On the use of ^{17}O NMR for the understanding of molecular and silica-grafted tungsten oxo siloxide complexes.

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Supporting Information

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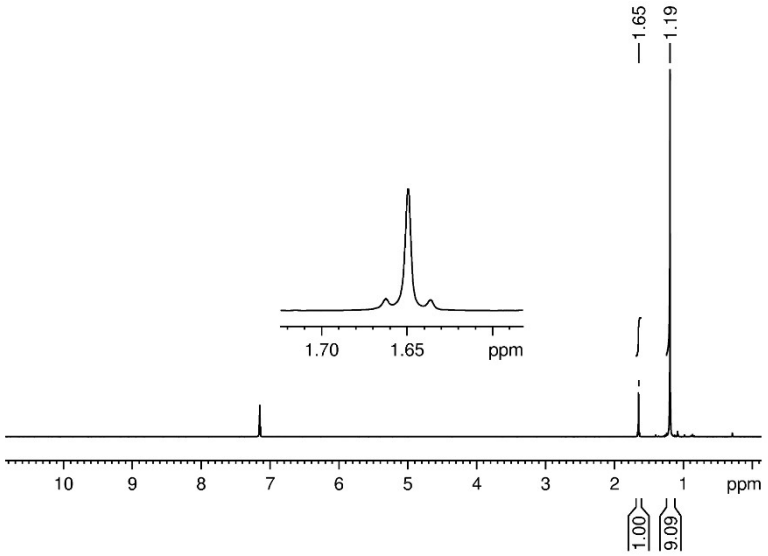


Figure S1. ^{1}H NMR spectrum of **1-Me** (300 MHz, C_6D_6)

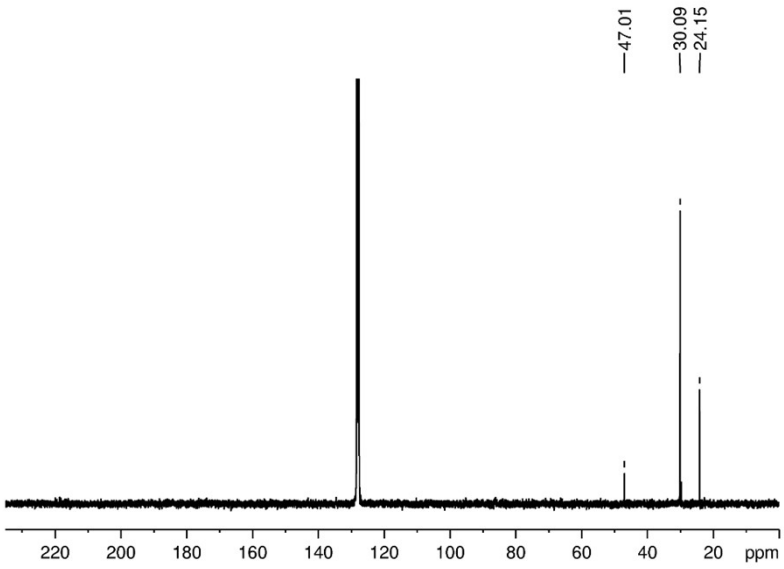
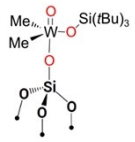
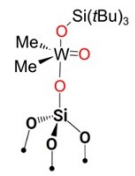
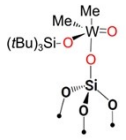
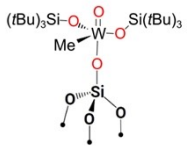
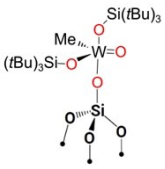
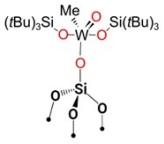


Figure S2. ^{13}C NMR spectrum of **1-Me** (75 MHz, C_6D_6)

Table S1. Calculated ^{17}O NMR parameters for all the possible species resulting from the **1-Me** grafting onto SiO_{2-700}

Species	CS (ppm)	C_Q (MHz)	η_Q	Δ_{CSA}	η_{CSA}
W−OSi*t*Bu$_3$ silanolysis products					
	**717**	**4.2**	**0.5**	**619**	**0.5**
	**621**	**0.3**	**0.9**	**484**	**0.5**
	**652**	**1.8**	**0.8**	**391**	**0.4**
W−CH$_3$ silanolysis products					
	**765**	**4.2**	**0.6**	**521**	**0.3**
	**734**	**1.2**	**0.7**	**545**	**0.5**
	**656**	**1.7**	**0.1**	**391**	**0.1**

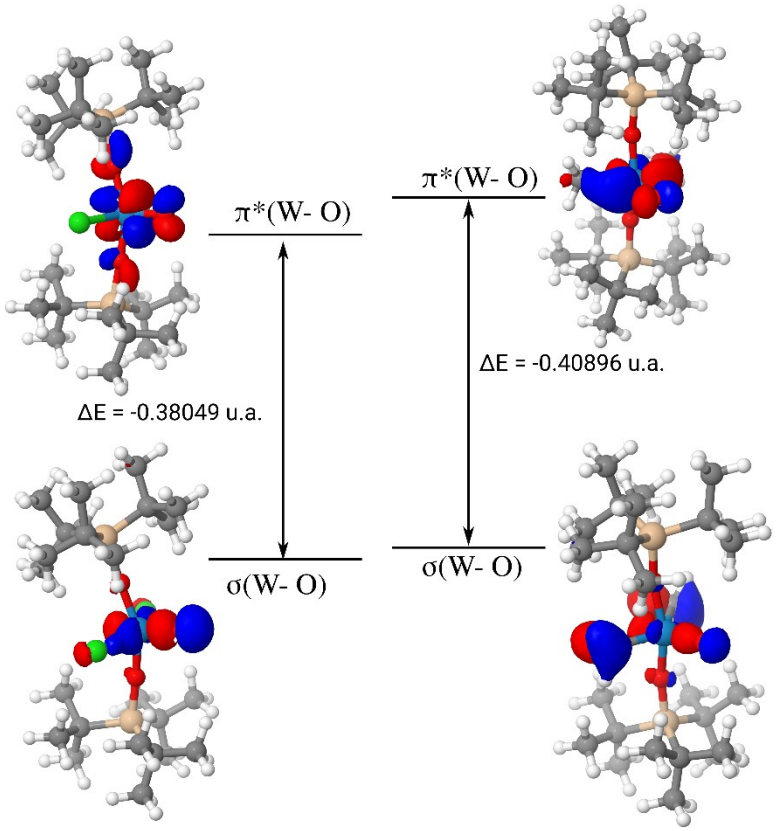


Figure S3. Energy difference between the σ(W-O) and π*(W-O) orbitals involved in the deshielding of the σ_{11} component of **1-Cl** and **1-Me**

Table S2. Canonical MO contributions in ppm to σ_{iso} in **1-Cl** and **1-Me**. For sake of clarity only the contributions above 1 ppm are indicated. The HOMO MO is the number 139 for **1-Cl** and 131 for **1-Me**.

1-Cl					**1-Me**			
Orbital	contribution	Orbital	contribution		Orbital	contribution	Orbital	contribution
3.	270.37	100.	3.09		3.	270.37	93.	-1.61
38.	1.77	102.	7.08		30.	1.73	94.	-4.71
39.	5.24	103.	6.61		31.	4.58	96.	-1.37
40.	-7.05	104.	-1.63		32.	-5.82	97.	1.81
41.	-4.73	106.	9.94		33.	-4.56	98.	-35.12
42.	-1.37	108.	32.28		34.	-1.76	99.	-1.69
44.	19.64	109.	1.77		36.	20.69	100.	-165.16
47.	-2.26	111.	46.67		37.	1.27	101.	-56.75
50.	1.18	113.	1.39		38.	1.47	102.	-58.04
51.	1.01	115.	68.82		41.	1.96	103.	-26.83
65.	-1.98	116.	72.15		42.	1.92	104.	-3.02
71.	-3.25	117.	-9.47		47.	1.28	105.	-2.93
72.	-4.88	118.	-113.01		48.	1.68	106.	-130.86
73.	-6.27	119.	9.69		51.	1.08	107.	-35.23
74.	-7.22	120.	1.45		52.	1.14	108.	-19.21
75.	-2.48	121.	10.36		53.	-1.26	109.	-1.15
76.	-20.55	122.	-81.94		54.	1.10	110.	44.17
78.	-2.51	123.	2.03		55.	1.08	111.	14.24
80.	3.87	124.	21.67		58.	1.13	112.	-5.55
81.	-57.70	125.	12.29		63.	-1.90	114.	11.96
83.	-7.69	126.	4.09		65.	-7.53	115.	14.22
85.	-26.45	127.	-3.99		68.	-4.09	116.	-6.99
86.	-6.44	128.	-6.60		69.	1.01	117.	6.78
87.	-51.36	129.	18.63		70.	-5.59	118.	10.62
88.	4.42	130.	25.60		72.	4.86	119.	-2.48
90.	-53.27	131.	-44.62		74.	-18.28	120.	16.29
91.	-440.62	132.	13.62		75.	-7.99	121.	1.87
92.	-55.50	133.	-74.66		77.	-14.09	122.	3.38
93.	-6.79	134.	8.11		81.	-1.55	124.	-3.62
94.	67.08	136.	-37.67		82.	-1.81	125.	-3.07
95.	-133.10	137.	15.78		83.	-14.30	126.	-146.14
98.	-1.05	138.	2.48		84.	-184.67	127.	62.89
99.	-3.24	139.	1.23		85.	20.70	128.	-1.28
					86.	34.43	129.	17.61
					89.	4.71	130.	-45.99
					91.	3.80	131.	54.38

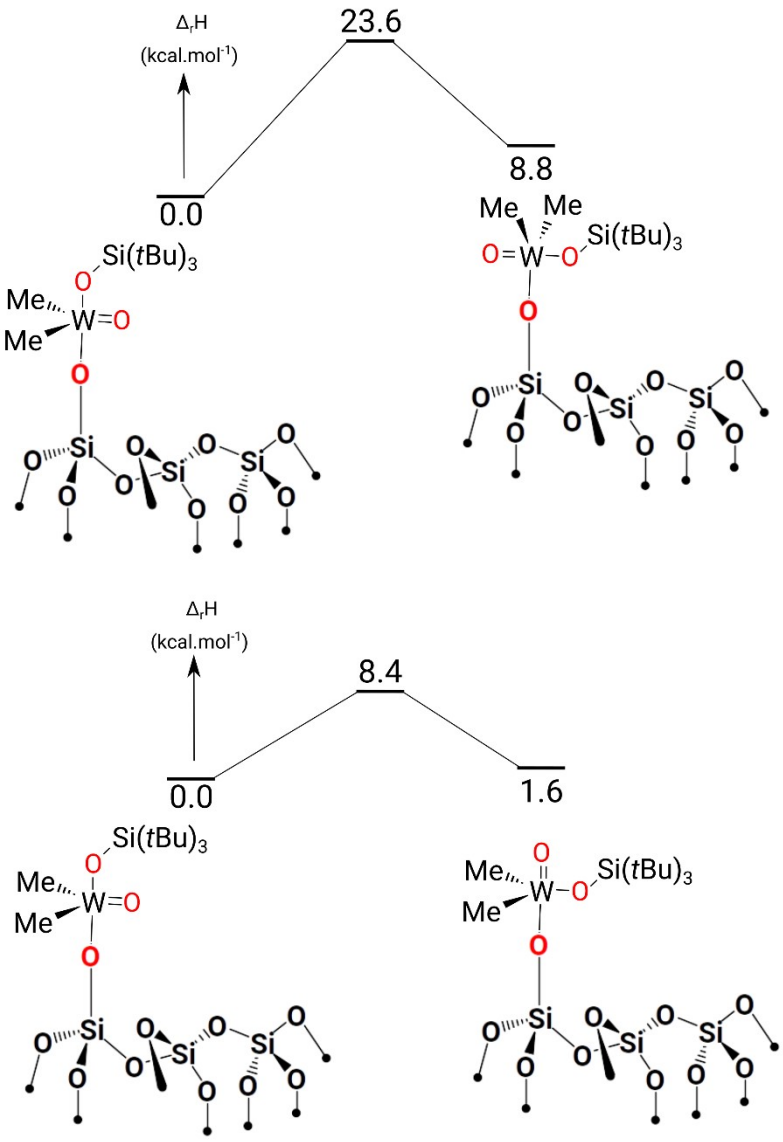


Figure S4. Interconversion barriers of the different isomeric structures within material **2**

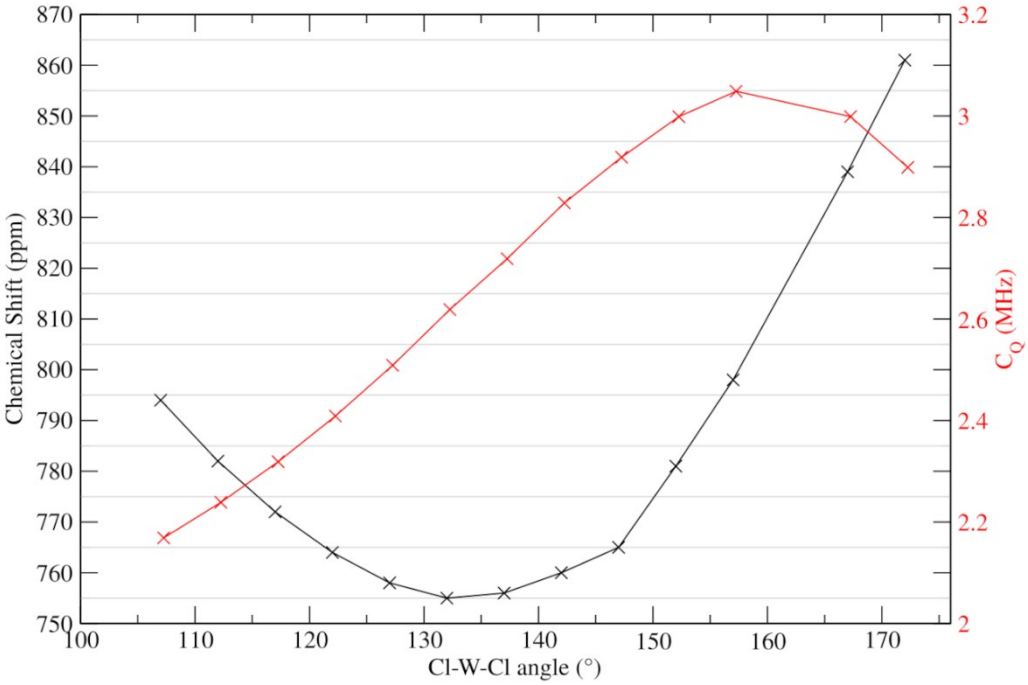


Figure S5. Chemical shift and CQ evolution as a function of the Cl-W-Cl angle in complex **1-Cl**

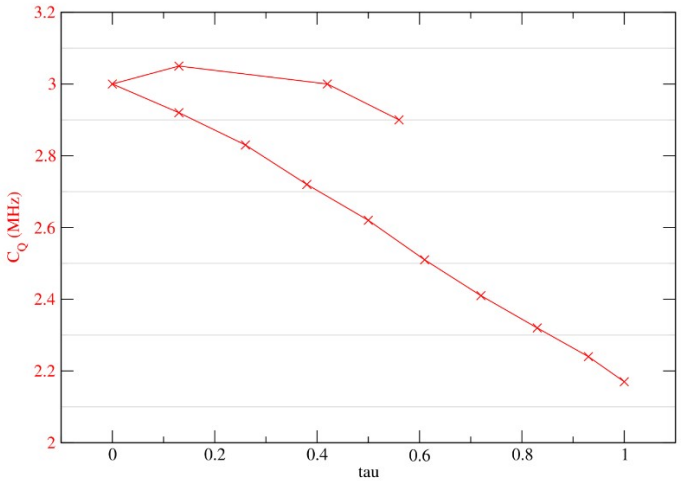


Figure S6. CQ evolution as a function of the τ in complex **1-Cl**

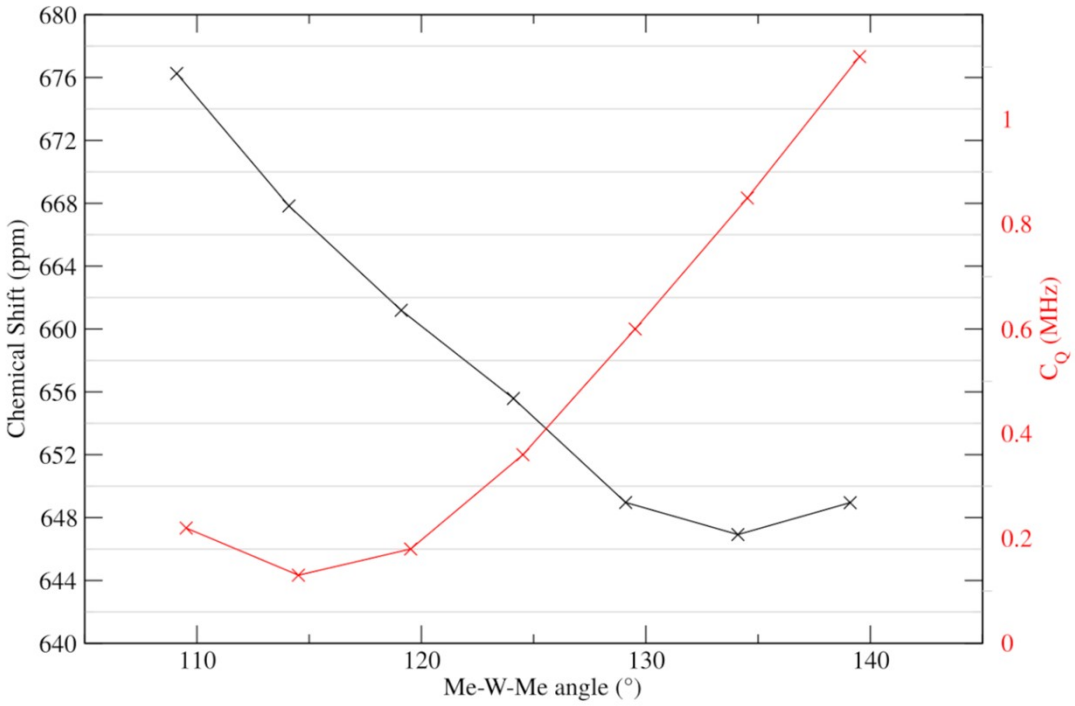


Figure S7. Chemical shift and CQ evolution as a function of the Me-W-Me angle in complex **1-Me**

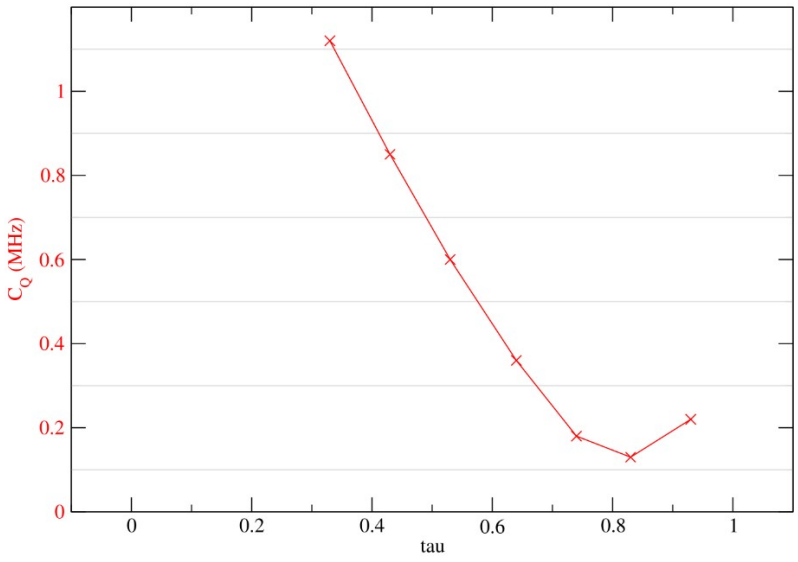


Figure S8. CQ evolution as a function of the τ in complex **1-Me**

Cartesian Coordinates :

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Silica model

O	0.19500	1.10992	9.54871
Si	0.38958	2.33464	8.46888
O	1.51654	3.41236	9.02634
Si	2.63487	4.49301	8.46638
O	1.96050	5.99946	8.33184
Si	0.48886	6.69735	8.06601
O	0.50126	8.10286	8.92078
O	-1.09303	3.04531	8.33080
Si	-1.75660	4.53762	8.06198
O	-0.74297	5.72784	8.59831
O	0.88785	1.74766	7.00215
Si	0.68344	2.04195	5.38809
O	-0.79429	2.74084	5.12489
Si	-1.47644	4.24112	4.98065
O	-2.71991	4.14286	3.92260
Si	-3.17302	5.00580	2.54195
O	-3.16216	4.67156	8.88761
Si	-4.27273	3.57825	9.54091
O	-2.05214	4.73714	6.44732
O	0.77408	0.63018	4.56536
Si	-0.35354	-0.45652	3.93252
O	1.89413	3.02383	4.83794
Si	2.91008	4.21171	5.38708
O	3.20921	3.99607	6.99835
O	3.87582	4.54588	9.53117
Si	4.67688	5.77880	10.36377
O	2.24124	5.70210	5.13735
Si	0.75026	6.40510	4.97827
O	0.28168	7.00125	6.45087

O	4.32098	4.14231	4.56116
Si	5.12346	2.94334	3.68263
O	0.80241	7.60937	3.85946
O	-0.35745	5.32123	4.41197
H	-5.49617	4.36805	9.85621
H	-3.71716	2.97364	10.78530
H	-4.59336	2.50841	8.55182
H	-0.97608	0.11518	2.70377
H	-1.40845	-0.76142	4.94258
H	5.10761	1.65165	4.42896
H	4.47405	2.76922	2.35141
H	-0.35731	8.52712	9.00973
H	6.52456	3.41927	3.50961
H	3.75722	6.41411	11.35066
H	5.18643	6.80394	9.40735
H	5.81551	5.12689	11.06980
H	1.51725	8.24163	3.97903
H	-2.16090	4.81512	1.46348
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H	-4.48613	4.44408	2.11779
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H	1.00488	0.65274	9.79369

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HOsitBu3

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Si	1.15819	-4.92429	-2.27230
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C	-0.00869	-6.54996	-4.38612
C	2.85465	-4.26283	-2.99334
C	2.69953	-2.78875	-3.41757
C	1.35480	-6.42937	-1.05247
C	1.95994	-5.93797	0.27808
C	3.95329	-4.28431	-1.91558
C	3.34447	-5.08506	-4.19665

C	-0.01420	-7.04362	-0.70757
C	2.24690	-7.53962	-1.63349
C	-0.15785	-4.08707	-4.72469
C	-1.60102	-5.16017	-3.03638
H	0.31949	-2.89289	-1.67093
H	-0.77262	-6.66792	-5.16812
H	0.96802	-6.63000	-4.87474
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H	-0.97978	-4.23269	-5.44023
H	-0.29447	-3.09028	-4.28851
H	0.77029	-4.07730	-5.30251
H	-2.36058	-5.24120	-3.82699
H	-1.77671	-5.97442	-2.33160
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H	3.48914	-6.14148	-3.94654
H	2.65760	-5.03654	-5.04698
H	4.86501	-3.81497	-2.31263
H	3.66075	-3.72359	-1.02189
H	4.22412	-5.29829	-1.60844

5

Methane

C	6.99098	-1.51536	-2.39461
H	7.38404	-2.01504	-3.28230
H	6.55672	-0.55500	-2.67934
H	7.80021	-1.35157	-1.68028
H	6.22199	-2.14018	-1.93593

86

1-Cl

Cl	-0.42170	-3.03824	4.11401
W	1.35478	-3.89457	2.81658
O	1.91908	-5.26199	3.62892
O	0.05240	-4.59948	1.70386
Si	-1.22273	-5.20585	0.67662
C	-2.17515	-6.50812	1.77998
C	-1.37412	-7.81356	1.93301
O	2.39196	-2.54836	3.55032
Si	3.40547	-1.28545	4.20637
C	3.29550	0.16359	2.89993
C	3.76099	1.49776	3.51362
Cl	2.68852	-3.67456	0.88243
C	2.59779	-0.85425	5.93437
C	1.31624	-0.01830	5.76362
C	5.17400	-2.10336	4.35298
C	5.23350	-3.09642	5.52786
C	2.19440	-2.13466	6.69115
C	3.58075	-0.05243	6.80889
C	-0.28953	-6.00711	-0.84363
C	0.91937	-6.83786	-0.36963
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C	-1.33782	-2.43440	-0.07461
C	0.25778	-4.93346	-1.80106
C	-1.23931	-6.92203	-1.63905
C	6.25087	-1.02421	4.57323
C	5.52646	-2.90436	3.08632
C	4.16437	-0.11646	1.66066

C	1.84686	0.31951	2.39878
C	-3.15398	-3.88345	-1.02284
C	-3.19510	-3.19022	1.36858
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C	-2.40433	-5.96758	3.20328
H	-4.04282	-7.61043	1.76417
H	-4.20889	-5.98246	1.11192
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H	-1.46179	-5.77272	3.72069
H	-2.99218	-5.04878	3.22982
H	-1.90827	-8.48248	2.62212
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H	-3.76127	-2.99209	-1.23320
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H	-3.96986	-3.92909	1.59053
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H	-1.94094	-1.55830	-0.35079
H	-0.75774	-2.15743	0.81157
H	-0.63787	-2.62042	-0.89146
H	-0.70893	-7.32318	-2.51382
H	-1.58339	-7.77971	-1.05366
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110
1-Bu
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W 0.08089 -3.09538 1.99876
O -0.20039 -2.36842 3.72006
Si -0.57503 -1.29315 5.01693
C -2.50890 -1.44308 5.30337
C -3.28367 -1.31152 3.97754
C -1.05441 -5.59142 3.31653

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C	-1.63837	-7.79116	4.47979
C	2.09522	-3.60021	2.65274
C	3.25196	-2.61071	2.47668
C	4.55673	-3.04169	3.16751
C	5.18354	-4.31817	2.61214
O	0.39989	-4.19464	0.49663
Si	0.51652	-4.75571	-1.12829
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C	1.09202	-7.39617	-2.22735
O	-0.22578	-1.65642	1.12485
C	-1.07875	-4.12527	-2.07699
C	-2.34025	-4.26326	-1.20588
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C	0.42320	-3.51502	6.56250
C	-0.04136	0.50992	4.46082
C	0.08297	1.44881	5.67555
C	-0.01412	-1.43475	7.87378
C	1.96535	-1.59996	6.36787
C	2.26263	-2.48677	-1.51460
C	3.40846	-4.65987	-1.23934
C	1.53824	-7.08513	0.21249
C	-0.78689	-7.28089	-0.59166
C	1.30614	0.48059	3.71796
C	-1.05647	1.12733	3.48149
C	-2.86786	-2.81244	5.90751
C	-3.02466	-0.35092	6.25913
H	-2.15363	-4.50831	-3.92224
H	-0.43340	-4.87716	-4.05104
H	-1.51525	-5.97773	-3.18800

H	-1.92155	-2.30203	-2.88089
H	-0.78289	-2.00786	-1.56022
H	-0.19226	-2.43277	-3.18108
H	-3.21611	-3.94569	-1.78948
H	-2.52877	-5.28585	-0.87118
H	-2.28990	-3.61678	-0.32591
H	1.08554	-8.48643	-2.08688
H	0.46074	-7.18011	-3.09491
H	2.11812	-7.11392	-2.48183
H	-0.69434	-8.35934	-0.39951
H	-1.20065	-6.82496	0.31376
H	-1.51753	-7.16284	-1.39675
H	1.51353	-8.17401	0.36040
H	2.57759	-6.80859	0.02654
H	1.23162	-6.61641	1.15174
H	3.23333	-2.10104	-1.85756
H	1.48769	-1.88961	-1.99639
H	2.19456	-2.30125	-0.44016
H	3.20062	-3.74963	-3.74511
H	2.19346	-5.19752	-3.69719
H	1.45151	-3.60487	-3.89954
H	4.31250	-4.14624	-1.59636
H	3.41292	-4.60284	-0.14652
H	3.50480	-5.71035	-1.52768
H	-2.36919	-3.91004	2.95520
H	-1.97162	-4.83214	1.50509
H	0.32551	2.46357	5.32965
H	-0.84485	1.52081	6.25224
H	0.88005	1.14823	6.36181
H	1.58802	1.50741	3.44441
H	2.12190	0.07225	4.31824
H	1.23326	-0.09268	2.78996
H	-0.66688	2.09115	3.12398
H	-1.21554	0.49453	2.60337

H	-2.02369	1.33226	3.94909
H	0.64079	-1.79814	8.67834
H	-0.00511	-0.34131	7.91986
H	-1.02735	-1.77241	8.11144
H	2.54513	-2.06800	7.17621
H	2.38418	-1.95447	5.42087
H	2.13942	-0.52275	6.43307
H	1.04669	-3.88025	7.39092
H	-0.58496	-3.90299	6.72177
H	0.81006	-3.95720	5.64034
H	-4.10359	-0.48596	6.42034
H	-2.54647	-0.38338	7.24254
H	-2.88708	0.65487	5.85175
H	-3.96098	-2.90565	5.97641
H	-2.50802	-3.64439	5.29407
H	-2.47312	-2.94159	6.91958
H	-4.34729	-1.52134	4.15982
H	-3.22247	-0.31074	3.54827
H	-2.93792	-2.01391	3.21644
H	2.32807	-4.54860	2.15371
H	1.97255	-3.82335	3.72263
H	-0.20381	-6.09603	2.83518
H	-0.68018	-5.20303	4.27297
H	-2.99065	-6.15170	4.08509
H	-2.50991	-7.03913	2.65069
H	-0.80104	-8.31727	4.00741
H	-2.42972	-8.52533	4.66331
H	-1.29205	-7.42676	5.45354
H	2.96508	-1.63075	2.87287
H	3.45190	-2.45739	1.40823
H	5.28081	-2.22039	3.08199
H	4.36591	-3.16782	4.24225
H	4.52221	-5.18237	2.73402
H	6.12301	-4.55146	3.12412

H 5.40600 -4.21676 1.54376

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1-Bu form2

C 2.84932 -3.28891 14.08102

C 2.32823 -4.63131 14.59439

C 2.84421 -4.97947 15.99653

C 2.32348 -6.32257 16.50329

W 2.28970 -2.74530 12.07092

C 0.44592 -3.25982 11.08331

C 0.45708 -4.33795 10.00571

C -0.93207 -4.61416 9.41955

C -0.92144 -5.70040 8.34578

O 1.15022 -1.39862 12.92593

Si 0.05761 -0.34311 13.70674

C -0.94100 -1.37064 15.05205

C -0.07514 -1.69907 16.28172

O 2.82301 -4.32468 11.64221

O 3.52651 -1.65711 11.21515

Si 4.80984 -1.29968 10.09581

C 4.08243 -1.72776 8.33330

C 2.60846 -1.29029 8.23446

C 1.17375 1.04997 14.52464

C 0.41707 1.86762 15.58678

C -1.12866 0.39142 12.31877

C -2.22068 -0.61033 11.90035

C 2.40821 0.41085 15.18671

C 1.70177 2.03389 13.46602

C -0.31477 0.72426 11.05400

C -1.84051 1.67464 12.78643

C -2.18369 -0.60868 15.54875

C -1.39905 -2.71799 14.46597

C 5.08665 0.61356 10.38455

C 5.13331 0.91900 11.89362

C 6.36498 -2.38056 10.58952

C	5.98686	-3.85012	10.85082
C	6.39009	1.11966	9.74095
C	3.91652	1.42600	9.80147
C	7.01605	-1.85715	11.88231
C	7.42279	-2.34211	9.47003
C	4.87479	-1.02670	7.21418
C	4.11592	-3.24460	8.07056
H	8.31403	-2.89890	9.79198
H	7.06927	-2.81374	8.54828
H	7.74964	-1.32653	9.22494
H	6.89352	-4.40321	11.13532
H	5.26447	-3.95871	11.66246
H	5.56443	-4.34842	9.97742
H	7.82564	-2.53840	12.17933
H	7.46221	-0.86618	11.76161
H	6.30680	-1.81450	12.71556
H	6.47736	2.20462	9.89332
H	7.27926	0.66367	10.18646
H	6.42709	0.94219	8.66137
H	5.17082	2.00700	12.04274
H	4.24552	0.54485	12.40882
H	6.00994	0.49636	12.38762
H	4.03837	2.48433	10.07151
H	3.87421	1.37891	8.70966
H	2.94968	1.09804	10.19547
H	3.60187	-3.45849	7.12284
H	5.13405	-3.63171	7.97189
H	3.60943	-3.81658	8.85432
H	4.47723	-1.33168	6.23614
H	4.79482	0.06337	7.26520
H	5.93821	-1.28533	7.22384
H	2.21153	-1.57839	7.25103
H	1.98638	-1.77814	8.99041
H	2.47135	-0.21224	8.33682

H	3.94877	-3.32836	14.01677
H	2.58662	-2.47200	14.75811
H	-0.20237	-3.56375	11.92131
H	0.01742	-2.32485	10.70108
H	-2.68695	-1.19684	16.32961
H	-1.93526	0.36203	15.98868
H	-2.91932	-0.43827	14.75771
H	-1.94567	-3.28629	15.23230
H	-2.06439	-2.60800	13.60717
H	-0.54683	-3.32916	14.15584
H	-0.64578	-2.34108	16.96805
H	0.83546	-2.24264	16.01300
H	0.21539	-0.80909	16.84637
H	-2.51366	2.03117	11.99357
H	-2.45288	1.51540	13.67925
H	-1.14353	2.48915	13.00102
H	-2.79559	-0.19078	11.06230
H	-1.80913	-1.56564	11.56383
H	-2.93406	-0.81492	12.70352
H	-0.99275	1.07665	10.26340
H	0.42269	1.51151	11.22256
H	0.21694	-0.14974	10.66815
H	1.06986	2.66318	15.97393
H	-0.47720	2.35333	15.18403
H	0.11038	1.26304	16.44519
H	2.42795	2.71554	13.93151
H	2.21439	1.52394	12.64612
H	0.91217	2.65676	13.03717
H	3.04453	1.19833	15.61534
H	2.15111	-0.27388	15.99833
H	3.01112	-0.14124	14.46064
H	1.22897	-4.62796	14.62037
H	2.61625	-5.42129	13.89119
H	3.94252	-4.99196	15.97919

H 2.56009 -4.18469 16.69941
H 2.70868 -6.55074 17.50253
H 1.22899 -6.32699 16.56040
H 2.62212 -7.13937 15.83676
H 1.13266 -4.04754 9.19007
H 0.87505 -5.26202 10.42163
H -1.61370 -4.90692 10.23031
H -1.34275 -3.68563 8.99923
H -1.92477 -5.88080 7.94583
H -0.27459 -5.42147 7.50605
H -0.54763 -6.64902 8.74731
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1-Bu form 3
O 1.05906 -1.40221 13.24932
W 2.32839 -2.57256 12.56055
O 2.21041 -4.22150 12.97707
Si -0.29633 -0.46817 13.83039
C 0.47458 0.94861 14.93409
C -1.13146 0.21751 12.20073
C -1.43290 -1.70855 14.82589
O 1.95179 -2.74165 10.68423
Si 1.89746 -3.65313 9.22011
C 0.50359 -5.01439 9.49997
C 3.69830 -2.36690 14.27100
C 4.16168 -1.69412 11.71084
C 1.41334 -2.32671 7.86460
C 3.64803 -4.47514 8.85743
C 1.54009 0.39109 15.89281
C 1.17887 2.00947 14.06884
C -0.61617 1.65164 15.76475
C -0.05087 0.66814 11.20015
C -2.06668 1.40529 12.49189
C -1.95575 -0.87180 11.49281
C -2.85288 -1.13539 14.99667

C	-1.52077	-3.06162	14.09510
C	-0.88021	-2.00366	16.23148
C	-0.02725	-5.57324	8.16717
C	1.01181	-6.19109	10.35577
C	-0.68003	-4.40544	10.27092
C	-0.05325	-1.88505	8.01268
C	1.60150	-2.84885	6.42896
C	2.28203	-1.06827	8.05020
C	3.49265	-5.61480	7.83008
C	4.68342	-3.49532	8.27516
C	4.25523	-5.06289	10.14582
H	1.29190	-2.07439	5.71256
H	2.64291	-3.09304	6.20121
H	0.99692	-3.73724	6.22153
H	1.96606	-0.29491	7.33555
H	2.17874	-0.65406	9.05679
H	3.34375	-1.25569	7.87408
H	-0.26186	-1.06870	7.30625
H	-0.75959	-2.68924	7.78714
H	-0.27320	-1.50988	9.01584
H	-0.78069	-6.34798	8.36869
H	-0.51378	-4.80568	7.55789
H	0.75490	-6.03642	7.55862
H	-1.44595	-5.17807	10.42952
H	-0.37199	-4.04725	11.25667
H	-1.15815	-3.58006	9.73919
H	0.17656	-6.87968	10.55013
H	1.79210	-6.77575	9.86135
H	1.39332	-5.85705	11.32498
H	5.64033	-4.02104	8.14658
H	4.39656	-3.11165	7.29243
H	4.87531	-2.64016	8.92832
H	4.48218	-6.03751	7.60579
H	2.87287	-6.43479	8.19939

H	3.06802	-5.27252	6.88076
H	5.19403	-5.57992	9.89982
H	4.49847	-4.28626	10.87579
H	3.60315	-5.78466	10.64021
H	4.60610	-2.93216	14.03032
H	4.01687	-1.32258	14.39842
C	3.12662	-2.92174	15.57995
H	5.07490	-1.99214	12.23434
H	4.25244	-2.01216	10.67078
C	4.04381	-0.16061	11.73371
H	-3.46073	-1.83736	15.58408
H	-2.85814	-0.18056	15.53238
H	-3.36914	-0.98712	14.04445
H	-2.16242	-3.74190	14.67251
H	-1.95237	-2.98430	13.09529
H	-0.54116	-3.54092	14.00667
H	-1.52371	-2.74788	16.72111
H	0.12889	-2.42416	16.20050
H	-0.86591	-1.12171	16.87762
H	-2.55367	1.72188	11.55896
H	-2.86245	1.15243	13.19967
H	-1.53321	2.27616	12.88319
H	-2.33781	-0.47447	10.54202
H	-1.35430	-1.75375	11.25730
H	-2.82359	-1.19612	12.07303
H	-0.53560	1.02570	10.28095
H	0.57208	1.48274	11.57439
H	0.60620	-0.16017	10.92081
H	-0.16713	2.48061	16.32935
H	-1.41206	2.07814	15.14625
H	-1.08146	0.98400	16.49601
H	1.67011	2.74200	14.72459
H	1.95388	1.57134	13.43259
H	0.48709	2.56652	13.43191

H	1.96654	1.21800	16.47765
H	1.14081	-0.33397	16.60412
H	2.36014	-0.08430	15.34933
C	4.08812	-2.76219	16.76467
H	2.17956	-2.42931	15.83213
H	2.89132	-3.98499	15.44482
C	3.53826	-3.34092	18.06708
H	5.04094	-3.24980	16.51790
H	4.31972	-1.69711	16.90301
H	4.24735	-3.21836	18.89276
H	2.60364	-2.84745	18.35763
H	3.32750	-4.41158	17.96611
C	5.24072	0.53368	11.06944
H	3.12845	0.16358	11.21747
H	3.96051	0.20490	12.76640
C	5.14267	2.05745	11.09315
H	6.16125	0.21340	11.57519
H	5.32511	0.18479	10.03198
H	6.01156	2.52189	10.61531
H	4.24840	2.40620	10.56397
H	5.08816	2.43602	12.12031

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1-Me

C	-0.51480	-2.19466	3.30208
W	1.13187	-3.30899	2.45661
O	1.66181	-4.70624	3.28368
O	-0.16434	-4.09966	1.35129
Si	-1.29632	-5.13734	0.57217
C	-1.94528	-6.35806	1.95838
C	-0.89192	-7.42821	2.29822
O	2.24228	-2.04069	3.28478
Si	3.41080	-1.16426	4.19509
C	3.66863	0.50404	3.20600
C	4.35507	1.58101	4.06503

C	2.15002	-2.76808	0.62920
C	2.60745	-0.89513	5.96214
C	1.51998	0.19378	5.92843
C	5.00117	-2.30502	4.24217
C	4.80251	-3.48567	5.21054
C	1.93092	-2.18784	6.45851
C	3.66706	-0.47025	6.99614
C	-0.28476	-6.04653	-0.83756
C	1.07739	-6.52858	-0.30209
C	-2.67692	-3.93684	-0.12397
C	-2.02022	-2.68336	-0.73447
C	0.00729	-5.10568	-2.02079
C	-1.05610	-7.26355	-1.38097
C	6.24709	-1.51648	4.68376
C	5.27410	-2.92660	2.85975
C	4.52893	0.28288	1.94901
C	2.30980	1.04280	2.71789
C	-3.54349	-4.61993	-1.19675
C	-3.61099	-3.44214	0.99477
C	-3.23591	-7.06979	1.51305
C	-2.22623	-5.60072	3.26970
H	2.01663	-3.50261	-0.16731
H	1.69190	-1.82391	0.29777
H	3.21647	-2.59037	0.78284
H	-0.72387	-1.38322	2.58862
H	-1.41945	-2.79750	3.40306
H	-0.27350	-1.74117	4.26492
H	-3.54925	-7.78142	2.28980
H	-4.06803	-6.37542	1.36221
H	-3.10588	-7.64075	0.58826
H	-2.60584	-6.31002	4.01878
H	-1.31431	-5.15791	3.67932
H	-2.97488	-4.81268	3.16384
H	-1.25621	-8.03656	3.13847

H	-0.70340	-8.11625	1.46933
H	0.05939	-6.98393	2.60702
H	-4.32645	-3.92706	-1.53623
H	-2.96862	-4.90816	-2.08144
H	-4.04878	-5.51553	-0.82054
H	-4.32371	-2.71620	0.57811
H	-4.20128	-4.24619	1.44279
H	-3.06258	-2.93395	1.79361
H	-2.80288	-1.98816	-1.06965
H	-1.40244	-2.15780	-0.00034
H	-1.39282	-2.90613	-1.59992
H	-0.48552	-7.72382	-2.19993
H	-1.20507	-8.03777	-0.62293
H	-2.03809	-6.99595	-1.78408
H	1.64441	-6.99111	-1.12234
H	1.67990	-5.70544	0.09027
H	0.98771	-7.27368	0.48979
H	0.64745	-5.62557	-2.74749
H	-0.89736	-4.80185	-2.55481
H	0.53770	-4.19985	-1.71163
H	2.47225	1.94854	2.11666
H	1.79367	0.31493	2.08458
H	1.63612	1.31367	3.53338
H	4.58641	1.22037	1.37762
H	5.55622	-0.00965	2.18330
H	4.09981	-0.47368	1.28489
H	4.51864	2.48591	3.46286
H	3.75379	1.87814	4.92942
H	5.33437	1.25966	4.43438
H	1.03916	0.25608	6.91495
H	1.92085	1.18678	5.70738
H	0.73412	-0.02344	5.19865
H	3.17998	-0.27670	7.96226
H	4.41896	-1.24596	7.16895

H 4.19083 0.44797 6.71095

H 1.45845 -1.99527 7.43218

H 1.14866 -2.53190 5.77721

H 2.63070 -3.01360 6.59614

H 7.10827 -2.19643 4.74686

H 6.51573 -0.72673 3.97567

H 6.12896 -1.05621 5.66973

H 6.17154 -3.55827 2.92211

H 4.44944 -3.56954 2.54083

H 5.45590 -2.18600 2.07807

H 5.67290 -4.15439 5.14708

H 4.72409 -3.16810 6.25384

H 3.91780 -4.07904 4.95865

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1-Me form 2

C 3.95339 -2.75052 14.03809

W 2.36809 -2.03998 12.78011

C 1.54290 -3.12408 11.12839

O 1.54153 -0.43848 13.19517

Si 1.45828 1.30405 13.17406

C 3.15979 1.90983 13.92194

C 4.28851 1.81121 12.87826

O 3.61539 -1.55996 11.69667

O 1.29897 -3.27996 13.84840

Si 0.49382 -4.53462 14.68347

C 0.90840 -6.23724 13.79412

C 2.40733 -6.30688 13.44856

C 1.17665 1.84414 11.31611

C 1.42663 3.35589 11.15319

C -0.08244 1.65680 14.31993

C 0.26301 1.36834 15.79229

C 2.10637 1.08547 10.35191

C -0.26266 1.54955 10.85592

C -1.25100 0.72468 13.94814

C	-0.56055	3.11629	14.21525
C	3.06783	3.37040	14.40233
C	3.58503	1.03053	15.11336
C	1.14720	-4.49629	16.53838
C	1.27276	-3.03788	17.02058
C	-1.41285	-4.08033	14.56541
C	-1.74322	-3.60036	13.13988
C	0.20338	-5.24414	17.49861
C	2.54134	-5.13613	16.67651
C	-1.77026	-2.92120	15.51254
C	-2.32868	-5.26833	14.90997
C	0.55614	-7.44295	14.68507
C	0.13942	-6.40304	12.47141
H	-3.37941	-4.94635	14.87582
H	-2.22818	-6.09761	14.20375
H	-2.14634	-5.66181	15.91490
H	-2.80610	-3.32520	13.08155
H	-1.15874	-2.71569	12.87103
H	-1.56594	-4.36587	12.38056
H	-2.80408	-2.59879	15.32288
H	-1.71485	-3.20371	16.56750
H	-1.12548	-2.05114	15.36046
H	0.61596	-5.21399	18.51727
H	-0.79250	-4.79537	17.54591
H	0.08189	-6.29890	17.23344
H	1.70991	-3.02124	18.02924
H	1.92182	-2.44734	16.36843
H	0.30949	-2.52707	17.07725
H	2.89820	-5.00697	17.70828
H	2.53349	-6.21115	16.47696
H	3.28396	-4.67721	16.01844
H	0.45066	-7.33910	11.98574
H	-0.94200	-6.46475	12.61836
H	0.34086	-5.59175	11.76706

H	0.76730	-8.37538	14.14231
H	1.14265	-7.47237	15.60724
H	-0.50283	-7.46531	14.96082
H	2.62411	-7.25877	12.94290
H	2.70140	-5.50413	12.76632
H	3.05267	-6.25265	14.32790
H	4.17102	-3.77902	13.72056
H	4.85705	-2.15134	13.90661
H	3.65251	-2.77336	15.08744
H	2.13716	-4.03888	11.00439
H	0.50237	-3.39834	11.31025
H	1.63866	-2.54062	10.20867
H	4.05202	3.69892	14.76437
H	2.77305	4.05955	13.60455
H	2.36488	3.49573	15.23185
H	4.55482	1.38400	15.49030
H	2.88207	1.06087	15.94782
H	3.71667	-0.01618	14.82469
H	5.24243	2.07909	13.35418
H	4.39426	0.79832	12.47710
H	4.14842	2.49927	12.04010
H	-1.39430	3.28064	14.91206
H	0.22228	3.83603	14.47412
H	-0.92828	3.36643	13.21522
H	-0.64120	1.48456	16.40600
H	0.62554	0.34578	15.93764
H	1.01027	2.05833	16.19418
H	-2.05632	0.84031	14.68675
H	-1.67931	0.94618	12.96906
H	-0.94660	-0.32473	13.95166
H	1.19486	3.65415	10.12121
H	0.79877	3.96448	11.81187
H	2.46952	3.63051	11.33591
H	-0.35514	1.78969	9.78749

H	-0.52913	0.49410	10.97436
H	-1.00664	2.15250	11.38321
H	1.92432	1.44423	9.32885
H	3.16683	1.22483	10.56397
H	1.91484	0.00991	10.35836

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1-Me form 3

O	0.88019	-1.19880	13.10820
W	2.24596	-2.34099	12.58295
O	2.25184	-3.93780	13.17378
Si	-0.51244	-0.38705	13.77393
C	0.17873	1.20748	14.66893
C	-1.59587	0.03976	12.20338
C	-1.34030	-1.67726	14.98514
O	1.90416	-2.69148	10.73490
Si	1.91599	-3.63322	9.29042
C	0.62422	-5.07574	9.61997
C	3.47475	-1.78028	14.30201
C	4.06120	-1.47965	11.73773
C	1.33819	-2.37607	7.90759
C	3.72393	-4.32780	8.95853
C	1.40785	0.87901	15.53329
C	0.63498	2.26969	13.65209
C	-0.89935	1.83623	15.57245
C	-0.69139	0.54933	11.06544
C	-2.65651	1.11106	12.51693
C	-2.32354	-1.20472	11.66775
C	-2.78573	-1.26884	15.32532
C	-1.35712	-3.08157	14.35117
C	-0.55367	-1.79897	16.30276
C	0.14238	-5.72733	8.31115
C	1.21330	-6.17568	10.52582
C	-0.60352	-4.52440	10.36582
C	-0.15947	-2.04834	8.03566

C	1.57961	-2.91396	6.48606
C	2.10300	-1.04920	8.07585
C	3.66490	-5.50404	7.96328
C	4.68399	-3.28419	8.35784
C	4.36508	-4.82750	10.26691
H	1.21742	-2.18347	5.74866
H	2.63879	-3.08262	6.27262
H	1.04795	-3.85188	6.29652
H	1.73852	-0.31900	7.33942
H	1.95155	-0.62214	9.07137
H	3.17877	-1.15606	7.91946
H	-0.42372	-1.26152	7.31450
H	-0.79906	-2.90813	7.81634
H	-0.41808	-1.67588	9.03059
H	-0.54624	-6.55207	8.54385
H	-0.40442	-5.02733	7.67189
H	0.96033	-6.14978	7.72012
H	-1.30988	-5.34454	10.55828
H	-0.32379	-4.10359	11.33543
H	-1.14218	-3.75990	9.80186
H	0.42604	-6.90811	10.75633
H	2.02898	-6.73096	10.05449
H	1.57366	-5.77464	11.47820
H	5.67904	-3.73803	8.24598
H	4.37667	-2.94499	7.36482
H	4.80629	-2.40381	8.99387
H	4.68510	-5.85899	7.75987
H	3.10243	-6.35680	8.35089
H	3.22600	-5.22035	7.00112
H	5.35254	-5.25691	10.04461
H	4.51883	-4.01539	10.98155
H	3.77899	-5.59982	10.76739
H	4.33149	-2.45396	14.39296
H	3.84516	-0.75220	14.30594

H 2.84191 -1.93353 15.18766
H 4.98692 -1.87093 12.16785
H 4.09005 -1.56590 10.65176
H 4.02018 -0.41197 11.99581
H -3.21416 -1.99206 16.03299
H -2.84556 -0.28297 15.79755
H -3.43711 -1.25848 14.44655
H -1.83165 -3.78431 15.05036
H -1.92186 -3.12616 13.41823
H -0.34843 -3.45757 14.15672
H -0.99690 -2.59611 16.91566
H 0.49438 -2.06752 16.13498
H -0.58291 -0.88380 16.90082
H -3.26870 1.29143 11.62234
H -3.34010 0.80810 13.31716
H -2.21416 2.07079 12.79859
H -2.85155 -0.94298 10.73999
H -1.63074 -2.01582 11.42791
H -3.07441 -1.59015 12.36304
H -1.30145 0.72446 10.16855
H -0.18988 1.48901 11.30294
H 0.07626 -0.18422 10.80441
H -0.50848 2.76295 16.01513
H -1.81231 2.09937 15.02950
H -1.17962 1.18149 16.40297
H 1.09673 3.10902 14.19053
H 1.38433 1.87902 12.95584
H -0.19158 2.68285 13.06824
H 1.75694 1.79780 16.02512
H 1.20297 0.15034 16.31931
H 2.23229 0.49671 14.92919

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1-Me graft adduct - green path.

W 0.84192 -3.20997 2.95901

O	0.16694	-3.18966	4.52545
O	-0.41680	-4.30012	2.09582
O	2.33806	-2.11645	3.25358
Si	3.64441	-1.15323	3.83660
C	4.09413	-1.87141	5.59939
C	4.10312	-3.41137	5.58629
O	-1.59666	0.82778	0.16819
Si	-1.14619	1.75591	-1.10573
O	-0.23997	0.87070	-2.17582
Si	0.00215	0.72574	-3.80190
O	1.27972	1.66597	-4.28232
Si	2.05845	3.05550	-3.83909
O	3.64325	2.89555	-4.22088
Si	5.09061	3.09796	-3.37574
C	0.19781	-1.66341	1.57707
C	2.26211	-4.78180	2.54147
Si	-1.73364	-5.27919	1.56317
C	-1.68535	-5.15915	-0.38829
C	-2.24152	-3.81324	-0.88646
C	5.06395	-1.38286	2.50573
C	6.14377	-0.29274	2.62647
C	2.94296	0.67251	3.90917
C	2.82152	1.27836	2.49938
C	4.46656	-1.34117	1.08590
C	5.75573	-2.74999	2.65037
O	-0.25289	3.06005	-0.60665
Si	0.92699	4.08584	-1.13214
O	1.91384	3.30547	-2.20883
O	-2.54858	2.27754	-1.80559
Si	-3.16355	3.56163	-2.64596
O	-3.00417	3.30915	-4.27357
Si	-2.02503	2.50589	-5.34052
O	-2.91328	2.01941	-6.62666
Si	-4.54051	2.15015	-7.05882

O	0.26116	5.42461	-1.84317
Si	-1.09182	5.88184	-2.67003
O	-1.33905	7.45851	-2.27581
O	1.83627	4.56060	0.14454
Si	2.04912	6.04222	0.93104
O	-2.38818	4.95688	-2.21634
O	-0.87313	5.72584	-4.30416
Si	0.01994	4.83999	-5.36953
O	1.43842	4.33950	-4.67413
O	-4.75832	3.71666	-2.31345
Si	-5.79051	3.10032	-1.12585
C	-3.33618	-4.48748	2.36386
C	-4.61479	-5.00663	1.68072
C	-1.34862	-7.07569	2.23987
C	-2.59870	-7.97417	2.18146
C	-3.42252	-4.80671	3.86744
C	-3.30651	-2.95180	2.25104
C	1.53336	0.68786	4.53201
C	3.85481	1.59400	4.74128
C	5.47518	-1.37188	6.06252
C	3.05195	-1.45792	6.65512
O	-1.36343	1.17347	-4.62049
O	0.33974	-0.84442	-4.12230
Si	1.29204	-1.63678	-5.26932
O	-0.82171	3.50568	-5.87449
O	0.32538	5.84211	-6.63714
C	-0.86122	-7.01277	3.70053
C	-0.23797	-7.76529	1.42595
C	-2.50512	-6.28225	-1.04904
C	-0.22842	-5.24334	-0.88206
H	-0.87075	-1.75366	1.37040
H	-7.07193	3.84812	-1.26531
H	-5.21354	3.31817	0.23188
H	-6.02161	1.64501	-1.35601

H	1.19129	-0.95837	-6.59433
H	0.77040	-3.02916	-5.36453
H	5.18923	2.09618	-2.27494
H	6.18252	2.87854	-4.36539
H	-1.98893	7.91489	-2.81837
H	5.17771	4.47757	-2.81472
H	2.95190	5.76761	2.08449
H	0.74031	6.56512	1.41760
H	2.68451	7.02749	0.00954
H	0.80715	5.43979	-7.36582
H	-4.67098	1.48349	-8.38483
H	-4.93411	3.58499	-7.16598
H	-5.40046	1.46169	-6.05295
H	2.71315	-1.65525	-4.81617
H	0.43353	-0.66990	1.96729
H	0.75669	-1.81684	0.64298
H	-0.93842	0.20058	0.49326
H	-2.33932	-8.98476	2.52700
H	-3.40385	-7.61400	2.82841
H	-3.00061	-8.07378	1.16805
H	-0.60061	-8.02611	4.03728
H	0.03004	-6.39032	3.81301
H	-1.61630	-6.62814	4.38771
H	-0.00175	-8.73478	1.88665
H	-0.53358	-7.96769	0.39294
H	0.68810	-7.18319	1.40403
H	-5.49579	-4.58194	2.18219
H	-4.67613	-4.71482	0.62790
H	-4.70999	-6.09589	1.73262
H	-4.27884	-4.27035	4.30009
H	-3.58184	-5.87016	4.06459
H	-2.52792	-4.48226	4.40833
H	-4.22812	-2.54171	2.68739
H	-2.47025	-2.52568	2.81211

H	-3.25143	-2.59155	1.22167
H	-2.49046	-6.15699	-2.14079
H	-2.10414	-7.27776	-0.83725
H	-3.55497	-6.27149	-0.73839
H	-0.20679	-5.13257	-1.97528
H	0.38400	-4.44168	-0.45855
H	0.25216	-6.19415	-0.64326
H	-2.12754	-3.75388	-1.97780
H	-3.30562	-3.68760	-0.66937
H	-1.70311	-2.96048	-0.46216
H	1.13542	1.71181	4.50078
H	0.83366	0.04805	3.98832
H	1.52327	0.36784	5.57491
H	2.33487	2.26088	2.56170
H	3.79294	1.43610	2.02331
H	2.21592	0.65988	1.83013
H	3.45807	2.61865	4.71857
H	3.90571	1.29570	5.79264
H	4.87808	1.63758	4.35423
H	3.29326	-1.94848	7.60887
H	3.04742	-0.38118	6.84542
H	2.03936	-1.76702	6.37745
H	5.67985	-1.74603	7.07533
H	6.28694	-1.72701	5.42064
H	5.53506	-0.27968	6.10421
H	4.38141	-3.77668	6.58494
H	3.11230	-3.81550	5.36162
H	4.81740	-3.83724	4.87829
H	6.93428	-0.47204	1.88405
H	5.75236	0.71125	2.43896
H	6.62362	-0.28670	3.61060
H	5.26124	-1.53290	0.35118
H	3.70018	-2.11037	0.95072
H	4.02071	-0.37654	0.83566

H 6.49900 -2.86694 1.84889

H 6.28974 -2.85786 3.59834

H 5.04967 -3.58080 2.55805

H 1.83064 -5.77737 2.66329

H 3.16202 -4.70200 3.15373

H 2.55022 -4.66623 1.48607

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1-Me graft TS - green path.

W 1.90041 -1.06800 11.83129

O 0.75824 -0.05948 12.57845

O 0.80844 -2.24817 10.87582

O 3.51554 -0.40104 12.49817

Si 4.82713 0.31994 13.38601

C 3.96636 1.44847 14.72707

C 2.80459 0.69678 15.40575

O 1.83485 0.63672 10.15762

Si 1.14673 1.91335 9.41969

O 1.42937 1.84010 7.78228

Si 0.68754 2.19319 6.35606

O 1.14815 3.69451 5.81857

Si 1.65907 5.13969 6.43860

O 2.69720 5.83040 5.37474

Si 4.35752 6.13189 5.36781

C 3.32453 -1.44317 9.87864

C 2.04353 -2.56576 13.34516

Si -0.33560 -3.36605 10.18700

C 0.66936 -5.00129 9.79649

C 1.57348 -4.84227 8.56124

C 5.85467 -1.16399 14.15267

C 7.25734 -0.68948 14.57982

C 5.85476 1.32578 12.05622

C 6.72267 0.40677 11.17774

C 6.00612 -2.29835 13.12183

C 5.18702 -1.77455 15.39817

O	1.77480	3.34173	9.99635
Si	2.10058	4.87787	9.50660
O	2.43262	4.90664	7.88216
O	-0.48969	1.91861	9.68440
Si	-1.77578	2.91613	9.92634
O	-2.55983	3.15613	8.48548
Si	-2.22361	3.14895	6.86502
O	-3.53454	2.61022	6.04315
Si	-5.16413	2.39369	6.42620
O	0.82924	5.89211	9.82711
Si	-0.81591	5.86342	10.00833
O	-1.27967	6.97093	11.13373
O	3.41890	5.42827	10.31246
Si	3.73979	6.84151	11.17788
O	-1.28195	4.37391	10.54286
O	-1.54047	6.24360	8.56685
Si	-1.25307	6.10317	6.94774
O	0.37074	6.15870	6.62504
O	-2.83170	2.22662	10.96910
Si	-3.27591	2.54574	12.56889
C	-0.99490	-2.46325	8.58721
C	-1.73008	-3.43888	7.64989
C	-1.72860	-3.63024	11.54616
C	-3.01845	-4.18143	10.90731
C	-1.95511	-1.31874	8.95573
C	0.16986	-1.82497	7.80837
C	4.90339	2.07798	11.10895
C	6.78485	2.35389	12.72796
C	4.96386	1.89728	15.81077
C	3.35572	2.70353	14.07701
O	-0.95842	2.14525	6.52501
O	1.14013	1.07250	5.24869
Si	1.44848	1.10947	3.59080
O	-1.86862	4.68508	6.35957

O	-2.00787	7.39529	6.26242
C	-2.04666	-2.29140	12.23839
C	-1.31180	-4.62035	12.64746
C	-0.28184	-6.18348	9.53225
C	1.59432	-5.36029	10.97369
H	2.93489	-1.84514	8.93993
H	-4.08977	3.79548	12.62522
H	-2.07193	2.68174	13.43606
H	-4.10290	1.38654	13.00748
H	0.39147	1.88309	2.87542
H	1.44438	-0.30725	3.12887
H	5.11967	4.86810	5.58762
H	4.67240	6.68960	4.02232
H	-1.62745	7.78403	10.75551
H	4.70760	7.12430	6.42526
H	5.19256	6.80526	11.50854
H	2.93166	6.87878	12.43059
H	3.43927	8.04379	10.34613
H	-1.91065	7.45941	5.30774
H	-5.85199	2.06697	5.14519
H	-5.73554	3.64377	7.00730
H	-5.32142	1.26795	7.39159
H	2.78356	1.72387	3.33355
H	4.27099	-0.92525	9.69790
H	3.58294	-2.31462	10.50155
H	2.53618	-0.24917	9.89130
H	-3.77043	-4.34542	11.69192
H	-3.46013	-3.49246	10.18301
H	-2.86345	-5.14304	10.40652
H	-2.82732	-2.45357	12.99527
H	-1.17429	-1.87314	12.74705
H	-2.41620	-1.53129	11.54782
H	-2.11513	-4.68462	13.39470
H	-1.14473	-5.63224	12.26962

H	-0.40931	-4.30501	13.17720
H	-2.12027	-2.88492	6.78483
H	-1.06971	-4.21811	7.25668
H	-2.58267	-3.93097	8.12762
H	-2.22554	-0.77066	8.04298
H	-2.88718	-1.67239	9.40414
H	-1.49592	-0.59890	9.63836
H	-0.22817	-1.30110	6.92923
H	0.70089	-1.08847	8.41437
H	0.89664	-2.55425	7.44448
H	0.30495	-7.07861	9.28246
H	-0.89485	-6.43657	10.40163
H	-0.95661	-5.99629	8.69142
H	2.14733	-6.27994	10.73560
H	2.33303	-4.57433	11.15473
H	1.05766	-5.53750	11.90802
H	2.16895	-5.75685	8.42965
H	1.00733	-4.69473	7.63763
H	2.27640	-4.01082	8.66786
H	5.49498	2.59503	10.34049
H	4.21099	1.40474	10.60052
H	4.30472	2.83630	11.61380
H	7.20301	1.00996	10.39479
H	7.52290	-0.08808	11.73449
H	6.13310	-0.36481	10.67417
H	7.36087	2.88041	11.95398
H	6.23222	3.11593	13.28478
H	7.50708	1.89523	13.41054
H	2.78802	3.26213	14.83429
H	4.11516	3.38357	13.68154
H	2.66224	2.45410	13.26838
H	4.45723	2.56799	16.51874
H	5.35583	1.05767	16.39300
H	5.81680	2.44787	15.40142

H	2.34930	1.35260	16.16140
H	2.02085	0.43508	14.69041
H	3.12318	-0.21170	15.92191
H	7.80356	-1.52776	15.03462
H	7.86106	-0.33447	13.74081
H	7.21802	0.11016	15.32664
H	6.56316	-3.13125	13.57351
H	5.03440	-2.68741	12.80544
H	6.54998	-1.99312	12.22589
H	5.79474	-2.61858	15.75405
H	5.11030	-1.06529	16.22666
H	4.18774	-2.16432	15.18906
H	1.09955	-3.10137	13.45181
H	2.28745	-2.09591	14.30005
H	2.82749	-3.29356	13.10584

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1-Me graft prod - green path.

W	0.69781	-2.50085	1.88905
O	-0.40390	-2.71394	3.16615
O	-0.09616	-3.71598	0.69403
O	1.92185	-1.41804	2.82201
Si	2.79973	-0.63909	4.09090
C	2.06991	1.17564	4.12282
C	0.53822	1.12821	3.97334
O	0.53098	-1.12413	0.53392
Si	0.01540	0.20658	-0.25174
O	-0.32954	-0.16073	-1.83241
Si	-1.33187	0.33957	-3.04380
O	-0.60516	1.50813	-3.96814
Si	0.49827	2.73447	-3.86347
O	1.24905	2.89573	-5.31048
Si	2.76875	2.47308	-5.91231
C	5.49147	-1.96561	-3.09711
C	2.26003	-3.97571	1.97448

Si	-1.05211	-4.92802	-0.07592
C	-0.22726	-5.16317	-1.83025
C	-0.51459	-3.95209	-2.73251
C	2.43411	-1.62626	5.74485
C	3.42243	-1.21489	6.85244
C	4.67489	-0.71200	3.53497
C	5.30721	-2.09167	3.79145
C	2.54271	-3.14809	5.53747
C	1.00310	-1.36172	6.24744
O	1.21301	1.35158	-0.22520
Si	1.84110	2.61567	-1.07234
O	1.62435	2.38850	-2.69999
O	-1.34273	0.80827	0.48161
Si	-2.09172	2.23256	0.83876
O	-3.18999	2.61433	-0.34392
Si	-3.44231	2.35150	-1.95904
O	-5.05074	2.28167	-2.25660
Si	-6.42680	2.05024	-1.30612
O	1.12745	4.04043	-0.62037
Si	-0.27918	4.62072	0.03520
O	0.02578	5.89753	1.02671
O	3.44740	2.68666	-0.75913
Si	4.58684	3.93045	-0.69599
O	-0.98520	3.45846	0.96814
O	-1.28103	5.11264	-1.18826
Si	-1.61762	4.73313	-2.75862
O	-0.26701	4.15897	-3.52702
O	-2.87918	2.04513	2.25943
Si	-3.52749	3.07779	3.42723
C	-2.84224	-4.13995	-0.12831
C	-3.75143	-4.86196	-1.13915
C	-0.96999	-6.54902	1.03088
C	-2.13041	-7.49921	0.67744
C	-3.51002	-4.18733	1.25880

C	-2.76580	-2.65279	-0.51813
C	4.77334	-0.45539	2.01847
C	5.52879	0.33184	4.27913
C	2.42005	1.91199	5.42890
C	2.60054	2.01657	2.94875
O	-2.74231	0.92614	-2.41191
O	-1.66768	-0.94754	-3.99992
Si	-1.93221	-1.13738	-5.65662
O	-2.81308	3.59298	-2.85201
O	-2.10740	6.14375	-3.44887
C	-1.05892	-6.19514	2.52731
C	0.33832	-7.33572	0.83328
C	-0.73462	-6.42739	-2.54487
C	1.30401	-5.24624	-1.68172
H	5.01983	-2.35509	-4.00150
H	-4.15402	4.26711	2.77804
H	-2.45447	3.52004	4.36241
H	-4.55877	2.29367	4.16236
H	-2.77644	-0.02507	-6.18296
H	-2.63719	-2.43840	-5.82736
H	3.04203	1.02691	-5.66875
H	2.72724	2.74761	-7.37602
H	0.06498	6.74703	0.57738
H	3.82558	3.30423	-5.26625
H	5.92452	3.28605	-0.81464
H	4.47930	4.65450	0.60300
H	4.37812	4.88663	-1.82347
H	-2.40456	6.06726	-4.36037
H	-7.56027	1.85762	-2.25340
H	-6.66866	3.25249	-0.45675
H	-6.26845	0.84415	-0.44243
H	-0.62662	-1.16588	-6.37753
H	6.39000	-1.40650	-3.36602
H	5.76314	-2.79612	-2.44236

H	4.79399	-1.30510	-2.57808
H	-2.04417	-8.41905	1.27307
H	-3.10988	-7.06713	0.89878
H	-2.12437	-7.79770	-0.37618
H	-1.00551	-7.11938	3.12042
H	-0.23635	-5.55104	2.84804
H	-1.98822	-5.68988	2.79490
H	0.34783	-8.19596	1.51771
H	0.44644	-7.73393	-0.17914
H	1.22819	-6.74040	1.05655
H	-4.76137	-4.43021	-1.09766
H	-3.39898	-4.74757	-2.16885
H	-3.85006	-5.93244	-0.93516
H	-4.46776	-3.64927	1.21544
H	-3.73338	-5.20455	1.59186
H	-2.89789	-3.70088	2.02519
H	-3.78217	-2.23502	-0.53664
H	-2.19335	-2.07466	0.21110
H	-2.32912	-2.48445	-1.50340
H	-0.27213	-6.50027	-3.53943
H	-0.48225	-7.34612	-2.00734
H	-1.81898	-6.41583	-2.69576
H	1.76253	-5.31760	-2.67817
H	1.70498	-4.34984	-1.19940
H	1.63711	-6.11547	-1.11060
H	0.04168	-4.06279	-3.67471
H	-1.57159	-3.86183	-2.99619
H	-0.19738	-3.01006	-2.27715
H	5.82400	-0.52984	1.70370
H	4.20317	-1.19557	1.44940
H	4.41370	0.53227	1.72410
H	6.33636	-2.09301	3.40523
H	5.36543	-2.34230	4.85428
H	4.77250	-2.89668	3.27832

H 6.57561 0.24918 3.95403

H 5.21281 1.35904 4.07771

H 5.51777 0.18520 5.36423

H 2.10307 2.99666 2.95672

H 3.67557 2.20510 3.01456

H 2.39022 1.55350 1.98216

H 2.03719 2.94100 5.38056

H 1.97034 1.44554 6.30991

H 3.49980 1.97876 5.59802

H 0.14443 2.15363 3.97960

H 0.24003 0.67210 3.02642

H 0.04044 0.58062 4.77567

H 3.17635 -1.75165 7.77960

H 4.45840 -1.46548 6.60456

H 3.38245 -0.14535 7.08092

H 2.36859 -3.65282 6.49852

H 1.78270 -3.51360 4.84236

H 3.52387 -3.46886 5.18039

H 0.81484 -1.97994 7.13702

H 0.84577 -0.32167 6.54455

H 0.25061 -1.62868 5.49918

H 2.88253 -3.79336 1.08713

H 1.86720 -4.99005 1.90552

H 2.88512 -3.87595 2.86035

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1-Me graft wo CH4 - green path.

C -2.74929 -2.90665 5.87234

C -3.99028 -3.54443 6.52519

C -3.78832 -3.58504 8.05117

Si -5.59014 -2.52212 6.04054

C -7.24443 -3.56243 6.17400

C -8.48860 -2.67163 6.00112

O -5.37271 -2.10242 4.37815

W -5.70249 -1.81989 2.54693

C	-4.92692	-3.81575	2.34484
O	-7.39981	-1.84564	2.63697
O	-5.56973	-1.77617	0.67295
Si	-5.86206	-1.82416	-1.02629
C	-6.89574	-3.44715	-1.41595
C	-6.02539	-4.71581	-1.47218
O	-4.67085	-0.18363	2.61975
Si	-3.94620	1.25622	2.84352
O	-5.06946	2.38539	3.30059
Si	-5.24515	3.71421	4.25938
O	-6.78021	3.73300	4.82347
Si	-7.61146	4.59153	6.01598
C	-5.70584	-0.79370	6.94822
C	-4.32631	-0.12191	7.06004
C	-6.59866	0.16488	6.13835
C	-6.28506	-0.92802	8.36871
O	-3.21047	1.75236	1.44099
Si	-2.82030	3.14950	0.65489
O	-2.85551	2.86074	-0.95755
Si	-2.02689	3.51076	-2.27742
O	-2.79174	1.11267	4.02498
Si	-1.34411	1.72188	4.51973
O	-0.52204	0.52904	5.28397
Si	0.56573	0.48165	6.57395
O	-1.29556	3.65266	1.06691
Si	-0.21865	3.60190	2.32011
O	-0.38057	4.95044	3.25996
Si	-1.53657	6.04084	3.72956
O	-0.84093	7.49155	4.07236
O	-3.91302	4.33595	1.01687
Si	-4.12002	5.60085	2.05901
O	-2.64813	6.19932	2.51398
O	1.30332	3.59358	1.71438
Si	2.46890	2.40129	1.44960

O	-0.45682	2.23062	3.21588
C	-4.08484	-1.85013	-1.83239
C	-3.19129	-2.86807	-1.09798
C	-6.87000	-0.17909	-1.35826
C	-6.25320	0.99150	-0.57029
C	-3.39955	-0.48125	-1.69033
C	-4.13379	-2.20640	-3.32817
C	-7.33341	-4.26215	7.54311
C	-7.33118	-4.63474	5.07141
C	-4.05456	-4.99807	6.02494
O	-1.56416	2.99209	5.55932
Si	-2.66780	4.17050	5.93143
O	-2.25799	5.56340	5.13486
O	-4.97544	5.09613	3.38317
O	-4.18408	3.66311	5.53000
O	-4.93601	6.80138	1.30246
Si	-6.55648	7.26545	1.20632
O	-2.68290	4.46220	7.55027
C	-6.88469	0.19262	-2.85164
C	-8.32319	-0.31291	-0.86578
C	-7.59653	-3.31742	-2.78280
C	-7.96476	-3.68642	-0.33354
H	-7.01020	5.94519	6.19965
H	-7.55808	3.83633	7.30018
H	-9.02243	4.71587	5.55416
H	-1.84127	4.98148	-2.10540
H	-2.86147	3.23809	-3.48084
H	1.87724	1.24771	0.71094
H	3.53911	3.03848	0.63217
H	-2.02445	5.09861	7.84436
H	3.02923	1.93530	2.75114
H	1.27603	-0.82437	6.48203
H	-0.17328	0.57477	7.86570
H	1.54506	1.60380	6.47123

H	-0.42822	7.93048	3.32270
H	-6.65645	8.20557	0.05508
H	-6.96063	7.95517	2.46582
H	-7.42816	6.07648	0.97775
H	-0.69845	2.84697	-2.41699
H	-8.13271	-4.25018	-3.00811
H	-8.33681	-2.51323	-2.80072
H	-6.89269	-3.14543	-3.60400
H	-8.53543	-4.59246	-0.58326
H	-7.52179	-3.83866	0.65371
H	-8.67884	-2.86611	-0.24566
H	-6.67213	-5.58565	-1.65490
H	-5.28790	-4.69110	-2.27881
H	-5.49343	-4.90693	-0.53568
H	-7.48381	1.10253	-2.99731
H	-5.88238	0.40607	-3.23575
H	-7.32560	-0.58713	-3.48018
H	-8.82917	0.65726	-0.97138
H	-8.90554	-1.03801	-1.44083
H	-8.37312	-0.59275	0.19160
H	-6.85520	1.89487	-0.74291
H	-6.25423	0.79928	0.50549
H	-5.22988	1.22266	-0.86836
H	-3.11928	-2.17118	-3.74989
H	-4.52009	-3.21302	-3.51298
H	-4.74521	-1.50370	-3.90344
H	-2.17549	-2.82815	-1.51615
H	-3.11677	-2.63650	-0.03119
H	-3.53979	-3.89837	-1.19628
H	-2.36680	-0.55304	-2.06122
H	-3.89560	0.29868	-2.27373
H	-3.35043	-0.14466	-0.65126
H	-1.85895	-3.49809	6.12960
H	-2.83182	-2.89168	4.78184

H -2.56726 -1.88202 6.20051

H -3.10842 -5.50512 6.26237

H -4.85331 -5.57586 6.49814

H -4.18665 -5.05625 4.94052

H -2.89434 -4.17899 8.28856

H -3.63534 -2.59176 8.48179

H -4.63064 -4.04975 8.57402

H -4.44917 0.88211 7.48937

H -3.64156 -0.66708 7.71573

H -3.84658 -0.00070 6.08583

H -6.29664 0.05915 8.85173

H -7.31487 -1.29660 8.37023

H -5.68962 -1.58980 9.00638

H -6.63796 1.13646 6.64885

H -6.19951 0.34111 5.13667

H -7.62669 -0.18592 6.02993

H -8.28842 -4.80126 7.61715

H -6.53835 -4.99947 7.68892

H -7.29539 -3.55929 8.38109

H -8.25160 -5.21885 5.21415

H -7.39172 -4.18213 4.07829

H -6.49862 -5.34193 5.08404

H -9.38759 -3.30455 6.01478

H -8.60384 -1.94169 6.80675

H -8.47947 -2.13933 5.04529

H -3.84428 -3.72873 2.51259

H -5.08707 -4.23050 1.35072

H -5.33022 -4.49009 3.10117

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1-Me graft adduct - blue path.

C -0.52900 -2.12128 3.22139

W 1.12296 -3.25315 2.41079

O 1.65557 -4.63155 3.26853

O -0.16427 -4.07299 1.32180

Si	-1.29336	-5.13603	0.56943
C	-1.91502	-6.33803	1.98499
C	-0.84900	-7.39254	2.33341
O	2.23051	-1.96942	3.23405
Si	3.40430	-1.15651	4.18913
C	3.70182	0.53631	3.24912
C	4.41479	1.57876	4.12734
C	2.14641	-2.74074	0.58210
C	2.59080	-0.91695	5.95545
C	1.52659	0.19514	5.94085
C	4.97722	-2.32056	4.22039
C	4.75596	-3.51784	5.16354
C	1.88292	-2.20840	6.40857
C	3.64784	-0.53963	7.01020
C	-0.28077	-6.05970	-0.82981
C	1.08701	-6.52641	-0.29547
C	-2.69231	-3.96484	-0.13547
C	-2.05720	-2.71602	-0.77739
C	-0.00094	-5.13165	-2.02622
C	-1.04687	-7.28911	-1.35233
C	6.23136	-1.55907	4.68559
C	5.24935	-2.91834	2.82743
C	4.54688	0.32225	1.98080
C	2.34939	1.11202	2.78671
C	-3.56131	-4.67924	-1.18589
C	-3.62132	-3.46017	0.98324
C	-3.20353	-7.07030	1.56729
C	-2.18953	-5.55943	3.28527
O	0.41606	0.81024	-0.22869
Si	-0.22348	1.98854	-1.18384
O	-1.83903	2.13534	-0.86124
Si	-3.01306	3.29682	-0.80969
O	-4.11708	2.91947	0.33592
Si	-4.22445	3.09883	2.01199

O	-0.02682	1.56613	-2.76756
Si	-0.76261	1.74499	-4.23429
O	-0.43263	0.42473	-5.14139
Si	-1.32648	-0.57885	-6.16323
O	0.56456	3.41067	-0.85459
Si	1.03091	4.80448	-1.61215
O	2.42777	5.31750	-0.92904
Si	2.91551	6.73614	-0.15229
O	-0.16828	3.08733	-4.99519
Si	0.50452	4.55984	-4.66761
O	-0.66953	5.72286	-4.64047
Si	-2.27995	5.87987	-4.28878
O	-2.93539	7.11018	-5.16162
O	-2.40441	1.88677	-4.05329
Si	-3.54502	3.06820	-3.86376
O	-3.04581	4.45091	-4.62076
O	1.56061	4.95467	-5.85366
Si	3.21486	4.72353	-6.10452
O	1.30112	4.50751	-3.21593
O	-0.12544	5.97612	-1.43601
Si	-1.76514	6.11064	-1.23655
O	-2.49705	6.30700	-2.70821
O	-3.80963	3.36599	-2.25630
O	-2.32207	4.76168	-0.46521
O	-4.93777	2.55962	-4.55611
Si	-6.51387	2.30706	-4.00189
O	-2.10878	7.41498	-0.29568
H	2.07073	-3.52123	-0.17800
H	-4.78591	4.44239	2.33270
H	-2.87941	2.94660	2.64041
H	-5.14221	2.03040	2.49680
H	-2.08065	0.23464	-7.16124
H	-2.27522	-1.40830	-5.36559
H	3.61578	3.34230	-5.70818

H	3.45219	4.93097	-7.56053
H	-2.42155	8.17965	-0.78828
H	3.98804	5.72361	-5.31278
H	4.35002	6.54097	0.19956
H	2.10907	6.95163	1.08376
H	2.76704	7.90559	-1.06650
H	-2.88090	7.00471	-6.11607
H	-7.29709	1.84849	-5.18340
H	-7.08494	3.57828	-3.47018
H	-6.52619	1.25960	-2.94031
H	-0.33967	-1.45341	-6.85632
H	1.63685	-1.84589	0.19443
H	3.19834	-2.49674	0.74381
H	1.10874	1.11913	0.36518
H	-0.76587	-1.35912	2.46387
H	-1.41962	-2.73557	3.37043
H	-0.28315	-1.60961	4.15342
H	-3.50229	-7.76875	2.36160
H	-4.04322	-6.38642	1.41085
H	-3.07760	-7.65906	0.65302
H	-2.55919	-6.25778	4.04963
H	-1.27649	-5.10539	3.67978
H	-2.94303	-4.77708	3.17208
H	-1.19966	-7.98893	3.18799
H	-0.66304	-8.09336	1.51470
H	0.10147	-6.93483	2.62466
H	-4.35659	-4.00237	-1.52895
H	-2.99153	-4.97455	-2.07169
H	-4.05078	-5.57493	-0.78917
H	-4.34649	-2.75120	0.55921
H	-4.19715	-4.26244	1.45310
H	-3.07122	-2.92896	1.76563
H	-2.85211	-2.03661	-1.11565
H	-1.43590	-2.16585	-0.06559

H	-1.43876	-2.94783	-1.64675
H	-0.47714	-7.75702	-2.16765
H	-1.18712	-8.05389	-0.58291
H	-2.03244	-7.03341	-1.75436
H	1.65389	-6.99255	-1.11382
H	1.68524	-5.69525	0.08611
H	1.00601	-7.26470	0.50370
H	0.64134	-5.65555	-2.74824
H	-0.91042	-4.84332	-2.56060
H	0.52136	-4.21660	-1.73071
H	2.52677	1.99246	2.15005
H	1.78184	0.36808	2.21782
H	1.71541	1.44109	3.61235
H	4.63093	1.27117	1.43156
H	5.56581	-0.00618	2.20246
H	4.09388	-0.40687	1.30148
H	4.58835	2.49737	3.54906
H	3.82690	1.86037	5.00606
H	5.39156	1.22989	4.47722
H	1.03207	0.23648	6.92168
H	1.95297	1.18573	5.75940
H	0.74724	0.01906	5.19315
H	3.15493	-0.36328	7.97667
H	4.38404	-1.33298	7.16877
H	4.19094	0.37635	6.75496
H	1.40855	-2.03515	7.38495
H	1.09770	-2.51271	5.71190
H	2.56320	-3.05360	6.52411
H	7.08122	-2.25343	4.74495
H	6.51935	-0.76204	3.99317
H	6.11128	-1.11327	5.67798
H	6.13875	-3.56196	2.88205
H	4.41854	-3.54435	2.49167
H	5.44364	-2.16540	2.06072

H	5.61862	-4.19574	5.09244
H	4.67379	-3.22108	6.21272
H	3.86586	-4.09435	4.89249

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1-Me graft TS - blue path.

W	1.93545	-1.07217	11.92064
C	0.52038	0.22284	12.85338
O	0.68597	-2.02384	10.89618
O	3.46387	-0.11249	12.42443
Si	4.93977	0.35410	13.21008
C	4.34756	1.54388	14.64704
C	3.15421	0.93234	15.40343
O	1.68385	0.67318	10.33061
Si	1.03112	1.93119	9.55418
O	1.53742	1.95174	7.97057
Si	1.00637	2.34303	6.46356
O	1.46963	3.88607	6.07614
Si	1.81636	5.32094	6.81905
O	2.95946	6.11448	5.95353
Si	4.64191	6.22083	6.03384
C	3.22007	-1.34457	9.88213
O	2.09821	-2.27068	13.12020
Si	-0.35205	-3.29362	10.32475
C	0.78962	-4.84046	9.92526
C	1.56168	-4.67288	8.60430
C	5.77160	-1.29417	13.85842
C	7.24656	-1.05621	14.23403
C	6.00424	1.26988	11.84482
C	6.71529	0.28573	10.89825
C	5.70428	-2.39562	12.78334
C	5.04752	-1.85103	15.09793
O	1.46917	3.36722	10.27325
Si	1.80740	4.93291	9.90352
O	2.37781	5.05203	8.35245

O	-0.63041	1.84340	9.58587
Si	-1.97352	2.78928	9.65931
O	-2.54516	3.06665	8.12811
Si	-1.98947	3.16070	6.57134
O	-3.14471	2.61010	5.54834
Si	-4.81569	2.39663	5.65644
O	0.45848	5.88510	10.06382
Si	-1.19181	5.77100	10.00487
O	-1.88446	6.77708	11.10743
O	2.96206	5.48362	10.93045
Si	3.12569	6.89529	11.84131
O	-1.65572	4.23743	10.40071
O	-1.71232	6.19571	8.49044
Si	-1.17965	6.14576	6.92848
O	0.46890	6.27925	6.85270
O	-3.12419	2.00371	10.52305
Si	-4.20763	2.48492	11.72711
C	-1.19875	-2.54398	8.73375
C	-1.87479	-3.62371	7.87059
C	-1.60480	-3.64381	11.78907
C	-2.82690	-4.43641	11.28935
C	-2.26382	-1.50068	9.11492
C	-0.14693	-1.80905	7.88347
C	5.08709	2.14863	10.97345
C	7.08784	2.16040	12.48046
C	5.47661	1.80686	15.66026
C	3.87221	2.89597	14.08407
O	-0.64502	2.22547	6.36350
O	1.68217	1.29739	5.39807
Si	1.27660	0.75309	3.85351
O	-1.63979	4.73404	6.19820
O	-1.88213	7.43890	6.19160
C	-2.10311	-2.32930	12.41753
C	-0.93371	-4.43794	12.92554

C	-0.06146	-6.11995	9.80337
C	1.84180	-5.05834	11.02813
H	2.74726	-1.71911	8.97128
H	-5.00906	3.65709	11.26857
H	-3.47161	2.82892	12.97726
H	-5.10362	1.31841	11.96574
H	0.70255	1.86347	3.03787
H	0.29039	-0.36132	3.95301
H	5.24410	4.87101	6.23805
H	5.08941	6.78992	4.73144
H	-2.07558	7.65738	10.77030
H	5.04139	7.12735	7.14932
H	4.52223	6.89742	12.36116
H	2.15822	6.89440	12.97634
H	2.90026	8.09830	10.98694
H	-1.61217	7.57779	5.27899
H	-5.29786	2.16042	4.26651
H	-5.46377	3.61552	6.22302
H	-5.12571	1.21465	6.51182
H	2.53795	0.26127	3.23077
H	4.11376	-0.76240	9.64084
H	3.58690	-2.22608	10.42629
H	2.42474	-0.22917	10.01451
H	0.96998	1.21520	12.94078
H	-0.35650	0.29756	12.20573
H	0.22219	-0.13589	13.84199
H	-3.48183	-4.67305	12.13974
H	-3.42770	-3.86762	10.57323
H	-2.55504	-5.38597	10.81890
H	-2.82101	-2.56459	13.21613
H	-1.28464	-1.76879	12.87308
H	-2.61028	-1.67157	11.70927
H	-1.63716	-4.52651	13.76573
H	-0.66309	-5.45633	12.63269

H	-0.03557	-3.93653	13.30001
H	-2.36267	-3.14981	7.00740
H	-1.16270	-4.35279	7.47308
H	-2.64884	-4.17521	8.41386
H	-2.65794	-1.03654	8.19979
H	-3.11659	-1.93941	9.64060
H	-1.85322	-0.69592	9.73057
H	-0.64198	-1.32876	7.02844
H	0.35044	-1.02470	8.45855
H	0.61913	-2.47536	7.48052
H	0.58722	-6.96268	9.52573
H	-0.55068	-6.39057	10.74300
H	-0.83461	-6.04178	9.03212
H	2.45143	-5.93769	10.77600
H	2.52152	-4.20754	11.11931
H	1.40749	-5.23205	12.01338
H	2.21660	-5.54377	8.45874
H	0.90682	-4.61852	7.73057
H	2.20216	-3.78681	8.60618
H	5.68196	2.61051	10.17289
H	4.28902	1.56646	10.50681
H	4.61359	2.95844	11.53066
H	7.23449	0.85324	10.11324
H	7.46959	-0.32351	11.40379
H	6.01854	-0.39067	10.39540
H	7.68012	2.63772	11.68722
H	6.66470	2.96486	13.08829
H	7.78585	1.59528	13.10716
H	3.45130	3.49885	14.90118
H	4.68502	3.47959	13.64337
H	3.09186	2.78231	13.32528
H	5.12384	2.51145	16.42645
H	5.78475	0.89558	16.18204
H	6.36617	2.24820	15.20135

H	2.82072	1.63736	16.17818
H	2.30612	0.74823	14.74207
H	3.39743	-0.00648	15.90282
H	7.67672	-1.98718	14.62937
H	7.85953	-0.76034	13.37792
H	7.36644	-0.29346	15.01023
H	6.22120	-3.29214	13.15403
H	4.66987	-2.68565	12.57996
H	6.17984	-2.11544	11.84120
H	5.49549	-2.81734	15.37058
H	5.14701	-1.19892	15.97040
H	3.98461	-2.02570	14.90734

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1-Me graft prod - blue path.

W	0.26428	-1.87173	2.50316
C	-1.00328	-0.41240	3.43673
O	-0.54589	-3.03342	1.31662
O	2.07350	-1.57833	2.64032
Si	3.76253	-1.39126	3.00261
C	3.89285	0.46290	3.59705
C	2.74588	0.79784	4.56904
O	0.21238	-0.47861	1.03039
Si	-0.40111	0.76759	0.21082
O	0.32452	0.88567	-1.27944
Si	-0.00536	1.27723	-2.84054
O	0.39320	2.86008	-3.12995
Si	0.53686	4.28667	-2.31092
O	1.74002	5.17452	-2.98157
Si	3.34220	5.50099	-2.56386
C	6.53914	-3.29019	-4.90978
O	0.04897	-2.81346	3.92566
Si	-1.37063	-4.45102	0.73229
C	0.01228	-5.81803	0.53997
C	0.91852	-5.53348	-0.67037

C	4.15354	-2.70254	4.39556
C	5.67155	-2.91602	4.53917
C	4.64619	-1.74432	1.29647
C	4.68134	-3.25008	0.98240
C	3.48636	-4.05197	4.06730
C	3.59406	-2.26613	5.76171
O	-0.15987	2.20722	1.01983
Si	0.10896	3.80465	0.72761
O	0.88981	4.00568	-0.71871
O	-2.04231	0.57864	-0.01135
Si	-3.44421	1.42728	-0.12263
O	-3.80378	1.71859	-1.71496
Si	-3.02903	1.89046	-3.16848
O	-3.98065	1.29948	-4.36425
Si	-5.62686	0.96668	-4.52413
O	-1.31768	4.65192	0.71246
Si	-2.92918	4.43671	0.39892
O	-3.84174	5.36570	1.40520
O	1.06478	4.41938	1.91076
Si	0.81444	5.54563	3.14202
O	-3.34749	2.86754	0.69181
O	-3.24950	4.87034	-1.16760
Si	-2.48961	4.90750	-2.63264
O	-0.86329	5.15627	-2.45118
O	-4.64774	0.53314	0.54267
Si	-6.02206	0.92542	1.44377
C	-2.10699	-3.84288	-0.96961
C	-2.55165	-5.02252	-1.85253
C	-2.72057	-4.88235	2.07476
C	-3.80256	-5.80123	1.47466
C	-3.31910	-2.92032	-0.75072
C	-1.05407	-3.01374	-1.73074
C	3.87351	-1.07117	0.14545
C	6.09335	-1.22016	1.30363

C	5.23552	0.72657	4.30292
C	3.76318	1.43674	2.41256
O	-1.61124	1.04599	-3.19040
O	0.89529	0.31552	-3.81512
Si	0.77617	-0.18719	-5.42037
O	-2.73346	3.49296	-3.45631
O	-3.16703	6.17306	-3.43795
C	-3.39463	-3.60081	2.60259
C	-2.11462	-5.58766	3.30230
C	-0.61487	-7.21213	0.35512
C	0.92509	-5.84264	1.77811
H	6.57717	-2.99127	-5.95915
H	-6.74448	2.07332	0.82182
H	-5.63621	1.26472	2.84344
H	-6.88780	-0.28759	1.43282
H	0.16423	0.88147	-6.26366
H	-0.04986	-1.42658	-5.49916
H	4.06295	4.24018	-2.22149
H	3.96423	6.13674	-3.75950
H	-4.02972	6.24543	1.06487
H	3.38852	6.44080	-1.40615
H	2.07011	5.57008	3.94430
H	-0.33375	5.13616	4.00160
H	0.55711	6.89723	2.56400
H	-2.78876	6.34772	-4.30480
H	-5.85971	0.69327	-5.97025
H	-6.44376	2.13700	-4.08772
H	-5.98898	-0.23214	-3.71363
H	2.16299	-0.47265	-5.88576
H	7.52810	-3.17287	-4.46225
H	6.22960	-4.33488	-4.84009
H	5.82177	-2.66155	-4.37859
H	-0.63107	0.59892	3.25295
H	-1.98158	-0.49687	2.94480

H	-1.12254	-0.60106	4.50426
H	-4.52846	-6.06809	2.25541
H	-4.36336	-5.32045	0.66761
H	-3.39172	-6.73845	1.08462
H	-4.19388	-3.88101	3.30327
H	-2.68724	-2.98065	3.15985
H	-3.84725	-2.98852	1.82035
H	-2.90625	-5.74735	4.04823
H	-1.70033	-6.57237	3.06708
H	-1.33679	-4.98254	3.77754
H	-2.97639	-4.63781	-2.79016
H	-1.71998	-5.67938	-2.12545
H	-3.32438	-5.63690	-1.37857
H	-3.66549	-2.54676	-1.72446
H	-4.16685	-3.43297	-0.28758
H	-3.06877	-2.04591	-0.14414
H	-1.51420	-2.59169	-2.63468
H	-0.68303	-2.18197	-1.12712
H	-0.19416	-3.60405	-2.05346
H	0.17972	-7.95519	0.19924
H	-1.18634	-7.53363	1.23056
H	-1.27759	-7.26219	-0.51460
H	1.68908	-6.62260	1.65003
H	1.45402	-4.89453	1.90868
H	0.39342	-6.05516	2.70682
H	1.73799	-6.26591	-0.68985
H	0.39108	-5.61960	-1.62417
H	1.37217	-4.53834	-0.62156
H	4.34252	-1.34475	-0.80999
H	2.82882	-1.39081	0.10646
H	3.87885	0.01810	0.20567
H	5.12346	-3.40138	-0.01224
H	5.28683	-3.82025	1.69241
H	3.67858	-3.68909	0.95782

H 6.57414 -1.45151 0.34296
H 6.14161 -0.13481 1.43156
H 6.70506 -1.67820 2.08794
H 3.74033 2.46732 2.79180
H 4.60390 1.37125 1.71593
H 2.83739 1.27920 1.85179
H 5.29895 1.78651 4.58553
H 5.34612 0.14321 5.22176
H 6.09792 0.51251 3.66327
H 2.82892 1.85037 4.87341
H 1.76783 0.67482 4.09581
H 2.75816 0.19491 5.47876
H 5.86530 -3.63087 5.35108
H 6.12398 -3.33155 3.63363
H 6.20684 -1.99382 4.78890
H 3.72817 -4.77286 4.86134
H 2.39716 -3.96296 4.03151
H 3.82871 -4.48595 3.12601
H 3.77400 -3.06582 6.49393
H 4.07512 -1.36462 6.15137
H 2.51318 -2.09855 5.72694

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1-Me graft wo CH4 - blue path.

W 0.26389 -1.87217 2.50438
C -1.00332 -0.41340 3.43932
O -0.54670 -3.03344 1.31770
O 2.07312 -1.57857 2.64079
Si 3.76247 -1.39096 3.00128
C 3.89281 0.46312 3.59604
C 2.74653 0.79754 4.56902
O 0.21078 -0.47837 1.03241
Si -0.40230 0.76773 0.21242
O 0.32405 0.88577 -1.27744
Si -0.00430 1.27668 -2.83901

O	0.39482	2.85935	-3.12867
Si	0.53777	4.28602	-2.30963
O	1.74148	5.17378	-2.97944
Si	3.34323	5.50031	-2.56012
O	0.04941	-2.81465	3.92651
Si	-1.37134	-4.45105	0.73322
C	0.01168	-5.81788	0.54045
C	0.91778	-5.53303	-0.66993
C	4.15510	-2.70247	4.39353
C	5.67327	-2.91569	4.53581
C	4.64463	-1.74331	1.29422
C	4.67992	-3.24898	0.97974
C	3.48791	-4.05196	4.06550
C	3.59667	-2.26651	5.76027
O	-0.16155	2.20744	1.02144
Si	0.10771	3.80472	0.72881
O	0.88943	4.00522	-0.71712
O	-2.04340	0.57865	-0.01038
Si	-3.44507	1.42747	-0.12325
O	-3.80319	1.71840	-1.71595
Si	-3.02768	1.89000	-3.16908
O	-3.97869	1.29879	-4.36523
Si	-5.62492	0.96668	-4.52619
O	-1.31881	4.65217	0.71249
Si	-2.93012	4.43696	0.39798
O	-3.84330	5.36626	1.40344
O	1.06292	4.41969	1.91233
Si	0.81192	5.54607	3.14333
O	-3.34887	2.86793	0.69093
O	-3.24932	4.87028	-1.16887
Si	-2.48851	4.90712	-2.63341
O	-0.86224	5.15564	-2.45105
O	-4.64937	0.53372	0.54119
Si	-6.02382	0.92630	1.44194

C	-2.10802	-3.84266	-0.96844
C	-2.55267	-5.02218	-1.85153
C	-2.72102	-4.88278	2.07581
C	-3.80295	-5.80174	1.47572
C	-3.32020	-2.92028	-0.74922
C	-1.05529	-3.01326	-1.72956
C	3.87073	-1.07010	0.14407
C	6.09165	-1.21880	1.30026
C	5.23598	0.72694	4.30090
C	3.76197	1.43725	2.41191
O	-1.60989	1.04553	-3.19026
O	0.89722	0.31436	-3.81207
Si	0.78330	-0.18946	-5.41720
O	-2.73203	3.49247	-3.45699
O	-3.16520	6.17265	-3.43938
C	-3.39521	-3.60142	2.60390
C	-2.11480	-5.58816	3.30318
C	-0.61537	-7.21200	0.35536
C	0.92462	-5.84268	1.77849
H	-6.74617	2.07396	0.81946
H	-5.63824	1.26609	2.84157
H	-6.88954	-0.28673	1.43126
H	0.17858	0.88048	-6.26410
H	-0.04660	-1.42610	-5.49856
H	4.06355	4.23960	-2.21646
H	3.96661	6.13552	-3.75535
H	-4.03046	6.24613	1.06302
H	3.38837	6.44061	-1.40277
H	2.06752	5.57131	3.94571
H	-0.33613	5.13618	4.00291
H	0.55394	6.89743	2.56504
H	-2.78603	6.34738	-4.30581
H	-5.85691	0.69316	-5.97243
H	-6.44164	2.13740	-4.09051

H	-5.98810	-0.23188	-3.71577
H	2.17116	-0.48010	-5.87633
H	-0.63127	0.59801	3.25574
H	-1.98186	-0.49772	2.94783
H	-1.12202	-0.60253	4.50683
H	-4.52871	-6.06882	2.25653
H	-4.36393	-5.32092	0.66882
H	-3.39203	-6.73883	1.08548
H	-4.19428	-3.88184	3.30469
H	-2.68782	-2.98120	3.16110
H	-3.84806	-2.98911	1.82181
H	-2.90631	-5.74805	4.04919
H	-1.70039	-6.57277	3.06779
H	-1.33699	-4.98298	3.77838
H	-2.97758	-4.63734	-2.78903
H	-1.72097	-5.67891	-2.12468
H	-3.32528	-5.63672	-1.37758
H	-3.66677	-2.54658	-1.72285
H	-4.16783	-3.43311	-0.28605
H	-3.06988	-2.04595	-0.14253
H	-1.51557	-2.59108	-2.63335
H	-0.68425	-2.18158	-1.12582
H	-0.19536	-3.60343	-2.05250
H	0.17927	-7.95496	0.19927
H	-1.18675	-7.53373	1.23078
H	-1.27816	-7.26194	-0.51432
H	1.68867	-6.62255	1.65017
H	1.45348	-4.89456	1.90924
H	0.39306	-6.05545	2.70721
H	1.73727	-6.26543	-0.68966
H	0.39024	-5.61896	-1.62369
H	1.37139	-4.53788	-0.62095
H	4.33878	-1.34336	-0.81193
H	2.82606	-1.38992	0.10604

H 3.87589 0.01916 0.20451

H 5.12100 -3.39984 -0.01545

H 5.28634 -3.81916 1.68894

H 3.67728 -3.68831 0.95607

H 6.57165 -1.44970 0.33908

H 6.13975 -0.13348 1.42848

H 6.70418 -1.67693 2.08389

H 3.73919 2.46771 2.79146

H 4.60213 1.37215 1.71456

H 2.83576 1.27966 1.85184

H 5.29939 1.78684 4.58365

H 5.34744 0.14343 5.21954

H 6.09792 0.51321 3.66052

H 2.82952 1.85004 4.87353

H 1.76814 0.67432 4.09657

H 2.75975 0.19444 5.47862

H 5.86786 -3.63054 5.34752

H 6.12498 -3.33113 3.62986

H 6.20864 -1.99341 4.78507

H 3.73045 -4.77298 4.85919

H 2.39867 -3.96313 4.03053

H 3.82964 -4.48567 3.12385

H 3.77733 -3.06637 6.49213

H 4.07792 -1.36504 6.14977

H 2.51574 -2.09908 5.72644

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1-Me graft adduct - red path.

C -1.55791 -4.80784 2.75842

W -0.16983 -3.29807 2.09688

O -0.81969 -1.98247 1.19811

O -0.35488 -2.59385 3.82162

Si -0.56301 -1.73747 5.30717

C 0.55192 -2.69005 6.60305

C 0.17848 -2.32107 8.05019

C	1.95127	-3.28236	2.47876
O	0.23715	-4.47046	0.69865
Si	0.55972	-5.51401	-0.64670
C	-1.01925	-5.39266	-1.79541
C	-1.05527	-6.56249	-2.79678
C	0.03797	0.08580	4.93766
C	1.34597	0.08104	4.12557
C	-2.47790	-1.85171	5.70540
C	-2.86657	-3.24420	6.23548
C	-0.99485	0.84548	4.08489
C	0.26929	0.87104	6.24187
C	2.17562	-4.78783	-1.47993
C	2.08544	-3.25171	-1.55956
C	0.82529	-7.28855	0.13780
C	1.67932	-7.17826	1.41527
C	3.44643	-5.12461	-0.67877
C	2.36250	-5.34359	-2.90453
C	-2.88740	-0.81408	6.76759
C	-3.31062	-1.60545	4.43273
C	2.04600	-2.37685	6.40856
C	0.39381	-4.21175	6.41692
C	-0.50363	-7.94464	0.55378
C	1.53054	-8.23651	-0.84985
C	-1.05293	-4.07668	-2.59337
C	-2.30609	-5.42181	-0.94994
O	-1.09102	-0.60955	-1.12911
Si	-0.59250	0.93145	-1.28638
O	0.91952	1.16147	-0.63296
Si	2.30840	1.99310	-0.92481
O	2.31669	3.40944	-0.06517
Si	1.25131	4.53783	0.51364
O	-0.18383	3.79475	0.86833
Si	-1.65005	3.47643	0.17196
O	-2.78387	3.49168	1.35552

Si	-4.30513	4.20276	1.51673
O	-1.63472	1.99696	-0.55092
O	-0.54858	1.24314	-2.91217
Si	-0.79134	2.45150	-4.00376
O	-1.87117	3.55916	-3.40848
Si	-1.87344	4.97187	-2.55077
O	-0.47817	5.81362	-2.84595
Si	1.02864	6.01668	-2.20529
O	1.44298	7.57560	-2.52698
O	-2.01774	4.65559	-0.93590
O	-3.15766	5.87230	-3.01969
Si	-3.34380	7.36712	-3.78327
O	-1.37207	1.83462	-5.40561
Si	-2.89413	1.34502	-5.94581
O	0.64790	3.18870	-4.35739
Si	2.11346	3.48812	-3.64918
O	2.09779	4.96552	-2.90793
O	3.57938	1.07996	-0.43141
Si	5.11755	0.79473	-1.06286
O	2.47955	2.31635	-2.54167
O	3.27815	3.48558	-4.80138
Si	3.26393	3.32782	-6.48262
O	1.02645	5.76231	-0.56967
O	1.87899	5.25778	1.85520
H	-5.18213	3.83776	0.36628
H	-4.17531	5.68645	1.60386
H	-4.88088	3.66967	2.78413
H	-3.60726	2.51088	-6.54426
H	-3.69789	0.78172	-4.82237
H	2.78411	1.96985	-6.87084
H	2.39232	4.37023	-7.09806
H	2.10279	4.65092	2.56670
H	4.67432	3.51546	-6.92620
H	5.85946	0.02892	-0.02121

H	5.81770	2.08304	-1.34143
H	5.02444	-0.01001	-2.31522
H	2.24297	7.87768	-2.08679
H	-4.80800	7.53839	-4.00194
H	-2.62771	7.37558	-5.09180
H	-2.82641	8.46127	-2.91186
H	-2.66529	0.30350	-6.98702
H	-0.99548	-1.03891	-0.25335
H	-1.92076	-6.44578	-3.46389
H	-0.16430	-6.60067	-3.43170
H	-1.16050	-7.53523	-2.30709
H	-1.99447	-4.02635	-3.15802
H	-1.01655	-3.19039	-1.95410
H	-0.24365	-4.00441	-3.32493
H	-3.17706	-5.36719	-1.61779
H	-2.41283	-6.33182	-0.35498
H	-2.36158	-4.56137	-0.27715
H	1.63861	-9.23039	-0.39335
H	0.96718	-8.36952	-1.77893
H	2.53530	-7.89547	-1.11447
H	-0.29471	-8.90610	1.04409
H	-1.06082	-7.33252	1.26920
H	-1.15757	-8.15600	-0.29619
H	1.81496	-8.17860	1.84990
H	2.67360	-6.76606	1.23308
H	1.19036	-6.55724	2.17212
H	3.00436	-2.86099	-2.01847
H	1.24768	-2.89863	-2.16242
H	1.99231	-2.79317	-0.57174
H	3.28972	-4.93962	-3.33441
H	2.44815	-6.43492	-2.92553
H	1.54926	-5.05675	-3.57654
H	4.30760	-4.62435	-1.14359
H	3.39380	-4.77890	0.35743

H	3.66918	-6.19516	-0.66804
H	-0.99130	-5.50832	3.38890
H	-2.35956	-4.38400	3.36648
H	-1.99162	-5.36252	1.92496
H	0.55608	1.90436	6.00119
H	-0.62628	0.92630	6.86899
H	1.07670	0.44833	6.84785
H	1.65921	1.11910	3.94563
H	2.17319	-0.41953	4.63351
H	1.20943	-0.38544	3.14640
H	-0.58749	1.82810	3.81019
H	-1.22498	0.32000	3.15297
H	-1.93161	1.03052	4.61684
H	0.83751	-2.85480	8.74925
H	0.29547	-1.25121	8.25149
H	-0.84851	-2.59841	8.30424
H	2.63705	-2.97802	7.11388
H	2.39352	-2.62815	5.40195
H	2.28813	-1.32831	6.60229
H	1.06310	-4.73559	7.11380
H	-0.61978	-4.56637	6.61440
H	0.66650	-4.52258	5.40378
H	-3.95390	-0.93368	7.00423
H	-2.33511	-0.92942	7.70585
H	-2.75120	0.21437	6.42180
H	-3.95700	-3.28947	6.36519
H	-2.58876	-4.04671	5.54575
H	-2.42160	-3.46640	7.20947
H	-4.37642	-1.73177	4.66912
H	-3.18635	-0.59984	4.02820
H	-3.06488	-2.31137	3.63536
H	2.52450	-3.18331	1.55420
H	2.20418	-4.25235	2.93067
H	2.24584	-2.48947	3.16731

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1-Me graft TS - red path.

C	0.51016	-1.77813	11.75061
W	2.48621	-0.92967	12.14497
O	3.01373	0.70030	12.17056
O	1.87472	-0.96924	13.88588
Si	1.44238	-0.61422	15.53040
C	1.72946	-2.31777	16.45105
C	0.98903	-2.36065	17.80022
C	4.22750	-1.92746	12.89717
O	3.09488	-2.07116	10.44953
Si	3.59264	-3.41495	9.44490
C	2.80538	-3.01172	7.68908
C	2.89856	-4.22746	6.74531
C	2.62506	0.81907	16.13858
C	4.07489	0.58207	15.67410
C	-0.43711	-0.07980	15.44963
C	-1.35536	-1.28484	15.17614
C	2.20760	2.18293	15.55956
C	2.60621	0.92022	17.67543
C	5.55657	-3.37671	9.40195
C	6.04438	-1.91542	9.36696
C	2.88234	-5.08359	10.19717
C	3.08724	-5.14714	11.71972
C	6.19811	-4.04702	10.63250
C	6.11299	-4.10388	8.16229
C	-0.88351	0.56855	16.77405
C	-0.66890	0.93004	14.30998
C	3.22242	-2.57553	16.72062
C	1.23332	-3.48213	15.57277
C	1.36962	-5.22787	9.95483
C	3.57465	-6.30680	9.56402
C	3.52470	-1.82928	7.01084
C	1.31530	-2.62204	7.78899

O	1.87977	-0.19159	10.04607
Si	2.10507	1.31785	9.43720
O	3.70893	1.72826	9.36301
Si	4.76559	2.61550	8.46530
O	4.88038	4.16499	9.04450
Si	3.96124	5.29523	9.83514
O	2.86720	4.52257	10.80540
Si	1.29948	3.99426	10.78167
O	0.65593	4.15015	12.28207
Si	-0.47763	5.22670	12.92216
O	1.23273	2.41809	10.31252
O	1.51719	1.31365	7.88024
Si	0.72946	2.27651	6.80118
O	-0.19160	3.40546	7.59325
Si	-0.07854	4.95250	8.16298
O	0.98466	5.82576	7.24125
Si	2.58374	6.23460	7.21677
O	2.64670	7.73116	6.53721
O	0.41533	4.93843	9.74046
O	-1.55755	5.65028	8.08157
Si	-2.17789	7.01566	7.30420
O	-0.24771	1.36560	5.85113
Si	-1.88944	0.97612	5.88043
O	1.82158	3.02828	5.80993
Si	3.38987	3.55939	5.84623
O	3.44484	5.14302	6.31983
O	6.24054	1.90521	8.56263
Si	7.81585	2.49086	8.70031
O	4.29144	2.64042	6.87989
O	4.03396	3.43662	4.34557
Si	3.45051	2.96132	2.83517
O	3.21188	6.28535	8.74827
O	4.92247	6.27661	10.74252
H	-1.82167	4.98193	12.32452

H	-0.05952	6.63734	12.67241
H	-0.51705	4.96469	14.38863
H	-2.69920	2.14337	5.42494
H	-2.31032	0.57253	7.25384
H	3.00889	1.53692	2.87331
H	2.31397	3.83322	2.41784
H	5.23210	5.88051	11.56260
H	4.58726	3.11704	1.88427
H	8.05367	3.00232	10.08228
H	8.06231	3.58125	7.71164
H	8.72039	1.33934	8.42514
H	3.51553	8.14340	6.55156
H	-3.62849	7.05813	7.64317
H	-2.00185	6.89691	5.82784
H	-1.50035	8.24778	7.80118
H	-2.06663	-0.16302	4.93596
H	2.51658	-1.16327	9.87846
H	2.53068	-3.94067	5.75036
H	3.91903	-4.59824	6.61669
H	2.27678	-5.06206	7.08279
H	3.00589	-1.58163	6.07489
H	3.52021	-0.92178	7.62152
H	4.56202	-2.05537	6.75131
H	0.93583	-2.43001	6.77557
H	0.69326	-3.40881	8.21944
H	1.15375	-1.70820	8.36374
H	3.13210	-7.22597	9.97310
H	3.44966	-6.34710	8.47808
H	4.64579	-6.34638	9.77875
H	1.00810	-6.13412	10.46138
H	0.80145	-4.38338	10.35544
H	1.12365	-5.33614	8.89571
H	2.70522	-6.10603	12.09780
H	4.13614	-5.07671	12.01727

H	2.52851	-4.35733	12.23041
H	7.14304	-1.89794	9.38747
H	5.73190	-1.38157	8.46752
H	5.68859	-1.33782	10.22380
H	7.21146	-4.08689	8.19556
H	5.81007	-5.15510	8.11901
H	5.81681	-3.62829	7.22404
H	7.28933	-3.92911	10.57436
H	5.87876	-3.60284	11.57757
H	5.99887	-5.12116	10.67959
H	0.37811	-2.64287	12.41503
H	-0.28304	-1.05770	11.97353
H	0.39193	-2.09072	10.71173
H	3.24075	1.75971	17.99223
H	1.60424	1.10724	18.07467
H	2.99815	0.02250	18.16299
H	4.70993	1.38855	16.06779
H	4.49857	-0.35962	16.03059
H	4.15270	0.61248	14.58397
H	2.94417	2.93958	15.86536
H	2.18101	2.17788	14.46625
H	1.23618	2.52095	15.93046
H	1.19817	-3.31460	18.30453
H	1.30516	-1.56253	18.47968
H	-0.09651	-2.29250	17.68596
H	3.34129	-3.56751	17.17895
H	3.81238	-2.57212	15.79934
H	3.66179	-1.85035	17.41093
H	1.42939	-4.43389	16.08626
H	0.16196	-3.43960	15.36655
H	1.75803	-3.51126	14.61352
H	-1.95268	0.81599	16.71590
H	-0.75385	-0.09399	17.63574
H	-0.35249	1.50161	16.98486

H -2.39000 -0.93096 15.06562

H -1.09059 -1.80469 14.25079

H -1.35500 -2.01329 15.99214

H -1.73887 1.17712 14.26240

H -0.12468 1.86495 14.44587

H -0.38495 0.52511 13.33625

H 5.05080 -1.77363 12.19761

H 4.05727 -2.99893 13.02115

H 4.49919 -1.49229 13.86005

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1-Me graft prod - red path.

C -2.23975 -1.76824 1.82939

W -0.50201 -0.68023 2.47018

O -0.71049 0.96997 2.83613

O -0.62528 -1.44688 4.14559

Si -0.73983 -1.77367 5.85329

C 0.04432 -3.55112 6.05884

C -0.32829 -4.17576 7.41578

C 1.53200 -1.34233 2.31769

O 0.18431 -3.59406 -0.03241

Si 0.66610 -4.78605 -1.16155

C -0.33744 -4.48218 -2.81596

C -0.36187 -5.73705 -3.70650

C 0.27819 -0.34509 6.71502

C 1.60492 -0.08314 5.97738

C -2.65666 -1.70521 6.23573

C -3.38004 -2.96600 5.72886

C -0.49344 0.98766 6.69914

C 0.58885 -0.70963 8.17894

C 2.60046 -4.59119 -1.39984

C 2.94989 -3.09989 -1.57724

C 0.16056 -6.42674 -0.23193

C 0.55005 -6.31946 1.25536

C 3.36412 -5.06607 -0.15057

C	3.12998	-5.37800	-2.61095
C	-2.90518	-1.59055	7.75149
C	-3.31401	-0.50188	5.53365
C	1.57978	-3.50520	5.95950
C	-0.44175	-4.47755	4.92819
C	-1.36394	-6.63591	-0.26665
C	0.83127	-7.67182	-0.83616
C	0.25929	-3.32708	-3.63975
C	-1.78636	-4.07927	-2.48115
O	-0.28597	-0.46088	0.52899
Si	-0.05113	0.83565	-0.44481
O	1.50338	1.37643	-0.25462
Si	2.73467	2.09633	-1.08228
O	2.68761	3.73979	-0.88293
Si	1.58368	4.93929	-0.58017
O	0.32802	4.30923	0.29194
Si	-1.18739	3.68618	0.06767
O	-2.10062	4.13156	1.34552
Si	-3.37777	3.50715	2.25417
O	-1.12259	2.04167	-0.07936
O	-0.29615	0.36978	-2.01956
Si	-0.83977	1.06475	-3.41930
O	-1.91801	2.27741	-3.09228
Si	-1.97968	3.92090	-2.91386
O	-0.76445	4.63586	-3.78255
Si	0.78862	5.15478	-3.57529
O	0.95569	6.46059	-4.56106
O	-1.84225	4.31964	-1.31724
O	-3.42537	4.43420	-3.48480
Si	-3.93692	5.76744	-4.38756
O	-1.58752	-0.08010	-4.32169
Si	-3.14425	-0.21763	-4.96332
O	0.43796	1.66087	-4.28458
Si	1.94702	2.31048	-4.07373

O	1.85295	3.95868	-3.99735
O	4.14080	1.51407	-0.47577
Si	5.73337	2.06982	-0.42405
O	2.63652	1.72424	-2.69168
O	2.89578	1.89359	-5.34121
Si	2.65253	1.05187	-6.78380
O	1.07357	5.59735	-2.00530
O	2.28717	6.16277	0.26656
H	-3.81305	2.18503	1.72139
H	-4.50542	4.48052	2.16342
H	-2.93554	3.38588	3.67058
H	-3.43529	0.93170	-5.86880
H	-4.15500	-0.27020	-3.86787
H	2.31818	-0.37395	-6.50011
H	1.55578	1.68150	-7.57529
H	2.23958	6.05862	1.22161
H	3.93696	1.13486	-7.53434
H	5.90904	2.97577	0.74848
H	6.07831	2.79707	-1.68054
H	6.60116	0.86847	-0.27113
H	1.77315	6.95309	-4.44183
H	-5.42503	5.77417	-4.30999
H	-3.50017	5.61939	-5.80577
H	-3.38688	7.02929	-3.81332
H	-3.16210	-1.49071	-5.73713
H	0.16281	-2.68004	-0.34115
H	-0.91047	-5.52428	-4.63509
H	0.64265	-6.06480	-3.99395
H	-0.86309	-6.58203	-3.22491
H	-0.37320	-3.14084	-4.51865
H	0.29700	-2.38769	-3.07879
H	1.26477	-3.54636	-4.00914
H	-2.33444	-3.88375	-3.41386
H	-2.33208	-4.85404	-1.93965

H	-1.82558	-3.16545	-1.88053
H	0.51217	-8.57014	-0.28850
H	0.56384	-7.82357	-1.88715
H	1.92275	-7.62919	-0.77346
H	-1.62614	-7.50717	0.35067
H	-1.90461	-5.77437	0.13853
H	-1.74216	-6.83421	-1.27375
H	0.19652	-7.21332	1.78927
H	1.62849	-6.25467	1.41172
H	0.08999	-5.44512	1.72354
H	4.03995	-2.98524	-1.65878
H	2.51280	-2.65735	-2.47461
H	2.62872	-2.50592	-0.71525
H	4.22134	-5.26457	-2.68214
H	2.92233	-6.45086	-2.53595
H	2.71069	-5.02346	-3.55730
H	4.43392	-4.84191	-0.27003
H	3.02483	-4.55518	0.75646
H	3.28046	-6.14432	0.01282
H	-1.86090	-2.67716	1.34166
H	-2.89435	-2.05013	2.65765
H	-2.80912	-1.19909	1.08924
H	1.11869	0.12485	8.65885
H	-0.31453	-0.89800	8.76769
H	1.23398	-1.58899	8.26610
H	2.15630	0.70709	6.50567
H	2.25803	-0.95678	5.93212
H	1.43594	0.27203	4.95717
H	0.14221	1.77354	7.13073
H	-0.75149	1.30196	5.68322
H	-1.40830	0.95684	7.29722
H	0.15788	-5.15612	7.51527
H	0.00039	-3.56645	8.26395
H	-1.40427	-4.34268	7.52055

H 1.97406 -4.52991 6.00426
H 1.91927 -3.07220 5.01340
H 2.04424 -2.94934 6.77857
H 0.04935 -5.45533 5.02619
H -1.51865 -4.65457 4.94952
H -0.18500 -4.08045 3.94227
H -3.98606 -1.61304 7.94785
H -2.45862 -2.41615 8.31492
H -2.52468 -0.65405 8.16949
H -4.46147 -2.84841 5.88428
H -3.22217 -3.13400 4.65908
H -3.07812 -3.87141 6.26247
H -4.39002 -0.50087 5.75708
H -2.91360 0.45911 5.85950
H -3.20819 -0.55369 4.44681
H 2.12085 -0.65512 1.70409
H 1.49628 -2.31563 1.80926
H 2.00539 -1.46015 3.29517

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1-Me graft wo HOSitBu3 - red path.

C -2.10187 -2.02460 2.52326
W -0.31506 -0.91342 2.99329
O -1.61681 0.46968 3.34835
Si -2.11409 1.69465 4.30710
O -3.45502 2.39081 3.63200
Si -4.85217 3.14615 4.08625
O -4.62637 4.78427 4.10515
Si -3.42002 5.89464 4.34487
O -3.71132 7.21306 3.41909
Si -4.89825 7.62991 2.29279
O 0.30259 -1.09128 4.56946
O 0.68854 -2.15377 2.05611
Si 1.81017 -3.32764 1.43530
C 1.00356 -5.05559 1.87115

C	0.45912	-5.05408	3.31291
C	0.58659	0.64687	1.81698
C	1.89361	-2.95894	-0.48182
C	0.48170	-2.67389	-1.03028
C	3.48115	-2.97935	2.38805
C	4.66511	-3.66927	1.68490
C	2.50210	-4.14457	-1.25302
C	2.74253	-1.71142	-0.78675
C	3.76191	-1.46686	2.46652
C	3.41606	-3.48521	3.84027
C	-0.18274	-5.37737	0.94415
C	2.03577	-6.19134	1.73775
O	-0.90162	2.81579	4.43428
Si	-0.68287	4.44380	4.58218
O	-1.95791	5.25727	3.91235
O	-2.49196	1.10852	5.80992
Si	-2.42922	1.57902	7.39473
O	-3.88109	2.23944	7.83660
Si	-5.17240	3.02631	7.17309
O	-6.54025	2.57639	7.95053
Si	-7.55522	3.30677	9.08648
O	-0.52040	4.86362	6.17652
Si	-1.01486	4.33389	7.66853
O	0.10897	4.71314	8.80942
O	0.69072	4.82687	3.77515
Si	1.76830	6.12502	3.80743
O	-1.22697	2.69358	7.61677
O	-2.39874	5.11557	8.11278
Si	-3.75676	5.77452	7.43190
O	-3.37500	6.35794	5.93042
O	-2.11026	0.29593	8.35548
Si	-2.16904	-1.38678	8.22623
O	-5.33018	2.61163	5.57945
O	-6.02716	2.81754	2.99383

Si	-7.33414	1.75073	2.94063
O	-4.97156	4.66347	7.31771
O	-4.33739	6.97270	8.39709
H	-3.21738	-1.80031	7.24837
H	-2.50829	-1.90561	9.58201
H	-0.83633	-1.89835	7.80152
H	-8.41406	2.21883	3.85677
H	-6.90332	0.37493	3.32613
H	-4.92184	6.64309	1.17458
H	-6.23697	7.68678	2.94858
H	0.81161	4.06329	8.90494
H	-4.52480	8.97752	1.77827
H	2.78367	5.90487	4.87827
H	1.04266	7.40530	4.05482
H	2.43503	6.16154	2.47548
H	-3.68184	7.61923	8.67503
H	-8.49773	2.24574	9.54084
H	-8.31210	4.42413	8.45175
H	-6.76317	3.81869	10.24190
H	-7.82167	1.75741	1.53263
H	-2.50706	-1.60245	1.59269
H	-1.92020	-3.09142	2.37473
H	-2.85542	-1.88690	3.30361
H	5.58463	-3.49484	2.26061
H	4.53594	-4.75359	1.60727
H	4.84104	-3.27993	0.67755
H	4.71937	-1.30677	2.98151
H	3.83825	-0.98862	1.48799
H	2.99520	-0.94455	3.04523
H	4.34151	-3.20109	4.36044
H	2.58347	-3.04160	4.39519
H	3.33664	-4.57373	3.90560
H	2.57189	-3.89275	-2.32030
H	3.51417	-4.38919	-0.91413

H 1.89572 -5.05176 -1.17885
H 2.70927 -1.50790 -1.86612
H 2.36285 -0.81929 -0.27952
H 3.79510 -1.83642 -0.51867
H 0.55044 -2.43417 -2.10040
H -0.19821 -3.52235 -0.93272
H 0.02143 -1.81582 -0.53136
H 1.54949 -7.15434 1.94672
H 2.46281 -6.25858 0.73196
H 2.86165 -6.09075 2.44793
H -0.65155 -6.31550 1.27176
H -0.95433 -4.60198 0.97196
H 0.11826 -5.51817 -0.09750
H -0.02429 -6.02005 3.51496
H 1.23790 -4.91858 4.06499
H -0.29109 -4.27467 3.46956
H 0.57603 1.59851 2.35449
H -0.02935 0.76291 0.91360
H 1.60921 0.40558 1.51824
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1-Me graft adduct - black path.
C -1.41935 -4.03073 2.27166
W 0.71710 -3.84626 2.51414
C 1.85623 -2.12208 1.87819
O 0.32710 -2.82915 4.04365
Si 0.10950 -2.18101 5.62460
C -0.35297 -3.70760 6.76242
C -0.97267 -3.23992 8.09144
O 1.54262 -5.13810 3.26719
O 0.84204 -4.42874 0.73194
Si 1.19174 -5.24477 -0.74238
C 0.88440 -3.90899 -2.13970
C 0.74919 -4.55050 -3.53223
C 1.82522 -1.36194 6.09920

C	2.99420	-2.29152	5.72081
C	-1.33711	-0.87559	5.43327
C	-2.71187	-1.55779	5.31477
C	2.05153	-0.03331	5.35445
C	1.90212	-1.07359	7.61047
C	3.05991	-5.81523	-0.59861
C	3.93072	-4.69308	-0.00250
C	-0.06296	-6.74671	-0.82307
C	-0.15480	-7.45137	0.54426
C	3.20320	-7.01899	0.35115
C	3.63282	-6.20431	-1.97338
C	-1.39128	0.09528	6.62617
C	-1.13492	-0.06904	4.13673
C	0.88104	-4.57278	7.07626
C	-1.35544	-4.62877	6.04355
C	-1.48617	-6.27933	-1.18064
C	0.37346	-7.77750	-1.88011
C	2.03370	-2.88759	-2.20047
C	-0.39658	-3.11149	-1.82913
O	0.33951	0.73940	-0.02525
Si	0.07384	2.05901	-0.97179
O	1.35037	3.10625	-0.82776
Si	2.12489	4.27351	-1.70482
O	1.45296	5.75264	-1.40068
Si	0.00676	6.44649	-0.98773
O	-0.86090	5.36984	-0.07737
Si	-2.03233	4.21944	-0.25845
O	-2.96344	4.23000	1.08568
Si	-4.59222	3.92906	1.41587
O	-1.33280	2.73339	-0.43984
O	-0.07891	1.62576	-2.56389
Si	-0.94409	2.03796	-3.90765
O	-2.39434	2.71585	-3.48298
Si	-3.05977	4.20251	-3.19618

O	-2.26965	5.35992	-4.07726
Si	-1.02322	6.43042	-3.91528
O	-1.43186	7.73130	-4.83346
O	-2.96936	4.55567	-1.58343
O	-4.63199	4.15644	-3.64566
Si	-5.62562	5.14923	-4.58637
O	-1.22189	0.68940	-4.79314
Si	-2.60596	-0.03033	-5.44216
O	-0.06748	3.10288	-4.82315
Si	1.09518	4.26775	-4.63759
O	0.38884	5.74985	-4.44904
O	3.69361	4.28797	-1.23622
Si	5.16789	4.51663	-2.02808
O	2.04296	3.93483	-3.32409
O	2.05610	4.29180	-5.96205
Si	1.95949	3.63374	-7.51457
O	-0.83131	6.89173	-2.33707
O	0.25891	7.83822	-0.14871
H	-4.68579	3.68313	2.88213
H	-5.06610	2.73269	0.66112
H	-5.40931	5.12030	1.04436
H	-3.30801	0.92438	-6.34879
H	-3.52456	-0.46377	-4.35060
H	2.14009	2.15438	-7.45428
H	0.64317	3.95967	-8.13644
H	0.63071	7.72016	0.73042
H	3.06498	4.25274	-8.29812
H	6.17564	4.78788	-0.96484
H	5.08430	5.67470	-2.96485
H	5.53638	3.28137	-2.77854
H	-0.87659	8.50631	-4.70659
H	-5.20748	5.08306	-6.01635
H	-5.56137	6.55720	-4.09957
H	-7.00717	4.61337	-4.43191

H	-2.13232	-1.21265	-6.21496
H	1.23461	0.38784	-0.05691
H	0.60786	-3.76548	-4.28838
H	1.63914	-5.11923	-3.82109
H	-0.11247	-5.22059	-3.60285
H	1.78909	-2.10769	-2.93546
H	2.19029	-2.38918	-1.23846
H	2.98224	-3.33465	-2.51000
H	-0.52914	-2.32632	-2.58648
H	-1.29715	-3.72845	-1.83906
H	-0.33862	-2.61895	-0.85449
H	-0.37430	-8.58081	-1.94182
H	0.46196	-7.34286	-2.88095
H	1.32842	-8.25008	-1.63372
H	-2.17157	-7.13709	-1.12881
H	-1.86312	-5.52092	-0.48786
H	-1.55881	-5.87622	-2.19481
H	-0.90052	-8.25678	0.48526
H	0.78720	-7.90415	0.85756
H	-0.47003	-6.76975	1.33856
H	4.97177	-5.04080	0.05746
H	3.93046	-3.77948	-0.60111
H	3.61670	-4.43909	1.01345
H	4.66572	-6.56070	-1.85401
H	3.06875	-7.00962	-2.45424
H	3.66565	-5.35910	-2.66796
H	4.27032	-7.24774	0.48352
H	2.78919	-6.80947	1.34255
H	2.73172	-7.92563	-0.03839
H	-1.94464	-4.09868	3.22627
H	-1.74292	-3.10911	1.76474
H	-1.70103	-4.87696	1.64179
H	2.46813	-1.70242	2.67976
H	2.48533	-2.32666	1.01036

H	1.09829	-1.37228	1.60699
H	2.85267	-0.57168	7.84006
H	1.09915	-0.41517	7.95672
H	1.87141	-1.98630	8.21254
H	3.94372	-1.79381	5.96399
H	2.97869	-3.24037	6.25892
H	3.00844	-2.52156	4.65260
H	3.05640	0.34526	5.58928
H	1.99334	-0.14875	4.26809
H	1.34159	0.74441	5.64921
H	-1.19217	-4.11231	8.72289
H	-0.30279	-2.58974	8.66312
H	-1.91542	-2.70368	7.94748
H	0.56325	-5.46226	7.63869
H	1.37773	-4.92310	6.16609
H	1.61637	-4.05192	7.69594
H	-1.61906	-5.46377	6.70818
H	-2.28616	-4.12587	5.77221
H	-0.92083	-5.06108	5.13826
H	-2.22883	0.79515	6.49587
H	-1.54855	-0.42021	7.57934
H	-0.48388	0.69909	6.71839
H	-3.48046	-0.79312	5.13321
H	-2.75325	-2.25969	4.47602
H	-3.00248	-2.09281	6.22319
H	-1.96806	0.63660	4.01095
H	-0.21386	0.51640	4.13393
H	-1.11934	-0.71904	3.25742

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1-Me graft TS - black path.

C	0.74615	-1.70626	12.23628
W	2.91704	-1.69916	12.23533
C	4.61854	-0.65608	11.40530
O	2.91353	-0.69120	13.76041

Si	2.89171	-0.10120	15.41734
C	2.70617	-1.70050	16.52273
C	2.29384	-1.31368	17.95596
O	3.46841	-3.20757	12.79052
O	2.67449	-2.48081	10.29152
Si	2.68374	-3.87804	9.24452
C	2.28242	-3.10720	7.48855
C	1.97662	-4.18739	6.43453
C	4.60840	0.80425	15.62541
C	5.74905	-0.02969	15.01392
C	1.35245	1.09660	15.47475
C	0.02715	0.31622	15.53739
C	4.62338	2.16581	14.90778
C	4.91190	1.04697	17.11638
C	4.48350	-4.65788	9.35005
C	5.54796	-3.54955	9.44502
C	1.30072	-5.13377	9.84284
C	1.33947	-5.33025	11.36947
C	4.67227	-5.53931	10.59962
C	4.79225	-5.52092	8.11158
C	1.41476	2.02277	16.70437
C	1.30585	1.96091	14.20078
C	4.02115	-2.49893	16.59337
C	1.64802	-2.66314	15.94899
C	-0.11749	-4.64953	9.49131
C	1.49569	-6.50723	9.17086
C	3.47202	-2.26515	6.99148
C	1.06461	-2.16363	7.55240
O	2.10838	-0.24956	10.37733
Si	1.94488	1.24535	9.79630
O	2.92668	2.30620	10.62592
Si	3.83379	3.65875	10.40681
O	2.96331	4.99479	10.85251
Si	1.39224	5.47800	10.96690

O	0.35736	4.20827	11.20161
Si	-0.51567	3.11819	10.31191
O	-1.82629	2.71755	11.21377
Si	-3.34945	2.08680	10.85209
O	0.37632	1.77912	9.97625
O	2.32819	1.32433	8.17664
Si	1.89302	2.12298	6.80625
O	0.31574	2.63071	6.87574
Si	-0.56670	3.95326	7.32088
O	0.31659	5.33912	7.10379
Si	1.31736	6.32483	7.96945
O	1.06882	7.84021	7.37623
O	-1.03215	3.82359	8.90145
O	-1.90356	4.02074	6.37706
Si	-2.62875	5.21928	5.43456
O	2.06369	1.09750	5.53790
Si	1.57835	1.13942	3.92264
O	2.86869	3.44202	6.56946
Si	3.78666	4.51300	7.42690
O	2.89831	5.87401	7.75484
O	5.16930	3.54840	11.35315
Si	6.77741	4.02078	11.14369
O	4.31729	3.81889	8.82883
O	5.10633	4.93113	6.55083
Si	5.48654	6.18533	5.48919
O	0.95488	6.28340	9.58350
O	1.30830	6.49005	12.26349
H	-3.84398	1.42841	12.09431
H	-3.26005	1.09219	9.74367
H	-4.27138	3.19450	10.46570
H	1.49552	2.54741	3.43401
H	0.24844	0.47841	3.78506
H	6.75364	5.79380	4.81064
H	4.40057	6.36929	4.48221

H	0.42329	6.58896	12.62681
H	5.68705	7.45361	6.24966
H	7.39979	4.00311	12.49750
H	6.84778	5.39628	10.56921
H	7.48093	3.05941	10.24690
H	1.49738	8.54158	7.87559
H	-1.73907	5.58877	4.29583
H	-2.92410	6.42552	6.26101
H	-3.89704	4.62955	4.92039
H	2.60151	0.38774	3.14227
H	2.33537	-1.38200	9.99387
H	1.81901	-3.70825	5.45799
H	2.78921	-4.90879	6.31194
H	1.06381	-4.74597	6.66456
H	3.19909	-1.76213	6.05447
H	3.74637	-1.47853	7.70157
H	4.35996	-2.86982	6.78817
H	0.90952	-1.71548	6.56180
H	0.14066	-2.67627	7.82440
H	1.20692	-1.33580	8.24949
H	0.68215	-7.18016	9.47669
H	1.47253	-6.45119	8.07811
H	2.43328	-6.98688	9.46261
H	-0.85261	-5.34003	9.92861
H	-0.33425	-3.65359	9.88938
H	-0.29980	-4.63181	8.41315
H	0.57457	-6.06704	11.65483
H	2.29998	-5.69591	11.73500
H	1.11661	-4.40407	11.90305
H	6.54676	-4.00885	9.43345
H	5.51056	-2.83349	8.62080
H	5.45585	-2.99376	10.37996
H	5.77931	-5.98876	8.23421
H	4.07013	-6.33016	7.96385

H	4.83157	-4.93285	7.19014
H	5.71872	-5.87470	10.64166
H	4.46400	-4.99446	11.52420
H	4.05381	-6.44083	10.58322
H	0.41636	-2.33420	13.07421
H	0.37527	-0.68892	12.38428
H	0.32329	-2.09097	11.30906
H	5.51819	-1.05182	11.89444
H	4.71778	-0.78639	10.32763
H	4.53102	0.41249	11.62108
H	5.84994	1.61181	17.20727
H	4.13425	1.63392	17.61607
H	5.04437	0.11680	17.67658
H	6.70071	0.49750	15.16861
H	5.85033	-1.02020	15.45988
H	5.61904	-0.15563	13.93685
H	5.62564	2.60642	15.00073
H	4.40899	2.08207	13.83873
H	3.92182	2.88215	15.34321
H	2.24204	-2.21843	18.57731
H	3.00712	-0.63550	18.43477
H	1.30643	-0.84391	17.99552
H	3.84980	-3.41855	17.17008
H	4.37080	-2.80062	15.60112
H	4.82488	-1.95457	17.09664
H	1.55703	-3.52877	16.62001
H	0.65491	-2.21824	15.86257
H	1.94283	-3.04860	14.96968
H	0.51850	2.65788	16.72647
H	1.43973	1.46892	17.64872
H	2.27911	2.69286	16.68453
H	-0.80951	1.02698	15.49193
H	-0.08809	-0.37224	14.69545
H	-0.08627	-0.25220	16.46476

H 0.41058 2.59621 14.22716

H 2.16847 2.62092 14.09770

H 1.24662 1.35144 13.29576

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1-Me graft prod - black path.

C -1.80008 -2.90671 1.52862

W -0.14750 -2.12291 2.61473

C 1.78269 -2.01216 1.72710

O -0.48905 -1.21494 4.17088

Si -0.56116 -0.82151 5.86409

C -0.85132 -2.50811 6.80469

C -1.33827 -2.24362 8.24133

O 0.22781 -3.70623 3.14814

O 0.55485 -3.69076 -1.23078

Si 1.15708 -4.91620 -2.26741

C -0.19438 -5.20045 -3.66212

C -0.01469 -6.55761 -4.36407

C 1.16981 0.00851 6.22664

C 2.29751 -0.80435 5.56393

C -2.07228 0.41106 5.94158

C -3.41386 -0.33552 5.83021

C 1.25549 1.43098 5.64661

C 1.43059 0.08690 7.74197

C 2.85497 -4.25616 -2.98587

C 2.69849 -2.78505 -3.41980

C 1.35176 -6.42758 -1.05398

C 1.96879 -5.96158 0.27982

C 3.95569 -4.27282 -1.91016

C 3.34484 -5.08574 -4.18472

C -2.07845 1.21590 7.25449

C -2.01335 1.39005 4.75314

C 0.43156 -3.35808 6.87196

C -1.90170 -3.36585 6.07151

C -0.01496 -7.04598 -0.70692

C	2.23996	-7.53100	-1.65562
C	-0.14693	-4.10051	-4.73796
C	-1.60194	-5.14049	-3.03751
O	-0.48790	-0.54591	1.42421
Si	-0.28874	0.64848	0.35659
O	1.22263	1.32432	0.51241
Si	2.42752	2.02722	-0.35938
O	2.27076	3.67461	-0.31014
Si	1.10598	4.81478	-0.06412
O	-0.16268	4.22687	0.82255
Si	-1.61672	3.46804	0.59689
O	-2.60896	3.93286	1.81703
Si	-4.24431	4.34837	1.88211
O	-1.42679	1.83400	0.60902
O	-0.45981	0.08976	-1.20589
Si	-1.01679	0.63316	-2.65904
O	-2.18891	1.78832	-2.46235
Si	-2.35288	3.43233	-2.41108
O	-1.15866	4.15867	-3.29909
Si	0.35224	4.78882	-3.08082
O	0.47231	6.03921	-4.14399
O	-2.29149	3.94975	-0.84162
O	-3.80954	3.82774	-3.04480
Si	-4.32318	4.90568	-4.24058
O	-1.67179	-0.63709	-3.46859
Si	-3.15212	-0.80538	-4.27368
O	0.23018	1.25292	-3.55028
Si	1.69659	1.99303	-3.36484
O	1.49990	3.63853	-3.40713
O	3.85455	1.58760	0.31231
Si	5.45195	1.50306	-0.22691
O	2.39508	1.52884	-1.94152
O	2.69453	1.53736	-4.58034
Si	3.09366	2.16882	-6.09351

O	0.55618	5.34606	-1.53617
O	1.79230	6.06511	0.75758
H	-4.59750	4.42997	3.32744
H	-5.07721	3.31058	1.20790
H	-4.46165	5.67364	1.23213
H	-3.34751	0.31583	-5.23822
H	-4.27092	-0.82979	-3.28820
H	3.78178	1.07733	-6.83787
H	1.86523	2.59571	-6.82506
H	1.21437	6.46284	1.41532
H	4.01292	3.33278	-5.93012
H	6.31806	1.65251	0.97617
H	5.73534	2.59830	-1.20066
H	5.69391	0.17951	-0.86939
H	1.21611	6.62845	-3.98727
H	-3.77751	4.50000	-5.56780
H	-3.88425	6.29251	-3.91115
H	-5.81108	4.82813	-4.25303
H	-3.08355	-2.10038	-5.00421
H	0.28990	-2.87961	-1.67728
H	-0.77435	-6.67572	-5.15026
H	0.96437	-6.65175	-4.84574
H	-0.13073	-7.40093	-3.67676
H	-0.96198	-4.26201	-5.45826
H	-0.28876	-3.09727	-4.32158
H	0.78569	-4.10290	-5.30874
H	-2.35859	-5.25056	-3.82750
H	-1.77811	-5.93070	-2.30560
H	-1.78294	-4.18362	-2.53779
H	2.30383	-8.37724	-0.95708
H	1.84624	-7.92084	-2.60024
H	3.26328	-7.18852	-1.83717
H	0.12450	-7.83081	0.04995
H	-0.70340	-6.30746	-0.28432

H	-0.50027	-7.51641	-1.56725
H	2.03049	-6.81794	0.96635
H	2.97987	-5.56451	0.16906
H	1.35648	-5.19714	0.76450
H	3.66231	-2.40587	-3.78728
H	1.97231	-2.64407	-4.22329
H	2.40634	-2.14573	-2.57971
H	4.31099	-4.69819	-4.53898
H	3.49612	-6.13958	-3.92774
H	2.65535	-5.04651	-5.03325
H	4.86602	-3.80569	-2.31280
H	3.66731	-3.70608	-1.01893
H	4.22708	-5.28502	-1.59742
H	-2.27676	-3.73467	2.05885
H	-2.52015	-2.12574	1.27543
H	-1.35274	-3.29610	0.60141
H	2.52601	-2.56692	2.30422
H	1.64792	-2.51865	0.75793
H	2.10438	-0.98353	1.55067
H	2.39388	0.58255	7.92580
H	0.66545	0.66589	8.26977
H	1.48469	-0.90074	8.20903
H	3.26439	-0.33497	5.79262
H	2.34749	-1.83837	5.90943
H	2.19785	-0.81618	4.47429
H	2.26907	1.82437	5.80611
H	1.06716	1.44896	4.56855
H	0.56306	2.12750	6.12726
H	-1.47057	-3.20004	8.76599
H	-0.62678	-1.65166	8.82659
H	-2.30380	-1.72916	8.26792
H	0.19989	-4.31563	7.35898
H	0.82059	-3.59017	5.87577
H	1.22594	-2.88783	7.45841

H -2.05926 -4.29474 6.63752

H -2.87253 -2.87622 5.97898

H -1.56160 -3.65343 5.07309

H -2.95447 1.87903 7.27400

H -2.13909 0.57657 8.14140

H -1.19520 1.85335 7.36049

H -4.23162 0.39785 5.79576

H -3.47762 -0.93347 4.91515

H -3.60838 -0.99132 6.68366

H -2.90101 2.03691 4.77639

H -1.14052 2.04421 4.78058

H -2.00771 0.86802 3.79276

101

1-Me graft wo HOSitBu3 - black path.

C -1.92423 -1.95257 1.47783

W -0.13720 -1.61389 2.59446

C 1.78924 -1.44721 1.68705

O -0.31756 -1.08382 4.33628

Si -0.44329 -1.02841 6.07138

C -0.98171 -2.82132 6.62562

C -1.52648 -2.79714 8.06580

O 0.09958 -3.30813 2.67160

C 1.35174 -0.51795 6.64832

C 2.41476 -1.33209 5.88670

C -1.80031 0.34787 6.35404

C -3.21085 -0.18781 6.04955

C 1.63833 0.96433 6.35090

C 1.52723 -0.75340 8.15947

C -1.77937 0.85966 7.80534

C -1.56371 1.53286 5.39708

C 0.19299 -3.81474 6.56543

C -2.07099 -3.37793 5.68775

O -0.34841 0.19966 1.78773

Si -0.24448 1.25389 0.55929

O	1.20531	2.06380	0.61682
Si	2.34217	2.70775	-0.38516
O	2.06221	4.32686	-0.59300
Si	0.79349	5.39046	-0.61398
O	-0.40132	4.83006	0.38371
Si	-1.79358	3.94063	0.31842
O	-2.83227	4.54385	1.43289
Si	-4.49529	4.83082	1.45692
O	-1.47930	2.35853	0.65798
O	-0.34677	0.44857	-0.89152
Si	-0.93549	0.63371	-2.41805
O	-2.21579	1.68763	-2.44149
Si	-2.50160	3.30269	-2.64710
O	-1.36350	3.96305	-3.65313
Si	0.08171	4.75650	-3.57029
O	0.10522	5.81077	-4.83303
O	-2.48018	4.07448	-1.18575
O	-3.98398	3.48226	-3.31810
Si	-4.57486	4.27454	-4.68821
O	-1.43983	-0.83412	-2.94239
Si	-2.64712	-1.37301	-3.99178
O	0.25544	1.19749	-3.41966
Si	1.65054	2.08073	-3.35205
O	1.32413	3.66794	-3.69981
O	3.81152	2.51180	0.31399
Si	5.35549	2.14204	-0.25933
O	2.34057	1.94663	-1.85711
O	2.72334	1.49886	-4.44345
Si	3.08220	1.83060	-6.05883
O	0.23311	5.59797	-2.15365
O	1.29087	6.88364	-0.13290
H	-4.85198	5.10253	2.87806
H	-5.24060	3.63661	0.96201
H	-4.82292	6.01716	0.61412

H	-2.72838	-0.49091	-5.19312
H	-3.96082	-1.38764	-3.28580
H	3.85035	0.66102	-6.56994
H	1.82936	2.00902	-6.84937
H	1.54255	6.94573	0.79328
H	3.91488	3.06547	-6.14723
H	6.29259	2.40421	0.86936
H	5.70401	3.01053	-1.42216
H	5.42543	0.70725	-0.65930
H	0.69083	6.56382	-4.71019
H	-3.97826	3.68557	-5.92167
H	-4.26595	5.73199	-4.61833
H	-6.04981	4.06297	-4.68199
H	-2.26945	-2.75580	-4.39729
H	-2.40530	-2.89229	1.75791
H	-2.61211	-1.10895	1.57894
H	-1.61507	-2.01365	0.42453
H	2.47977	-2.19725	2.07969
H	1.63518	-1.64947	0.61668
H	2.19699	-0.43877	1.79098
H	2.53101	-0.43137	8.46936
H	0.80835	-0.18550	8.75944
H	1.43170	-1.80845	8.43234
H	3.41421	-1.02126	6.22152
H	2.33710	-2.40801	6.05135
H	2.36643	-1.15142	4.80863
H	2.68350	1.18756	6.60630
H	1.50453	1.20513	5.29143
H	1.01474	1.64378	6.93862
H	-1.79078	-3.81770	8.37553
H	-0.79438	-2.42163	8.78850
H	-2.43179	-2.18971	8.15969
H	-0.17306	-4.81706	6.82809
H	0.62275	-3.88231	5.56114

H 0.99182 -3.57287 7.27214

H -2.36963 -4.37469 6.04139

H -2.97255 -2.76349 5.65708

H -1.69947 -3.49939 4.66647

H -2.56218 1.61873 7.94019

H -1.97100 0.06604 8.53509

H -0.82762 1.33180 8.06595

H -3.93629 0.63147 6.14871

H -3.29438 -0.56927 5.02653

H -3.52496 -0.97761 6.73765

H -2.37910 2.25957 5.51808

H -0.63069 2.06336 5.59454

H -1.55327 1.21871 4.34973

101

Interconversion : O-Si ax.

C 0.76704 -0.23262 2.98471

W -0.65664 -1.77046 2.47940

O -2.11553 -1.75008 3.35602

O -1.13598 -0.51617 1.10748

Si -1.59459 0.45000 -0.12212

O -1.27775 2.02439 0.27536

Si -0.85531 3.44951 -0.44513

O 0.06683 4.30718 0.60234

Si 1.59021 5.02960 0.51688

C -0.57144 -3.13261 0.80925

O 0.34558 -2.97335 3.46378

Si 1.06935 -4.06726 4.60430

C 2.99294 -3.86712 4.31992

C 3.30201 -3.78611 2.81215

O -3.21582 0.24878 -0.38696

Si -4.54444 1.11228 -0.86698

O -5.87076 0.55034 -0.09221

Si -6.13089 -0.57467 1.14445

O -0.75329 0.03859 -1.48836

Si	-0.96036	-0.03374	-3.12480
O	-0.08723	-1.29026	-3.70912
Si	-0.45542	-2.64480	-4.64841
O	0.01875	3.16012	-1.82317
Si	-0.21200	2.96572	-3.44877
O	1.11091	3.54417	-4.22030
Si	2.14388	2.95705	-5.41956
O	-2.20981	4.32839	-0.79729
Si	-3.80291	4.11208	-1.19943
O	-4.69816	5.39429	-0.68882
O	-1.53899	3.82482	-3.92789
Si	-3.16018	3.61798	-4.19615
O	-3.66113	4.51604	-5.47937
O	-0.40359	1.36214	-3.81891
O	-3.98958	4.07469	-2.83868
O	-3.47005	2.04720	-4.59552
Si	-3.90425	0.62485	-3.86805
O	-4.81149	-0.26247	-4.90041
Si	-5.90070	0.10370	-6.13938
O	-4.34559	2.71304	-0.50003
C	0.45261	-3.45451	6.35600
C	0.52667	-1.91925	6.45569
C	0.38084	-5.82746	4.10128
C	0.62314	-6.85525	5.22289
C	1.30782	-4.06702	7.48082
C	-1.01834	-3.83635	6.60073
O	-4.76754	0.94382	-2.49637
O	-2.55669	-0.26209	-3.50133
C	-1.13231	-5.75955	3.81724
C	1.05569	-6.35369	2.82143
C	3.53135	-2.56880	4.94805
C	3.77127	-5.04765	4.92882
H	-6.76001	1.26076	-5.75525
H	-5.45304	-0.12840	2.39433

H	-5.62575	-1.91578	0.73228
H	-7.60633	-0.62407	1.34731
H	-1.03358	-2.22628	-5.95831
H	-1.41629	-3.52937	-3.92814
H	2.94213	1.81152	-4.89423
H	1.36322	2.52531	-6.61534
H	-4.78828	5.46990	0.26571
H	3.04727	4.08616	-5.77855
H	1.78386	5.74295	1.81062
H	1.64441	5.99913	-0.61552
H	2.64593	3.98938	0.34510
H	-3.72588	5.46013	-5.30722
H	-5.15066	0.41779	-7.38938
H	-6.73584	-1.11424	-6.33762
H	0.83402	-3.35969	-4.86438
H	0.33519	-2.88809	0.23793
H	-0.51430	-4.17781	1.12124
H	-1.43050	-2.99962	0.14620
H	0.25448	-7.83951	4.90216
H	1.68389	-6.97334	5.46647
H	0.09280	-6.60187	6.14524
H	-1.48114	-6.75019	3.49385
H	-1.72034	-5.47910	4.69231
H	-1.37236	-5.05245	3.01912
H	0.58454	-7.30243	2.52966
H	0.94586	-5.66426	1.97896
H	2.12172	-6.55567	2.95747
H	0.91861	-3.74037	8.45507
H	1.28888	-5.16167	7.47918
H	2.35393	-3.75017	7.43258
H	-1.34534	-3.40521	7.55729
H	-1.68227	-3.44330	5.82441
H	-1.16806	-4.91706	6.67244
H	0.20410	-1.60919	7.45940

H 1.53285 -1.52314 6.30398

H -0.14465 -1.43706 5.73986

H 4.84926 -4.89482 4.78087

H 3.60593 -5.14791 6.00661

H 3.51661 -6.00281 4.46109

H 4.59970 -2.46916 4.71091

H 3.02986 -1.67959 4.55360

H 3.44420 -2.55622 6.03774

H 4.38146 -3.63616 2.67165

H 3.02782 -4.69069 2.26613

H 2.79002 -2.94146 2.34174

H 1.57986 -0.28491 2.24613

H 0.31188 0.75856 2.91129

H 1.19120 -0.36821 3.98231

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Interconversion : O-Si ax. TS

W 0.75280 -1.59549 2.44058

O 1.27910 -0.04691 1.27359

Si 1.31734 0.76349 -0.12001

O -0.15409 0.68138 -0.89686

O 2.49363 0.17144 -1.13990

O 1.66198 2.35791 0.19196

Si 2.46855 3.65530 -0.42068

O 3.70063 3.16229 -1.41684

Si 3.96047 2.82369 -3.01294

O 2.95883 3.74567 -3.94886

Si 1.49035 3.66109 -4.70915

O 0.33796 4.32204 -3.72255

Si 0.01679 4.50571 -2.11374

O 1.42040 4.63626 -1.24298

C 0.84922 0.14190 3.72898

C 0.92351 -2.46732 0.46988

O 1.83100 -2.73407 3.37284

Si 2.62911 -3.97383 4.33610

C	3.10819	-3.03890	5.97938
C	4.15209	-3.84453	6.77612
O	-0.89040	-1.92699	2.66261
Si	-1.13258	1.62687	-1.83569
O	-0.85930	3.22840	-1.53054
Si	2.80138	-0.04606	-2.74127
O	1.39820	-0.17329	-3.61432
Si	0.34170	0.79367	-4.44154
O	1.13805	2.09379	-5.08807
C	1.27974	-5.36526	4.56927
C	-0.09215	-4.75248	4.91294
C	4.15377	-4.50298	3.24027
C	5.26273	-3.43581	3.26504
C	1.08781	-6.18358	3.27994
C	1.69187	-6.33107	5.69627
O	3.10957	4.53090	0.80941
Si	4.67453	4.77843	1.38589
O	-0.86043	1.31644	-3.43800
O	-2.70211	1.29654	-1.50186
Si	-3.49695	0.23113	-0.46053
O	-0.30037	-0.10388	-5.65068
Si	-0.85249	0.22745	-7.21183
O	3.70686	1.21560	-3.31918
O	3.65768	-1.43445	-2.92291
Si	3.56210	-2.72134	-4.01096
O	5.51652	3.19705	-3.36587
Si	6.79372	2.37142	-4.09618
O	-0.85032	5.90034	-2.00418
O	1.52453	4.46998	-6.14102
C	4.74778	-5.83075	3.74650
C	3.73854	-4.67040	1.76632
C	1.87868	-2.82275	6.87937
C	3.68559	-1.64442	5.66983
H	-1.65585	1.48421	-7.22983

H	-3.17530	0.56092	0.95758
H	-3.10578	-1.17671	-0.76105
H	-4.95396	0.41880	-0.71072
H	3.59795	-2.22397	-5.41735
H	2.31252	-3.50231	-3.78142
H	7.19013	1.19541	-3.26799
H	6.41031	1.91851	-5.46529
H	-1.17080	6.10664	-1.12120
H	7.92298	3.34025	-4.17789
H	4.53634	5.56064	2.64708
H	5.47847	5.54975	0.39402
H	5.34184	3.47342	1.66991
H	1.52291	5.42832	-6.05929
H	0.30690	0.35078	-8.14186
H	-1.70266	-0.93013	-7.60962
H	4.75308	-3.57765	-3.74508
H	1.91742	-2.31833	0.03940
H	0.71829	-3.54163	0.58312
H	0.18132	-2.04298	-0.21168
H	0.94334	-7.13028	5.78546
H	2.65648	-6.81381	5.50792
H	1.74794	-5.83738	6.67118
H	-0.82687	-5.56288	5.01600
H	-0.09285	-4.19759	5.85244
H	-0.45828	-4.08503	4.12800
H	0.27813	-6.91022	3.43278
H	0.79974	-5.55684	2.42969
H	1.97880	-6.75227	3.00068
H	4.37698	-3.32138	7.71555
H	3.79970	-4.84633	7.04262
H	5.09803	-3.95297	6.23715
H	2.17367	-2.22790	7.75457
H	1.08089	-2.27347	6.36940
H	1.46085	-3.75985	7.25680

H	3.90890	-1.13202	6.61568
H	4.61344	-1.67968	5.09669
H	2.97344	-1.02190	5.12253
H	5.63020	-6.08968	3.14549
H	5.07477	-5.77695	4.79006
H	4.04533	-6.66469	3.65713
H	6.06462	-3.73532	2.57653
H	4.90255	-2.45663	2.93319
H	5.71813	-3.31813	4.25210
H	4.61955	-4.95872	1.17684
H	2.98218	-5.44221	1.61335
H	3.35777	-3.73673	1.34429
H	1.84246	0.59852	3.69863
H	0.12262	0.89181	3.40758
H	0.60377	-0.18343	4.75022

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Interconversion : O ax.

C	-1.34218	0.14044	3.19487
W	-0.62792	-1.78969	2.61852
O	-1.71779	-2.47275	3.74873
O	-0.01739	-0.75392	1.03119
Si	-0.07160	0.29307	-0.20601
O	0.45652	1.78875	0.28638
Si	1.30797	3.08526	-0.26922
O	2.16225	3.71424	0.98108
Si	3.71954	4.34606	1.13634
C	-1.53769	-2.97193	1.09100
O	1.02782	-2.32026	3.18368
Si	2.44038	-2.89378	4.02377
C	3.86337	-2.60002	2.71959
C	3.38917	-3.00979	1.31100
O	-1.62962	0.43973	-0.77341
Si	-2.60677	1.57521	-1.47408
O	-4.15323	1.35067	-0.98100

Si	-5.20399	0.03776	-0.85399
O	0.91303	-0.24597	-1.42772
Si	1.03758	-0.27984	-3.07013
O	1.74525	-1.68263	-3.53467
Si	1.22134	-3.05023	-4.37369
O	2.36201	2.63139	-1.46505
Si	2.42343	2.49767	-3.11187
O	3.95902	2.79876	-3.59546
Si	5.10278	1.93748	-4.49057
O	0.26967	4.23955	-0.84180
Si	-1.22785	4.35473	-1.54034
O	-1.92978	5.79264	-1.15738
O	1.41748	3.61418	-3.79841
Si	-0.12767	3.74702	-4.37903
O	-0.17703	4.73498	-5.69267
O	1.99483	0.96894	-3.58521
O	-1.10158	4.35320	-3.18588
O	-0.66538	2.27670	-4.90213
Si	-1.50751	0.97117	-4.33032
O	-2.37754	0.30864	-5.54763
Si	-2.92315	0.85948	-7.04910
O	-2.16584	3.09745	-1.00854
C	2.54634	-1.76001	5.60948
C	2.25027	-0.29168	5.24990
C	2.07516	-4.77335	4.40027
C	3.07963	-5.33118	5.42585
C	3.94423	-1.84499	6.25026
C	1.50233	-2.17778	6.66024
O	-2.52848	1.44760	-3.12219
O	-0.46304	-0.17960	-3.76601
C	0.64743	-4.96095	4.94806
C	2.17059	-5.62355	3.12002
C	4.24844	-1.11212	2.63285
C	5.12395	-3.40391	3.08594

H	-3.56018	2.20117	-6.91269
H	-4.98052	-0.65227	0.45043
H	-4.98428	-0.92270	-1.97475
H	-6.58806	0.58528	-0.90714
H	0.85651	-2.69077	-5.77454
H	0.04841	-3.66591	-3.68640
H	5.47364	0.67992	-3.77909
H	4.56859	1.61532	-5.84560
H	-2.20174	5.87710	-0.23875
H	6.29195	2.82758	-4.60805
H	3.76878	5.01210	2.46860
H	3.99391	5.33910	0.05722
H	4.72654	3.24678	1.08034
H	-0.05863	5.66925	-5.49712
H	-1.78441	0.92986	-8.00930
H	-3.92514	-0.13915	-7.51729
H	2.36813	-4.00168	-4.37300
H	-0.85999	-3.10036	0.24334
H	-1.87454	-3.93565	1.48002
H	-2.41634	-2.40926	0.74569
H	2.88565	-6.40083	5.58563
H	4.11871	-5.23866	5.09295
H	2.99407	-4.84301	6.40152
H	0.45786	-6.03442	5.08716
H	0.49133	-4.47968	5.91453
H	-0.11563	-4.58002	4.26399
H	1.89193	-6.66015	3.35479
H	1.48593	-5.27436	2.34009
H	3.17985	-5.65098	2.70084
H	3.97061	-1.23110	7.16114
H	4.21075	-2.86585	6.54310
H	4.73127	-1.47044	5.58885
H	1.52165	-1.46160	7.49351
H	0.48471	-2.17964	6.25593

H 1.70330 -3.16516 7.08528
H 2.28608 0.31625 6.16436
H 2.96932 0.13447 4.54858
H 1.25127 -0.16995 4.82034
H 5.91771 -3.19622 2.35519
H 5.51893 -3.14030 4.07314
H 4.95047 -4.48396 3.07165
H 4.99213 -0.97983 1.83495
H 3.39162 -0.47866 2.38290
H 4.70009 -0.73604 3.55524
H 4.19836 -2.82049 0.59225
H 3.13008 -4.06743 1.23262
H 2.52403 -2.42245 0.99097
H -0.63356 0.92995 2.93333
H -2.26360 0.29869 2.61488
H -1.59945 0.17135 4.25637
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Interconversion : O-Si trans Silica surface
O -0.25095 -2.16525 2.16871
W 1.39531 -1.79981 1.94004
C 2.14280 -0.06456 2.97674
O 1.21115 -0.54871 0.48859
Si 0.38629 0.45563 -0.50079
O -1.23752 0.27229 -0.25387
Si -2.63874 1.14856 -0.22653
O -3.63333 0.59857 0.94702
Si -4.21232 -0.91092 1.44141
C 2.44368 -2.93461 0.43793
O 2.17827 -2.85309 3.24682
Si 2.57762 -3.89712 4.57613
C 2.51197 -5.70208 3.82459
C 3.73620 -5.99272 2.93811
O 0.75406 0.08305 -2.07221
Si 0.02470 0.07728 -3.55431

O	0.63987	-1.14876	-4.44898
Si	0.01439	-2.59526	-5.05593
O	0.83451	2.01528	-0.17117
Si	1.01786	3.46826	-0.93650
O	2.22976	4.29873	-0.21101
Si	3.77392	4.78514	-0.68914
O	0.34352	1.49915	-4.33783
Si	0.66093	3.08912	-3.99971
O	-0.74100	3.96273	-3.99591
Si	-2.36503	3.76270	-3.73882
O	-3.24015	4.70130	-4.76716
O	-1.60967	-0.13426	-3.39398
Si	-2.99726	0.75962	-3.28643
O	-2.80559	2.20665	-4.06855
O	1.66581	3.69108	-5.14370
Si	2.32032	3.08530	-6.57790
O	1.40619	3.23002	-2.53013
C	4.37337	-3.33641	5.10850
C	5.05679	-4.40087	5.98602
C	1.20166	-3.56079	5.92365
C	-0.13887	-4.21111	5.53380
C	5.23988	-3.08463	3.85866
C	4.34711	-2.01543	5.89794
C	0.92492	-2.05200	6.06188
C	1.63026	-4.11338	7.29531
C	2.47516	-6.75941	4.94392
C	1.26361	-5.88230	2.93948
O	-0.36857	4.35667	-0.80462
Si	-2.00879	4.15528	-0.68076
O	-2.71220	4.17188	-2.17314
O	-3.38368	1.02288	-1.70174
O	-2.31498	2.73395	0.10882
O	-4.19716	-0.09017	-4.00530
Si	-5.53067	0.31846	-4.95890

O	-2.67696	5.42135	0.12972
H	-3.74597	-1.15563	2.83432
H	-3.72857	-1.98476	0.52768
H	-5.70255	-0.84886	1.40988
H	-1.04176	-2.31453	-6.07109
H	-0.55061	-3.42287	-3.95057
H	3.20069	1.91609	-6.29032
H	1.23286	2.68342	-7.51680
H	-2.44582	5.47171	1.06191
H	3.12070	4.19482	-7.16816
H	4.40851	5.39328	0.51419
H	3.68303	5.79430	-1.78371
H	4.57191	3.61046	-1.14772
H	-3.20097	5.64432	-4.58196
H	-5.08137	0.66681	-6.33748
H	-6.27047	1.46592	-4.35814
H	-6.40111	-0.89044	-4.99562
H	1.15860	-3.30606	-5.69283
H	2.62101	-3.97238	0.72870
H	1.91254	-2.90603	-0.51702
H	3.41537	-2.44078	0.29219
H	2.47926	-7.76389	4.49838
H	3.34111	-6.70065	5.61136
H	1.57232	-6.68648	5.55691
H	1.27371	-6.89252	2.50708
H	0.32778	-5.77546	3.48984
H	1.23991	-5.17262	2.10851
H	3.62031	-6.98312	2.47648
H	3.84561	-5.26715	2.12638
H	4.67168	-6.01190	3.50364
H	0.82494	-3.94762	8.02425
H	1.82749	-5.18982	7.27403
H	2.52271	-3.61652	7.68714
H	-0.90145	-3.92784	6.27288

H -0.49359 -3.87102 4.55569

H -0.09547 -5.30371 5.52809

H 0.16487 -1.89813 6.84047

H 1.80448 -1.47407 6.35249

H 0.52536 -1.62918 5.13612

H 6.04823 -4.04228 6.29566

H 4.49309 -4.61663 6.89961

H 5.21035 -5.34556 5.45645

H 5.37862 -1.70741 6.11886

H 3.88343 -1.20284 5.33001

H 3.82893 -2.10295 6.85694

H 6.22839 -2.71950 4.17032

H 5.40256 -3.98178 3.25835

H 4.79844 -2.32265 3.20928

H 3.18075 0.07507 2.64052

H 1.58489 0.83702 2.71260

H 2.14334 -0.19347 4.06160

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Interconversion : O-Si trans Silica surface TS

O -1.86423 -0.30323 3.42224

W -0.22315 -0.11712 3.06607

C 0.10612 1.24535 4.73128

O 0.11565 1.07796 1.68591

Si -0.40788 2.02320 0.41159

O -1.98957 1.66304 0.14011

Si -3.37352 2.42293 -0.38507

O -4.67035 1.80405 0.38448

Si -5.36996 0.27440 0.57740

C -0.18750 -1.94331 1.86981

O 1.14920 -1.08728 4.03027

Si 2.28142 -2.11282 4.79580

C 1.48076 -3.91100 4.87979

C 1.56656 -4.65171 3.53219

O 0.52855 1.63204 -0.88303

Si	0.39104	1.56294	-2.53725
O	1.39338	0.40740	-3.10917
Si	1.24247	-1.21333	-3.56762
O	-0.21094	3.59327	0.85359
Si	0.11847	5.06526	0.15574
O	0.91726	5.99358	1.23689
Si	2.52903	6.45033	1.46740
O	0.84980	3.00788	-3.19080
Si	0.90523	4.62283	-2.82099
O	-0.47125	5.37037	-3.34460
Si	-2.05917	5.03055	-3.66927
O	-2.58712	5.87315	-4.97737
O	-1.17392	1.20633	-2.93780
Si	-2.57541	1.97974	-3.36204
O	-2.22308	3.43621	-4.06290
O	2.20502	5.30237	-3.54259
Si	3.29220	4.82572	-4.74604
O	1.05742	4.82786	-1.18633
C	3.88948	-2.04949	3.66686
C	4.86583	-3.19313	3.99599
C	2.62808	-1.41253	6.60539
C	1.40407	-1.63699	7.51393
C	3.51311	-2.14257	2.17783
C	4.64246	-0.71903	3.84248
C	2.90440	0.10239	6.61744
C	3.84787	-2.09437	7.25579
C	2.16680	-4.81445	5.92199
C	-0.01234	-3.80134	5.24706
O	-1.29357	5.82231	-0.23600
Si	-2.84772	5.47556	-0.69915
O	-2.96939	5.42052	-2.34314
O	-3.51302	2.20636	-2.01914
O	-3.28568	4.02976	-0.02079
O	-3.38251	1.03660	-4.42486

Si	-4.08585	1.28289	-5.94336
O	-3.86676	6.67343	-0.22334
H	-5.63293	0.08142	2.02918
H	-4.45155	-0.78212	0.06294
H	-6.64939	0.25321	-0.18775
H	0.48539	-1.30547	-4.84889
H	0.54189	-1.98835	-2.50319
H	4.17142	3.73577	-4.23362
H	2.55357	4.35952	-5.95521
H	-3.98743	6.75407	0.72750
H	4.10390	6.03136	-5.07146
H	2.58932	7.09662	2.80754
H	2.93676	7.41739	0.40835
H	3.41501	5.25058	1.43128
H	-2.72653	6.81262	-4.82528
H	-3.02868	1.58294	-6.95136
H	-5.06774	2.40320	-5.88160
H	-4.77659	0.00879	-6.28713
H	2.62944	-1.72331	-3.75062
H	-0.58009	-2.81348	2.39840
H	-0.86887	-1.73103	1.03081
H	0.80745	-2.17483	1.48391
H	1.71876	-5.81770	5.88352
H	3.23862	-4.93556	5.73348
H	2.04302	-4.45209	6.94576
H	-0.46213	-4.80458	5.25319
H	-0.17573	-3.36902	6.23664
H	-0.57094	-3.19614	4.52889
H	1.02937	-5.60798	3.61136
H	1.11182	-4.09390	2.71200
H	2.59546	-4.89140	3.24953
H	3.95331	-1.73743	8.29034
H	3.76912	-3.18348	7.29852
H	4.78041	-1.84449	6.74021

H 1.57171 -1.14484 8.48255

H 0.48982 -1.21098 7.08733

H 1.21748 -2.69348 7.72394

H 3.10060 0.41919 7.65200

H 3.77541 0.38844 6.02556

H 2.05102 0.67703 6.26044

H 5.76882 -3.09798 3.37599

H 5.19091 -3.18239 5.04039

H 4.44032 -4.17915 3.79017

H 5.45402 -0.65744 3.10312

H 3.99333 0.14934 3.68582

H 5.10486 -0.62648 4.82889

H 4.42697 -2.10474 1.56755

H 2.99231 -3.06866 1.92430

H 2.88304 -1.30255 1.87032

H 1.12748 1.63787 4.70316

H -0.60528 2.07179 4.58184

H -0.08073 0.80401 5.71234

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Interconversion : O-Si cis Silica surface

O -2.43737 -2.42948 1.88356

W -0.80354 -2.55683 2.41050

C -1.49952 -2.07943 4.36125

O 0.01249 -1.25573 1.32222

Si -0.26237 -0.10636 0.16364

O -1.84355 -0.11091 -0.28931

Si -3.04101 0.93493 -0.75687

O -4.47999 0.46692 -0.14954

Si -5.41245 -0.94650 -0.16176

C -0.85590 -4.58888 1.79017

O 0.85138 -3.03626 3.29535

Si 2.38184 -3.38284 3.97380

C 2.22487 -5.13524 4.83864

C 2.20162 -6.28018 3.81003

O	0.70212	-0.47379	-1.12621
Si	0.67218	-0.30689	-2.77409
O	1.49325	-1.54678	-3.45706
Si	1.05325	-3.04681	-4.09820
O	0.16244	1.35007	0.81245
Si	0.79295	2.80649	0.34274
O	1.65822	3.41977	1.58937
Si	3.23630	3.99851	1.75835
O	1.42498	1.09934	-3.20323
Si	1.72848	2.61813	-2.61545
O	0.54694	3.66042	-3.11173
Si	-1.04563	3.65972	-3.56662
O	-1.31236	4.74717	-4.77051
O	-0.89367	-0.31596	-3.30963
Si	-2.10208	0.74141	-3.71001
O	-1.45529	2.18780	-4.19088
O	3.17944	3.13261	-3.17001
Si	4.21204	2.64343	-4.41485
O	1.79178	2.59880	-0.96290
C	3.61903	-3.37900	2.45291
C	4.96313	-4.04098	2.80397
C	2.74945	-1.94012	5.25240
C	1.95760	-2.11129	6.56123
C	2.99604	-4.12717	1.25979
C	3.89671	-1.94604	1.96373
C	2.32595	-0.58463	4.65364
C	4.24365	-1.87026	5.61805
C	3.38761	-5.40266	5.81047
C	0.89651	-5.21421	5.61443
O	-0.42909	3.85507	-0.02522
Si	-1.97942	3.85692	-0.61255
O	-1.97591	4.04154	-2.25214
O	-3.10038	0.96949	-2.41254
O	-2.71754	2.44454	-0.16866

O	-2.95690	0.09038	-4.94326
Si	-3.62418	0.69050	-6.37543
O	-2.81075	5.14986	-0.02813
H	-5.72674	-1.30147	1.24850
H	-4.68115	-2.05178	-0.84283
H	-6.67221	-0.64180	-0.90154
H	0.48671	-2.86565	-5.46560
H	0.05161	-3.71523	-3.21705
H	4.85411	1.34398	-4.06374
H	3.45698	2.50887	-5.69444
H	-3.04192	5.09467	0.90383
H	5.24618	3.70863	-4.53876
H	3.34588	4.49826	3.15751
H	3.48676	5.10981	0.79537
H	4.21596	2.89741	1.52920
H	-1.30570	5.66731	-4.49052
H	-2.54109	0.97210	-7.36108
H	-4.40539	1.93195	-6.10593
H	-4.52164	-0.37986	-6.89378
H	2.30159	-3.85697	-4.16416
H	-1.28635	-5.13814	2.64136
H	-1.51323	-4.72638	0.92928
H	0.14405	-4.97899	1.59464
H	3.27469	-6.39995	6.25881
H	4.36195	-5.38278	5.31135
H	3.42059	-4.68410	6.63421
H	0.78802	-6.21490	6.05623
H	0.83321	-4.49138	6.43036
H	0.03837	-5.05060	4.95536
H	2.04015	-7.23450	4.33163
H	1.38951	-6.16894	3.08502
H	3.14089	-6.37419	3.25796
H	4.40618	-1.07100	6.35515
H	4.61023	-2.79959	6.06605

H	4.87739	-1.64134	4.75645
H	2.12140	-1.23286	7.20140
H	0.87948	-2.18977	6.39144
H	2.27172	-2.98615	7.13707
H	2.49940	0.21039	5.39279
H	2.88493	-0.31859	3.75481
H	1.26341	-0.56586	4.39572
H	5.63982	-3.98686	1.93932
H	5.47042	-3.54903	3.63997
H	4.85373	-5.09977	3.05713
H	4.50496	-1.98543	1.04888
H	2.97337	-1.41293	1.71731
H	4.45515	-1.35026	2.69106
H	3.69781	-4.10964	0.41397
H	2.77533	-5.17544	1.47348
H	2.07420	-3.64323	0.92551
H	-0.70776	-1.68126	4.99707
H	-2.35966	-1.40782	4.32707
H	-1.83145	-3.04170	4.78084