587	7.15596	7.57291
H	0.57468	6.17622	6.10249
H	-0.11735	5.56991	7.61322
H	1.60906	2.95023	7.35964
H	3.36800	3.05869	7.18352
H	2.99248	-1.58806	5.81045
H	1.47361	-1.27621	6.69866
H	3.85168	-5.51868	7.13700
H	3.02496	-5.21841	5.60099
H	4.44520	-4.26484	6.03564
H	3.71927	-3.43379	9.46370
H	4.32825	-2.17886	8.37303
H	2.81373	-1.92613	9.25804
H	1.13814	-4.99624	8.76866
H	0.22758	-3.50971	8.44927
H	0.30447	-4.78067	7.22443
H	4.46840	0.78030	0.86943
H	3.47229	0.61638	-1.39227
H	1.07645	0.02775	-1.64346
H	4.20104	1.01884	3.18062
H	2.64180	0.77043	3.99157
H	3.67366	-0.61244	3.61793
H	-0.98043	-0.52044	-0.80161
H	-1.01771	-1.47404	0.69070
H	-1.36045	0.24710	0.74767

102

Product without TMS

C	1.38707	-0.00290	-0.57144
C	0.63497	-0.30294	0.55882
C	1.20035	-0.26132	1.83631
C	2.56763	0.07608	1.95369

C	3.33173	0.42975	0.82206
C	2.71814	0.37135	-0.43349
C	0.33340	-0.53853	3.03581
S	3.23750	0.19705	3.61046
W	4.94674	-1.38364	4.01553
O	4.87569	-0.54861	5.81745
Si	4.67889	-0.01896	7.34086
O	6.15059	0.43747	7.96215
Si	6.79899	1.54535	8.99540
O	6.95590	0.88165	10.50417
Si	6.24134	-0.27123	11.45612
O	7.37599	-0.95574	12.41788
Si	9.05701	-0.85195	12.52932
C	4.76581	0.87159	0.91099
C	4.66782	-3.24676	4.95331
Si	3.63051	-4.65471	4.18168
C	3.45881	-6.00415	5.50684
C	6.91308	-0.67965	3.86398
Si	8.38755	-1.82077	4.33997
C	9.94983	-0.77872	4.06598
O	4.92821	-2.03609	2.43372
C	4.51656	-5.35805	2.66636
C	1.90986	-4.03249	3.70319
C	8.30851	-2.33204	6.15950
C	8.42800	-3.32921	3.19798
O	4.05009	-1.24363	8.27069
Si	4.10941	-1.82114	9.81253
O	2.87051	-1.19567	10.71825
Si	1.92624	0.16446	10.79920
O	0.43578	-0.20727	11.38969
O	3.65497	1.28294	7.38381
Si	2.49071	1.96582	8.33141
O	3.16881	3.14874	9.27623
Si	4.61858	3.53188	9.97124
O	4.78170	5.15991	10.00248
Si	4.75175	6.33614	11.21503
O	3.95068	-3.45116	9.73328
Si	3.56747	-4.65466	10.85284
O	5.56002	-1.44770	10.51685
O	1.31519	2.62303	7.40148
Si	1.13703	4.08602	6.57632
O	1.78219	0.81471	9.28438
O	5.86001	2.90843	9.07308
O	8.28900	1.95695	8.44877
Si	9.05992	3.42738	8.14100
O	4.68369	2.94403	11.51732
Si	4.06201	1.71730	12.42992
O	3.91173	2.32801	13.94919
O	2.58001	1.24313	11.86352
O	5.08395	0.41494	12.41532
H	4.00222	-4.25697	12.22365
H	0.56714	5.10892	7.50068
H	0.19006	3.83202	5.45475
H	2.45056	4.55603	6.04832
H	9.04791	4.28914	9.35883

H	8.39037	4.13482	7.01134
H	9.68740	-1.21800	11.22754
H	9.46476	0.52919	12.91857
H	-0.18527	-0.52919	10.72965
H	9.46389	-1.82158	13.58478
H	2.09433	-4.89138	10.83804
H	4.28291	-5.88944	10.42443
H	3.45388	1.75516	14.57148
H	5.92879	6.17346	12.11632
H	3.48867	6.24000	12.00219
H	4.82152	7.65013	10.51579
H	10.46301	3.08840	7.77056
H	5.48573	-5.79009	2.93789
H	4.68307	-4.57793	1.91845
H	3.91667	-6.15200	2.20826
H	1.97752	-3.29437	2.89844
H	1.28354	-4.85927	3.35122
H	1.40629	-3.57146	4.55937
H	4.43807	-6.38375	5.81696
H	2.87594	-6.85041	5.12672
H	2.95098	-5.61872	6.39709
H	4.36793	-3.07130	5.99273
H	5.70988	-3.62020	4.98037
H	7.09573	-0.38739	2.82240
H	6.98648	0.20821	4.50451
H	9.29491	-3.96028	3.42144
H	7.52824	-3.94317	3.29874
H	8.49790	-3.01876	2.15044
H	10.84633	-1.36275	4.30157
H	10.02954	-0.44376	3.02683
H	9.94761	0.10685	4.70940
H	9.21438	-2.88367	6.43388
H	8.24062	-1.45051	6.80407
H	7.44970	-2.97221	6.38151
H	3.30097	0.63495	-1.31258
H	0.93063	-0.04184	-1.55670
H	-0.41433	-0.56862	0.45819
H	5.06066	1.40063	0.00063
H	4.93087	1.53426	1.76611
H	5.43008	0.00936	1.03016
H	-0.68287	-0.79149	2.72196
H	0.72009	-1.36473	3.63855
H	0.27611	0.33344	3.69671