Supplementary Information (SI) for Environmental Science: Advances.

Aqueous Solution Degradation Pathways of Trimethylsiloxane Surfactants

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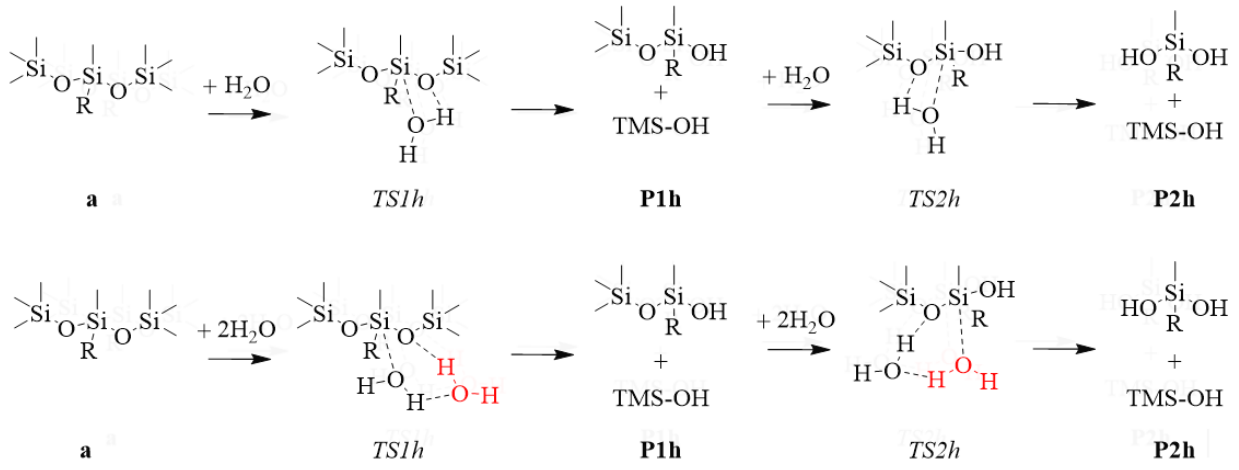


Figure S1. Pathways of the neutral hydrolysis of TriSil-1n (**a**) via attack by one water molecule (top) or with an assisting water molecule (bottom). The assisting water is shown in red. *TS* and **P** refer to the transition state and product complex, respectively.

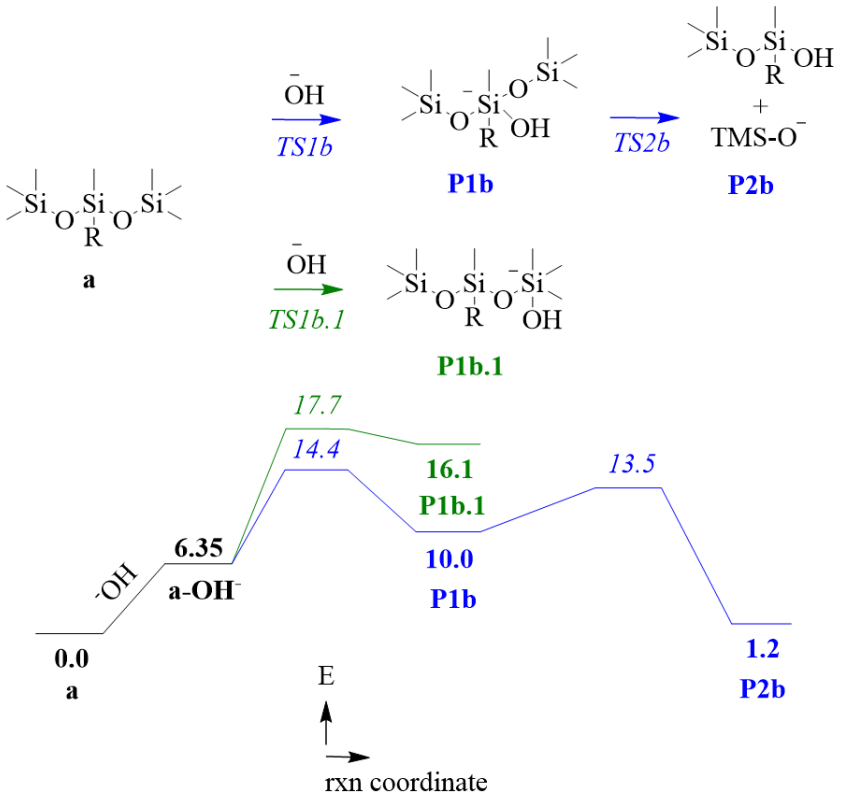


Figure S2. Potential energy surfaces for the hydrolysis reactions of TriSil-1n in basic pH conditions, computed at the ωb97X-D/6-311+G(2d,2p) level of theory. All energies are presented in kcal/mol and are normalized to TriSil-1n (a). Transition state energy barriers are in italics and product reaction free energies are in bold.

Table S1. Partial atomic charges for TriSil-1n (neutral, reactant complex) and in basic conditions, where the hydroxyl radical is either attacking the central silicon (Si-46) or terminal silicon (Si-6 or Si-7) atom (transition state complex). All values are presented in a.u. and all optimization and NBO calculations were performed at the ωb97X-D/6-311+G(2d,2p) level of theory in the gas phase.

Atom label	**TriSil-1n**		
	Neutral	**OH attack at the central Si**	**OH attack at the terminal Si**
Si-6 (terminal)	1.91	1.94	1.94
Si-7 (terminal)	1.90	1.92	1.91
Si-46 (central)	2.18	2.20	2.20

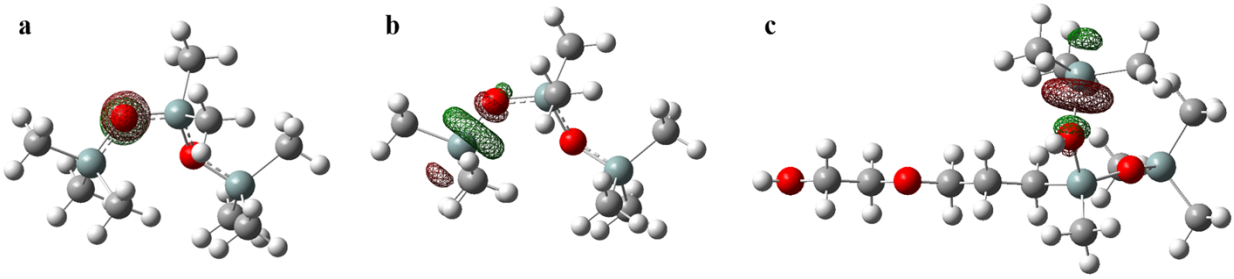


Figure S3. a) Highest occupied molecular orbital (HOMO) of PDMS and lowest unoccupied molecular orbital (LUMO) of b) PDMS and c) protonated TriSil-1n. Oxygen atoms are red, silicon atoms are pale blue, carbon atoms are gray, and hydrogen atoms are white. NBO analyses were computed at the ωb97X-D/6-311+G(2d,2p) level of theory with SMD water solvation. The molecular orbital isovalue is 0.1 a.u..

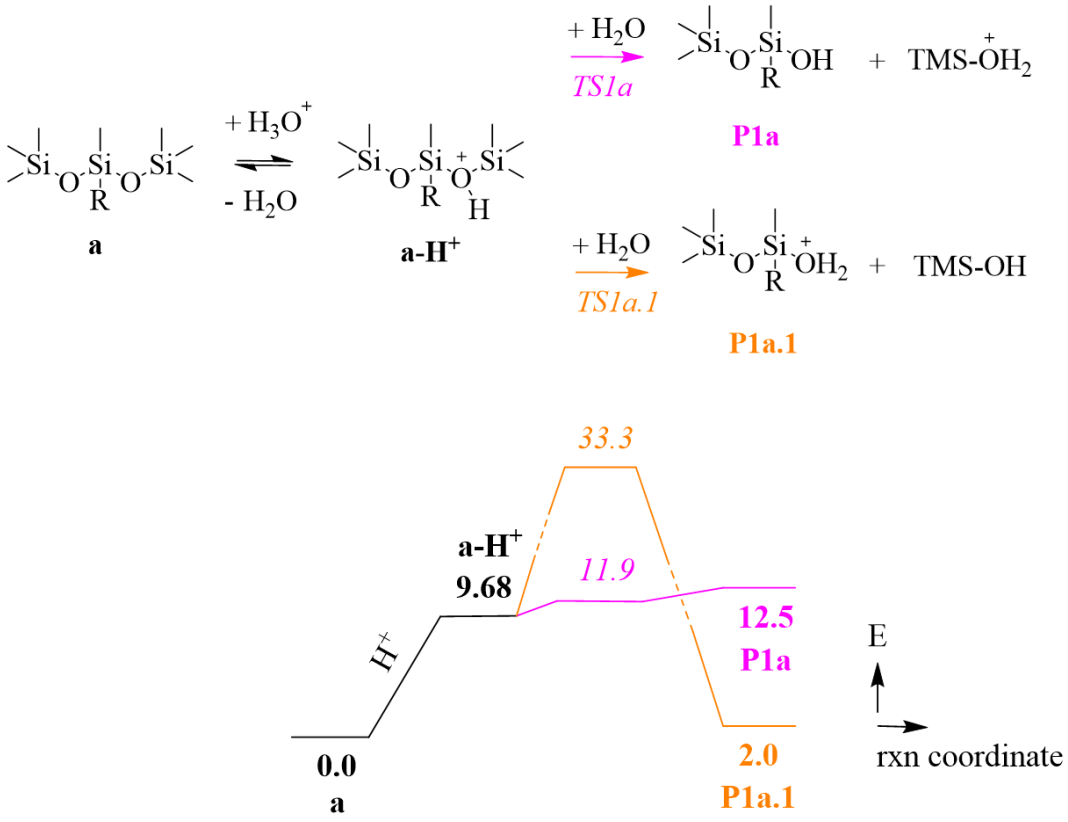


Figure S4. Potential energy surfaces for the hydrolysis reactions of TriSil-1n in acidic pH conditions, computed at the ωb97X-D/6-311+G(2d,2p) level of theory. All energies are presented in kcal/mol and are normalized to TriSil-1n (a). Transition state energy barriers are in italics and product reaction free energies are in bold.

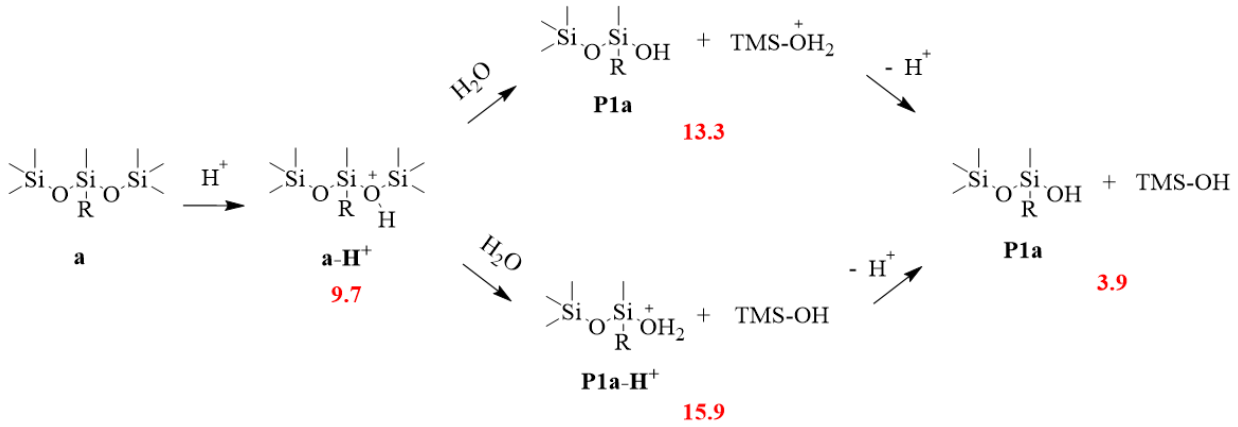


Figure S5. Pathways of the hydrolysis of TriSil-1n (**a**) in acidic pH conditions. Reaction energies (shown in red) are presented in kcal/mol and are normalized to the first reaction.

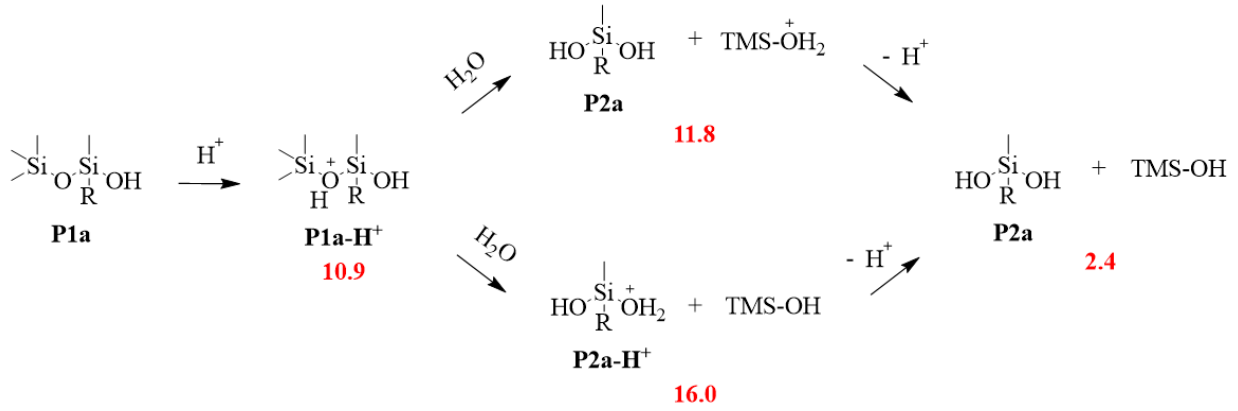


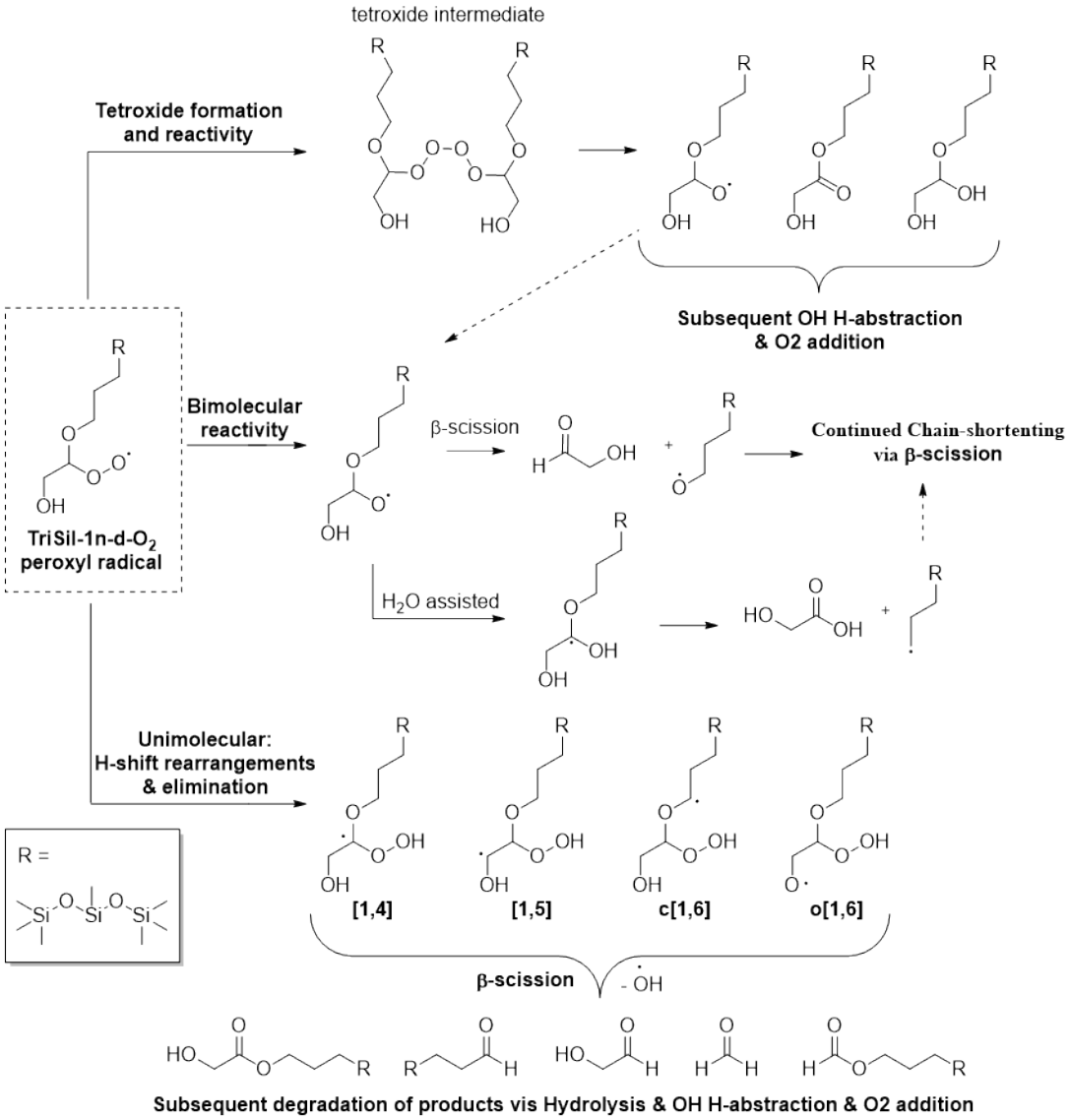
Figure S6. Proposed hydrolysis mechanism of TriSil-1n degradation product **P1a** in acidic pH conditions. Reaction energies (shown in red) are presented in kcal/mol and are normalized to the first reaction.

Table S2. Transition state energy barriers, product free energies, reaction free energies, and bond dissociation energies (BDEs) for the H-atom abstractions of TriSil-1n via hydroxyl radical at positions a-g (refer to **Figure 1** for atom labels). Calculations were performed at the ωb97X-D/6-311+G(2d,2p) level of theory in the gas phase. The * indicates the reactant and product calculations were performed in the solution phase (implicit SMD water solvation).

Radical	Transition state energy barrier (kcal/mol)	Product free energy (kcal/mol)	Reaction free energy (kcal/mol)	Reaction free energy* (kcal/mol)	BDE (kcal/mol)	BDE* (kcal/mol)
a	6.41	-17.5	-21.6	-23.7	88.0	89.8
b	6.38	-18.8	-21.9	-24.4	87.7	89.1
c	5.36	-19.9	-23.9	-26.7	85.7	86.7
d	4.84	-22.1	-24.0	-27.6	85.6	85.8
e	5.35	-20.0	-22.7	-25.9	86.9	87.5
f	7.51	-11.9	-15.5	-17.1	94.1	96.3
g	9.23	-12.4	-15.8	-18.4	93.8	95.0

Table S3. Reaction free energies for the addition of O_2 to TriSil-1n radicals (a-e) (refer to **Figure 1** for atom labels). Calculations were performed at the ωb97X-D/6-311+G(2d,2p) level of theory in the solution phase (implicit SMD water solvation).

Radical	Reaction free energy (kcal/mol)
a	-20.5
b	-22.2
c	-27.7
d	-23.1
e	-26.0



Scheme S1. Proposed reaction diagram for reaction channels leading to degradation of TriSil-1n-d-O_2 peroxyl radical. Similar reactions are expected for peroxyl radicals at all positions along the PEG chain (a-f).

i) $a_{(aq)} \rightarrow a^{+}_{(aq)} + e^{-}_{(aq)}$

ii) $a_{(aq)} + e^{-}_{(aq)} \rightarrow a^{-}_{(aq)}$

Scheme S2. Half reaction for the i) oxidation and ii) reduction of TriSil-1n (**a**).

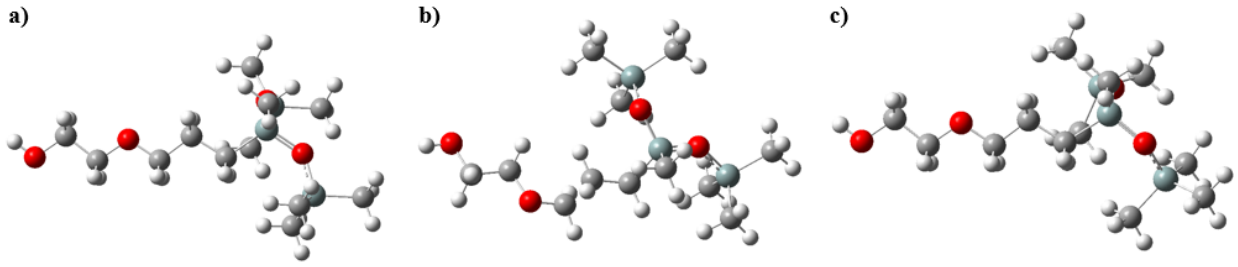


Figure S7. Structures of a) neutral b) oxidized and c) reduced TriSil-1n at ωb97X-D/6-311+G(2d,2p) level of theory. Oxygen atoms are red, silicon atoms are pale blue, carbon atoms are gray, and hydrogen atoms are white.

Table S4. Selected bond lengths within oxidized, neutral, and reduced PEG-3n, PDMS, and TriSil-1n molecules performed at various levels of theory (ωb97X-D, M062X, and B3LYP) with the 6-311+G(2d,2p) basis set and SMD water solvation. Refer to **Figure 1** for atom labels. The change in bond lengths between the oxidized and reduced structures compared to that of the neutral molecule is shown in parentheses, where a positive reflects an increase in bond length and a negative value reflects a decrease in bond length. Changes of 0.004 Å or less were rounded to 0 Å.

Level of Theory	**Molecule**	**Bond**	**Bond Length (Å)**		
			Oxidized	**Neutral**	**Reduced**
ωB97X-D	PEG-3n	C_a-C_b	1.77 **(+0.26)**	1.51	1.51 **(0)**
		C_a-O	1.33 **(-0.09)**	1.41	1.42 **(0)**
		C_b-O	1.33 **(-0.09)**	1.41	1.42 **(0)**
	PDMS	Si_1-O_1	1.59 **(-0.06)**	1.65	1.65 **(0)**
		Si_2-O_2	1.70 **(+0.04)**	1.66	1.67 **(0)**
		Si_1-C_a	2.16 **(+0.31)**	1.86	1.86 **(0)**
	TriSil-1n	Si_1-O_1	1.62 **(-0.03)**	1.65	1.65 **(0)**
		Si_2-O	1.68 **(+0.02)**	1.66	1.66 **(0)**
		Si_1-C_a	1.96 **(+0.10)**	1.87	1.87 **(0)**
		C_a-C_b	1.46 **(-0.07)**	1.53	1.53 **(0)**
		C_b-C_c	1.69 **(+0.18)**	1.51	1.51 **(0)**
		C_c-O	1.35 **(-0.07)**	1.42	1.42 **(0)**
		O-C_d	1.43 **(+0.02)**	1.41	1.41 **(0)**
		C_d-C_e	1.51 **(0)**	1.51	1.51 **(0)**
M062-X	PEG-3n	C_a-C_b	1.77 **(+0.26)**	1.51	1.51 **(0)**
		C_a-O	1.33 **(-0.09)**	1.42	1.42 **(0)**
		C_b-O	1.33 **(-0.09)**	1.42	1.42 **(0)**

	PDMS	Si_1-O_1	1.59 **(-0.06)**	1.65	1.65 **(0)**
		Si_2-O_2	1.71 **(+0.04)**	1.67	1.66 **(0)**
		Si_1-C_a	2.20 **(+0.34)**	1.86	1.86 **(0)**
	TriSil-1n	Si_1-O_1	1.65 **(0)**	1.65	1.65 **(0)**
		Si_2-O	1.67 **(0)**	1.67	1.66 **(0)**
		Si_1-C_a	1.87 **(0)**	1.87	1.87 **(0)**
		C_a-C_b	1.53 **(0)**	1.53	1.53 **(0)**
		C_b-C_c	1.51 **(0)**	1.51	1.51 **(0)**
		C_c-O	1.44 **(+0.02)**	1.42	1.42 **(0)**
		O-C_d	1.32 **(-0.09)**	1.41	1.41 **(0)**
		C_d-C_e	1.78 **(+0.27)**	1.51	1.51 **(0)**
B3LYP	PEG-3n	C_a-C_b	1.73 **(+0.22)**	1.52	1.51 **(0)**
		C_a-O	1.35 **(-0.08)**	1.42	1.43 **(0)**
		C_b-O	1.35 **(-0.08)**	1.42	1.43 **(0)**
	PDMS	Si_1-O_1	1.60 **(-0.05)**	1.65	1.65 **(0)**
		Si_2-O_2	1.71 **(+0.04)**	1.67	1.67 **(0)**
		Si_1-C_a	2.10 **(+0.24)**	1.87	1.87 **(0)**
	TriSil-1n	Si_1-O_1	1.62 **(-0.03)**	1.65	1.65 **(0)**
		Si_2-O	1.69 **(+0.02)**	1.67	1.67 **(0)**
		Si_1-C_a	2.01 **(+0.13)**	1.88	1.88 **(0)**
		C_a-C_b	1.47 **(-0.06)**	1.54	1.54 **(0)**
		C_b-C_c	1.63 **(+0.11)**	1.52	1.52 **(0)**
		C_c-O	1.39 **(-0.05)**	1.43	1.43 **(0)**
		O-C_d	1.43 **(+0.01)**	1.42	1.42 **(0)**
		C_d-C_e	1.51 **(0)**	1.52	1.52 **(0)**

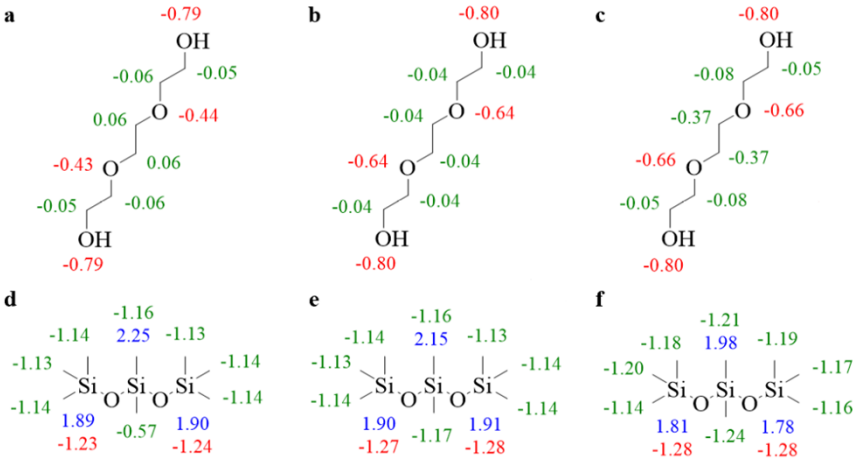


Figure S8. Partial atomic charges for a) oxidized b) neutral and c) reduced PEG-3n and d) oxidized e) neutral and f) reduced PDMS, where green represents carbon, red represents oxygen, and blue represents silicon. All values are presented in a.u. and were computed at the ωb97X-D/6-311+G(2d,2p) level of theory.

Table S5. Reaction free energies (kcal/mol) for the oxidation of TriSil-1n, PDMS, and PEG (1n-8n). All values were computed at the ωb97X-D/6-311+G(2d,2p) level of theory with SMD implicit water solvation. Reaction energies were calculated using a hydroxyl radical as the oxidant and hydroxide anion as a product. The * indicates the Gibbs free energies of the methyl radical and PDMS cationic fragments (separately calculated) were substituted for the oxidized PDMS product (containing both fragments) in the calculation. Values with ** correspond to neutral molecules with one imaginary frequency.

Molecule	**Reaction Energy (kcal/mol)**
TriSil-1n	24.6
PDMS	32.2/38.9*
PEG-1n	26.1
PEG-2n	24.7
PEG-3n	24.4
PEG-4n	31.5**
PEG-5n	22.6**
PEG-6n	34.4
PEG-7n	23.5**
PEG-8n	32.6

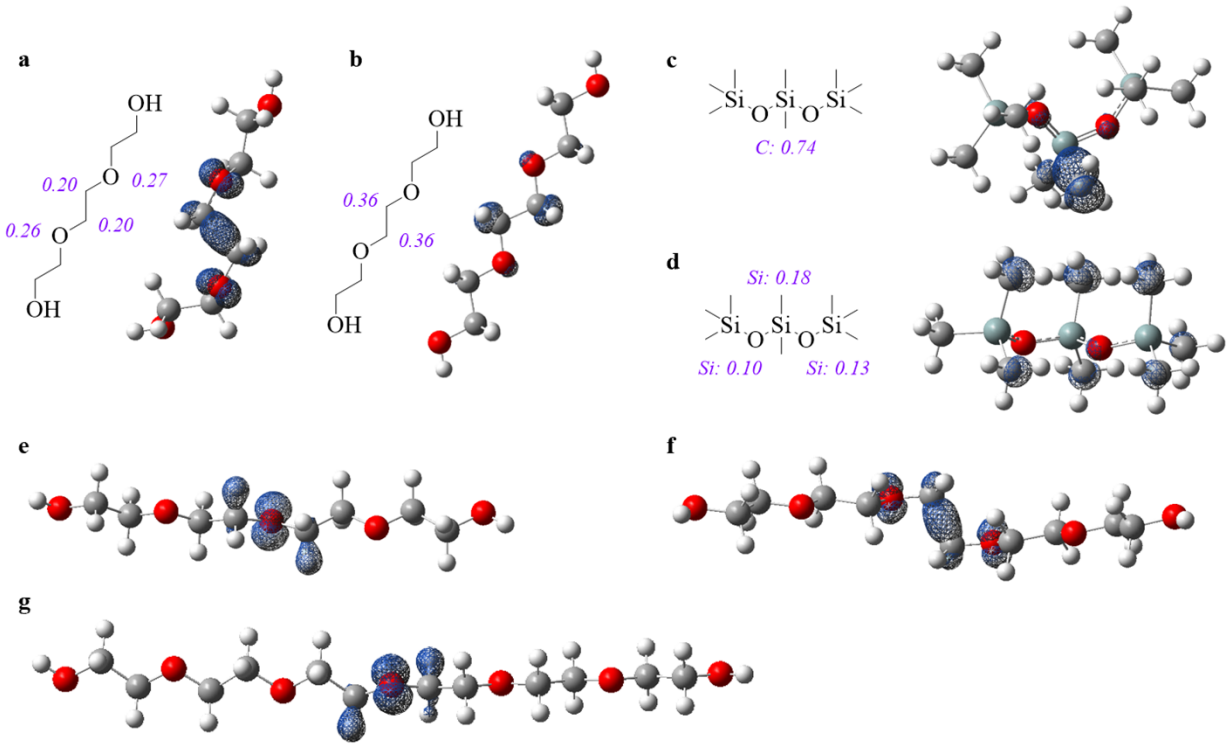


Figure S9. Chemical structures (left) and NBO spin density isosurfaces (right) for a) oxidized and b) reduced PEG-3n and c) oxidized and d) reduced PDMS. NBO spin density isosurfaces of oxidized e) PEG-4n f) PEG-5n and g) PEG-6n. Computations performed at the ωb97X-D/6-311+G(2d,2p) level of theory with SMD implicit water solvation. Oxygen atoms are red, silicon atoms are pale blue, carbon atoms are gray, and hydrogen atoms are white. The isovalue for the spin density surfaces is 0.01 a.u. for all plots except for reduced PEG-3n (isovalue = 0.003 a.u.) and reduced PDMS (isovalue = 0.001 a.u.). In the chemical structures, only spin densities greater than 0.10 a. u. are reported.

Table S6. Standard reduction potentials (Volts) of TriSil-1n, PDMS, and PEG-1n at different positions and reaction free energies (kcal/mol), computed at the ωb97X-D/6-311+G(2d,2p) level of theory with SMD water solvation. Refer to **Figure 1** in-text for atomic positions for TriSil-1n and below for PDMS and PEG-1n. Standard reduction potentials were calculated using the methods provided by Van Hoomissen et al. (SHE = 4.44 V) where position 0 refers to reduced molecule (TriSil-1n, PDMS, or PEG) in which no bonds were altered before optimization.[48] Reaction energies of the parent molecule were calculated using a solvated electron as the reductant. Values with * correspond to neutral molecules with one imaginary frequency. Reaction energies for PEG-1n (positions a and b) were calculated using the PEG radical and hydrogen anion as products.

Molecule	Position	$E^{o}_{s,com.}$ (Volts)	$E^{o}_{s,sep.}$ (Volts)	Reaction Energy (kcal/mol)
TriSil-1n	0	-4.30	-	22.2
	a	-4.35	-4.13	23.3
	b	-4.20	-4.07	20.0
	c	-4.18	-4.02	19.5
	d	-4.11	-3.98	17.9
	e	-4.12	-3.92	18.1
	f	-3.89	-4.38	12.8
	g	-4.55	-4.30	27.9
PDMS	0	-4.47	-	26.0
	a	-4.58	-4.36	28.6
	b	-4.57	-4.33	28.3
	c	-4.52	-4.32	27.3
PEG-1n	0	-4.70	-	31.4
	a	-	-4.42	24.9
	b	-4.23	-3.97	14.6
PEG-2n	0	-3.95	-	14.1
PEG-3n	0	-4.82	-	34.2
PEG-4n	0	-4.55*	-	28.0*
PEG-5n	0	-4.56*	-	28.2*
PEG-6n	0	-4.57	-	28.3
PEG-7n	0	-3.97*	-	14.6*
PEG-8n	0	-3.94	-	13.8

Optimized coordinates for all species presented in the manuscript

TriSil-1n-neutral-B3LYP.log Energy: -1033243.6834284

C	-0.51128	-0.76511	0.00574
H	-0.48294	-1.85670	0.08720
H	-0.39552	-0.53842	-1.05814
O	2.36469	-0.60861	0.16162
O	0.98513	1.56237	0.85484
Si	3.09664	-2.00285	-0.39614
Si	1.36039	2.78344	-0.22402
C	2.92826	-3.36446	0.88067
H	1.88322	-3.63108	1.04957
H	3.44841	-4.26406	0.54303
H	3.36184	-3.06828	1.83767
C	4.89748	-1.57525	-0.67020
H	5.44729	-2.43714	-1.05444
H	5.00285	-0.76262	-1.39177
H	5.37362	-1.26237	0.26121
C	2.29235	-2.51891	-2.00762
H	1.24413	-2.78668	-1.86443
H	2.33850	-1.71561	-2.74557
H	2.80366	-3.38801	-2.42822
C	0.49782	4.31911	0.40873
H	0.82998	4.56707	1.41894
H	0.71096	5.17673	-0.23305
H	-0.58491	4.18101	0.43435
C	0.74394	2.34202	-1.93831
H	-0.33367	2.16822	-1.94074
H	0.95072	3.15901	-2.63379
H	1.23395	1.44673	-2.32490
C	3.21627	3.03641	-0.24149
H	3.59033	3.26049	0.75960
H	3.73545	2.14786	-0.60433
H	3.48504	3.87116	-0.89295
C	-1.86601	-0.24272	0.50748
H	-1.99236	-0.46947	1.56867
H	-1.90940	0.84376	0.40724
C	-3.02582	-0.84912	-0.26210
H	-2.93595	-0.62479	-1.33063
H	-3.03719	-1.93858	-0.14708

C	-5.39171	-0.81893	-0.45831
H	-5.44427	-1.90728	-0.34802
H	-5.32144	-0.58626	-1.52616
C	-6.62798	-0.17444	0.13475
H	-6.70175	-0.41466	1.19767
H	-6.57174	0.91087	0.02526
O	-4.25665	-0.30817	0.23163
O	-7.76346	-0.69062	-0.57505
Si	0.98604	-0.08869	0.91057
C	1.00557	-0.57247	2.71077
H	0.15368	-0.14273	3.24093
H	0.96213	-1.65643	2.82892
H	1.91649	-0.21607	3.19559
H	-8.55523	-0.28881	-0.20231

TriSil-1n-neutral-M062X.log Energy: -1032943.9563920

C	-0.30061	-0.87296	0.14600
H	-0.25629	-1.95089	0.33418
H	-0.17781	-0.74113	-0.93196
O	2.53267	-0.35082	0.20850
O	0.91549	1.57740	1.02713
Si	3.16362	-1.73571	-0.47343
Si	0.94822	2.68421	-0.22107
C	2.88273	-3.16885	0.68667
H	1.81769	-3.35047	0.84590
H	3.31678	-4.07949	0.26868
H	3.34915	-2.98625	1.65626
C	4.97972	-1.42013	-0.72064
H	5.46250	-2.28541	-1.17806
H	5.13618	-0.56035	-1.37442
H	5.47312	-1.21919	0.23156
C	2.32466	-2.05100	-2.10784
H	1.27300	-2.30825	-1.97441
H	2.38523	-1.17270	-2.75301
H	2.81063	-2.88146	-2.62433
C	-0.22787	4.04802	0.24550
H	0.07013	4.51324	1.18652
H	-0.24696	4.82172	-0.52391
H	-1.24123	3.65981	0.36230
C	0.40818	1.86465	-1.80863

H	-0.61225	1.48347	-1.73563
H	0.43876	2.59291	-2.62202
H	1.06891	1.03697	-2.07544
C	2.68804	3.32610	-0.39376
H	3.03077	3.77813	0.53842
H	3.37299	2.51661	-0.65231
H	2.74461	4.08265	-1.17852
C	-1.65919	-0.31816	0.58556
H	-1.81129	-0.47913	1.65574
H	-1.69667	0.76090	0.41475
C	-2.79275	-0.96971	-0.17649
H	-2.67259	-0.79738	-1.25230
H	-2.79779	-2.05206	-0.00623
C	-5.12688	-0.97547	-0.43964
H	-5.16356	-2.05869	-0.28357
H	-5.03254	-0.78515	-1.51390
C	-6.38691	-0.33286	0.09176
H	-6.47983	-0.53258	1.16118
H	-6.34206	0.74756	-0.06057
O	-4.02860	-0.41724	0.25459
O	-7.47960	-0.89817	-0.62374
Si	1.12897	-0.05546	1.02303
C	1.26330	-0.60687	2.78654
H	0.37373	-0.31589	3.34772
H	1.36277	-1.69153	2.84768
H	2.13210	-0.15492	3.26756
H	-8.29360	-0.51965	-0.27929

TriSil-1n-neutral-wB97XD.log Energy: -1033051.4127575

C	-0.38061	-0.82014	0.17989
H	-0.36710	-1.90319	0.33991
H	-0.23472	-0.66574	-0.89186
O	2.48376	-0.51994	0.39005
O	0.98301	1.56721	1.02537
Si	3.02987	-1.83060	-0.47777
Si	1.21680	2.63334	-0.23685
C	2.52291	-3.39434	0.40345
H	1.43592	-3.47748	0.46804
H	2.89418	-4.27245	-0.12987
H	2.92791	-3.41943	1.41715

C	4.88299	-1.67231	-0.54776
H	5.31982	-2.49828	-1.11330
H	5.17385	-0.73920	-1.03485
H	5.31559	-1.68241	0.45456
C	2.31036	-1.77884	-2.19680
H	1.22679	-1.90627	-2.18370
H	2.53825	-0.82912	-2.68510
H	2.73547	-2.58005	-2.80623
C	0.33332	4.20225	0.23532
H	0.72576	4.60671	1.17053
H	0.45711	4.96229	-0.53917
H	-0.73594	4.02248	0.36435
C	0.50411	1.92525	-1.80967
H	-0.55585	1.68919	-1.69642
H	0.60316	2.65310	-2.61866
H	1.02874	1.01674	-2.11259
C	3.04511	2.92940	-0.44473
H	3.49111	3.30065	0.48012
H	3.55759	2.00667	-0.72359
H	3.22772	3.66856	-1.22811
C	-1.73430	-0.24538	0.60396
H	-1.90427	-0.41306	1.67042
H	-1.74916	0.83521	0.44295
C	-2.86886	-0.87007	-0.17881
H	-2.72929	-0.69393	-1.25224
H	-2.89335	-1.95434	-0.01745
C	-5.20276	-0.83216	-0.46748
H	-5.26021	-1.91685	-0.32232
H	-5.09737	-0.63577	-1.54050
C	-6.45646	-0.17209	0.06031
H	-6.56036	-0.37749	1.12863
H	-6.39262	0.90975	-0.08184
O	-4.10032	-0.30050	0.23861
O	-7.55797	-0.70909	-0.66321
Si	1.06432	-0.07622	1.09709
C	1.06918	-0.57354	2.88189
H	0.15206	-0.25625	3.38168
H	1.14318	-1.65996	2.96694
H	1.91631	-0.13207	3.40987
H	-8.36201	-0.31870	-0.31602

TriSil-1n-oxidized-B3LYP.log Energy: -1033094.9447460

C	-0.46544	-1.22827	-0.25671
H	-0.03178	-2.22737	-0.23444
H	-0.34825	-0.76122	-1.23442
O	2.24625	-0.38299	0.00177
O	0.37605	1.36255	0.77899
Si	3.53545	-1.41538	-0.35655
Si	0.64410	2.77223	-0.12069
C	3.95077	-2.41823	1.16408
H	3.12779	-3.07478	1.45094
H	4.82355	-3.04543	0.96815
H	4.18653	-1.77402	2.01285
C	4.94366	-0.29247	-0.84663
H	5.82348	-0.88011	-1.11763
H	4.67397	0.32396	-1.70586
H	5.22282	0.36991	-0.02542
C	2.99890	-2.50863	-1.77301
H	2.15625	-3.14182	-1.49022
H	2.70363	-1.91444	-2.63953
H	3.81992	-3.16146	-2.07801
C	-0.54695	4.03079	0.57213
H	-0.35917	4.20727	1.63284
H	-0.44299	4.98439	0.05020
H	-1.58047	3.69801	0.46055
C	0.28318	2.40127	-1.91732
H	-0.74105	2.04902	-2.05112
H	0.40638	3.30502	-2.51851
H	0.96107	1.64338	-2.31331
C	2.42011	3.29662	0.12705
H	2.63824	3.45428	1.18495
H	3.11511	2.54788	-0.25620
H	2.61388	4.23477	-0.39790
C	-1.80706	-1.11150	0.33958
H	-1.89639	-1.59229	1.30957
H	-2.17741	-0.08948	0.37981
C	-2.85765	-1.89555	-0.63406
H	-2.80067	-1.44826	-1.62377
H	-2.56629	-2.94107	-0.63118
C	-4.88558	-0.63988	-0.44713

H	-4.91094	-0.55434	-1.53499
H	-4.40534	0.25120	-0.03389
C	-6.27645	-0.80442	0.13008
H	-6.75636	-1.68738	-0.29591
H	-6.21773	-0.92330	1.21393
O	-4.12657	-1.79962	-0.08425
O	-7.00180	0.38116	-0.21279
Si	0.86735	-0.17968	0.82220
C	0.85718	-0.85476	2.54868
H	-0.09378	-0.62625	3.02895
H	1.00801	-1.93318	2.54677
H	1.66240	-0.38467	3.11600
H	-7.91057	0.27277	0.08716

TriSil-1n-oxidized-M062X.log Energy: -1032788.2724975

C	-0.46288	-0.69598	0.26845
H	-0.52243	-1.76883	0.47908
H	-0.39768	-0.59342	-0.81753
O	2.40432	-0.51335	0.15727
O	1.07776	1.62161	0.98472
Si	2.83527	-1.98789	-0.49300
Si	1.25249	2.65991	-0.31145
C	2.47751	-3.32646	0.75504
H	1.41157	-3.37672	0.98751
H	2.77910	-4.29907	0.36104
H	3.02389	-3.15335	1.68373
C	4.65309	-1.88429	-0.86987
H	5.00931	-2.81578	-1.31291
H	4.85468	-1.07526	-1.57414
H	5.22860	-1.69757	0.03809
C	1.85464	-2.27642	-2.05140
H	0.79246	-2.40144	-1.83643
H	1.97033	-1.44205	-2.74543
H	2.20499	-3.18143	-2.55222
C	0.36175	4.22742	0.14646
H	0.78375	4.66386	1.05323
H	0.44193	4.96537	-0.65352
H	-0.69730	4.03139	0.32303
C	0.49274	1.89083	-1.83271
H	-0.56781	1.67869	-1.68297

H	0.58322	2.57971	-2.67533
H	0.99697	0.96107	-2.10468
C	3.06751	2.97371	-0.58525
H	3.53145	3.38125	0.31447
H	3.58469	2.04929	-0.84766
H	3.21622	3.68869	-1.39656
C	-1.72008	0.00976	0.78351
H	-1.81795	-0.10907	1.86416
H	-1.66989	1.07950	0.57120
C	-2.94909	-0.56242	0.11466
H	-2.91270	-0.40735	-0.96681
H	-3.08506	-1.62137	0.33171
C	-5.25465	-0.50045	0.65475
H	-6.00917	0.05038	1.20670
H	-5.18429	-1.57338	0.82007
C	-5.95760	-0.47609	-0.98533
H	-6.01577	0.59120	-1.17342
H	-5.20258	-1.03942	-1.52523
O	-4.11042	0.15671	0.58495
O	-7.11876	-1.12958	-0.92131
Si	1.10105	-0.02321	1.03798
C	1.26334	-0.52989	2.81160
H	0.45233	-0.10631	3.40642
H	1.22652	-1.61548	2.91184
H	2.20898	-0.17863	3.22733
H	-7.84270	-0.52920	-0.68876

TriSil-1n-oxidized-wB97XD.log Energy: -1032896.8999777

C	-0.06720	-1.30654	0.03995
H	0.38781	-2.28399	0.20290
H	0.07240	-0.96873	-0.98635
O	2.44603	0.02036	0.22880
O	0.33215	1.37673	1.08106
Si	3.51525	-1.03830	-0.51679
Si	0.05939	2.54815	-0.09579
C	3.63549	-2.57768	0.52319
H	2.66703	-3.07515	0.61026
H	4.33454	-3.28520	0.07177
H	3.99270	-2.34478	1.52805
C	5.13719	-0.13922	-0.61321

H	5.88956	-0.75913	-1.10542
H	5.03498	0.78562	-1.18418
H	5.50464	0.11245	0.38334
C	2.84359	-1.41625	-2.21029
H	1.90635	-1.97223	-2.15213
H	2.66357	-0.49672	-2.77067
H	3.55757	-2.02052	-2.77466
C	-1.38462	3.54513	0.51372
H	-1.16778	3.99816	1.48293
H	-1.62065	4.34692	-0.18911
H	-2.27102	2.91648	0.62005
C	-0.34507	1.69907	-1.70502
H	-1.20561	1.03448	-1.59925
H	-0.59045	2.44718	-2.46236
H	0.50058	1.11577	-2.07587
C	1.60044	3.57548	-0.25623
H	1.86223	4.04150	0.69554
H	2.44275	2.96118	-0.57970
H	1.45637	4.36873	-0.99309
C	-1.43161	-1.17551	0.53953
H	-1.60756	-1.59461	1.52560
H	-1.86739	-0.18449	0.43084
C	-2.42213	-2.09222	-0.48551
H	-2.26072	-1.68069	-1.47985
H	-2.07478	-3.11034	-0.34332
C	-4.43160	-0.84746	-0.50847
H	-4.41119	-0.84852	-1.59923
H	-3.96714	0.07161	-0.14108
C	-5.83781	-0.98577	0.02725
H	-6.28397	-1.91187	-0.34140
H	-5.81352	-1.01635	1.11895
O	-3.68353	-1.96689	-0.02926
O	-6.55847	0.14539	-0.43574
Si	1.06066	-0.07133	1.06572
C	1.25042	-0.74585	2.76797
H	0.28530	-0.76709	3.27572
H	1.64992	-1.75983	2.73148
H	1.93535	-0.12155	3.34425
H	-7.46816	0.05867	-0.14424

TriSil-1n-reduced-B3LYP.log Energy: -1033255.7251845

C	-0.53370	-0.76612	-0.14521
H	-0.47245	-1.85953	-0.15413
H	-0.45965	-0.45549	-1.19220
O	2.32113	-0.60834	-0.11941
O	0.97679	1.51770	0.79484
Si	3.33142	-1.91983	-0.35413
Si	1.13888	2.86909	-0.17439
C	4.39545	-2.17361	1.16940
H	3.79620	-2.45360	2.03975
H	5.12326	-2.97198	0.99204
H	4.95100	-1.26443	1.41603
C	4.40054	-1.51401	-1.83659
H	5.09833	-2.33288	-2.04569
H	3.79156	-1.35146	-2.73134
H	4.98802	-0.60681	-1.66145
C	2.31205	-3.46069	-0.68167
H	1.67731	-3.71375	0.17190
H	1.67250	-3.33738	-1.55912
H	2.97374	-4.31220	-0.86818
C	0.16504	4.22866	0.66968
H	0.53995	4.40794	1.68008
H	0.24214	5.16557	0.11277
H	-0.89335	3.96808	0.74332
C	0.44883	2.54077	-1.88726
H	-0.60554	2.25673	-1.84876
H	0.52977	3.44273	-2.50042
H	0.99854	1.74598	-2.39727
C	2.95066	3.33698	-0.27873
H	3.37560	3.49143	0.71697
H	3.53785	2.55894	-0.77438
H	3.07724	4.26341	-0.84715
C	-1.88380	-0.32569	0.43900
H	-1.97017	-0.64584	1.47998
H	-1.95979	0.76377	0.43504
C	-3.05044	-0.89882	-0.34589
H	-3.00685	-0.57163	-1.39042
H	-3.02105	-1.99392	-0.33595
C	-5.42061	-0.93103	-0.46970
H	-5.43316	-2.02621	-0.47291

H	-5.39264	-0.58641	-1.50876
C	-6.65845	-0.39744	0.22199
H	-6.68889	-0.74600	1.25672
H	-6.64420	0.69461	0.22173
O	-4.28139	-0.45353	0.23718
O	-7.79769	-0.88275	-0.50368
Si	0.99327	-0.13281	0.74269
C	1.08006	-0.72241	2.51135
H	0.23411	-0.33802	3.08660
H	1.05764	-1.81285	2.56999
H	1.99749	-0.37586	2.99161
H	-8.58910	-0.51736	-0.09459

TriSil-1n-reduced-M062X.log Energy: -1032955.3596007

C	-0.29755	-0.84955	-0.15336
H	-0.15436	-1.93491	-0.15030
H	-0.27608	-0.54243	-1.20372
O	2.52334	-0.32800	-0.17265
O	0.91179	1.55330	0.84404
Si	3.56978	-1.60680	-0.37162
Si	0.52670	2.83062	-0.15294
C	4.63420	-1.80065	1.14949
H	4.03318	-2.03767	2.02934
H	5.35428	-2.61039	1.00182
H	5.19035	-0.88285	1.35298
C	4.63707	-1.25800	-1.85778
H	5.33614	-2.08358	-2.02417
H	4.02584	-1.13267	-2.75491
H	5.21070	-0.33875	-1.71593
C	2.58361	-3.17099	-0.63667
H	1.95836	-3.39825	0.22989
H	1.93593	-3.08221	-1.51171
H	3.25691	-4.01711	-0.79636
C	-0.60252	3.92777	0.84513
H	-0.10822	4.26292	1.75882
H	-0.89136	4.81081	0.27213
H	-1.51169	3.39297	1.12687
C	-0.35522	2.26415	-1.69873
H	-1.27228	1.71626	-1.47200
H	-0.62499	3.14428	-2.28910

H	0.28667	1.63147	-2.31635
C	2.07712	3.76161	-0.60928
H	2.65184	4.02099	0.28383
H	2.72093	3.15966	-1.25514
H	1.82174	4.68591	-1.13591
C	-1.64945	-0.49820	0.47498
H	-1.71113	-0.89597	1.49056
H	-1.76702	0.58626	0.54867
C	-2.79345	-1.05541	-0.34404
H	-2.76599	-0.64346	-1.35948
H	-2.71458	-2.14558	-0.42087
C	-5.13425	-1.19320	-0.46938
H	-5.09222	-2.28459	-0.54902
H	-5.12477	-0.77385	-1.48090
C	-6.39398	-0.77425	0.25198
H	-6.40092	-1.19652	1.25896
H	-6.43013	0.31442	0.32818
O	-4.02851	-0.71287	0.26987
O	-7.49325	-1.26354	-0.50818
Si	1.15827	-0.06905	0.71291
C	1.34986	-0.73278	2.43656
H	0.45969	-0.51325	3.03014
H	1.49264	-1.81554	2.42604
H	2.21083	-0.27883	2.93142
H	-8.30640	-0.99856	-0.06884

H2O.log Energy: -47971.9724678

O	-0.00000	0.00000	0.11743
H	0.00000	-0.75902	-0.46970
H	0.00000	0.75902	-0.46970

P1a-H+_Fig_S5.log Energy: -776833.3282783

C	0.03758	-0.04764	-0.00550
H	-0.09743	-0.75079	-0.83322
H	-0.09044	-0.62569	0.91425
O	-2.80710	0.59065	-0.05351
O	-1.26701	2.06405	1.49496
Si	-3.54883	-0.92571	-0.03767
C	-3.08993	-1.79061	-1.61788
H	-2.01105	-1.94706	-1.67994

H	-3.57484	-2.76778	-1.67193
H	-3.40308	-1.20920	-2.48704
C	-5.36948	-0.58339	0.06685
H	-5.93232	-1.51923	0.06784
H	-5.61352	-0.04127	0.98232
H	-5.70453	0.01189	-0.78448
C	-2.93492	-1.85756	1.44956
H	-1.87224	-2.08996	1.36254
H	-3.08861	-1.28218	2.36450
H	-3.47677	-2.80083	1.54965
C	1.43561	0.57739	-0.06078
H	1.56568	1.12792	-0.99456
H	1.56730	1.29078	0.75631
C	2.51079	-0.48400	0.03578
H	2.42489	-1.02939	0.98280
H	2.40317	-1.20809	-0.78029
C	4.84263	-0.79129	0.03761
H	4.76958	-1.52254	-0.77515
H	4.80195	-1.33202	0.98975
C	6.14068	-0.02346	-0.06907
H	6.17861	0.50718	-1.02373
H	6.20310	0.70958	0.73926
O	3.78170	0.13931	-0.04384
O	7.20348	-0.96467	0.02462
Si	-1.31887	1.19674	-0.09871
C	-1.09864	2.59852	-1.25588
H	-0.17921	3.14260	-1.03412
H	-1.02961	2.22158	-2.27792
H	-1.94076	3.28837	-1.19668
H	8.03156	-0.48714	-0.05189
H	-0.60139	2.75605	1.62108
H	-1.31678	1.54044	2.30795

P1a-H+_Fig_S6.log Energy: -776833.3308009

C	-0.04695	0.14099	-0.38627
H	0.16060	-0.73455	0.23605
H	-0.00457	-0.19736	-1.42516
O	2.79980	0.49823	-0.47393
O	1.28420	2.49058	-1.31607
Si	3.43284	-1.09521	0.07904

C	2.90738	-1.18475	1.84409
H	1.82257	-1.19245	1.95577
H	3.28690	-2.12023	2.26263
H	3.32172	-0.36117	2.42588
C	5.24507	-0.89406	-0.19284
H	5.75983	-1.82166	0.06566
H	5.45949	-0.67193	-1.23973
H	5.64899	-0.09333	0.42751
C	2.62688	-2.33292	-1.02614
H	1.54766	-2.36161	-0.87422
H	2.82906	-2.10585	-2.07386
H	3.02668	-3.32655	-0.81135
C	-1.43641	0.69651	-0.05140
H	-1.47203	1.02631	0.98934
H	-1.65993	1.56440	-0.67504
C	-2.50414	-0.35461	-0.26992
H	-2.50095	-0.68806	-1.31419
H	-2.31068	-1.22877	0.36282
C	-4.81931	-0.73461	-0.12346
H	-4.65892	-1.61119	0.51416
H	-4.85871	-1.07140	-1.16538
C	-6.11467	-0.05049	0.25069
H	-6.06805	0.28547	1.28967
H	-6.27093	0.82081	-0.39025
O	-3.77018	0.19675	0.05132
O	-7.16307	-0.99640	0.07576
Si	1.29458	1.37233	-0.12224
C	1.47720	2.07409	1.56313
H	0.64696	2.75393	1.76358
H	1.46100	1.28796	2.31823
H	2.41015	2.63131	1.65602
H	-7.99151	-0.56805	0.29888
H	1.70916	3.33327	-1.13915
H	3.30548	0.89663	-1.19690

P1a.log Energy: -776570.5353135

C	0.03774	-0.01278	0.22558
H	-0.14661	-0.77053	-0.54309
H	-0.01215	-0.53011	1.18854
O	-2.78505	0.53007	0.50071

O	-1.17913	2.34133	1.39578
Si	-3.52145	-0.87443	-0.02022
C	-3.28668	-1.03389	-1.86356
H	-2.22936	-1.12497	-2.12201
H	-3.79780	-1.92580	-2.23338
H	-3.69396	-0.16828	-2.38954
C	-5.32254	-0.71814	0.41653
H	-5.86844	-1.61526	0.11655
H	-5.45360	-0.58805	1.49261
H	-5.77515	0.13759	-0.08819
C	-2.74453	-2.32363	0.85669
H	-1.69577	-2.43744	0.57639
H	-2.79725	-2.20070	1.94024
H	-3.26485	-3.24841	0.59659
C	1.42718	0.60021	0.02689
H	1.49260	1.07999	-0.95261
H	1.61136	1.37471	0.77620
C	2.51554	-0.44648	0.13365
H	2.48489	-0.92622	1.11905
H	2.36975	-1.22615	-0.62345
C	4.84635	-0.75342	0.05464
H	4.74275	-1.54603	-0.69500
H	4.84543	-1.21862	1.04685
C	6.13821	0.00157	-0.16240
H	6.13790	0.45731	-1.15578
H	6.23210	0.79417	0.58427
O	3.78076	0.16834	-0.05533
O	7.20496	-0.93205	-0.03905
Si	-1.34305	1.23677	0.16098
C	-1.39382	2.10203	-1.47975
H	-0.49776	2.70922	-1.62487
H	-1.44468	1.37769	-2.29499
H	-2.26319	2.75819	-1.54886
H	8.02994	-0.46049	-0.16793
H	-0.38012	2.87108	1.36525

P2a-H+.log Energy: -520353.1604327

C	-1.24285	-0.73582	-0.21269
H	-1.22440	-1.07378	-1.25337
H	-1.22722	-1.63495	0.40951

O	-4.12056	-1.09480	-0.34732
O	-3.11518	0.32170	1.65195
C	-0.02149	0.14418	0.08143
H	-0.04665	1.04949	-0.52903
H	-0.02375	0.45676	1.12734
C	1.26202	-0.60620	-0.20549
H	1.31168	-1.51867	0.40016
H	1.30146	-0.90039	-1.26082
C	3.60230	-0.40282	-0.16594
H	3.67644	-0.66104	-1.22824
H	3.68982	-1.32587	0.41794
C	4.70716	0.55742	0.21247
H	4.60935	1.47966	-0.36582
H	4.63612	0.80329	1.27498
O	2.36578	0.22903	0.09917
O	5.94441	-0.08490	-0.07268
Si	-2.84176	0.12609	0.05871
C	-3.27940	1.53422	-1.02381
H	-2.54657	2.33359	-0.90184
H	-3.27471	1.22521	-2.07046
H	-4.26689	1.92511	-0.77657
H	6.65341	0.51592	0.16314
H	-3.80744	0.93027	1.92196
H	-4.30357	-1.78218	0.31101
H	-4.13454	-1.50184	-1.22658

P2a.log Energy: -520091.8618257

C	-1.30400	-0.80522	-0.23913
H	-1.26264	-1.13767	-1.28101
H	-1.27110	-1.71293	0.37215
O	-4.18424	-0.99993	-0.44829
O	-3.03970	0.31469	1.65378
C	-0.09605	0.08325	0.07161
H	-0.12612	0.98945	-0.53817
H	-0.11574	0.39868	1.11692
C	1.20454	-0.64312	-0.19776
H	1.27031	-1.54730	0.41910
H	1.25687	-0.95051	-1.24899
C	3.54204	-0.40279	-0.14969
H	3.61909	-0.69038	-1.20433

H	3.64697	-1.30742	0.45988
C	4.63213	0.58576	0.19761
H	4.51984	1.48797	-0.40898
H	4.55832	0.86349	1.25204
O	2.29545	0.21443	0.09983
O	5.87912	-0.04612	-0.06906
Si	-2.95142	0.01390	0.01976
C	-3.19553	1.56860	-0.95401
H	-2.44460	2.31292	-0.68469
H	-3.11154	1.37231	-2.02431
H	-4.18124	1.99767	-0.76371
H	6.57939	0.57129	0.14930
H	-3.77331	0.86408	1.93726
H	-4.14836	-1.88969	-0.09105

TMS-OH.log Energy: -304445.1068209

O	0.09379	-0.07705	1.69889
Si	0.00688	0.00014	0.02239
C	-1.04636	-1.40314	-0.60847
H	-2.06237	-1.33680	-0.21289
H	-1.11059	-1.37477	-1.69866
H	-0.63083	-2.37017	-0.31885
C	1.76959	-0.15678	-0.54803
H	2.19342	-1.12048	-0.25951
H	1.82483	-0.07685	-1.63585
H	2.39185	0.63262	-0.12203
C	-0.73018	1.63033	-0.50212
H	-1.74443	1.74590	-0.11389
H	-0.13102	2.47018	-0.14524
H	-0.78114	1.69029	-1.59185
H	-0.75477	-0.06797	2.14593

TMS_+OH2.log Energy: -304710.2144385

O	-0.05504	-0.12575	1.66578
Si	0.00640	0.00058	-0.15555
C	-1.59435	-0.78850	-0.60498
H	-2.43343	-0.24669	-0.16555
H	-1.71448	-0.76958	-1.69024
H	-1.63008	-1.82701	-0.27493
C	1.53289	-0.95809	-0.52494

H	1.43127	-1.99841	-0.21512
H	1.72147	-0.93667	-1.60042
H	2.39845	-0.52104	-0.02451
C	0.11472	1.80848	-0.49342
H	-0.76387	2.32948	-0.11046
H	1.00719	2.23777	-0.03584
H	0.16959	1.97948	-1.57063
H	-0.85986	0.18166	2.10742
H	0.70485	0.19767	2.17185

TriSil-1n_H+.log Energy: -1033315.7661941

C	-0.51873	-0.99652	0.22916
H	-0.57119	-2.07427	0.41344
H	-0.32066	-0.87595	-0.83755
O	2.35942	-0.62525	0.53486
O	0.81682	1.42191	1.04492
Si	3.18341	-1.62462	-0.53498
Si	1.29756	2.49965	-0.30958
C	4.10715	-2.86931	0.48917
H	3.41667	-3.48536	1.06865
H	4.69500	-3.53082	-0.15079
H	4.78981	-2.37571	1.18338
C	4.33583	-0.52098	-1.48732
H	4.90357	-1.10882	-2.21225
H	3.78569	0.24829	-2.03280
H	5.04772	-0.02798	-0.82292
C	1.96579	-2.45866	-1.66780
H	1.25047	-3.06660	-1.11122
H	1.41076	-1.73442	-2.26639
H	2.50484	-3.11748	-2.35291
C	0.23157	3.97259	0.00572
H	0.42953	4.39735	0.99129
H	0.43800	4.74300	-0.73986
H	-0.82515	3.70967	-0.05924
C	0.85320	1.55802	-1.83343
H	-0.21364	1.33235	-1.85761
H	1.08762	2.18104	-2.70001
H	1.41542	0.63034	-1.93487
C	3.10295	2.78887	-0.07354
H	3.28940	3.31817	0.86196

H	3.65452	1.84937	-0.06073
H	3.48696	3.39976	-0.89345
C	-1.84715	-0.33086	0.60362
H	-2.05132	-0.45552	1.66944
H	-1.80004	0.74258	0.40597
C	-2.99314	-0.92315	-0.18823
H	-2.82211	-0.78673	-1.26260
H	-3.07456	-1.99902	0.00554
C	-5.31709	-0.77843	-0.51681
H	-5.42950	-1.85355	-0.33770
H	-5.18810	-0.62195	-1.59366
C	-6.54239	-0.04043	-0.02699
H	-6.66807	-0.20559	1.04593
H	-6.42307	1.03179	-0.20276
O	-4.19874	-0.27850	0.18851
O	-7.66123	-0.54555	-0.74649
Si	0.91630	-0.34375	1.19148
C	0.84062	-0.60635	3.00712
H	-0.09081	-0.21097	3.41636
H	0.87770	-1.67523	3.22557
H	1.67857	-0.12097	3.50827
H	-8.44959	-0.11282	-0.41369
H	0.36199	1.86844	1.77183

TS1a-IRC-prod.log Energy: -1081288.9122126

C	-0.76714	-1.16565	0.16211
H	-0.91407	-2.24664	0.25407
H	-0.53679	-0.97443	-0.88716
O	2.11292	-1.16849	0.57962
O	0.78901	1.01247	1.23966
Si	2.86705	-2.03998	-0.63279
Si	1.54233	2.32217	0.03486
C	3.71455	-3.47958	0.18307
H	2.98949	-4.13203	0.67365
H	4.25794	-4.07299	-0.55544
H	4.42923	-3.13778	0.93412
C	4.09320	-0.89397	-1.43418
H	4.64675	-1.42353	-2.21317
H	3.59077	-0.04265	-1.89724
H	4.81288	-0.51417	-0.70710

C	1.60903	-2.62363	-1.87476
H	0.84022	-3.24347	-1.41052
H	1.12101	-1.78603	-2.37618
H	2.10999	-3.22444	-2.63779
C	0.58111	3.68710	0.85449
H	0.78395	3.69161	1.92802
H	0.82728	4.67129	0.46294
H	-0.48868	3.51888	0.71776
C	0.86190	1.49234	-1.48293
H	-0.22433	1.42215	-1.40406
H	1.10509	2.03464	-2.39388
H	1.25661	0.48143	-1.58482
C	3.32415	2.07352	0.50898
H	3.44618	1.23972	1.19792
H	3.93443	1.88539	-0.37389
H	3.70335	2.97685	0.99037
C	-2.04477	-0.42416	0.56646
H	-2.27629	-0.60306	1.61917
H	-1.90704	0.65264	0.44412
C	-3.22196	-0.86842	-0.27493
H	-3.02347	-0.67902	-1.33656
H	-3.39228	-1.94441	-0.15204
C	-5.52698	-0.53942	-0.60312
H	-5.72661	-1.60767	-0.46213
H	-5.37474	-0.35779	-1.67296
C	-6.69458	0.27772	-0.09820
H	-6.83358	0.10068	0.97141
H	-6.49530	1.34117	-0.25204
O	-4.37994	-0.15500	0.12780
O	-7.84741	-0.12705	-0.82749
Si	0.69300	-0.72055	1.20929
C	0.51944	-1.18601	2.98337
H	-0.36583	-0.72289	3.42307
H	0.41370	-2.26850	3.07486
H	1.39449	-0.87617	3.55616
H	-8.58660	0.41203	-0.54000
H	0.47677	1.40889	2.06085
O	2.33595	3.92922	-1.37585
H	2.85177	4.57986	-0.88834
H	2.94849	3.54916	-2.01425

TS1a-IRC-prod_-H.log Energy: -1081024.1636646

C	-0.42998	-1.07236	-0.12072
H	-0.32307	-1.72604	-0.99191
H	-0.29606	-0.05415	-0.49507
O	2.36002	-0.82408	0.44187
O	0.71378	-0.70605	2.52031
Si	3.37972	-1.13086	-0.83574
Si	0.77164	3.07133	0.16752
C	4.46801	-2.57477	-0.38443
H	3.86883	-3.47053	-0.20740
H	5.17373	-2.79469	-1.18870
H	5.04155	-2.36525	0.52066
C	4.37683	0.42201	-1.07892
H	5.12046	0.28618	-1.86735
H	3.73454	1.25836	-1.36023
H	4.90330	0.69043	-0.16069
C	2.37519	-1.53818	-2.35393
H	1.78769	-2.44677	-2.20398
H	1.69120	-0.72805	-2.61345
H	3.03743	-1.70684	-3.20650
C	-0.84006	2.56274	0.94840
H	-0.87038	1.49188	1.15302
H	-0.98864	3.08609	1.89530
H	-1.68101	2.79984	0.29362
C	1.01003	2.30037	-1.51390
H	0.11905	2.41761	-2.13383
H	1.85027	2.76502	-2.03490
H	1.22454	1.23470	-1.42398
C	2.22424	2.66624	1.26371
H	2.32865	1.58638	1.38441
H	3.15438	3.04250	0.83136
H	2.10557	3.11130	2.25364
C	-1.82949	-1.21934	0.47993
H	-2.02177	-2.25994	0.75176
H	-1.91213	-0.62862	1.39523
C	-2.89055	-0.75177	-0.49239
H	-2.71826	0.29914	-0.75621
H	-2.85129	-1.34034	-1.41676
C	-5.20569	-0.43591	-0.74962

H	-5.21280	-1.01694	-1.67877
H	-5.05316	0.61843	-1.00671
C	-6.51989	-0.60604	-0.02161
H	-6.67011	-1.65891	0.23009
H	-6.50777	-0.02481	0.90387
O	-4.17223	-0.88609	0.10242
O	-7.54916	-0.14577	-0.88986
Si	0.96912	-1.44729	1.05316
C	1.14005	-3.25595	1.40964
H	0.23022	-3.65262	1.86418
H	1.31789	-3.80405	0.48188
H	1.97506	-3.44970	2.08495
H	-8.38981	-0.25623	-0.44216
H	0.60075	0.24689	2.48728
O	0.63391	4.73739	-0.00220
H	1.38167	5.15976	-0.42897

TS1a-IRC-react.log Energy: -1081289.9951684

C	-0.76129	-1.26291	0.07089
H	-0.89667	-2.34305	-0.04237
H	-0.51821	-0.87751	-0.92113
O	2.12240	-1.21621	0.48727
O	0.72718	0.74595	1.50274
Si	2.90299	-1.94845	-0.80781
Si	1.34165	2.08535	0.47395
C	3.72952	-3.47490	-0.14572
H	2.99221	-4.17454	0.25304
H	4.28363	-3.98345	-0.93762
H	4.43116	-3.22565	0.65240
C	4.14027	-0.71321	-1.43838
H	4.67511	-1.12766	-2.29607
H	3.65158	0.20884	-1.75887
H	4.87617	-0.46367	-0.67198
C	1.66100	-2.37928	-2.12422
H	0.89599	-3.06046	-1.74766
H	1.16728	-1.49093	-2.52136
H	2.17436	-2.87568	-2.95129
C	0.41399	3.52636	1.15762
H	0.61575	3.65363	2.22263
H	0.72821	4.43701	0.64355

H	-0.66047	3.40576	1.01349
C	0.84787	1.61802	-1.24218
H	-0.23412	1.49954	-1.31563
H	1.14564	2.42663	-1.91390
H	1.32931	0.70525	-1.59039
C	3.15833	2.12628	0.79206
H	3.60841	1.14739	0.63221
H	3.64054	2.83841	0.11919
H	3.35759	2.43842	1.81833
C	-2.05135	-0.61820	0.58800
H	-2.31689	-1.02324	1.56701
H	-1.91243	0.45864	0.70899
C	-3.19643	-0.85631	-0.37290
H	-2.95554	-0.43782	-1.35734
H	-3.37307	-1.93089	-0.49873
C	-5.47128	-0.38831	-0.73494
H	-5.68455	-1.45083	-0.89691
H	-5.25488	0.06966	-1.70666
C	-6.66219	0.28911	-0.09559
H	-6.88093	-0.17908	0.86742
H	-6.43897	1.34559	0.07349
O	-4.36677	-0.23666	0.13425
O	-7.76334	0.14522	-0.98524
Si	0.68730	-1.00002	1.18585
C	0.54321	-1.72089	2.86806
H	-0.36263	-1.36772	3.36410
H	0.48637	-2.80877	2.79762
H	1.40516	-1.45810	3.48196
H	-8.52648	0.56573	-0.58487
H	0.27213	1.03191	2.30642
O	2.67380	4.85024	-1.64338
H	2.98080	4.96571	-0.74090
H	2.99524	3.98172	-1.89727

TS1a.1-IRC-prod.log Energy: -1081294.7503285

C	-0.65560	-0.97799	-0.10136
H	-0.61188	-1.71255	-0.91043
H	-0.46247	-0.00647	-0.56343
O	2.16451	-0.67036	0.35638
O	2.32573	1.78258	0.77314

Si	3.24939	-1.39161	-0.83944
Si	1.24781	2.89089	0.03917
C	4.25617	-2.64313	0.07306
H	3.63965	-3.46641	0.43342
H	5.01591	-3.05371	-0.59585
H	4.76473	-2.18706	0.92372
C	4.23499	0.05309	-1.43440
H	4.97271	-0.29537	-2.16050
H	3.60373	0.79583	-1.92208
H	4.77076	0.53065	-0.61299
C	2.13404	-2.11889	-2.12349
H	1.54981	-2.95504	-1.73542
H	1.45235	-1.36477	-2.51993
H	2.74087	-2.49627	-2.94984
C	-0.38161	2.80806	0.93105
H	-0.25462	3.03473	1.99165
H	-1.06684	3.54903	0.51241
H	-0.85558	1.82922	0.84424
C	1.14177	2.28857	-1.71312
H	0.97983	1.20990	-1.75934
H	0.30850	2.77473	-2.22466
H	2.05505	2.52118	-2.26264
C	1.99956	4.58139	0.17806
H	2.12842	4.86805	1.22362
H	2.97326	4.61982	-0.31294
H	1.35055	5.32190	-0.29460
C	-2.04435	-0.97301	0.54523
H	-2.27973	-1.95679	0.95683
H	-2.07413	-0.25994	1.37250
C	-3.10218	-0.59000	-0.46716
H	-2.89468	0.41038	-0.86594
H	-3.09853	-1.29357	-1.30801
C	-5.40558	-0.21644	-0.73356
H	-5.43430	-0.89328	-1.59488
H	-5.22909	0.80004	-1.10295
C	-6.71763	-0.27474	0.01545
H	-6.89649	-1.29264	0.37076
H	-6.68067	0.39432	0.87891
O	-4.37587	-0.59922	0.15594
O	-7.73957	0.12860	-0.88877

Si	0.72087	-1.32352	1.08448
C	0.61608	-0.51294	2.72794
H	-0.23687	-0.90735	3.28252
H	1.52124	-0.69688	3.30791
H	0.48215	0.56439	2.62242
H	-8.58012	0.08282	-0.42978
H	2.49180	1.91998	1.71035
O	1.03331	-2.92241	1.26369
H	2.27501	0.35114	0.51760
H	0.80800	-3.49798	0.52911

TS1a.1-IRC-react.log Energy: -1081288.1398237

C	-0.37939	-0.88717	-0.14212
H	-0.35589	-1.92279	-0.48748
H	-0.22180	-0.27026	-1.02520
O	2.51606	-1.17677	0.62883
O	1.48097	1.17510	0.41362
Si	3.43558	-1.21475	-0.77377
Si	0.68769	2.65609	-0.05689
C	4.62161	0.22033	-0.72732
H	5.19550	0.22907	0.20127
H	5.32771	0.14919	-1.55794
H	4.09841	1.17474	-0.81823
C	2.32485	-1.08523	-2.26316
H	2.92860	-1.15394	-3.17130
H	1.58610	-1.88797	-2.28932
H	1.79784	-0.12942	-2.28328
C	4.34183	-2.83733	-0.74586
H	4.97086	-2.91796	0.14278
H	3.64143	-3.67482	-0.74530
H	4.98400	-2.93319	-1.62392
C	-0.30583	3.24199	1.39243
H	0.32247	3.36779	2.27547
H	-0.75866	4.20798	1.15670
H	-1.11056	2.54589	1.63385
C	-0.36506	2.28847	-1.53400
H	-1.26602	1.73124	-1.27660
H	-0.67932	3.24100	-1.96849
H	0.18906	1.73911	-2.29639
C	2.11940	3.76361	-0.45404

H	2.79283	3.85915	0.40002
H	2.68717	3.37692	-1.30195
H	1.76113	4.76213	-0.71205
C	-1.74291	-0.58088	0.48522
H	-1.91033	-1.21140	1.36206
H	-1.78478	0.45619	0.82700
C	-2.86091	-0.81125	-0.50778
H	-2.72875	-0.16518	-1.38395
H	-2.85441	-1.85156	-0.85374
C	-5.19591	-0.70706	-0.76312
H	-5.21874	-1.73884	-1.13130
H	-5.10716	-0.03736	-1.62589
C	-6.46269	-0.40199	0.00385
H	-6.54954	-1.07893	0.85743
H	-6.43097	0.62522	0.37591
O	-4.10270	-0.52371	0.11399
O	-7.55570	-0.57859	-0.88988
Si	1.03066	-0.65727	1.04917
C	0.76241	-0.02993	2.77074
H	0.51209	-0.81499	3.48060
H	1.66443	0.47757	3.11733
H	-0.04442	0.70421	2.76452
H	-8.36619	-0.40542	-0.40749
H	2.36613	1.36858	0.74663
O	0.72757	-2.61859	1.77290
H	0.90696	-3.27050	1.08607
H	-0.17425	-2.78939	2.06833

TS1a.1.log Energy: -1081264.6678509

C	-0.42880	-1.07193	-0.08138
H	-0.43413	-2.10852	-0.42670
H	-0.25075	-0.45788	-0.96324
O	2.58528	-1.18905	0.54853
O	1.38197	1.07405	0.46808
Si	3.52894	-0.93630	-0.88330
Si	0.54852	2.52622	0.01382
C	4.55182	0.58322	-0.60491
H	5.07970	0.53079	0.34863
H	5.29915	0.66122	-1.39817
H	3.95121	1.49328	-0.62468

C	2.36239	-0.77004	-2.31231
H	2.93486	-0.71641	-3.24119
H	1.69181	-1.62825	-2.37848
H	1.76386	0.13731	-2.23189
C	4.55093	-2.47899	-0.96802
H	5.18042	-2.58003	-0.08239
H	3.91429	-3.36251	-1.04240
H	5.20044	-2.45427	-1.84522
C	-0.41856	3.10890	1.48516
H	0.23209	3.26627	2.34698
H	-0.90436	4.05893	1.25016
H	-1.19605	2.39545	1.76267
C	-0.54784	2.14535	-1.42891
H	-1.42820	1.56904	-1.14664
H	-0.89727	3.09842	-1.83504
H	-0.01787	1.62031	-2.22393
C	1.92135	3.68954	-0.43637
H	2.63217	3.80061	0.38492
H	2.46144	3.33428	-1.31545
H	1.51429	4.67711	-0.66333
C	-1.78778	-0.72967	0.54177
H	-1.97023	-1.34390	1.42639
H	-1.80978	0.31268	0.86819
C	-2.90403	-0.95323	-0.45564
H	-2.73473	-0.34945	-1.35518
H	-2.93585	-2.00576	-0.76064
C	-5.22573	-0.75118	-0.75380
H	-5.30524	-1.79707	-1.07073
H	-5.07868	-0.13301	-1.64650
C	-6.48584	-0.32932	-0.03275
H	-6.63129	-0.95222	0.85338
H	-6.39808	0.71281	0.28472
O	-4.13972	-0.58991	0.13694
O	-7.56989	-0.48760	-0.94087
Si	0.96966	-0.87892	1.12248
C	0.76678	-0.19494	2.82621
H	0.40083	-0.95903	3.50988
H	1.72633	0.16946	3.19869
H	0.07228	0.64393	2.82289
H	-8.37620	-0.22950	-0.49050

H	2.20053	1.31503	0.91877
O	1.27010	-2.63549	1.59907
H	2.31810	-2.24705	0.96898
H	0.78546	-3.28856	1.08674

TS1a.log Energy: -1081288.8741353

C	-0.74142	-1.21099	0.15052
H	-0.88246	-2.29376	0.22795
H	-0.51033	-1.00329	-0.89552
O	2.14434	-1.13627	0.55747
O	0.76251	0.97678	1.27500
Si	2.92153	-1.98574	-0.65809
Si	1.44651	2.29013	0.09333
C	3.79122	-3.41494	0.15190
H	3.07553	-4.08305	0.63512
H	4.34771	-3.99415	-0.58809
H	4.49672	-3.06559	0.90810
C	4.12661	-0.80580	-1.44098
H	4.69667	-1.31503	-2.22158
H	3.60772	0.03843	-1.89879
H	4.83316	-0.41722	-0.70567
C	1.67746	-2.58247	-1.90739
H	0.92066	-3.22146	-1.44928
H	1.17311	-1.75019	-2.40150
H	2.19054	-3.16649	-2.67533
C	0.44988	3.64384	0.88363
H	0.70571	3.71996	1.94319
H	0.61642	4.61552	0.42558
H	-0.61340	3.40695	0.81135
C	0.81831	1.50299	-1.46540
H	-0.26529	1.38623	-1.40818
H	1.05421	2.10315	-2.34122
H	1.25784	0.51611	-1.61136
C	3.24830	2.13355	0.52179
H	3.42700	1.28204	1.17656
H	3.84987	2.00993	-0.37799
H	3.58703	3.03715	1.03118
C	-2.02258	-0.48008	0.56424
H	-2.25543	-0.67628	1.61358
H	-1.88782	0.59903	0.45929

C	-3.19771	-0.91242	-0.28610
H	-2.99637	-0.70893	-1.34455
H	-3.36993	-1.98966	-0.17798
C	-5.50219	-0.57366	-0.61280
H	-5.70839	-1.64187	-0.48135
H	-5.34645	-0.38372	-1.68068
C	-6.66572	0.24645	-0.10326
H	-6.80662	0.06272	0.96500
H	-6.46007	1.30976	-0.24936
O	-4.35479	-0.20194	0.12406
O	-7.82033	-0.14622	-0.83622
Si	0.71268	-0.76499	1.20457
C	0.55753	-1.26901	2.96820
H	-0.34218	-0.84311	3.41625
H	0.48629	-2.35589	3.03860
H	1.42275	-0.94184	3.54599
H	-8.55524	0.39883	-0.54902
H	0.35101	1.35635	2.06065
O	2.25501	4.05321	-1.36433
H	2.68603	4.72046	-0.82170
H	2.95187	3.70836	-1.93069

4water-anion3.log Energy: -191916.6352938

O	1.00912	-0.30068	1.91999
H	1.85288	-0.60602	1.57125
O	1.68374	-0.21323	-1.57596
O	-1.77437	-1.66456	-0.35408
O	-1.05653	2.18711	-0.15007
H	-0.70797	1.25364	-0.16662
H	0.46524	-0.15092	1.10222
H	-1.08836	-0.94392	-0.29618
H	-2.13987	-1.69758	0.53577
H	2.34782	-0.45266	-0.92127
H	0.85935	-0.09952	-1.03070
H	-0.48472	2.62785	0.48654

4water-neutral-from-anion4.log Energy: -191901.4936102

O	0.52855	-1.89066	-0.05689
H	1.07603	-1.08081	-0.04938
O	1.88592	0.52804	-0.14123

O	-1.88672	-0.52886	0.07643
O	-0.53253	1.88896	-0.05694
H	-1.07692	1.07949	0.00602
H	0.66480	-2.29487	0.80296
H	-2.34658	-0.65778	-0.75613
H	-1.07930	-1.07592	0.01200
H	2.34733	0.65275	0.69113
H	1.07922	1.07562	-0.07223
H	-0.62637	2.32161	0.79469

P1b.1.log Energy: -1080701.0549728

C	-1.05805	-0.68531	-0.48427
H	-1.05994	-1.76719	-0.32247
H	-1.04618	-0.53760	-1.56915
O	1.83012	-0.68209	-0.51300
O	0.52912	1.61213	-0.16785
Si	2.93174	-1.96638	-0.11692
Si	1.72927	2.76129	-0.15096
C	3.58478	-1.99729	1.67617
H	3.75516	-0.98186	2.04283
H	2.91921	-2.50642	2.37647
H	4.55359	-2.50562	1.70431
C	3.70551	-3.10577	-1.44566
H	3.50945	-4.16169	-1.24816
H	3.23449	-2.87126	-2.40716
H	4.78010	-2.96754	-1.57352
C	1.45308	-3.23733	0.19507
H	0.73204	-2.90617	0.94971
H	0.89151	-3.44579	-0.72365
H	1.86158	-4.19301	0.54571
C	0.88084	4.41772	-0.05434
H	0.29204	4.50368	0.86119
H	1.61433	5.22714	-0.06107
H	0.21109	4.56379	-0.90438
C	2.72558	2.63831	-1.72293
H	2.08774	2.78103	-2.59788
H	3.50435	3.40412	-1.74556
H	3.20653	1.66248	-1.81070
C	2.83455	2.52062	1.33586
H	2.26765	2.61092	2.26453

H	3.32241	1.54366	1.33221
H	3.61655	3.28377	1.34350
C	-2.32416	-0.06919	0.11505
H	-2.33909	-0.21486	1.19819
H	-2.34209	1.00866	-0.06244
C	-3.57586	-0.68358	-0.47402
H	-3.60016	-0.53301	-1.55996
H	-3.59318	-1.76372	-0.28566
C	-5.92555	-0.63417	-0.37958
H	-5.96741	-1.70827	-0.16589
H	-5.99041	-0.49909	-1.46521
C	-7.07564	0.07369	0.30042
H	-7.00092	-0.05670	1.38304
H	-7.03797	1.14241	0.07505
O	-4.72135	-0.08299	0.11264
O	-8.28083	-0.50083	-0.19186
Si	0.53761	-0.00575	0.20656
C	0.58169	-0.15875	2.06614
H	-0.17535	0.49000	2.51198
H	0.37988	-1.18147	2.38810
H	1.55396	0.13475	2.46396
H	-9.01734	-0.05038	0.22512
O	4.29630	-0.74031	-0.58879
H	4.02813	0.12606	-0.28120

TS1b.1-IRC-react.log Energy: -1080713.1661628

C	-1.22055	-0.66264	-0.38462
H	-1.26526	-1.74898	-0.25215
H	-1.17685	-0.48699	-1.46404
O	1.63111	-0.84737	-0.38577
O	0.54624	1.52928	0.03122
Si	2.48343	-2.25238	-0.12232
Si	1.92290	2.46759	-0.09176
C	3.57945	-2.04407	1.37060
H	4.28047	-1.21902	1.22663
H	2.99590	-1.84807	2.27169
H	4.16258	-2.95290	1.53814
C	3.50755	-2.52352	-1.65177
H	4.11806	-3.42416	-1.55737
H	2.87403	-2.63399	-2.53407

H	4.17847	-1.67682	-1.81504
C	1.27451	-3.64814	0.14499
H	0.65646	-3.47054	1.02795
H	0.61347	-3.76440	-0.71614
H	1.80479	-4.59168	0.29295
C	1.36599	4.23897	0.04467
H	0.87646	4.42312	1.00305
H	2.22030	4.91512	-0.03327
H	0.66312	4.49174	-0.75174
C	2.72740	2.15848	-1.74466
H	2.03959	2.39147	-2.56050
H	3.61455	2.78485	-1.86193
H	3.03317	1.11559	-1.84460
C	3.08844	2.03469	1.29947
H	2.63115	2.23780	2.27006
H	3.37178	0.98072	1.27011
H	4.00205	2.62880	1.22538
C	-2.47428	-0.01314	0.20560
H	-2.53120	-0.20707	1.27944
H	-2.43536	1.07108	0.07721
C	-3.73168	-0.53835	-0.45338
H	-3.70914	-0.33445	-1.53050
H	-3.80640	-1.62417	-0.31971
C	-6.07509	-0.34884	-0.46370
H	-6.18471	-1.43269	-0.34456
H	-6.08134	-0.12048	-1.53553
C	-7.21584	0.36564	0.22501
H	-7.21038	0.12898	1.29191
H	-7.10033	1.44612	0.10735
O	-4.86678	0.08922	0.12368
O	-8.42406	-0.07894	-0.38145
Si	0.38059	-0.07745	0.35833
C	0.42938	-0.35370	2.19533
H	-0.36560	0.21401	2.68317
H	0.28452	-1.40901	2.43636
H	1.38276	-0.03269	2.61727
H	-9.15660	0.35250	0.06175
O	5.83657	0.48777	-0.61341
H	4.88633	0.43553	-0.49808

TS1b-IRC-prod.log Energy: -1080707.2809147

C	-0.49343	-1.11565	0.22715
H	-0.60822	-2.19941	0.29128
H	-0.27241	-0.90428	-0.82558
O	2.48740	-0.21735	0.34132
O	0.59974	1.15404	1.20301
Si	3.33679	-0.92689	-0.87391
Si	0.66545	2.32393	0.07064
C	4.62998	-2.10788	-0.21008
H	4.18422	-3.01386	0.20380
H	5.31265	-2.40690	-1.00965
H	5.22436	-1.63252	0.57371
C	4.22022	0.45450	-1.77824
H	4.82354	0.05423	-2.59686
H	3.50750	1.16590	-2.20102
H	4.88657	1.00268	-1.10844
C	2.24732	-1.82725	-2.10215
H	1.71343	-2.65570	-1.63570
H	1.51152	-1.15942	-2.55386
H	2.86578	-2.23255	-2.90757
C	-0.67014	3.58575	0.46329
H	-0.54085	3.99800	1.46697
H	-0.64541	4.41742	-0.24556
H	-1.66330	3.13257	0.41281
C	0.34666	1.71621	-1.67746
H	-0.63989	1.25508	-1.76334
H	0.38288	2.55908	-2.37305
H	1.09120	0.98707	-1.99674
C	2.31535	3.21965	0.09144
H	2.49469	3.67473	1.06891
H	3.13847	2.53495	-0.11642
H	2.33783	4.01678	-0.65622
C	-1.82329	-0.45781	0.59283
H	-2.05756	-0.63242	1.64722
H	-1.76782	0.62234	0.45730
C	-2.95749	-0.99598	-0.25255
H	-2.75964	-0.80848	-1.31555
H	-3.05862	-2.07982	-0.11916
C	-5.27578	-0.84216	-0.62938
H	-5.38882	-1.92343	-0.49018

H	-5.12327	-0.64992	-1.69770
C	-6.51682	-0.12700	-0.14513
H	-6.66460	-0.32520	0.91934
H	-6.40198	0.95084	-0.28594
O	-4.17665	-0.36377	0.11757
O	-7.61698	-0.61760	-0.90335
Si	1.06918	-0.60581	1.20011
C	1.13735	-0.60292	3.09932
H	2.06235	-1.06583	3.45378
H	1.05171	0.38615	3.54923
H	0.31926	-1.22021	3.48349
H	-8.41593	-0.20493	-0.57049
O	1.54585	-2.40798	1.20823
H	2.42601	-2.49546	1.57694

TS1b-IRC-react.log Energy: -1080713.8656665

C	-0.36338	-0.89301	0.13901
H	-0.31026	-1.98428	0.20907
H	-0.21038	-0.64845	-0.91443
O	2.46976	-0.86173	0.60186
O	1.13554	1.42916	1.01559
Si	3.30480	-1.03658	-0.82824
Si	0.65876	2.68669	0.03911
C	4.71643	-2.19021	-0.45244
H	4.34402	-3.15461	-0.10047
H	5.32025	-2.36498	-1.34552
H	5.36697	-1.77431	0.31958
C	3.93710	0.62452	-1.38932
H	4.62284	0.49839	-2.23075
H	3.12077	1.26724	-1.72137
H	4.47536	1.13553	-0.58912
C	2.18737	-1.76720	-2.13014
H	1.68329	-2.66160	-1.75834
H	1.42820	-1.05212	-2.45195
H	2.77426	-2.04923	-3.00766
C	-0.73032	3.59173	0.89161
H	-0.41154	3.96317	1.86774
H	-1.04847	4.44893	0.29360
H	-1.59738	2.94560	1.04057
C	0.08896	2.05525	-1.62260

H	-0.86708	1.53427	-1.54560
H	-0.04404	2.89826	-2.30508
H	0.81498	1.37346	-2.06985
C	2.12259	3.82349	-0.15173
H	2.46963	4.17126	0.82360
H	2.95612	3.32804	-0.65161
H	1.84676	4.70048	-0.74186
C	-1.74032	-0.40488	0.59403
H	-1.93611	-0.72459	1.62010
H	-1.78215	0.68688	0.58803
C	-2.83733	-0.93102	-0.30554
H	-2.66828	-0.60407	-1.33878
H	-2.84455	-2.02740	-0.29796
C	-5.16412	-0.90729	-0.64894
H	-5.20853	-2.00202	-0.62670
H	-5.03017	-0.59164	-1.68985
C	-6.44306	-0.32565	-0.09027
H	-6.56772	-0.63962	0.94907
H	-6.39764	0.76598	-0.12110
O	-4.09182	-0.44363	0.14587
O	-7.51659	-0.80619	-0.89134
Si	1.05601	-0.20945	1.13572
C	0.90212	-0.63466	2.93275
H	0.86259	-1.71755	3.06682
H	1.75461	-0.25211	3.49720
H	-0.00686	-0.20477	3.35756
H	-8.33534	-0.46079	-0.53109
O	1.65255	-4.07395	1.13049
H	1.90000	-3.16837	0.93536

TS1b.1.log Energy: -1080699.0824156

C	-1.05408	-0.71101	-0.44914
H	-1.05282	-1.79213	-0.28182
H	-1.04578	-0.56746	-1.53445
O	1.82831	-0.72433	-0.48703
O	0.55277	1.58312	-0.16541
Si	2.78340	-2.06523	-0.09698
Si	1.75225	2.73641	-0.14070
C	3.63197	-1.98448	1.58486
H	3.78356	-0.95142	1.89952

H	3.04989	-2.49804	2.35368
H	4.61701	-2.45390	1.53495
C	3.57968	-2.97439	-1.54380
H	3.19029	-3.98977	-1.64330
H	3.36663	-2.44170	-2.47338
H	4.66370	-3.02578	-1.44283
C	1.38815	-3.33368	0.28837
H	0.73109	-3.03349	1.10906
H	0.76233	-3.52315	-0.58923
H	1.84277	-4.28876	0.57400
C	0.90315	4.38803	0.00493
H	0.32763	4.45211	0.93060
H	1.63585	5.19818	0.00634
H	0.22147	4.55257	-0.83208
C	2.71841	2.63784	-1.73149
H	2.06886	2.81710	-2.59092
H	3.51342	3.38681	-1.74755
H	3.17621	1.65399	-1.85083
C	2.87488	2.45828	1.32580
H	2.32648	2.56311	2.26400
H	3.33039	1.46581	1.31159
H	3.68073	3.19602	1.32237
C	-2.31772	-0.09250	0.15354
H	-2.33976	-0.25645	1.23386
H	-2.32453	0.98827	-0.00609
C	-3.57157	-0.68298	-0.45505
H	-3.58743	-0.50719	-1.53727
H	-3.60086	-1.76692	-0.29153
C	-5.92071	-0.57664	-0.40588
H	-5.98980	-1.66047	-0.25903
H	-5.96308	-0.37420	-1.48211
C	-7.06696	0.11554	0.29641
H	-7.02796	-0.09798	1.36752
H	-6.98864	1.19635	0.15373
O	-4.71377	-0.08353	0.13857
O	-8.27498	-0.37891	-0.27018
Si	0.53720	-0.02190	0.23361
C	0.60145	-0.17411	2.09031
H	-0.13819	0.48978	2.54279
H	0.38008	-1.19219	2.41440

H	1.58312	0.09927	2.47882
H	-9.00917	0.04569	0.17693
O	4.48597	-0.57525	-0.68118
H	4.17021	0.23787	-0.28621

TS1b.log Energy: -1080702.4828894

C	-0.46678	-1.06921	0.22045
H	-0.54087	-2.14321	0.37985
H	-0.25451	-0.92944	-0.84399
O	2.46278	-0.31972	0.39338
O	0.63692	1.26723	1.21277
Si	3.29201	-0.98544	-0.86889
Si	0.70438	2.44346	0.06027
C	4.60193	-2.16434	-0.24624
H	4.17810	-3.10551	0.10613
H	5.30518	-2.39413	-1.05076
H	5.16936	-1.71612	0.57246
C	4.15449	0.42908	-1.73799
H	4.74531	0.05171	-2.57646
H	3.43810	1.15352	-2.13033
H	4.83223	0.95466	-1.06178
C	2.17755	-1.84387	-2.09839
H	1.62775	-2.66430	-1.63744
H	1.45797	-1.15412	-2.54295
H	2.78737	-2.25407	-2.90787
C	-0.60750	3.70709	0.48019
H	-0.45214	4.12021	1.47919
H	-0.58964	4.53525	-0.23231
H	-1.60336	3.25922	0.45018
C	0.35645	1.77560	-1.65338
H	-0.64391	1.34200	-1.71423
H	0.41370	2.58908	-2.38118
H	1.07649	1.01307	-1.94988
C	2.38457	3.26288	0.08533
H	2.56198	3.75032	1.04681
H	3.17932	2.53320	-0.07442
H	2.45924	4.02369	-0.69534
C	-1.80365	-0.40703	0.56198
H	-2.02350	-0.52107	1.62736
H	-1.76762	0.66441	0.35996

C	-2.93878	-1.00919	-0.23708
H	-2.75387	-0.88387	-1.31118
H	-3.02592	-2.08351	-0.03599
C	-5.26003	-0.87603	-0.60705
H	-5.37514	-1.94876	-0.41450
H	-5.11182	-0.73613	-1.68395
C	-6.49595	-0.13313	-0.15219
H	-6.64074	-0.28036	0.92095
H	-6.37599	0.93631	-0.34374
O	-4.15637	-0.36411	0.11077
O	-7.60119	-0.65278	-0.88287
Si	1.00694	-0.40175	1.18380
C	1.09933	-0.70117	3.02899
H	2.06099	-1.13273	3.30770
H	0.96083	0.22752	3.58512
H	0.32723	-1.40644	3.33994
H	-8.39582	-0.21488	-0.57265
O	1.56210	-2.85571	1.21540
H	2.48331	-2.79670	1.46941

TS2b-IRC-prod.log Energy: -1080713.2448902

C	-0.58637	-0.91574	-0.06948
H	-0.52448	-1.55006	-0.95856
H	-0.39433	0.10729	-0.40436
O	2.25082	-0.97331	0.45764
O	-0.24616	2.73223	0.89682
Si	3.19367	-1.45426	-0.82594
Si	1.13620	3.05675	0.14765
C	4.10068	-3.00820	-0.33821
H	3.39750	-3.81324	-0.11486
H	4.75486	-3.34525	-1.14548
H	4.71678	-2.83932	0.54732
C	4.38363	-0.05803	-1.14420
H	5.08951	-0.32584	-1.93369
H	3.85434	0.84408	-1.45520
H	4.95609	0.17537	-0.24416
C	2.12273	-1.77803	-2.31856
H	1.42902	-2.60142	-2.13661
H	1.54241	-0.89540	-2.59323
H	2.74726	-2.05022	-3.17290

C	1.36017	4.90310	-0.20109
H	1.34331	5.48412	0.72517
H	2.31288	5.10117	-0.70037
H	0.56213	5.28370	-0.84458
C	1.28309	2.19789	-1.53156
H	0.42068	2.42568	-2.16425
H	2.18176	2.51954	-2.06532
H	1.33426	1.11351	-1.41861
C	2.66062	2.53647	1.13930
H	2.70131	3.06435	2.09637
H	2.65391	1.46508	1.34920
H	3.58211	2.76445	0.59564
C	-1.98721	-0.99717	0.54261
H	-2.20720	-2.01800	0.86371
H	-2.04879	-0.36016	1.42818
C	-3.04135	-0.55380	-0.44895
H	-2.85357	0.48063	-0.76064
H	-3.01202	-1.18482	-1.34533
C	-5.35096	-0.21301	-0.72168
H	-5.36078	-0.82761	-1.62907
H	-5.18640	0.82947	-1.01673
C	-6.66980	-0.34278	0.00621
H	-6.83229	-1.38414	0.29550
H	-6.65542	0.27176	0.90982
O	-4.32544	-0.64251	0.15030
O	-7.69057	0.09616	-0.88301
Si	0.79094	-1.38147	1.08874
C	0.66833	-0.55114	2.74147
H	0.64958	0.53332	2.61568
H	-0.24148	-0.84884	3.26521
H	1.52364	-0.80751	3.36988
H	-8.53300	0.02064	-0.43150
O	0.68891	-3.03880	1.24631
H	1.32307	-3.43423	1.84791

TS2b-IRC-react.log Energy: -1080707.3506937

C	-0.67803	-0.68095	-0.21348
H	-0.67279	-1.66615	-0.68520
H	-0.55553	0.05720	-1.00937
O	2.36246	-0.44556	0.42341

O	0.63417	1.31623	0.94090
Si	3.23902	-1.36834	-0.61761
Si	1.31512	2.43165	-0.02748
C	4.07867	-2.79083	0.26221
H	3.35701	-3.53023	0.61241
H	4.77890	-3.29338	-0.40993
H	4.64497	-2.43292	1.12524
C	4.56748	-0.25308	-1.32235
H	5.19697	-0.80387	-2.02576
H	4.13254	0.59682	-1.85239
H	5.21264	0.13713	-0.53195
C	2.19645	-2.02653	-2.02659
H	1.47926	-2.76996	-1.67691
H	1.64151	-1.22674	-2.52132
H	2.83792	-2.49939	-2.77480
C	0.33196	4.02482	0.14205
H	0.34008	4.38740	1.17291
H	0.74830	4.81209	-0.49186
H	-0.70991	3.87508	-0.15185
C	1.29262	1.96833	-1.84911
H	0.27029	1.90695	-2.22934
H	1.81934	2.72643	-2.43511
H	1.77670	1.00846	-2.02855
C	3.08827	2.82258	0.45547
H	3.14433	3.13458	1.50158
H	3.73687	1.95565	0.32696
H	3.48423	3.63781	-0.15606
C	-2.03430	-0.45982	0.46347
H	-2.19230	-1.20592	1.24762
H	-2.06040	0.51967	0.94776
C	-3.18152	-0.54372	-0.52031
H	-3.06917	0.21700	-1.30245
H	-3.19588	-1.52559	-1.00864
C	-5.52606	-0.41836	-0.70351
H	-5.56611	-1.40239	-1.18450
H	-5.45279	0.34275	-1.48882
C	-6.77345	-0.19462	0.12135
H	-6.84051	-0.95585	0.90267
H	-6.73128	0.78883	0.59640
O	-4.41249	-0.33994	0.16184

O	-7.88949	-0.27959	-0.75784
Si	0.77527	-0.52169	1.00913
C	0.56171	-0.38400	2.89361
H	1.24992	0.35999	3.30100
H	-0.44870	-0.02403	3.11076
H	0.70128	-1.32025	3.43577
H	-8.68720	-0.16114	-0.23906
O	0.80730	-2.37111	1.09099
H	1.45929	-2.65193	1.73478

TS2b.log Energy: -1080703.2678975

C	-0.71047	-0.58149	-0.21026
H	-0.72725	-1.46770	-0.85209
H	-0.52106	0.28061	-0.84627
O	2.23508	-0.61305	0.42600
O	0.61143	1.62105	1.01565
Si	3.13263	-1.48589	-0.65607
Si	1.49297	2.54787	0.04632
C	3.91136	-2.95551	0.19481
H	3.15550	-3.66550	0.53453
H	4.58624	-3.47922	-0.48658
H	4.49340	-2.63680	1.06245
C	4.48302	-0.35817	-1.28159
H	5.10515	-0.88647	-2.00836
H	4.07198	0.52785	-1.76845
H	5.12948	-0.02803	-0.46594
C	2.08117	-2.06280	-2.09010
H	1.33665	-2.79249	-1.76877
H	1.55895	-1.23034	-2.56565
H	2.71315	-2.53646	-2.84555
C	0.87538	4.33791	0.03730
H	0.91680	4.77821	1.03738
H	1.48096	4.96313	-0.62543
H	-0.16070	4.39527	-0.30789
C	1.44406	2.01600	-1.76802
H	0.43837	2.14035	-2.17936
H	2.12443	2.62250	-2.37271
H	1.72461	0.97000	-1.89166
C	3.31000	2.65968	0.55515
H	3.40222	3.14524	1.53111

H	3.76661	1.67238	0.63059
H	3.88984	3.24810	-0.16171
C	-2.06996	-0.43482	0.47785
H	-2.25022	-1.27763	1.15099
H	-2.08418	0.47075	1.08880
C	-3.20211	-0.37129	-0.52445
H	-3.07628	0.49073	-1.19067
H	-3.21167	-1.27532	-1.14505
C	-5.54524	-0.23550	-0.71294
H	-5.56627	-1.14497	-1.32422
H	-5.47845	0.62688	-1.38596
C	-6.80123	-0.14605	0.12419
H	-6.85892	-1.00743	0.79443
H	-6.77909	0.76417	0.72876
O	-4.43933	-0.26112	0.16550
O	-7.91049	-0.12923	-0.76716
Si	0.69586	-0.81051	1.01032
C	0.53975	-0.46524	2.84460
H	1.27895	0.26238	3.17554
H	-0.44653	-0.05309	3.06721
H	0.65897	-1.38045	3.42831
H	-8.71257	-0.08161	-0.24383
O	0.56733	-2.54413	1.03720
H	1.13395	-2.94012	1.70123

assist_TS1h-IRC_prod.log Energy: -1128999.3170169

Si	-1.65927	0.00946	-0.34411
O	-1.59163	0.62643	1.21438
O	2.39318	1.99548	0.11228
H	-1.92359	0.04274	1.90168
Si	2.11974	3.61755	-0.19201
C	1.95453	3.80973	-2.03856
H	1.87148	4.86565	-2.30576
H	2.82960	3.40373	-2.55083
H	1.06975	3.29397	-2.41582
C	3.57341	4.61639	0.41700
H	4.49732	4.30580	-0.07556
H	3.42360	5.67871	0.21035
H	3.70699	4.49818	1.49438
C	0.56204	4.15416	0.68691

H	0.69088	4.12946	1.77103
H	0.30717	5.17905	0.40663
H	-0.28299	3.51369	0.42862
C	-0.90514	1.30394	-1.42221
H	-1.44437	2.24937	-1.35155
H	0.13205	1.47125	-1.13115
H	-0.91462	0.98006	-2.46468
C	-0.73196	-1.60414	-0.39450
H	-1.11393	-2.24596	0.40538
H	-0.96842	-2.11102	-1.33471
O	-3.22692	-0.22187	-0.77526
Si	-4.55439	-0.89474	-0.01770
C	0.78413	-1.43528	-0.25530
H	1.17461	-0.84337	-1.08607
H	1.02538	-0.89368	0.66216
C	1.49214	-2.77256	-0.23280
H	1.27412	-3.33506	-1.14849
H	1.14759	-3.37167	0.61848
O	2.89184	-2.56081	-0.12800
C	-5.24620	0.35616	1.17700
H	-4.51677	0.59505	1.95372
H	-5.51351	1.28243	0.66467
H	-6.14345	-0.03207	1.66427
C	-5.78077	-1.30064	-1.35510
H	-5.36637	-2.02317	-2.06079
H	-6.68783	-1.73057	-0.92473
H	-6.06334	-0.40427	-1.91065
C	-4.02379	-2.42918	0.90034
H	-4.88898	-2.89824	1.37479
H	-3.57080	-3.15901	0.22690
H	-3.30192	-2.19405	1.68595
C	3.61493	-3.77380	-0.07806
H	3.30703	-4.36420	0.79235
H	3.42419	-4.36777	-0.97911
C	5.08535	-3.43545	0.01936
H	5.26716	-2.83469	0.91406
H	5.39088	-2.85719	-0.85623
O	5.80233	-4.66297	0.08562
H	6.73672	-4.45923	0.15551
H	0.06730	1.01136	1.94034

O	0.93730	1.17073	2.34609
H	0.84302	2.00738	2.80834
H	1.90813	1.65374	0.88459

assist_TS1h-IRC_react.log Energy: -1129007.7952785

Si	0.94451	-0.38959	1.08247
O	-1.80589	3.17154	-1.00882
O	1.06636	0.92512	0.08222
H	-1.06420	3.60841	-0.58437
Si	2.10405	2.23956	0.05984
C	1.53815	3.45362	1.35423
H	2.12605	4.37271	1.30021
H	0.48773	3.71577	1.20960
H	1.65040	3.04059	2.35833
C	1.96233	2.96161	-1.64831
H	0.94730	3.31295	-1.84400
H	2.64055	3.81007	-1.76218
H	2.21955	2.21814	-2.40552
C	3.84270	1.66462	0.40529
H	4.19308	0.98014	-0.36905
H	4.51912	2.52240	0.42796
H	3.91294	1.15672	1.36905
C	0.91637	0.15501	2.85295
H	1.86564	0.61532	3.13391
H	0.12037	0.88183	3.02287
H	0.74560	-0.69806	3.51256
C	-0.60093	-1.27565	0.54826
H	-0.49808	-1.50114	-0.51919
H	-0.65474	-2.23976	1.06159
O	2.26114	-1.35262	0.87487
Si	2.86804	-2.16222	-0.45359
C	-1.88168	-0.47227	0.79414
H	-2.06240	-0.37581	1.86705
H	-1.78195	0.53957	0.39313
C	-3.07957	-1.13158	0.14628
H	-3.20449	-2.15408	0.52238
H	-2.93601	-1.19033	-0.94006
O	-4.24576	-0.37510	0.43009
C	2.47342	-1.22194	-2.01599
H	1.39605	-1.11669	-2.15715

H	2.91559	-0.22468	-2.01100
H	2.87161	-1.76357	-2.87761
C	4.70720	-2.28347	-0.20045
H	4.94204	-2.82651	0.71718
H	5.17849	-2.80869	-1.03404
H	5.15218	-1.28868	-0.13085
C	2.07329	-3.84664	-0.51387
H	2.47139	-4.43308	-1.34498
H	2.25475	-4.40110	0.40894
H	0.99338	-3.75757	-0.65079
C	-5.39898	-0.92222	-0.17607
H	-5.28268	-0.94098	-1.26559
H	-5.55823	-1.95025	0.16855
C	-6.58047	-0.05909	0.20486
H	-6.41465	0.96596	-0.13624
H	-6.69645	-0.04988	1.29152
O	-7.73291	-0.61510	-0.41794
H	-8.49116	-0.08220	-0.17192
H	-1.41998	2.37975	-1.42262
O	-0.65498	0.86666	-2.18636
H	-1.29348	0.16841	-2.01870
H	-0.01229	0.78974	-1.46150

assist_TS1h.log Energy: -1128960.2935961

Si	-0.72296	-0.30596	-0.55706
O	-0.74105	-0.84223	1.32185
O	-0.68909	1.32363	0.20047
H	-0.33836	-1.70555	1.41853
Si	-1.60310	2.73500	-0.10433
C	-0.83167	3.72089	-1.47845
H	-1.23653	4.73568	-1.45683
H	0.24918	3.78998	-1.34114
H	-1.02768	3.29895	-2.46287
C	-1.49875	3.68898	1.49063
H	-0.46707	3.94421	1.73930
H	-2.05988	4.62089	1.39302
H	-1.92553	3.12458	2.32180
C	-3.36247	2.24829	-0.45002
H	-3.79031	1.74094	0.41602
H	-3.95428	3.14735	-0.63858

H	-3.45851	1.59396	-1.31594
C	-0.74814	0.44039	-2.32552
H	-1.62774	1.04419	-2.55702
H	0.13941	1.04918	-2.52051
H	-0.73810	-0.38961	-3.03790
C	0.93643	-1.21112	-0.74015
H	0.93266	-2.16081	-0.19727
H	1.07351	-1.45723	-1.79653
O	-2.16889	-1.11666	-0.76463
Si	-3.19967	-2.06864	0.11597
C	2.12214	-0.36260	-0.26932
H	2.14462	0.58810	-0.80919
H	2.02105	-0.12555	0.79173
C	3.43976	-1.07587	-0.48397
H	3.58094	-1.30703	-1.54650
H	3.45289	-2.02259	0.06935
O	4.50606	-0.25179	-0.03447
C	-4.11156	-1.07040	1.40388
H	-3.42660	-0.55821	2.07992
H	-4.75296	-0.32371	0.93153
H	-4.75086	-1.72653	2.00024
C	-4.43839	-2.71004	-1.12884
H	-3.95123	-3.32847	-1.88609
H	-5.20071	-3.31941	-0.63773
H	-4.94268	-1.88617	-1.63857
C	-2.33064	-3.53753	0.88431
H	-3.05092	-4.34116	1.05645
H	-1.55867	-3.92351	0.21456
H	-1.86510	-3.29790	1.84045
C	5.76440	-0.87568	-0.18834
H	5.80253	-1.80282	0.39494
H	5.93836	-1.12688	-1.24079
C	6.82585	0.08533	0.29749
H	6.63908	0.34418	1.34288
H	6.79709	1.00093	-0.29840
O	8.08472	-0.56385	0.15886
H	8.76839	0.04885	0.43565
H	-0.13970	0.06681	2.10797
O	0.25796	1.05085	2.37555
H	-0.31635	1.42705	3.04934

H	-0.19920	1.34805	1.28287

assist_TS2h-IRC-prod.log Energy: -872523.1261022

Si	-3.16282	-0.95071	-0.22167
O	-3.19430	-1.10852	1.44358
O	-0.37232	2.68920	0.97658
H	-3.00927	-1.98666	1.78505
Si	0.76946	2.54455	-0.23353
C	0.01346	1.78286	-1.76219
H	0.76403	1.70746	-2.55297
H	-0.37002	0.78067	-1.57002
H	-0.81024	2.39380	-2.13708
C	2.19503	1.49986	0.36035
H	2.93300	1.36854	-0.43444
H	2.69415	1.96727	1.21173
H	1.85363	0.50996	0.66652
C	1.31704	4.28592	-0.60355
H	1.77293	4.75179	0.27221
H	2.05431	4.28950	-1.40948
H	0.47385	4.90401	-0.91885
C	-3.27637	0.87326	-0.50111
H	-2.44259	1.39106	-0.02508
H	-3.25611	1.10143	-1.56769
H	-4.20441	1.26990	-0.08407
C	-1.63070	-1.74966	-0.90611
H	-1.81962	-2.80973	-1.09280
H	-1.43832	-1.29791	-1.88496
O	-4.44040	-1.75416	-0.91110
C	-0.40776	-1.58646	0.00283
H	-0.33269	-0.56334	0.37985
H	-0.50800	-2.23437	0.87577
C	0.87550	-1.91950	-0.72603
H	1.05291	-1.18085	-1.51698
H	0.81066	-2.90730	-1.19772
O	1.95517	-1.89815	0.19350
H	-5.30447	-1.35690	-0.78317
C	3.21261	-1.89530	-0.44890
H	3.27156	-1.06175	-1.15805
H	3.36336	-2.82833	-1.00392
C	4.27713	-1.73945	0.61310

H	4.21208	-2.56259	1.32930
H	4.12495	-0.79831	1.14810
O	5.53872	-1.74515	-0.04543
H	6.22157	-1.61660	0.61528
H	-1.88805	0.00465	2.23608
O	-1.21670	0.58607	2.62965
H	-0.63681	1.87915	1.44557
H	-1.69262	1.10812	3.28002

assist_TS2h-IRC-react.log Energy: -872495.1339339

Si	-1.91040	-1.35978	-0.22086
O	-2.05757	-1.74293	1.62503
O	-1.82263	0.29412	0.41767
H	-1.86914	-2.67169	1.79737
Si	-1.80934	1.81371	-0.21598
C	-0.91068	1.89052	-1.85521
H	-0.92099	2.91774	-2.22859
H	0.13184	1.58302	-1.74950
H	-1.37860	1.25683	-2.61068
C	-0.90787	2.90448	1.00869
H	-0.87306	3.93444	0.64612
H	-1.40644	2.91043	1.98085
H	0.12119	2.56780	1.15574
C	-3.54976	2.46518	-0.43070
H	-4.11780	2.36816	0.49723
H	-3.52337	3.52479	-0.69714
H	-4.09119	1.93602	-1.21611
C	-3.41911	-0.99241	-1.29286
H	-4.25953	-0.70027	-0.65787
H	-3.22020	-0.14991	-1.95757
H	-3.73050	-1.83892	-1.90444
C	-0.15969	-1.39248	-0.92390
H	0.08886	-2.41157	-1.22379
H	-0.20046	-0.80594	-1.84880
O	-2.09917	-3.12863	-0.33237
C	0.95475	-0.83577	-0.03640
H	0.71910	0.17953	0.28504
H	1.05774	-1.44023	0.86844
C	2.27962	-0.81251	-0.76706
H	2.20323	-0.18625	-1.66467

H	2.56363	-1.82206	-1.08736
O	3.28537	-0.28899	0.08897
H	-3.02069	-3.39099	-0.34937
C	4.54501	-0.21994	-0.54697
H	4.48961	0.42504	-1.43135
H	4.86292	-1.21738	-0.87139
C	5.53929	0.34433	0.44256
H	5.60013	-0.30662	1.31830
H	5.21488	1.33614	0.76777
O	6.79877	0.41918	-0.21589
H	7.44201	0.75982	0.40818
H	-1.56601	-1.15754	2.25786
O	-0.66019	0.05964	2.95950
H	-0.82287	0.49902	2.10829
H	-1.20392	0.53805	3.59118

assist_TS2h.log Energy: -872489.1591778

Si	-1.92251	-1.41523	-0.19646
O	-2.11097	-1.80218	1.51609
O	-1.76107	0.36583	0.45837
H	-2.01080	-2.74598	1.65917
Si	-1.71090	1.87843	-0.19991
C	-0.81712	1.91203	-1.84233
H	-0.81301	2.93372	-2.23094
H	0.22043	1.58793	-1.73917
H	-1.30254	1.27588	-2.58468
C	-0.78104	2.95158	1.01921
H	-0.70189	3.97673	0.65042
H	-1.28772	2.98290	1.98663
H	0.23105	2.57268	1.17928
C	-3.43317	2.57100	-0.43203
H	-4.01318	2.49387	0.49026
H	-3.37856	3.62766	-0.70601
H	-3.97788	2.04879	-1.21990
C	-3.45241	-0.90047	-1.16973
H	-4.17395	-0.41001	-0.51440
H	-3.17435	-0.17276	-1.93600
H	-3.94619	-1.73339	-1.67028
C	-0.16823	-1.36721	-0.90118
H	0.09089	-2.36902	-1.24770

H	-0.21749	-0.74259	-1.79932
O	-2.08032	-3.16001	-0.54965
C	0.95018	-0.84722	0.00301
H	0.72080	0.15549	0.36363
H	1.05504	-1.48669	0.88342
C	2.27241	-0.80305	-0.73172
H	2.19528	-0.14501	-1.60631
H	2.55149	-1.80155	-1.08889
O	3.28436	-0.31428	0.13782
H	-2.99631	-3.44132	-0.53631
C	4.54228	-0.23251	-0.49994
H	4.48861	0.44288	-1.36148
H	4.85166	-1.22048	-0.85965
C	5.54448	0.28972	0.50459
H	5.60400	-0.39186	1.35679
H	5.22879	1.27194	0.86559
O	6.80191	0.37818	-0.15617
H	7.45273	0.68071	0.47957
H	-1.54793	-1.02535	2.36637
O	-1.05200	-0.08931	2.76743
H	-1.25304	0.36691	1.85199
H	-1.62772	0.31411	3.42664

TS1h-IRC-prod.log Energy: -1081024.1755810

Si	-0.11177	0.23831	0.62192
O	-0.60168	-0.70881	-0.66606
O	-2.39031	-2.80775	-0.16204
H	-0.64097	-0.29441	-1.53057
Si	-3.91978	-2.12643	-0.19722
H	-1.69871	-2.15375	-0.35335
C	-5.09726	-3.50806	0.21356
H	-6.12764	-3.14584	0.19962
H	-5.01790	-4.32201	-0.50970
H	-4.89751	-3.91303	1.20758
C	-4.24809	-1.45250	-1.90683
H	-5.18686	-0.89508	-1.93706
H	-3.44734	-0.77939	-2.21859
H	-4.31130	-2.26268	-2.63640
C	-4.03431	-0.76194	1.07081
H	-3.27032	-0.00077	0.90702

H	-5.01039	-0.27359	1.01782
H	-3.90898	-1.15637	2.08134
C	-0.25869	-0.86805	2.09540
H	-1.30067	-1.14247	2.26805
H	0.31870	-1.78325	1.95613
H	0.11376	-0.36562	2.98999
C	1.61563	0.86039	0.31798
H	1.62134	1.41564	-0.62486
H	1.85290	1.58727	1.10112
O	-1.12990	1.51198	0.81090
Si	-1.74009	2.73713	-0.14245
C	2.67789	-0.24136	0.28387
H	2.68323	-0.79303	1.22693
H	2.45146	-0.96052	-0.50671
C	4.05872	0.33059	0.04428
H	4.32450	1.03080	0.84517
H	4.08312	0.88121	-0.90363
O	5.00608	-0.72554	0.00347
C	-2.89227	2.00234	-1.40938
H	-2.36660	1.29722	-2.05634
H	-3.72437	1.47852	-0.93636
H	-3.30593	2.79103	-2.04257
C	-2.65451	3.87990	1.00523
H	-1.98290	4.30609	1.75299
H	-3.10628	4.70331	0.44787
H	-3.45249	3.34753	1.52688
C	-0.33363	3.61600	-0.99444
H	0.41496	3.95676	-0.27673
H	0.15880	2.96417	-1.71889
H	-0.70869	4.48963	-1.53282
C	6.32174	-0.25691	-0.21204
H	6.37995	0.29071	-1.15948
H	6.62036	0.42225	0.59453
C	7.24254	-1.45558	-0.24880
H	6.94219	-2.12713	-1.05698
H	7.17971	-1.99934	0.69724
O	8.56384	-0.97256	-0.46330
H	9.15302	-1.72754	-0.51215

TS1h-IRC-react.log Energy: -1081029.6239885

Si	-0.92551	-0.22819	-1.07681
O	0.54967	0.22202	2.45856
O	-1.05106	0.89794	0.13115
H	1.20701	-0.39659	2.13063
Si	-1.59903	2.47742	0.21621
H	0.00599	0.42919	1.68350
C	-0.40424	3.56593	-0.70954
H	-0.64635	4.61932	-0.55095
H	0.61808	3.39837	-0.36425
H	-0.43871	3.37101	-1.78272
C	-1.62974	2.89829	2.02786
H	-2.05158	3.89402	2.18090
H	-2.24303	2.18288	2.57973
H	-0.62512	2.88915	2.45417
C	-3.30718	2.59705	-0.51821
H	-4.02826	2.01813	0.06004
H	-3.63520	3.63941	-0.51857
H	-3.33018	2.24133	-1.54975
C	-0.90757	0.56433	-2.75250
H	-1.81717	1.13331	-2.94904
H	-0.05319	1.23556	-2.85318
H	-0.81988	-0.20775	-3.51999
C	0.64585	-1.16323	-0.73353
H	0.54844	-1.63913	0.24663
H	0.74571	-1.97516	-1.45945
O	-2.22733	-1.22992	-0.99559
Si	-3.03106	-1.95370	0.27678
C	1.89219	-0.27261	-0.75987
H	2.08153	0.08138	-1.77573
H	1.74146	0.61171	-0.13527
C	3.10965	-1.01750	-0.25784
H	3.29248	-1.90879	-0.86984
H	2.94862	-1.34893	0.77582
O	4.24311	-0.16508	-0.31028
C	-4.07264	-0.68405	1.15696
H	-3.45041	0.09187	1.60615
H	-4.77850	-0.20810	0.47419
H	-4.64599	-1.16081	1.95572
C	-4.10086	-3.27864	-0.47402
H	-3.49550	-4.02153	-0.99717

H	-4.67241	-3.79400	0.30099
H	-4.80886	-2.85223	-1.18751
C	-1.79750	-2.69100	1.46522
H	-1.14236	-3.40793	0.96695
H	-1.17643	-1.91877	1.92385
H	-2.32454	-3.21507	2.26620
C	5.41455	-0.80740	0.15072
H	5.28680	-1.13010	1.19022
H	5.62691	-1.69324	-0.45845
C	6.55868	0.17594	0.04991
H	6.34591	1.05582	0.66236
H	6.68082	0.49542	-0.98807
O	7.73037	-0.48652	0.51213
H	8.46717	0.12245	0.43665

TS1h.log Energy: -1080983.9841580

Si	0.72958	-0.20974	0.54075
O	0.81091	-0.46985	-1.46834
O	0.75009	1.44153	-0.28269
H	-0.00949	-0.84152	-1.79521
Si	1.76478	2.82827	-0.15629
H	0.74451	0.89951	-1.19665
C	1.06416	3.90956	1.17607
H	1.58321	4.87093	1.17155
H	0.00350	4.09946	1.00314
H	1.18142	3.46783	2.16520
C	1.64438	3.60902	-1.83470
H	2.26545	4.50592	-1.88060
H	1.98831	2.92001	-2.60851
H	0.61615	3.89620	-2.06077
C	3.48446	2.23309	0.20865
H	3.82655	1.55254	-0.57345
H	4.17183	3.08139	0.24353
H	3.53898	1.71379	1.16616
C	0.72093	0.57374	2.26813
H	1.62137	1.15461	2.47862
H	-0.14377	1.22686	2.41066
H	0.66448	-0.22054	3.01696
C	-0.91364	-1.12616	0.56983
H	-0.87885	-1.99550	-0.09141

H	-1.05677	-1.50398	1.58648
O	2.14754	-1.04351	0.69532
Si	2.99278	-2.18937	-0.16300
C	-2.10011	-0.23183	0.19305
H	-2.13822	0.64296	0.84733
H	-1.98716	0.13842	-0.82905
C	-3.41242	-0.97837	0.29952
H	-3.56501	-1.33448	1.32523
H	-3.40700	-1.85322	-0.36157
O	-4.47959	-0.11589	-0.06578
C	4.02472	-1.38096	-1.49012
H	3.41061	-0.85763	-2.22252
H	4.71936	-0.66336	-1.04794
H	4.61669	-2.13436	-2.01590
C	4.13612	-2.98015	1.08465
H	3.57154	-3.46663	1.88298
H	4.76319	-3.73691	0.60743
H	4.79437	-2.23675	1.53942
C	1.85885	-3.50281	-0.85175
H	1.20609	-3.89258	-0.06732
H	1.23476	-3.12512	-1.66095
H	2.44991	-4.33786	-1.23612
C	-5.73648	-0.75582	0.02214
H	-5.76760	-1.62544	-0.64409
H	-5.91504	-1.10319	1.04607
C	-6.79908	0.24241	-0.37854
H	-6.61801	0.58548	-1.40034
H	-6.76568	1.10639	0.28996
O	-8.05776	-0.41519	-0.28578
H	-8.74051	0.21133	-0.53222

TS2h-IRC-prod.log Energy: -824544.2727721

Si	-1.97507	-2.16250	0.02361
O	-2.51660	-1.09000	1.16496
O	-1.40860	1.46565	1.32391
H	-2.11137	-0.20484	1.16465
Si	-1.62512	2.50670	0.01047
H	-1.84146	1.75192	2.13159
C	-0.26853	2.08541	-1.18681
H	-0.29443	2.77931	-2.03026

H	0.71352	2.16063	-0.71663
H	-0.38218	1.07579	-1.58263
C	-1.49167	4.25948	0.62301
H	-1.64569	4.96314	-0.19798
H	-2.24553	4.46561	1.38592
H	-0.50770	4.45251	1.05428
C	-3.30346	2.18684	-0.73097
H	-4.09550	2.40816	-0.01247
H	-3.46283	2.81367	-1.61131
H	-3.40293	1.14356	-1.03647
C	-2.38190	-1.55149	-1.68140
H	-3.46037	-1.44112	-1.81113
H	-1.91997	-0.57996	-1.86603
H	-2.01559	-2.24825	-2.43799
C	-0.16013	-2.50357	0.24288
H	0.00350	-2.85159	1.26737
H	0.12204	-3.32967	-0.41657
O	-2.75649	-3.59256	0.34180
C	0.71641	-1.28159	-0.04652
H	0.59177	-0.96906	-1.08569
H	0.41447	-0.43729	0.57787
C	2.18125	-1.56718	0.20188
H	2.52282	-2.39417	-0.43199
H	2.34185	-1.85687	1.24707
O	2.93756	-0.40147	-0.08884
H	-3.67943	-3.62716	0.08351
C	4.32057	-0.59001	0.12995
H	4.69955	-1.39878	-0.50514
H	4.50682	-0.86037	1.17548
C	5.02492	0.70561	-0.20402
H	4.64512	1.50718	0.43446
H	4.83440	0.97163	-1.24691
O	6.41633	0.50532	0.01662
H	6.86938	1.33057	-0.16587

TS2h-IRC-react.log Energy: -824548.1452586

Si	1.67106	1.54302	-0.11572
O	0.97922	-0.35442	3.06831
O	2.10594	0.04182	0.42956
H	1.24375	-1.24237	3.31870

Si	2.49913	-1.42475	-0.28014
H	1.35500	-0.23242	2.18383
C	1.06531	-2.02199	-1.30875
H	1.31860	-2.97636	-1.77697
H	0.17610	-2.17359	-0.69467
H	0.81708	-1.31568	-2.10292
C	2.82640	-2.59583	1.12857
H	3.18572	-3.55388	0.74637
H	3.58426	-2.19683	1.80544
H	1.91770	-2.78552	1.70306
C	4.02066	-1.21148	-1.33342
H	4.82370	-0.72950	-0.77246
H	4.38096	-2.18804	-1.66546
H	3.81429	-0.61210	-2.22115
C	1.98738	1.69849	-1.93692
H	3.05442	1.64022	-2.15833
H	1.47790	0.91711	-2.50304
H	1.62101	2.66426	-2.29059
C	-0.09864	1.83711	0.36100
H	-0.15429	1.94423	1.44839
H	-0.40997	2.79771	-0.06078
O	2.55310	2.67379	0.72144
C	-1.04190	0.72454	-0.10402
H	-0.95336	0.57129	-1.18287
H	-0.76936	-0.21806	0.37514
C	-2.48344	1.04407	0.22680
H	-2.79360	1.96881	-0.27401
H	-2.60215	1.19164	1.30685
O	-3.31157	-0.02693	-0.19981
H	3.47338	2.75830	0.46400
C	-4.67870	0.21670	0.06147
H	-5.01265	1.11564	-0.46904
H	-4.83889	0.37339	1.13418
C	-5.46504	-0.98549	-0.41023
H	-5.13705	-1.87711	0.12999
H	-5.29385	-1.14285	-1.47822
O	-6.84001	-0.72240	-0.15592
H	-7.34687	-1.48545	-0.43905

TS2h.log Energy: -824507.2706409

Si	1.71198	-1.54271	0.04688
O	1.60478	-1.45540	-1.96778
O	2.11086	0.14307	-0.48892
H	0.68855	-1.47052	-2.25034
Si	2.31833	1.77659	-0.00938
H	1.90824	-0.20189	-1.48861
C	0.77437	2.33717	0.85164
H	0.88843	3.38107	1.15411
H	-0.09366	2.26794	0.19479
H	0.58002	1.74760	1.74861
C	2.58531	2.66036	-1.61819
H	2.71380	3.73079	-1.44575
H	3.47757	2.28881	-2.12504
H	1.72979	2.52494	-2.28254
C	3.80073	1.86313	1.10150
H	4.65680	1.35262	0.65754
H	4.07430	2.90971	1.25570
H	3.59992	1.42187	2.07779
C	2.11656	-1.18761	1.86712
H	3.15674	-0.88981	2.01602
H	1.47816	-0.39653	2.26938
H	1.93707	-2.08359	2.46764
C	-0.11429	-1.97775	0.13759
H	-0.37106	-2.68353	-0.65635
H	-0.28431	-2.49302	1.08734
O	2.83111	-2.76090	-0.23664
C	-1.02791	-0.75050	0.05851
H	-0.81651	-0.07076	0.88675
H	-0.84243	-0.19506	-0.86477
C	-2.48952	-1.13956	0.10628
H	-2.71085	-1.68071	1.03390
H	-2.73516	-1.79980	-0.73395
O	-3.29065	0.03105	0.03785
H	3.30655	-2.98829	0.56484
C	-4.67232	-0.26526	0.05648
H	-4.93484	-0.79785	0.97756
H	-4.93532	-0.90379	-0.79445
C	-5.43090	1.04024	-0.02245
H	-5.16262	1.56836	-0.94094
H	-5.17078	1.67162	0.83091

O	-6.81919	0.72776	-0.01075
H	-7.31010	1.54954	-0.06605

TriSil-1n-aH-O2.log Energy: -1126997.7914981

C	0.76832	-0.29330	2.06521
H	0.80800	-1.36654	2.25709
O	0.99362	-0.72130	-0.76006
O	1.44050	1.71554	0.15496
Si	0.85999	-2.29586	-1.29193
Si	0.65975	2.54586	-1.07190
C	2.32069	-2.64707	-2.38984
H	3.25336	-2.54592	-1.83046
H	2.27421	-3.66235	-2.78956
H	2.35155	-1.95196	-3.23116
C	-0.75035	-2.37373	-2.21960
H	-0.91387	-3.36968	-2.63677
H	-1.58729	-2.14237	-1.55681
H	-0.75903	-1.65686	-3.04313
C	0.84592	-3.43958	0.17884
H	1.75967	-3.34024	0.76906
H	-0.00717	-3.23470	0.82844
H	0.77457	-4.47774	-0.15365
C	-1.10121	1.95484	-1.23747
H	-1.62917	1.99703	-0.28301
H	-1.63529	2.59468	-1.94436
H	-1.14334	0.93139	-1.61297
C	1.58956	2.26143	-2.66122
H	1.58173	1.20336	-2.93024
H	1.13114	2.82136	-3.47950
H	2.62878	2.58400	-2.57180
C	0.70439	4.33709	-0.57179
H	0.17801	4.49074	0.37243
H	1.73175	4.68582	-0.45036
H	0.22382	4.95822	-1.33077
C	-0.66358	0.21894	2.15382
H	-1.01831	0.10624	3.18006
H	-0.70252	1.27913	1.89818
C	-1.58453	-0.54918	1.22522
H	-1.23479	-0.48981	0.19356
H	-1.62220	-1.60761	1.50664

C	-3.73186	-0.48505	0.29768
H	-3.82770	-1.57303	0.38644
H	-3.31668	-0.25628	-0.69055
C	-5.08410	0.17170	0.45506
H	-5.50153	-0.06645	1.43647
H	-4.97793	1.25670	0.37501
O	-2.88046	0.01801	1.30846
O	-5.91954	-0.32969	-0.58170
Si	1.69214	0.12714	0.44329
C	3.49410	-0.24836	0.58748
H	3.97730	0.37007	1.34454
H	3.65145	-1.29673	0.84770
H	3.98075	-0.05747	-0.37133
H	-6.79075	0.05658	-0.47734
O	1.48616	0.33911	3.17341
O	2.44860	-0.39241	3.65185

TriSil-1n-bH-O2.log Energy: -1127001.5936595

C	0.11289	1.72768	0.05203
H	0.24401	2.55328	-0.65503
H	0.91706	1.80781	0.78655
O	2.04619	0.26253	-1.35437
O	0.17043	-1.19807	-0.09856
Si	3.57494	0.23689	-0.70161
Si	0.08482	-1.81413	1.44428
C	4.73280	0.65951	-2.09760
H	4.51027	1.64793	-2.50470
H	5.76845	0.66272	-1.75074
H	4.65077	-0.06816	-2.90757
C	3.94641	-1.46776	-0.04563
H	5.00613	-1.54504	0.20959
H	3.37288	-1.68879	0.85465
H	3.72348	-2.23300	-0.79151
C	3.71475	1.50316	0.66043
H	3.43935	2.49766	0.30397
H	3.07864	1.25534	1.51184
H	4.74672	1.54776	1.01729
C	-1.70778	-1.96109	1.93129
H	-2.27214	-2.51189	1.17621
H	-1.79139	-2.50310	2.87653

H	-2.17349	-0.98349	2.06067
C	0.98674	-0.70211	2.64003
H	0.55679	0.30064	2.66748
H	0.91415	-1.12135	3.64679
H	2.04556	-0.61380	2.39340
C	0.86378	-3.50498	1.39132
H	0.31670	-4.15882	0.70875
H	1.90156	-3.45829	1.05746
H	0.84600	-3.96400	2.38234
C	-1.20622	1.89642	0.76056
H	-1.31629	1.21525	1.60307
C	-2.45181	1.81453	-0.10880
H	-3.27067	2.36497	0.36355
H	-2.26398	2.24408	-1.09896
C	-3.86924	0.20622	-1.07680
H	-3.66164	0.60479	-2.07621
H	-4.77330	0.69278	-0.69516
C	-4.05968	-1.29218	-1.14120
H	-3.13778	-1.76149	-1.49579
H	-4.28483	-1.67870	-0.14410
O	-2.77957	0.44835	-0.21223
O	-5.13464	-1.54862	-2.03607
Si	0.45819	0.17179	-0.94710
C	-0.46652	0.09416	-2.54825
H	-1.53603	-0.03641	-2.39522
H	-0.30840	1.00814	-3.12374
H	-0.10219	-0.74558	-3.14377
H	-5.27982	-2.49599	-2.06434
O	-1.15542	3.24606	1.35379
O	-2.03383	3.41472	2.29550

TriSil-1n-cH-O2.log Energy: -1127004.6582589

C	-0.15323	-0.68715	0.27014
H	-0.12439	-1.76370	0.45868
H	-0.04455	-0.55663	-0.80876
O	2.70587	-0.36971	0.35385
O	1.22126	1.72863	0.99826
Si	3.22483	-1.73846	-0.44075
Si	1.39779	2.76062	-0.30213
C	2.79038	-3.23371	0.58590

H	1.70981	-3.32326	0.71725
H	3.14429	-4.14646	0.10116
H	3.25104	-3.17656	1.57417
C	5.06788	-1.56290	-0.62768
H	5.48722	-2.42661	-1.14818
H	5.31575	-0.66897	-1.20384
H	5.55474	-1.48572	0.34643
C	2.40425	-1.82787	-2.11200
H	1.32860	-1.98768	-2.02236
H	2.56907	-0.90779	-2.67645
H	2.81953	-2.65625	-2.69103
C	0.49170	4.32364	0.14521
H	0.89942	4.76665	1.05605
H	0.57779	5.06078	-0.65608
H	-0.56943	4.12474	0.30866
C	0.65704	1.98811	-1.83113
H	-0.39599	1.74070	-1.68227
H	0.72361	2.69003	-2.66592
H	1.18760	1.07775	-2.11802
C	3.21279	3.08838	-0.56651
H	3.67315	3.49800	0.33480
H	3.73853	2.16864	-0.82981
H	3.35936	3.80632	-1.37669
C	-1.48675	-0.10045	0.72846
H	-1.65779	-0.27477	1.79292
H	-1.50402	0.97946	0.57038
C	-2.66282	-0.65138	-0.03770
H	-2.54875	-0.57146	-1.12031
C	-4.96005	-0.30485	-0.43123
H	-5.17915	-1.37116	-0.51561
H	-4.74441	0.09461	-1.42529
C	-6.12752	0.42317	0.19349
H	-6.32501	0.01816	1.18888
H	-5.89097	1.48571	0.28920
O	-3.83377	-0.09684	0.42100
O	-7.24662	0.23032	-0.66126
Si	1.32126	0.09027	1.11410
C	1.39310	-0.36089	2.90855
H	0.49314	-0.03170	3.43148
H	1.47224	-1.44450	3.01931

H	2.25697	0.09580	3.39466
H	-8.00129	0.67271	-0.26822
O	-2.74324	-2.11068	0.22919
O	-2.54739	-2.83489	-0.83170

TriSil-1n-dH-O2.log Energy: -1127003.6173775

C	-0.07116	-1.16938	0.25344
H	-0.10617	-2.25747	0.35683
H	0.04494	-0.96645	-0.81538
O	2.74908	-1.44058	0.67679
O	1.73068	1.02632	0.73266
Si	3.90546	-1.27985	-0.51192
Si	1.23197	2.30297	-0.20310
C	4.75391	-2.93227	-0.63883
H	4.05067	-3.71247	-0.93705
H	5.55289	-2.89608	-1.38269
H	5.19637	-3.21960	0.31714
C	5.11608	0.04771	-0.01630
H	5.88190	0.17366	-0.78523
H	4.61198	1.00591	0.11885
H	5.61754	-0.20920	0.91906
C	3.08897	-0.83862	-2.13014
H	2.26103	-1.51407	-2.35449
H	2.70672	0.18241	-2.11861
H	3.81281	-0.91085	-2.94545
C	0.28939	3.47443	0.89712
H	0.90651	3.81725	1.72991
H	-0.04080	4.35170	0.33638
H	-0.59613	2.98488	1.30882
C	0.13651	1.75745	-1.61292
H	-0.82778	1.38601	-1.26381
H	-0.05573	2.62054	-2.25586
H	0.60171	0.98395	-2.22527
C	2.77440	3.10379	-0.87483
H	3.44246	3.40801	-0.06667
H	3.31962	2.41864	-1.52724
H	2.52106	3.99319	-1.45641
C	-1.37349	-0.55562	0.77709
H	-1.57915	-0.92135	1.78491
H	-1.29659	0.53281	0.84532

C	-2.53653	-0.89859	-0.12291
H	-2.38040	-0.49651	-1.12771
H	-2.66447	-1.98089	-0.19470
C	-4.84368	-0.46242	-0.34577
C	-5.92514	0.49983	0.08522
H	-6.85131	0.22892	-0.42495
H	-6.06974	0.41161	1.16473
O	-3.72870	-0.31187	0.42595
O	-5.49978	1.80100	-0.27741
Si	1.44743	-0.54130	1.13096
C	1.27860	-0.65856	2.97291
H	0.43998	-0.05277	3.32146
H	1.10376	-1.69026	3.28428
H	2.18392	-0.30173	3.46762
H	-6.16562	2.42384	0.02117
H	-4.63942	-0.41625	-1.41704
O	-5.35292	-1.83297	-0.09373
O	-6.06055	-2.28307	-1.08494

TriSil-1n-eH-O2.log Energy: -1127004.6252519

C	0.25836	-1.15050	0.35986
H	0.32530	-2.21980	0.58444
H	0.42337	-1.05546	-0.71556
O	3.08943	-0.94437	0.80411
O	1.64412	1.31623	0.97425
Si	3.94038	-1.31738	-0.57563
Si	1.23389	2.41752	-0.20171
C	5.31407	-2.45427	-0.03923
H	4.91438	-3.36782	0.40567
H	5.93377	-2.73737	-0.89283
H	5.95697	-1.96992	0.69858
C	4.63462	0.24547	-1.31680
H	5.32892	-0.00046	-2.12404
H	3.84529	0.86973	-1.73774
H	5.17714	0.83074	-0.57213
C	2.83641	-2.16760	-1.81556
H	2.31331	-3.01628	-1.37112
H	2.09343	-1.48212	-2.22681
H	3.44076	-2.54119	-2.64596
C	-0.21201	3.41518	0.42100

H 0.03633 3.92226 1.35559
H -0.49095 4.17694 -0.31083
H -1.08459 2.78352 0.59782
C 0.77081 1.54853 -1.78717
H -0.17115 1.00689 -1.68267
H 0.64434 2.28792 -2.58187
H 1.53926 0.84237 -2.10697
C 2.70535 3.53085 -0.45930
H 2.96412 4.04712 0.46761
H 3.58059 2.97019 -0.79071
H 2.48211 4.28827 -1.21421
C -1.13428 -0.62868 0.72006
H -1.33682 -0.78432 1.78217
H -1.19977 0.44630 0.53704
C -2.20507 -1.32040 -0.09377
H -2.03497 -1.15497 -1.16395
H -2.18803 -2.40109 0.08793
C -4.51917 -1.40823 -0.46089
H -4.57340 -2.48040 -0.25129
H -4.38170 -1.27036 -1.53918
C -5.82607 -0.79088 -0.03851
H -5.96101 -0.76713 1.04151
O -3.47913 -0.80053 0.26692
O -6.86336 -1.41606 -0.69934
Si 1.64920 -0.30266 1.26813
C 1.50787 -0.52434 3.10302
H 0.57991 -0.08617 3.47513
H 1.51303 -1.58331 3.36801
H 2.34052 -0.04043 3.61713
H -7.68647 -1.23584 -0.23666
O -5.75790 0.62176 -0.45913
O -6.71290 1.32128 0.07802

gas_hydroxyl_radical.log Energy: -47525.1728309
O 0.00000 0.00000 0.10773
H 0.00000 0.00000 -0.86187

gas_H_radical.log Energy: -315.4291426
H 0.00000 0.00000 0.00000
53

gas_TriSil-1n-aH-OH-IRC-forward-reactant.log Energy: -1080600.5846011

C	-0.33323	-1.12335	1.59856
H	-0.21479	-2.19890	1.71618
H	-0.46522	-2.65164	-1.24103
O	1.91457	-0.71462	-0.03337
O	0.68043	1.44509	0.97642
Si	3.46080	-1.00972	-0.58441
Si	0.19247	2.34650	-0.33000
C	4.59310	0.39910	-0.11527
H	4.78999	0.42412	0.95663
H	5.55229	0.29028	-0.62545
H	4.16578	1.35855	-0.40844
C	3.33439	-1.16740	-2.43428
H	4.29220	-1.47004	-2.86151
H	2.58462	-1.91055	-2.70933
H	3.04778	-0.22023	-2.89339
C	4.05272	-2.60340	0.18508
H	4.08315	-2.52577	1.27317
H	3.39098	-3.42979	-0.07841
H	5.05755	-2.85433	-0.15956
C	-1.16737	1.46966	-1.25769
H	-2.06244	1.35548	-0.64351
H	-1.44418	2.04706	-2.14250
H	-0.85228	0.47954	-1.59367
C	1.65874	2.61412	-1.45534
H	2.02420	1.66077	-1.83857
H	1.38493	3.23654	-2.30911
H	2.47524	3.10801	-0.92637
C	-0.41709	3.96754	0.35871
H	-1.25621	3.80632	1.03707
H	0.37210	4.47690	0.91329
H	-0.75242	4.63065	-0.44081
C	-1.73194	-0.61532	1.69390
H	-2.16053	-0.85235	2.67461
H	-1.76183	0.46913	1.58810
C	-2.63591	-1.22681	0.62903
H	-2.20219	-1.07112	-0.36505
H	-2.72915	-2.31062	0.78827
C	-4.77741	-1.04188	-0.30107
H	-4.96755	-2.11952	-0.22355

H	-4.35459	-0.84440	-1.29334
C	-6.07639	-0.28331	-0.13738
H	-6.48059	-0.47308	0.86160
H	-5.88044	0.78904	-0.23209
O	-3.89950	-0.61250	0.70987
O	-6.95674	-0.74067	-1.14782
Si	1.15429	-0.08255	1.29158
C	2.31155	-0.04747	2.74603
H	1.77948	0.29677	3.63359
H	2.71474	-1.03872	2.95882
H	3.14284	0.63541	2.56949
H	-7.78255	-0.26513	-1.07969
O	-0.02257	-1.98568	-1.76580
H	0.60670	-1.56961	-1.16181

gas_TriSil-1n-aH-OH-opt-product.log Energy: -1080600.5846011

C	-0.33382	-1.12244	1.59835
H	-0.21582	-2.19805	1.71596
H	-0.46710	-2.65144	-1.23832
O	1.91442	-0.71478	-0.03307
O	0.68107	1.44557	0.97637
Si	3.46053	-1.01023	-0.58423
Si	0.19361	2.34668	-0.33045
C	4.59334	0.39794	-0.11435
H	4.79026	0.42226	0.95756
H	5.55247	0.28909	-0.62461
H	4.16634	1.35772	-0.40693
C	3.33414	-1.16714	-2.43418
H	4.29185	-1.47002	-2.86146
H	2.58412	-1.90995	-2.70946
H	3.04792	-0.21971	-2.89300
C	4.05176	-2.60450	0.18456
H	4.08196	-2.52746	1.27270
H	3.38979	-3.43051	-0.07954
H	5.05658	-2.85560	-0.15999
C	-1.16542	1.46928	-1.25881
H	-2.06101	1.35547	-0.64533
H	-1.44150	2.04614	-2.14419
H	-0.85006	0.47896	-1.59394
C	1.66047	2.61459	-1.45495

H	2.02611	1.66133	-1.83823
H	1.38711	3.23721	-2.30870
H	2.47670	3.10832	-0.92542
C	-0.41687	3.96762	0.35769
H	-1.25630	3.80621	1.03562
H	0.37185	4.47732	0.91264
H	-0.75197	4.63051	-0.44210
C	-1.73237	-0.61391	1.69330
H	-2.16107	-0.85026	2.67414
H	-1.76195	0.47048	1.58690
C	-2.63648	-1.22581	0.62879
H	-2.20288	-1.07046	-0.36542
H	-2.72966	-2.30957	0.78845
C	-4.77817	-1.04150	-0.30097
H	-4.96815	-2.11912	-0.22289
H	-4.35562	-0.84445	-1.29345
C	-6.07721	-0.28301	-0.13734
H	-6.48116	-0.47238	0.86181
H	-5.88141	0.78932	-0.23256
O	-3.90006	-0.61151	0.70954
O	-6.95771	-0.74092	-1.14739
Si	1.15422	-0.08226	1.29169
C	2.31122	-0.04769	2.74635
H	1.77912	0.29655	3.63389
H	2.71411	-1.03910	2.95902
H	3.14274	0.63497	2.57004
H	-7.78359	-0.26550	-1.07926
O	-0.02236	-1.98793	-1.76445
H	0.60657	-1.57105	-1.16069

gas_TriSil-1n-aH-OH-radical.log Energy: -1032629.8713741

C	0.53530	-0.30162	2.38992
H	0.86325	-0.99652	3.15623
O	1.57637	-0.57504	-0.27564
O	1.24075	1.83219	0.69642
Si	1.57811	-2.13806	-0.80486
Si	0.59720	2.53335	-0.66197
C	3.24031	-2.49034	-1.57573
H	4.03973	-2.37125	-0.84240
H	3.28894	-3.50910	-1.96452

H	3.43772	-1.80427	-2.40069
C	0.21561	-2.29183	-2.06993
H	0.19857	-3.28897	-2.51336
H	-0.76151	-2.10996	-1.61898
H	0.35383	-1.56799	-2.87477
C	1.27396	-3.29731	0.63019
H	2.04578	-3.19136	1.39495
H	0.30920	-3.09791	1.09874
H	1.27809	-4.33612	0.29455
C	-0.94368	1.61977	-1.19609
H	-1.67533	1.55255	-0.38844
H	-1.41648	2.13198	-2.03661
H	-0.69197	0.60803	-1.51736
C	1.86523	2.48545	-2.03178
H	2.12881	1.45138	-2.25870
H	1.48103	2.94840	-2.94261
H	2.77526	3.01334	-1.74266
C	0.18140	4.28940	-0.19301
H	-0.54844	4.30955	0.61769
H	1.07179	4.82299	0.14219
H	-0.24019	4.83215	-1.04105
C	-0.92046	0.04095	2.35547
H	-1.39821	-0.09749	3.32619
H	-1.04710	1.08929	2.07199
C	-1.66768	-0.78701	1.31059
H	-1.11907	-0.76601	0.36223
H	-1.74162	-1.83554	1.62801
C	-3.64853	-0.84597	0.06948
H	-3.82335	-1.91006	0.27042
H	-3.07737	-0.76590	-0.86388
C	-4.97186	-0.12912	-0.08364
H	-5.52882	-0.19494	0.85584
H	-4.78314	0.92679	-0.30017
O	-2.95140	-0.24006	1.12936
O	-5.66714	-0.75990	-1.14374
Si	1.70215	0.31758	1.10175
C	3.46125	0.29988	1.69210
H	3.59868	0.97055	2.54063
H	3.75699	-0.70433	2.00245
H	4.13108	0.61741	0.89190

H	-6.50412	-0.31784	-1.27342

gas_TriSil-1n-aH-OH-TS.log Energy: -1080575.3560598

C	-0.42292	-0.93927	0.28835
H	-0.32427	-2.02544	0.36560
H	-0.32303	-0.75301	-0.86584
O	2.30899	-0.42105	-0.07648
O	0.83819	1.54262	0.94846
Si	3.41895	-1.63701	-0.28355
Si	0.74477	2.79051	-0.14598
C	4.73351	-1.49990	1.03306
H	4.30874	-1.63460	2.02890
H	5.50495	-2.25934	0.89300
H	5.21424	-0.52118	1.00061
C	4.13794	-1.38947	-1.98408
H	4.91674	-2.12449	-2.19418
H	3.36931	-1.49208	-2.75234
H	4.57742	-0.39516	-2.07549
C	2.53504	-3.27886	-0.16847
H	2.09551	-3.42690	0.81996
H	1.73324	-3.33278	-0.90713
H	3.22018	-4.10811	-0.35292
C	-0.86206	2.66931	-1.08410
H	-1.72110	2.75035	-0.41630
H	-0.93448	3.47364	-1.81911
H	-0.92340	1.71975	-1.61886
C	2.19095	2.69028	-1.32294
H	2.14497	1.78191	-1.92402
H	2.19287	3.54555	-2.00135
H	3.13594	2.68446	-0.77829
C	0.81780	4.36166	0.85439
H	-0.00382	4.40176	1.57089
H	1.75401	4.42575	1.41059
H	0.74633	5.23925	0.20930
C	-1.79229	-0.46102	0.73514
H	-1.95339	-0.74140	1.78074
H	-1.85123	0.62635	0.68973
C	-2.91165	-1.04840	-0.10176
H	-2.78565	-0.75150	-1.15105
H	-2.87975	-2.14621	-0.06451

C	-5.24244	-1.04612	-0.34732
H	-5.29319	-2.14188	-0.32872
H	-5.16903	-0.73097	-1.39522
C	-6.49607	-0.46837	0.27268
H	-6.55609	-0.78039	1.31977
H	-6.44214	0.62397	0.24093
O	-4.14318	-0.58158	0.39432
O	-7.59508	-0.95503	-0.47645
Si	1.08407	-0.06406	0.96271
C	1.49206	-0.58718	2.69722
H	0.66430	-0.35092	3.36713
H	1.67969	-1.66050	2.75735
H	2.37738	-0.06191	3.05736
H	-8.40209	-0.59212	-0.11625
O	0.13132	-0.59083	-2.22523
H	1.05678	-0.46289	-1.96468

gas_TriSil-1n-bH-OH-opt-product_re.log Energy: -1080603.6326907

C	-0.11657	-2.26891	0.68824
H	0.45794	-3.14751	1.01620
H	-0.27661	-2.37672	-0.38708
O	2.47676	-1.22359	0.26094
O	0.47155	0.51120	0.23942
Si	3.44039	-0.53280	-0.89948
Si	0.03774	2.09721	0.47750
C	4.83294	-1.73184	-1.20769
H	4.44849	-2.68436	-1.57490
H	5.52977	-1.33991	-1.95074
H	5.38953	-1.92455	-0.28956
C	4.09976	1.09016	-0.24583
H	4.77116	1.56056	-0.96653
H	3.28282	1.78594	-0.04907
H	4.65225	0.94355	0.68358
C	2.45257	-0.24087	-2.45531
H	1.94052	-1.14971	-2.77479
H	1.69945	0.53198	-2.29977
H	3.10132	0.08318	-3.27136
C	-1.79742	2.16216	0.77642
H	-2.09069	1.50429	1.59545
H	-2.12357	3.17717	1.01096

H	-2.32343	1.82641	-0.11714
C	0.47705	2.99158	-1.09766
H	-0.04363	2.53883	-1.94357
H	0.18330	4.04153	-1.04585
H	1.54901	2.95174	-1.29681
C	0.97557	2.81123	1.92775
H	0.67192	2.35209	2.86898
H	2.05276	2.67731	1.81702
H	0.77948	3.88280	2.00165
C	-1.39981	-2.17472	1.41930
H	-1.38369	-2.04442	2.49421
H	-0.55860	-0.02611	-1.50588
C	-2.71930	-2.25141	0.74982
H	-2.68197	-2.95216	-0.09430
H	-3.48576	-2.60090	1.44982
C	-4.40715	-1.00263	-0.33040
H	-5.15139	-1.31308	0.41126
H	-4.43724	-1.71436	-1.16312
C	-4.73510	0.38660	-0.83376
H	-4.67347	1.09568	-0.00246
H	-4.00465	0.67790	-1.59462
O	-3.11855	-0.96775	0.25023
O	-6.04552	0.32877	-1.36724
Si	1.05964	-0.83323	0.97269
C	1.33431	-0.54801	2.78847
H	0.41586	-0.23730	3.28867
H	1.68511	-1.46630	3.26182
H	2.08867	0.22234	2.94957
H	-6.23561	1.15220	-1.81293
O	-1.38267	-0.28764	-1.92409
H	-1.95144	-0.49249	-1.16884

gas_TriSil-1n-bH-OH-opt-reactant-re.log Energy: -1080580.3591928

C	-0.15210	-1.18552	0.39178
H	-0.12086	-2.24221	0.67605
H	0.04220	-1.15523	-0.68347
O	2.67428	-0.75551	0.64610
O	1.02916	1.32387	1.05790
Si	3.54037	-1.44369	-0.57409
Si	1.03258	2.41147	-0.19000

C	4.72357	-2.66059	0.19833
H	4.18299	-3.44988	0.72295
H	5.35538	-3.12973	-0.55805
H	5.37285	-2.16240	0.91957
C	4.47998	-0.10277	-1.47026
H	5.11731	-0.53120	-2.24626
H	3.80380	0.60737	-1.94843
H	5.11741	0.45198	-0.78015
C	2.40808	-2.32890	-1.77159
H	1.78909	-3.06846	-1.26151
H	1.74610	-1.63610	-2.29326
H	3.00018	-2.85103	-2.52598
C	-0.30125	3.66307	0.14874
H	-0.14600	4.13760	1.11882
H	-0.30136	4.44589	-0.61240
H	-1.28885	3.19818	0.15023
C	0.67774	1.51546	-1.79741
H	-0.31660	1.06551	-1.78190
H	0.71371	2.21081	-2.63801
H	1.40667	0.72602	-1.98814
C	2.71447	3.21588	-0.26064
H	2.91726	3.76041	0.66273
H	3.49712	2.46707	-0.38683
H	2.78097	3.92191	-1.09046
C	-1.53227	-0.59287	0.68221
H	-1.75862	-0.63966	1.74979
H	-1.54703	0.46441	0.40900
C	-2.62805	-1.30907	-0.07875
H	-2.42092	-1.28759	-1.15632
H	-2.68784	-2.35997	0.22806
C	-4.96159	-1.30705	-0.45611
H	-5.04690	-2.34428	-0.11589
H	-4.82494	-1.31403	-1.54303
C	-6.22042	-0.54541	-0.09936
H	-6.33508	-0.52975	0.98887
H	-6.13535	0.48692	-0.45149
O	-3.86974	-0.67358	0.17868
O	-7.29459	-1.22126	-0.72467
Si	1.23775	-0.28353	1.26704
C	1.23969	-0.61645	3.09107

H	0.30120	-0.29731	3.54621
H	1.37842	-1.67874	3.29618
H	2.05021	-0.06851	3.57250
H	-8.10002	-0.72820	-0.57891
O	-3.76172	2.11731	-0.14899
H	-3.79870	1.14938	0.01821

gas_TriSil-1n-bH-OH-radical.log Energy: -1032628.3516529

C	-0.26955	-0.83899	-1.50441
H	-0.25226	-1.93400	-1.52330
H	0.54576	-0.48768	-2.14165
O	1.67383	-0.78747	0.61883
O	0.10934	1.33068	0.33529
Si	3.00388	-1.66839	0.20994
Si	1.22398	2.52021	0.05126
C	2.94969	-3.28603	1.13841
H	2.06940	-3.86698	0.85790
H	3.83257	-3.89182	0.92622
H	2.90860	-3.11354	2.21474
C	4.49853	-0.66873	0.70680
H	5.42197	-1.20666	0.48483
H	4.52702	0.28277	0.17305
H	4.48312	-0.45258	1.77612
C	3.04023	-1.99300	-1.63135
H	2.17877	-2.57866	-1.95468
H	3.04870	-1.06395	-2.20354
H	3.94079	-2.55225	-1.89316
C	0.27558	4.11061	-0.15678
H	-0.30822	4.32985	0.73820
H	0.94943	4.95038	-0.33604
H	-0.41452	4.04263	-0.99884
C	2.17148	2.11575	-1.51240
H	1.49605	2.00282	-2.36230
H	2.88404	2.90669	-1.75331
H	2.73155	1.18628	-1.39804
C	2.39758	2.61996	1.49812
H	1.86241	2.87274	2.41461
H	2.88968	1.65847	1.64901
H	3.16632	3.37766	1.33538
C	-1.57464	-0.31246	-1.95664

H	-1.62469	0.69246	-2.35507
C	-2.85914	-0.96716	-1.61483
H	-3.50346	-1.05517	-2.50163
H	-2.68367	-1.98213	-1.23329
C	-4.76176	-0.79705	-0.23830
H	-4.59277	-1.79957	0.17542
H	-5.44598	-0.89640	-1.09013
C	-5.38363	0.08911	0.81875
H	-4.69130	0.18192	1.66128
H	-5.55102	1.08579	0.39993
O	-3.54893	-0.20484	-0.62979
O	-6.60042	-0.51933	1.21285
Si	0.15047	-0.30107	0.26051
C	-1.04338	-0.99797	1.49052
H	-2.05148	-0.65380	1.25718
H	-1.03230	-2.08902	1.47036
H	-0.78294	-0.67356	2.49841
H	-7.01480	0.02044	1.88349

gas_TriSil-1n-bH-OH-TS.log Energy: -1080575.9104456

C	-0.36155	-1.05025	0.31573
H	-0.34875	-2.11810	0.56846
H	-0.18880	-0.99321	-0.76160
O	2.47429	-0.77830	0.57470
O	0.96905	1.38069	1.03621
Si	3.27400	-1.69097	-0.53966
Si	1.36018	2.44877	-0.17405
C	4.17094	-3.04979	0.37124
H	3.46744	-3.70031	0.89343
H	4.75291	-3.66665	-0.31597
H	4.85445	-2.63203	1.11169
C	4.48570	-0.58691	-1.42935
H	5.06064	-1.15566	-2.16265
H	3.97172	0.21834	-1.95643
H	5.18879	-0.13434	-0.72859
C	2.07782	-2.43449	-1.77056
H	1.33143	-3.06000	-1.27900
H	1.55346	-1.66528	-2.33963
H	2.62092	-3.05997	-2.48202
C	0.34492	3.98269	0.09506

H	0.56050	4.42341	1.06952
H	0.55581	4.73219	-0.67015
H	-0.71574	3.73319	0.05468
C	0.96282	1.66364	-1.82456
H	-0.10386	1.44177	-1.88609
H	1.21742	2.33535	-2.64646
H	1.52329	0.73755	-1.96737
C	3.18763	2.81576	-0.05390
H	3.42126	3.30304	0.89400
H	3.76591	1.89297	-0.10928
H	3.51457	3.47370	-0.86134
C	-1.72415	-0.46973	0.64284
H	-1.90412	-0.34052	1.71141
H	-1.75860	0.63464	0.21986
C	-2.87439	-1.19279	-0.01128
H	-2.68721	-1.29808	-1.08741
H	-2.97065	-2.20227	0.41222
C	-5.19541	-1.07412	-0.37526
H	-5.35985	-2.07001	0.05147
H	-5.06576	-1.18578	-1.45799
C	-6.39254	-0.19328	-0.09045
H	-6.50941	-0.08306	0.99177
H	-6.22253	0.79862	-0.52142
O	-4.06459	-0.46549	0.20347
O	-7.51631	-0.82402	-0.67368
Si	1.07073	-0.23540	1.21379
C	1.03101	-0.62218	3.02755
H	0.11889	-0.24180	3.48924
H	1.08318	-1.69763	3.20298
H	1.87943	-0.15460	3.52810
H	-8.29328	-0.29235	-0.51042
O	-2.27065	1.75189	-0.44935
H	-3.19306	1.46374	-0.36935

gas_TriSil-1n-cH-OH-opt-product.log Energy: -1080600.7135418

C	-0.48522	-0.24866	-0.06794
H	-0.61881	-1.33324	-0.11568
H	-0.29895	0.08596	-1.09287
O	2.30199	-0.73620	0.27524
O	1.41372	1.68416	0.88394

Si	2.53258	-2.21169	-0.44014
Si	2.29719	2.58758	-0.18980
C	1.62696	-3.52564	0.53121
H	0.54715	-3.36188	0.52685
H	1.81013	-4.51359	0.10430
H	1.96534	-3.54245	1.56879
C	4.37056	-2.52232	-0.43400
H	4.61064	-3.47518	-0.90903
H	4.89635	-1.73390	-0.97479
H	4.75656	-2.54540	0.58598
C	1.88777	-2.14399	-2.19227
H	0.81503	-1.94673	-2.20849
H	2.38690	-1.35909	-2.76304
H	2.06006	-3.09188	-2.70566
C	1.87450	4.37371	0.13794
H	2.12010	4.64601	1.16532
H	2.42925	5.03620	-0.52907
H	0.80954	4.55567	-0.01323
C	1.81776	2.10818	-1.93403
H	0.75665	2.28899	-2.11450
H	2.38533	2.68340	-2.66777
H	2.01707	1.04946	-2.10933
C	4.11411	2.26730	0.08492
H	4.40724	2.53788	1.10039
H	4.33144	1.20815	-0.05833
H	4.72776	2.84424	-0.60945
C	-1.76274	0.39798	0.47407
H	-1.92103	0.12001	1.52055
H	-1.65822	1.49133	0.47112
C	-2.96468	-0.00160	-0.30671
H	-2.91068	-0.09299	-1.39053
H	-2.76944	-2.10727	0.12264
C	-5.28400	0.11506	-0.59960
H	-5.38931	-0.96459	-0.73393
H	-5.17606	0.57991	-1.58374
C	-6.49797	0.67532	0.10839
H	-6.58896	0.20919	1.09416
H	-6.37007	1.75311	0.24725
O	-4.15153	0.40046	0.20343
O	-7.61386	0.38445	-0.70970

Si	1.04963	0.08911	0.94176
C	0.81893	-0.40438	2.71624
H	0.06975	0.21984	3.20472
H	0.49656	-1.44484	2.78584
H	1.75567	-0.29857	3.26428
H	-8.40460	0.72269	-0.29335
O	-2.51435	-3.00082	0.39639
H	-2.94363	-3.13282	1.24129

gas_TriSil-1n-cH-OH-opt-reactant.log Energy: -1080579.9259164

C	-0.26459	-0.77631	-0.07433
H	-0.24447	-1.86944	-0.00585
H	-0.06463	-0.53202	-1.12236
O	2.56556	-0.56195	0.29175
O	1.08812	1.55586	0.86605
Si	3.22512	-1.90825	-0.40169
Si	1.66078	2.64257	-0.24776
C	2.82257	-3.40069	0.64975
H	1.74398	-3.55665	0.71766
H	3.26175	-4.30675	0.22845
H	3.20902	-3.27906	1.66285
C	5.06425	-1.62518	-0.48572
H	5.57436	-2.47588	-0.94095
H	5.29028	-0.73905	-1.08086
H	5.47935	-1.47475	0.51167
C	2.51775	-2.12659	-2.11750
H	1.44070	-2.29683	-2.08339
H	2.70053	-1.24250	-2.73058
H	2.97560	-2.98099	-2.61968
C	0.77763	4.25262	0.06864
H	0.96695	4.60317	1.08408
H	1.11273	5.02653	-0.62434
H	-0.30035	4.13501	-0.05063
C	1.27804	2.00924	-1.96739
H	0.20400	1.87267	-2.10640
H	1.62814	2.70848	-2.72880
H	1.76866	1.04976	-2.14134
C	3.50408	2.82681	-0.03223
H	3.74391	3.19504	0.96630
H	3.99209	1.85982	-0.16124

H	3.92124	3.52547	-0.75977
C	-1.64067	-0.24763	0.33522
H	-1.86246	-0.52067	1.36940
H	-1.65195	0.84329	0.29106
C	-2.73964	-0.78350	-0.55848
H	-2.56167	-0.48840	-1.59977
H	-2.76458	-1.87994	-0.52244
C	-5.07108	-0.69289	-0.93135
H	-5.15872	-1.78464	-0.90971
H	-4.91966	-0.38298	-1.97073
C	-6.33648	-0.06306	-0.38910
H	-6.49254	-0.38517	0.64453
H	-6.22816	1.02594	-0.39655
O	-3.98787	-0.26545	-0.13203
O	-7.39241	-0.48519	-1.23114
Si	1.14049	-0.07676	0.94586
C	1.02706	-0.59389	2.72273
H	0.10272	-0.23444	3.17660
H	1.05094	-1.68118	2.81344
H	1.86365	-0.18609	3.29086
H	-8.21956	-0.16126	-0.87905
O	-4.43720	-0.13401	2.64600
H	-4.25439	-0.14007	1.68128

gas_TriSil-1n-cH-OH-radical.log Energy: -1032630.5329825

C	-0.52955	-0.71213	0.11928
H	-0.55431	-1.80271	0.21169
H	-0.39311	-0.50079	-0.94578
O	2.32597	-0.60937	0.28628
O	0.98538	1.57935	0.92668
Si	2.86777	-1.99457	-0.43155
Si	1.50985	2.62392	-0.24869
C	2.45619	-3.45472	0.66124
H	1.37720	-3.55497	0.79505
H	2.82353	-4.38589	0.22612
H	2.90893	-3.34247	1.64768
C	4.71094	-1.81034	-0.63281
H	5.14642	-2.69080	-1.10857
H	4.94551	-0.94251	-1.25117
H	5.19464	-1.67351	0.33522

C	2.04458	-2.19136	-2.09724
H	0.96438	-2.30314	-1.99358
H	2.23523	-1.32432	-2.73190
H	2.42431	-3.07402	-2.61550
C	0.71458	4.27260	0.10317
H	0.99303	4.63151	1.09494
H	1.02513	5.02191	-0.62727
H	-0.37295	4.19441	0.06671
C	0.97491	1.98090	-1.92301
H	-0.11039	1.87790	-1.97678
H	1.28794	2.65793	-2.71987
H	1.41928	1.00333	-2.11884
C	3.37003	2.74174	-0.17632
H	3.69891	3.11683	0.79391
H	3.81033	1.75454	-0.32291
H	3.75628	3.41144	-0.94693
C	-1.85829	-0.12003	0.59826
H	-2.01225	-0.33092	1.66128
H	-1.81828	0.97571	0.52020
C	-3.01677	-0.64742	-0.16674
H	-2.93068	-0.86305	-1.22966
C	-5.33096	-0.68795	-0.49892
H	-5.38220	-1.77983	-0.48779
H	-5.22835	-0.35561	-1.53676
C	-6.58590	-0.10109	0.10906
H	-6.67379	-0.43470	1.14733
H	-6.51461	0.99080	0.10244
O	-4.23348	-0.23982	0.27149
O	-7.67189	-0.55529	-0.67638
Si	0.96781	-0.05418	1.02454
C	0.96428	-0.53787	2.81604
H	0.09601	-0.12466	3.33080
H	0.94055	-1.62350	2.92473
H	1.86075	-0.16442	3.31194
H	-8.48546	-0.20972	-0.31370

gas_TriSil-1n-cH-OH-TS.log Energy: -1080575.7125040

C	-0.40435	-0.50446	-0.01659
H	-0.50003	-1.59506	0.00835
H	-0.22043	-0.23537	-1.06149

O	2.43870	-0.64320	0.26367
O	1.25122	1.62310	0.93946
Si	2.88852	-2.04792	-0.48305
Si	1.95110	2.66043	-0.14837
C	2.30202	-3.50073	0.53594
H	1.21336	-3.51214	0.61900
H	2.60812	-4.44515	0.08236
H	2.71705	-3.46195	1.54437
C	4.74781	-2.01918	-0.60103
H	5.12616	-2.91810	-1.09088
H	5.08351	-1.15515	-1.17663
H	5.19827	-1.95802	0.39051
C	2.12526	-2.11036	-2.18712
H	1.03603	-2.13279	-2.13157
H	2.41641	-1.24020	-2.77787
H	2.45058	-3.00286	-2.72508
C	1.29062	4.36177	0.23130
H	1.53529	4.65135	1.25414
H	1.71728	5.10717	-0.44236
H	0.20535	4.39044	0.12394
C	1.47225	2.14206	-1.88182
H	0.38846	2.15394	-2.01081
H	1.90562	2.81383	-2.62493
H	1.82897	1.13228	-2.09276
C	3.80479	2.59688	0.04787
H	4.09989	2.89643	1.05456
H	4.16170	1.57986	-0.11977
H	4.30217	3.26028	-0.66208
C	-1.70649	0.13383	0.46868
H	-1.90638	-0.14760	1.50517
H	-1.62979	1.22309	0.44932
C	-2.88614	-0.29221	-0.37530
H	-2.76500	0.02452	-1.42046
H	-2.92987	-1.41317	-0.40159
C	-5.20729	-0.07983	-0.62708
H	-5.32630	-1.16256	-0.74916
H	-5.10574	0.36486	-1.62348
C	-6.41831	0.49998	0.07068
H	-6.51550	0.04803	1.06283
H	-6.27957	1.57800	0.19639

O	-4.07586	0.20817	0.16359
O	-7.54037	0.21152	-0.74147
Si	1.10185	-0.00636	0.97158
C	0.97830	-0.55684	2.73925
H	0.13594	-0.07828	3.24026
H	0.84210	-1.63795	2.79934
H	1.88685	-0.29574	3.28274
H	-8.32372	0.57539	-0.33297
O	-3.25136	-2.85236	0.55414
H	-3.70667	-2.29665	1.20454

gas_TriSil-1n-dH-OH-IRC-forward-reactant.log Energy: -1080579.3275673

C	0.10653	-1.34048	-0.12462
H	0.10008	-2.43365	-0.09378
H	0.06695	-1.00923	0.91813
O	-2.73177	-1.50351	-0.22825
O	-1.62436	0.85642	-0.77398
Si	-3.97330	-1.02411	0.75605
Si	-1.02107	2.25284	-0.13842
C	-4.96023	-2.55468	1.15283
H	-4.34198	-3.29367	1.66435
H	-5.80831	-2.31787	1.79793
H	-5.34657	-3.01216	0.24102
C	-5.02459	0.23709	-0.13186
H	-5.84215	0.58513	0.50227
H	-4.42121	1.09960	-0.41716
H	-5.45892	-0.18720	-1.03847
C	-3.26653	-0.28249	2.32055
H	-2.59030	-0.98295	2.81342
H	-2.70943	0.62884	2.10103
H	-4.05915	-0.02687	3.02619
C	-0.01537	3.11799	-1.45102
H	-0.62325	3.31912	-2.33424
H	0.37057	4.07024	-1.08238
H	0.83664	2.51048	-1.76067
C	0.05260	1.89914	1.35237
H	0.95986	1.35980	1.07762
H	0.35654	2.83732	1.82109
H	-0.47726	1.31024	2.10234
C	-2.48330	3.29936	0.35930

H	-3.12770	3.49359	-0.49954
H	-3.08437	2.80293	1.12268
H	-2.15778	4.26088	0.76039
C	1.38766	-0.83738	-0.79466
H	1.50244	-1.28865	-1.78211
H	1.34708	0.24300	-0.95369
C	2.62063	-1.14643	0.02785
H	2.53924	-0.67873	1.01888
H	2.71230	-2.22982	0.18367
C	4.95007	-0.88359	0.06272
H	5.12166	-1.95636	0.21483
H	4.91578	-0.40584	1.05123
C	6.08024	-0.29614	-0.75503
H	6.10853	-0.77670	-1.73531
H	5.91451	0.77512	-0.89097
O	3.76018	-0.65558	-0.64245
O	7.29021	-0.53866	-0.04181
Si	-1.46446	-0.76495	-0.95280
C	-1.48463	-1.15988	-2.76567
H	-0.64969	-0.68106	-3.27928
H	-1.41867	-2.23577	-2.93291
H	-2.41002	-0.80195	-3.21834
H	8.02657	-0.19534	-0.54602
O	6.94463	0.38630	2.63387
H	7.18206	0.04977	1.74441

gas_TriSil-1n-dH-OH-opt-product.log Energy: -1080605.4019349

C	-0.05631	-1.62912	0.11188
H	0.14025	-2.70317	0.16107
H	0.05208	-1.34537	-0.94004
O	2.73107	-1.27974	0.56836
O	1.17138	0.87880	0.72468
Si	3.84416	-0.79389	-0.55678
Si	0.45705	2.15016	-0.05535
C	5.05114	-2.19956	-0.76310
H	4.54464	-3.09952	-1.11458
H	5.82895	-1.94476	-1.48537
H	5.53544	-2.43435	0.18574
C	4.70880	0.74147	0.05480
H	5.41882	1.11858	-0.68357

H	3.98146	1.52657	0.26245
H	5.25656	0.53553	0.97568
C	2.96866	-0.44822	-2.17421
H	2.44110	-1.33571	-2.52830
H	2.24009	0.35533	-2.05954
H	3.67738	-0.14804	-2.94816
C	-0.58439	3.09266	1.16477
H	-0.01143	3.33895	2.05989
H	-0.93948	4.02562	0.72242
H	-1.46639	2.51922	1.45346
C	-0.60925	1.54852	-1.47020
H	-1.53135	1.09759	-1.10099
H	-0.89624	2.39771	-2.09399
H	-0.08866	0.83110	-2.10644
C	1.83897	3.22197	-0.71305
H	2.47831	3.57188	0.09911
H	2.46521	2.67959	-1.42306
H	1.43493	4.09871	-1.22270
C	-1.47386	-1.31848	0.59806
H	-1.65533	-1.78800	1.56672
H	-1.59949	-0.24254	0.74083
C	-2.51994	-1.78847	-0.38796
H	-2.36532	-1.30593	-1.35780
H	-2.47520	-2.87263	-0.52625
C	-4.83950	-1.61402	-0.75316
H	-4.59661	-1.85557	-1.78101
H	-3.66689	0.54798	0.92089
C	-6.10306	-0.94753	-0.39650
H	-6.93129	-1.45995	-0.89127
H	-6.24904	-0.99800	0.68615
O	-3.81214	-1.43169	0.10226
O	-6.07448	0.43266	-0.82092
Si	1.27418	-0.71690	1.05800
C	1.12016	-0.96630	2.88942
H	0.15783	-0.60260	3.25259
H	1.21016	-2.02164	3.15031
H	1.90607	-0.41937	3.41119
H	-6.91001	0.83921	-0.58635
O	-3.76042	1.46942	0.66931
H	-4.49372	1.42935	0.04476

gas_TriSil-1n-dH-OH-radical.log Energy: -1032630.6100406

C	-0.50726	-1.31099	-0.00177
H	-0.51346	-2.40459	0.00952
H	-0.37195	-1.02069	-1.04861
O	2.30683	-1.50516	0.35957
O	1.19382	0.88817	0.71747
Si	3.64015	-1.08204	-0.52570
Si	0.67216	2.26745	-0.02038
C	4.62956	-2.64146	-0.77699
H	4.04608	-3.38924	-1.31585
H	5.53647	-2.44181	-1.35070
H	4.92380	-3.07082	0.18166
C	4.63158	0.19512	0.40707
H	5.50892	0.50584	-0.16337
H	4.02220	1.07747	0.60573
H	4.97534	-0.20144	1.36371
C	3.08965	-0.38857	-2.17294
H	2.44621	-1.09592	-2.69878
H	2.53356	0.53959	-2.03744
H	3.94677	-0.17298	-2.81354
C	-0.43565	3.19215	1.16255
H	0.09233	3.41854	2.08993
H	-0.77218	4.13464	0.72660
H	-1.32163	2.60706	1.41463
C	-0.26552	1.86937	-1.58967
H	-1.20314	1.35304	-1.38051
H	-0.50990	2.79228	-2.11952
H	0.32194	1.24512	-2.26438
C	2.18989	3.27627	-0.41988
H	2.75402	3.49853	0.48728
H	2.85215	2.74187	-1.10277
H	1.91784	4.22400	-0.88798
C	-1.83480	-0.76898	0.53404
H	-2.03776	-1.17493	1.52697
H	-1.79565	0.31705	0.64781
C	-2.99276	-1.10817	-0.37891
H	-2.83494	-0.68016	-1.37463
H	-3.09049	-2.19415	-0.48929
C	-5.30666	-0.81258	-0.54710

C	-6.55938	-0.34470	0.09351
H	-6.85147	-1.01316	0.91938
H	-6.38882	0.64874	0.52470
O	-4.18783	-0.57909	0.17393
O	-7.57394	-0.31902	-0.89633
Si	0.99346	-0.72258	0.94119
C	0.84523	-1.04956	2.76142
H	-0.02370	-0.54059	3.18109
H	0.74664	-2.11747	2.96077
H	1.73262	-0.68765	3.28193
H	-8.42093	-0.23060	-0.46242
H	-5.31603	-1.67375	-1.20854

gas_TriSil-1n-dH-OH-TS.log Energy: -1080577.6378412

C	-0.16207	-1.37045	0.08077
H	-0.14150	-2.46229	0.02340
H	-0.10637	-1.01248	-0.95226
O	2.67559	-1.49906	0.23972
O	1.52286	0.83285	0.81796
Si	3.92887	-0.98359	-0.71114
Si	0.91620	2.23446	0.19464
C	4.94450	-2.49280	-1.11759
H	4.34676	-3.22987	-1.65557
H	5.80172	-2.23195	-1.74099
H	5.31918	-2.96279	-0.20727
C	4.94557	0.27377	0.22140
H	5.77059	0.64445	-0.38982
H	4.32556	1.12288	0.51111
H	5.36781	-0.16235	1.12812
C	3.24211	-0.22158	-2.27450
H	2.58706	-0.92208	-2.79510
H	2.66640	0.67654	-2.04875
H	4.04476	0.06034	-2.95846
C	-0.12195	3.06460	1.50448
H	0.46732	3.25512	2.40254
H	-0.51084	4.01953	1.14607
H	-0.97375	2.44348	1.78641
C	-0.12459	1.89692	-1.32196
H	-1.03578	1.35054	-1.07601
H	-0.42428	2.84021	-1.78298

H	0.42331	1.32239	-2.07012
C	2.37720	3.30474	-0.25464
H	3.00284	3.48941	0.62005
H	2.99803	2.82912	-1.01545
H	2.04907	4.27016	-0.64403
C	-1.46190	-0.89821	0.73721
H	-1.59465	-1.38056	1.70762
H	-1.43411	0.17710	0.92903
C	-2.67051	-1.19067	-0.12490
H	-2.57773	-0.68693	-1.09467
H	-2.75684	-2.26777	-0.31567
C	-4.99144	-0.90069	-0.19882
H	-5.11736	-1.93361	-0.54615
H	-4.95787	-0.26166	-1.15619
C	-6.17513	-0.43170	0.61337
H	-6.31754	-1.09128	1.47432
H	-5.97610	0.58071	0.97404
O	-3.83372	-0.72644	0.53610
O	-7.30530	-0.46220	-0.24543
Si	1.38411	-0.79382	0.95457
C	1.37196	-1.23295	2.75742
H	0.51994	-0.77822	3.26487
H	1.31793	-2.31344	2.89708
H	2.28254	-0.87361	3.23815
H	-8.07561	-0.17156	0.23983
O	-5.45437	0.60166	-2.31162
H	-6.38197	0.48146	-2.05338

gas_TriSil-1n-eH-OH-IRC-forward-product.log Energy: -1080602.6984044

C	-0.13215	-1.24483	0.40764
H	-0.06439	-2.31880	0.60894
H	0.01930	-1.12846	-0.66880
O	2.69662	-0.91444	0.67334
O	1.12327	1.22936	1.10921
Si	3.53680	-1.34373	-0.67724
Si	0.87331	2.40049	-0.03308
C	4.86842	-2.52986	-0.13203
H	4.43225	-3.42294	0.31788
H	5.48646	-2.84315	-0.97538
H	5.51880	-2.06417	0.60969

C	4.29820	0.17767	-1.44624
H	4.94085	-0.09607	-2.28536
H	3.53344	0.85887	-1.82150
H	4.90485	0.71883	-0.71877
C	2.40788	-2.17424	-1.91667
H	1.86803	-3.00725	-1.46396
H	1.67350	-1.47900	-2.32610
H	2.99229	-2.56653	-2.75147
C	-0.52942	3.47954	0.54501
H	-0.35236	3.83593	1.56082
H	-0.63592	4.35010	-0.10568
H	-1.47300	2.93235	0.51932
C	0.43053	1.61104	-1.67063
H	-0.55693	1.14890	-1.61832
H	0.39326	2.36887	-2.45565
H	1.15825	0.85610	-1.97349
C	2.44639	3.39609	-0.17778
H	2.68452	3.86971	0.77597
H	3.29144	2.76748	-0.45909
H	2.34320	4.18259	-0.92782
C	-1.51398	-0.71229	0.79013
H	-1.70662	-0.85924	1.85511
H	-1.56340	0.36291	0.60787
C	-2.61356	-1.38464	-0.00464
H	-2.42250	-1.27336	-1.07955
H	-2.65623	-2.45721	0.22131
C	-4.94244	-1.36104	-0.37349
H	-4.98557	-2.43931	-0.14596
H	-4.81548	-1.26452	-1.46006
C	-6.18127	-0.66172	0.04456
H	-6.37169	-0.47505	1.09557
H	-4.00092	2.25697	-1.11304
O	-3.85650	-0.78077	0.31652
O	-7.24697	-0.88781	-0.77271
Si	1.27677	-0.38596	1.29116
C	1.27730	-0.74495	3.11106
H	0.35161	-0.40270	3.57550
H	1.38399	-1.81384	3.30025
H	2.10738	-0.22960	3.59528
H	-8.03591	-0.50450	-0.39119

O	-3.25805	1.68950	-0.91333
H	-3.62126	0.95344	-0.39973

gas_TriSil-1n-eH-OH-IRC-reverse-reactant.log Energy: -1080580.3683733

C	-0.11928	-1.17103	0.34119
H	-0.09234	-2.23183	0.60999
H	0.08388	-1.12973	-0.73265
O	2.68297	-1.08448	0.82227
O	1.35853	1.25193	0.82484
Si	3.62826	-1.43569	-0.48442
Si	0.95717	2.39992	-0.29276
C	4.96815	-2.58237	0.11721
H	4.53946	-3.49733	0.52844
H	5.64279	-2.85943	-0.69479
H	5.55903	-2.10665	0.90107
C	4.36168	0.13685	-1.17269
H	5.09283	-0.08521	-1.95237
H	3.58821	0.76776	-1.61176
H	4.86054	0.71100	-0.39109
C	2.60137	-2.27046	-1.80728
H	2.06964	-3.13528	-1.40776
H	1.86377	-1.58697	-2.23144
H	3.23908	-2.61507	-2.62375
C	-0.46054	3.41797	0.35733
H	-0.20718	3.84131	1.33079
H	-0.67346	4.24757	-0.32030
H	-1.38094	2.84287	0.46763
C	0.47748	1.56559	-1.90039
H	-0.44470	0.99289	-1.78851
H	0.31097	2.31058	-2.68061
H	1.25834	0.88731	-2.24960
C	2.44931	3.49142	-0.54305
H	2.73485	3.96096	0.39961
H	3.30795	2.92937	-0.90993
H	2.23095	4.28506	-1.26019
C	-1.50228	-0.58818	0.63371
H	-1.73765	-0.67078	1.69697
H	-1.52653	0.47695	0.39291
C	-2.58432	-1.29190	-0.15858
H	-2.38817	-1.20232	-1.23467

H	-2.60486	-2.36005	0.08805
C	-4.91674	-1.33593	-0.53601
H	-4.96437	-2.39906	-0.27829
H	-4.78422	-1.25253	-1.62015
C	-6.20034	-0.65017	-0.11873
H	-6.31089	-0.72356	0.96761
H	-6.15459	0.40903	-0.38841
O	-3.84415	-0.71704	0.14447
O	-7.25178	-1.31394	-0.79347
Si	1.29334	-0.32736	1.23567
C	1.10725	-0.43777	3.07699
H	0.19507	0.06061	3.40771
H	1.07197	-1.47690	3.40648
H	1.95191	0.04564	3.56878
H	-8.07466	-0.86638	-0.60459
O	-3.91637	2.07775	0.34485
H	-3.88352	1.09609	0.31419

gas_TriSil-1n-eH-OH-radical.log Energy: -1032629.9933494

C	-0.36936	-1.11903	0.34721
H	-0.36376	-2.18732	0.58572
H	-0.18165	-1.05402	-0.72857
O	2.44608	-1.10117	0.79098
O	1.17305	1.25821	0.85965
Si	3.36863	-1.40944	-0.54226
Si	0.74431	2.43661	-0.21080
C	4.71139	-2.58443	-0.00460
H	4.28366	-3.51138	0.37990
H	5.37127	-2.83539	-0.83696
H	5.31752	-2.14087	0.78646
C	4.10118	0.18412	-1.18299
H	4.81740	-0.01176	-1.98326
H	3.32391	0.83553	-1.58373
H	4.61652	0.72523	-0.38860
C	2.31638	-2.18831	-1.87875
H	1.78642	-3.06474	-1.50298
H	1.57496	-1.48601	-2.26367
H	2.93830	-2.50482	-2.71847
C	-0.66532	3.42846	0.50592
H	-0.38260	3.85027	1.47163

H	-0.92835	4.25523	-0.15697
H	-1.56005	2.82273	0.65325
C	0.22551	1.66288	-1.83495
H	-0.69546	1.08829	-1.72401
H	0.04607	2.43553	-2.58489
H	0.99662	0.99534	-2.22408
C	2.22140	3.54896	-0.45552
H	2.53327	3.97817	0.49790
H	3.07096	3.00772	-0.87180
H	1.97873	4.37145	-1.13112
C	-1.73352	-0.51173	0.67801
H	-1.96539	-0.64099	1.73722
H	-1.73065	0.56397	0.49218
C	-2.84794	-1.12879	-0.14137
H	-2.64367	-0.99402	-1.21345
H	-2.90331	-2.21048	0.04594
C	-5.15551	-1.02356	-0.52748
H	-5.22349	-2.11739	-0.38477
H	-5.02799	-0.85412	-1.60661
C	-6.38887	-0.34662	-0.05921
H	-6.52623	-0.14544	0.99735
O	-4.06674	-0.51291	0.19854
O	-7.49127	-0.63112	-0.81081
Si	1.07359	-0.33088	1.23915
C	0.91507	-0.47174	3.08108
H	0.01515	0.03343	3.43431
H	0.86757	-1.51632	3.39118
H	1.77470	-0.01120	3.56887
H	-8.26346	-0.23002	-0.41430

gas_TriSil-1n-eH-OH-TS.log Energy: -1080576.7938660

C	0.01077	-1.26665	0.38438
H	0.09731	-2.33009	0.62798
H	0.17609	-1.19327	-0.69441
O	2.82317	-1.02480	0.76220
O	1.36370	1.22477	0.87483
Si	3.74157	-1.24439	-0.59245
Si	0.82232	2.37492	-0.17649
C	5.17950	-2.31980	-0.09525
H	4.83111	-3.28173	0.28330

H	5.84110	-2.50861	-0.94250
H	5.76456	-1.84136	0.69131
C	4.33588	0.40910	-1.22313
H	5.04497	0.27999	-2.04302
H	3.50190	1.00530	-1.59461
H	4.82829	0.97603	-0.43223
C	2.72496	-2.08534	-1.91898
H	2.27233	-3.00506	-1.54545
H	1.92410	-1.43770	-2.28005
H	3.35208	-2.34233	-2.77495
C	-0.65077	3.24093	0.57481
H	-0.38176	3.69108	1.53155
H	-1.00495	4.03729	-0.08257
H	-1.48540	2.56138	0.74951
C	0.34134	1.57314	-1.79868
H	-0.52498	0.92046	-1.67948
H	0.08193	2.33394	-2.53712
H	1.15976	0.97819	-2.20833
C	2.19803	3.60686	-0.43394
H	2.48879	4.05285	0.51843
H	3.08260	3.14177	-0.86885
H	1.87660	4.41176	-1.09767
C	-1.38725	-0.75610	0.73435
H	-1.59495	-0.89767	1.79692
H	-1.45756	0.31729	0.54612
C	-2.46753	-1.44711	-0.07055
H	-2.28316	-1.31105	-1.14472
H	-2.46632	-2.52593	0.13124
C	-4.78879	-1.43820	-0.46459
H	-4.89123	-2.51187	-0.26523
H	-4.63115	-1.30282	-1.54077
C	-6.04632	-0.71025	-0.05368
H	-6.26787	-0.85219	1.00799
H	-5.82722	0.42216	-0.17229
O	-3.72088	-0.89390	0.27225
O	-7.08870	-1.10804	-0.88692
Si	1.40728	-0.36725	1.24819
C	1.30100	-0.52904	3.09184
H	0.37088	-0.10109	3.46823
H	1.34711	-1.57517	3.39684

H	2.13011	-0.00100	3.56379
H	-7.90937	-0.73160	-0.57125
O	-5.04218	1.68288	-0.14935
H	-4.22788	1.22261	0.10908

gas_TriSil-1n-fH-OH-opt-product.log Energy: -1080592.3039799

C	-0.06478	-0.88726	0.61113
H	-0.15204	-1.90202	1.01210
H	0.04999	-1.00425	-0.47033
O	2.76536	-1.10622	0.87640
O	1.72882	1.36217	0.68384
Si	3.54758	-1.72677	-0.43783
Si	1.37962	2.39942	-0.54885
C	4.77913	-2.96670	0.20865
H	4.27460	-3.76439	0.75560
H	5.34554	-3.42065	-0.60643
H	5.48656	-2.48922	0.88795
C	4.41509	-0.35293	-1.35809
H	5.04820	-0.75675	-2.15047
H	3.69527	0.32345	-1.82017
H	5.04305	0.23235	-0.68530
C	2.31982	-2.55983	-1.57704
H	1.72263	-3.29876	-1.04078
H	1.63665	-1.83800	-2.02781
H	2.84020	-3.07256	-2.38844
C	0.12525	3.64674	0.04839
H	0.50302	4.18035	0.92183
H	-0.08509	4.38326	-0.72968
H	-0.81841	3.17557	0.32574
C	0.69055	1.44933	-2.00770
H	-0.27767	1.00549	-1.77023
H	0.55021	2.11361	-2.86249
H	1.36311	0.64762	-2.31802
C	2.95430	3.27969	-1.02125
H	3.35831	3.81857	-0.16285
H	3.71769	2.58298	-1.36745
H	2.76998	4.00421	-1.81678
C	-1.33164	-0.08794	0.91981
H	-1.49212	-0.02318	1.99805
H	-1.23448	0.93826	0.55989

C	-2.56115	-0.69990	0.28207
H	-2.43341	-0.75620	-0.80767
H	-2.71061	-1.72474	0.64680
C	-4.87647	-0.40314	0.03427
H	-5.09584	-1.41595	0.39210
H	-4.81628	-0.44792	-1.05957
C	-5.98640	0.54582	0.45316
H	-6.03837	0.63339	1.55343
H	-5.76300	1.58094	0.13787
O	-3.68725	0.09129	0.59269
O	-7.22666	0.23205	0.00314
Si	1.51118	-0.14229	1.29080
C	1.47716	-0.01099	3.13985
H	0.65996	0.63140	3.47050
H	1.35181	-0.99192	3.59983
H	2.41165	0.41753	3.50331
H	-7.27494	-1.40104	-1.08832
O	-7.02754	-2.19957	-1.56991
H	-7.84043	-2.54158	-1.93876

gas_TriSil-1n-fH-OH-opt-reactant.log Energy: -1080576.6841334

C	0.15670	-1.17260	0.36865
H	0.21158	-2.24511	0.58034
H	0.30239	-1.07499	-0.71116
O	2.98231	-1.06506	0.71753
O	1.63359	1.24694	0.87554
Si	3.87163	-1.30313	-0.65264
Si	1.11948	2.43597	-0.14401
C	5.27665	-2.43590	-0.18936
H	4.89894	-3.38836	0.18499
H	5.91770	-2.63980	-1.04884
H	5.89100	-1.98768	0.59268
C	4.51737	0.33421	-1.27567
H	5.20931	0.18810	-2.10729
H	3.70020	0.96409	-1.62854
H	5.04132	0.87456	-0.48645
C	2.80529	-2.09079	-1.97283
H	2.32279	-2.99613	-1.60164
H	2.02472	-1.40911	-2.31515
H	3.40982	-2.36263	-2.84040

C	-0.29807	3.35235	0.65321
H	0.00708	3.76286	1.61694
H	-0.62110	4.18297	0.02244
H	-1.16107	2.70741	0.82192
C	0.56700	1.68504	-1.76802
H	-0.32480	1.06996	-1.63729
H	0.32677	2.46919	-2.48843
H	1.34809	1.06037	-2.20545
C	2.54204	3.61117	-0.41422
H	2.87622	4.02526	0.53830
H	3.39376	3.11560	-0.87999
H	2.24091	4.44225	-1.05486
C	-1.21639	-0.62687	0.76322
H	-1.40381	-0.78932	1.82658
H	-1.26183	0.45205	0.60342
C	-2.33536	-1.26885	-0.03014
H	-2.17677	-1.10220	-1.10531
H	-2.34384	-2.35511	0.13428
C	-4.66298	-1.24289	-0.32474
H	-4.73600	-2.32712	-0.17365
H	-4.56307	-1.06335	-1.40552
C	-5.91750	-0.56614	0.19751
H	-6.03311	-0.77688	1.25897
H	-5.84156	0.51563	0.07267
O	-3.56576	-0.70927	0.36687
O	-7.07705	-1.07557	-0.44381
Si	1.60169	-0.35105	1.22770
C	1.50974	-0.53211	3.07043
H	0.60604	-0.06442	3.46345
H	1.50749	-1.58332	3.36111
H	2.36949	-0.05204	3.53877
H	-7.10353	-0.75245	-1.34602
O	-8.59002	0.81434	-0.75704
H	-9.06576	0.22392	-0.15646

gas_TriSil-1n-fH-OH-radical.log Energy: -1032622.4995874

C	-0.37662	-1.12620	0.33115
H	-0.36945	-2.19522	0.56617
H	-0.18099	-1.05678	-0.74290
O	2.43493	-1.09971	0.79210

O	1.15069	1.25452	0.86740
Si	3.36944	-1.40113	-0.53492
Si	0.73461	2.43635	-0.20402
C	4.70800	-2.57780	0.00843
H	4.27771	-3.50695	0.38463
H	5.37516	-2.82420	-0.81947
H	5.30708	-2.13781	0.80679
C	4.10533	0.19659	-1.16085
H	4.82734	0.00591	-1.95713
H	3.33069	0.85009	-1.56328
H	4.61491	0.73307	-0.35963
C	2.32797	-2.17378	-1.88343
H	1.79616	-3.05282	-1.51642
H	1.58894	-1.47018	-2.27061
H	2.95657	-2.48536	-2.71998
C	-0.68648	3.42189	0.49941
H	-0.41581	3.84306	1.46881
H	-0.94597	4.24885	-0.16462
H	-1.57996	2.81190	0.63683
C	0.23522	1.66730	-1.83664
H	-0.68416	1.08798	-1.73716
H	0.05995	2.44218	-2.58525
H	1.01284	1.00464	-2.22097
C	2.21151	3.55267	-0.42701
H	2.51003	3.98030	0.53136
H	3.06767	3.01449	-0.83358
H	1.97567	4.37624	-1.10369
C	-1.74498	-0.52444	0.65417
H	-1.98272	-0.65555	1.71183
H	-1.74469	0.55144	0.46887
C	-2.85104	-1.14613	-0.17259
H	-2.64363	-1.00810	-1.24313
H	-2.90364	-2.22750	0.01340
C	-5.16382	-1.04924	-0.56748
H	-5.28837	-2.12461	-0.38907
H	-5.02012	-0.90212	-1.64528
C	-6.41058	-0.30752	-0.11233
H	-6.55155	-0.41277	0.97791
H	-6.28730	0.78184	-0.24483
O	-4.07841	-0.53850	0.16083

O	-7.55615	-0.68535	-0.72791
Si	1.05811	-0.33720	1.23702
C	0.88738	-0.48958	3.07671
H	-0.01663	0.01004	3.42740
H	0.84227	-1.53610	3.38051
H	1.74192	-0.02852	3.57286

gas_TriSil-1n-fH-OH-TS.log Energy: -1080572.4246368

C	0.06023	-1.11555	0.49142
H	0.08337	-2.18245	0.73494
H	0.15398	-1.05720	-0.59692
O	2.90271	-1.10794	0.69035
O	1.64997	1.25788	0.85248
Si	3.70740	-1.42040	-0.71670
Si	1.13366	2.43581	-0.17880
C	5.08838	-2.59786	-0.29421
H	4.69305	-3.52329	0.12686
H	5.67382	-2.85151	-1.17975
H	5.76124	-2.15484	0.44123
C	4.38482	0.17120	-1.41949
H	5.02614	-0.02602	-2.28061
H	3.57627	0.82460	-1.74869
H	4.97031	0.71056	-0.67405
C	2.54191	-2.19861	-1.95610
H	2.04505	-3.07367	-1.53465
H	1.77122	-1.49546	-2.27662
H	3.08821	-2.51745	-2.84602
C	-0.20753	3.43108	0.65563
H	0.15882	3.85565	1.59155
H	-0.52731	4.25598	0.01576
H	-1.08597	2.82625	0.88300
C	0.47479	1.66096	-1.75072
H	-0.43295	1.08636	-1.55953
H	0.23055	2.43271	-2.48305
H	1.20890	0.99291	-2.20502
C	2.58576	3.54553	-0.55053
H	2.97983	3.97368	0.37244
H	3.39515	3.00328	-1.03921
H	2.28679	4.36879	-1.20219
C	-1.26795	-0.50168	0.93635

H	-1.40580	-0.62214	2.01285
H	-1.27868	0.57251	0.74210
C	-2.45105	-1.12201	0.22302
H	-2.34415	-0.99499	-0.86348
H	-2.49309	-2.20139	0.42356
C	-4.78719	-1.00686	0.04097
H	-4.91018	-2.07708	0.25054
H	-4.73066	-0.87794	-1.04759
C	-5.97558	-0.23654	0.58409
H	-6.05132	-0.36954	1.66650
H	-5.84526	0.83413	0.40199
O	-3.63635	-0.50104	0.66490
O	-7.19692	-0.68399	0.06012
Si	1.57823	-0.32813	1.25043
C	1.57773	-0.45650	3.09997
H	0.71492	0.05693	3.52633
H	1.55087	-1.49876	3.42020
H	2.47906	0.00123	3.50874
H	-7.17340	-0.73117	-1.00368
O	-7.17307	-0.09811	-2.12131
H	-7.95558	0.46406	-2.08118

gas_TriSil-1n-gH-OH-radical.log Energy: -1032622.8411220

C	-0.33898	-1.10187	0.37224
H	-0.34530	-2.16637	0.62651
H	-0.14226	-1.05300	-0.70318
O	2.47003	-1.09873	0.81144
O	1.18956	1.27346	0.89654
Si	3.39579	-1.43970	-0.51219
Si	0.81202	2.43973	-0.20740
C	4.71146	-2.63389	0.04860
H	4.26322	-3.54870	0.43875
H	5.37329	-2.90578	-0.77561
H	5.31916	-2.19344	0.84016
C	4.16338	0.13397	-1.16057
H	4.88184	-0.08282	-1.95340
H	3.40338	0.79821	-1.57327
H	4.68374	0.67036	-0.36621
C	2.33814	-2.21291	-1.84728
H	1.79164	-3.07678	-1.46615

H	1.61061	-1.50267	-2.24378
H	2.95984	-2.54806	-2.67990
C	-0.60168	3.46222	0.45571
H	-0.33726	3.89956	1.41966
H	-0.83944	4.27869	-0.22910
H	-1.50568	2.86804	0.59347
C	0.32378	1.64706	-1.83176
H	-0.60535	1.08331	-1.73412
H	0.17005	2.41089	-2.59633
H	1.09640	0.96647	-2.19406
C	2.31348	3.52307	-0.42945
H	2.60222	3.96864	0.52370
H	3.16643	2.95848	-0.80589
H	2.10642	4.33358	-1.13088
C	-1.69778	-0.47570	0.68728
H	-1.92285	-0.56554	1.75215
H	-1.68894	0.59265	0.46284
C	-2.81932	-1.11539	-0.10456
H	-2.61814	-1.02448	-1.18176
H	-2.88296	-2.18802	0.12542
C	-5.13009	-1.00782	-0.48640
H	-5.25992	-2.07432	-0.26435
H	-4.98989	-0.90537	-1.56975
C	-6.36530	-0.24513	-0.05936
H	-6.50110	-0.35617	1.02060
H	-6.22667	0.81718	-0.28191
O	-4.03364	-0.47866	0.21391
O	-7.45921	-0.78660	-0.77776
Si	1.10785	-0.31729	1.26252
C	0.96000	-0.46212	3.08688
H	0.49010	0.30052	3.69588
H	1.30855	-1.33142	3.63138
H	-8.25692	-0.32668	-0.52303

gas_TriSil-1n-gH-OH-TS-IRC-product-re3.log Energy: -1080594.8090416

C	-0.54290	-0.82512	0.03473
H	-0.46694	-1.91505	-0.02765
H	-0.46041	-0.45802	-0.99481
O	2.31440	-0.68924	0.31765
O	0.91617	1.48564	0.89285

Si	2.87257	-2.03971	-0.47652
Si	0.85481	2.56758	-0.37190
C	2.41619	-3.55031	0.52360
H	1.33431	-3.63973	0.63969
H	2.77291	-4.46096	0.03916
H	2.86009	-3.50431	1.51920
C	4.71671	-1.83581	-0.60180
H	5.17187	-2.68120	-1.12053
H	4.96790	-0.92701	-1.15088
H	5.16844	-1.75990	0.38803
C	2.09402	-2.11942	-2.17103
H	1.00828	-2.20487	-2.11022
H	2.33359	-1.22408	-2.74647
H	2.46678	-2.98313	-2.72496
C	1.65095	4.14288	0.21920
H	2.71745	3.99151	0.39064
H	1.54201	4.93398	-0.52492
H	1.19453	4.48818	1.14781
C	-0.93833	2.85331	-0.81496
H	-1.51080	3.18956	0.05070
H	-1.02478	3.61516	-1.59208
H	-1.40366	1.94071	-1.19191
C	1.77058	1.86849	-1.84066
H	2.81192	1.67877	-1.57832
H	1.32439	0.93259	-2.18149
H	1.74847	2.57241	-2.67479
C	-1.89476	-0.42551	0.63321
H	-2.03456	-0.90774	1.60262
H	-1.93260	0.65070	0.81230
C	-3.04929	-0.80146	-0.27216
H	-2.94543	-0.29386	-1.24228
H	-3.04261	-1.88303	-0.46842
C	-5.38514	-0.72381	-0.44635
H	-5.44972	-1.80007	-0.64912
H	-5.33767	-0.20255	-1.41050
C	-6.61371	-0.27486	0.31442
H	-6.65417	-0.79895	1.27403
H	-6.54244	0.79912	0.51076
O	-4.25908	-0.42760	0.33977
O	-7.73725	-0.58131	-0.49134

Si	0.91397	-0.14499	0.98938
C	0.86563	-0.60586	2.76511
H	0.47336	0.05269	3.53016
H	1.19777	-1.57343	3.12300
H	3.64879	1.98765	1.47519
H	-8.53095	-0.30545	-0.03668
H	3.66357	0.73262	0.63472
O	4.19225	1.51030	0.84793

gas_TriSil-1n-gH-OH-TS-IRC-reactant.log Energy: -1080579.8729044

C	-0.52507	-0.81492	0.00935
H	-0.43979	-1.90132	-0.09075
H	-0.44655	-0.41197	-1.00639
O	2.33981	-0.65723	0.33288
O	0.92588	1.48271	0.91877
Si	2.89307	-1.99412	-0.48971
Si	0.85171	2.60938	-0.30204
C	2.40257	-3.52694	0.45818
H	1.31750	-3.61728	0.53663
H	2.77357	-4.42598	-0.03710
H	2.81332	-3.50609	1.46872
C	4.74301	-1.80905	-0.57448
H	5.19740	-2.64355	-1.11115
H	5.01568	-0.88865	-1.09421
H	5.17880	-1.77216	0.42485
C	2.14922	-2.01229	-2.20073
H	1.06216	-2.09413	-2.16423
H	2.40338	-1.09790	-2.73875
H	2.52902	-2.85792	-2.77723
C	1.71603	4.13423	0.31861
H	2.76240	3.91228	0.53365
H	1.68401	4.93405	-0.42333
H	1.25014	4.50079	1.23419
C	-0.94770	2.94744	-0.67687
H	-1.48442	3.26178	0.21938
H	-1.04573	3.73828	-1.42296
H	-1.44194	2.05688	-1.06996
C	1.69691	1.93928	-1.82827
H	2.74498	1.72004	-1.62119
H	1.21766	1.02545	-2.18403

H	1.65563	2.67234	-2.63631
C	-1.88368	-0.44935	0.61641
H	-2.03120	-0.97793	1.56009
H	-1.92823	0.61730	0.84575
C	-3.03020	-0.78733	-0.31392
H	-2.92387	-0.23114	-1.25664
H	-3.01439	-1.85769	-0.56383
C	-5.36562	-0.71758	-0.49769
H	-5.42189	-1.78310	-0.75282
H	-5.31609	-0.14975	-1.43501
C	-6.60140	-0.31395	0.27669
H	-6.64268	-0.88289	1.21038
H	-6.53935	0.75009	0.52368
O	-4.24589	-0.45288	0.30866
O	-7.71831	-0.59059	-0.54873
Si	0.91485	-0.14704	0.99730
C	0.84716	-0.66040	2.77582
H	-0.05658	-0.28561	3.25729
H	0.85745	-1.74799	2.86643
H	1.70825	-0.26488	3.31533
H	-8.51624	-0.33864	-0.08762
H	3.63382	0.73480	0.55060
O	4.32370	1.42829	0.59718

gas_TriSil-1n-gH-OH-TS.log Energy: -1080571.8281075

C	-0.47764	-0.72278	-0.15940
H	-0.35108	-1.80081	-0.29849
H	-0.45553	-0.28438	-1.16372
O	2.38478	-0.42198	0.02718
O	0.86260	1.59245	0.84305
Si	2.98427	-1.72312	-0.81108
Si	0.76092	2.79105	-0.30122
C	2.56878	-3.28291	0.12810
H	1.49037	-3.44199	0.18735
H	3.00635	-4.16012	-0.35151
H	2.95912	-3.22241	1.14572
C	4.82830	-1.48086	-0.90588
H	5.29984	-2.28242	-1.47707
H	5.07058	-0.53389	-1.39025
H	5.27265	-1.47679	0.09085

C	2.22475	-1.74274	-2.51620
H	1.14159	-1.86325	-2.46500
H	2.43767	-0.81090	-3.04250
H	2.62463	-2.56485	-3.11257
C	1.46287	4.33603	0.46319
H	2.50846	4.19011	0.73714
H	1.40681	5.17785	-0.22917
H	0.91298	4.60297	1.36660
C	-1.03650	3.02630	-0.75389
H	-1.63565	3.26112	0.12704
H	-1.15326	3.84374	-1.46797
H	-1.44935	2.12463	-1.21022
C	1.73238	2.28594	-1.81646
H	2.76819	2.06614	-1.55616
H	1.30881	1.39061	-2.27560
H	1.72432	3.08155	-2.56375
C	-1.82184	-0.43110	0.51390
H	-1.89022	-0.95716	1.46845
H	-1.91426	0.63344	0.73709
C	-2.99319	-0.84388	-0.35332
H	-2.96364	-0.29765	-1.30728
H	-2.93286	-1.91569	-0.58964
C	-5.33532	-0.90077	-0.41984
H	-5.34521	-1.97103	-0.66068
H	-5.36489	-0.34349	-1.36434
C	-6.55081	-0.55542	0.41267
H	-6.51477	-1.11577	1.35171
H	-6.53385	0.51299	0.64777
O	-4.19272	-0.56430	0.32529
O	-7.69109	-0.89988	-0.35318
Si	0.98022	-0.03212	0.78418
C	1.07199	-0.68162	2.52295
H	0.54516	-0.10105	3.27730
H	0.84768	-1.74273	2.62454
H	2.23208	-0.60441	2.83194
H	-8.47730	-0.69182	0.14820
H	3.70204	-0.32316	1.94659
O	3.57695	-0.57105	2.87470

gas_TriSil-1n-neutral.log Energy: -1033046.7327919

C	-0.48082	-0.77779	0.09179
H	-0.45954	-1.86992	0.17754
H	-0.33753	-0.55418	-0.97004
O	2.36775	-0.56197	0.29385
O	0.92917	1.56340	0.93502
Si	2.97982	-1.91365	-0.43091
Si	1.41781	2.64056	-0.22671
C	2.61995	-3.40259	0.64138
H	1.54505	-3.55145	0.76228
H	3.03224	-4.31193	0.20041
H	3.05675	-3.28197	1.63397
C	4.81524	-1.64653	-0.60646
H	5.29490	-2.50177	-1.08570
H	5.01905	-0.76257	-1.21274
H	5.28045	-1.49918	0.36905
C	2.18688	-2.12858	-2.10903
H	1.11147	-2.28935	-2.02112
H	2.34655	-1.24684	-2.73186
H	2.61213	-2.98753	-2.63174
C	0.55392	4.25153	0.13608
H	0.81228	4.61192	1.13272
H	0.83732	5.01993	-0.58551
H	-0.52927	4.12929	0.09288
C	0.91923	1.99178	-1.91012
H	-0.16093	1.84759	-1.97215
H	1.21073	2.68740	-2.69909
H	1.40250	1.03394	-2.11153
C	3.27130	2.83168	-0.14125
H	3.57881	3.21154	0.83412
H	3.75145	1.86396	-0.29264
H	3.63551	3.52253	-0.90385
C	-1.83397	-0.23832	0.56074
H	-2.00384	-0.48512	1.61115
H	-1.84874	0.85106	0.49066
C	-2.98222	-0.79484	-0.25590
H	-2.84934	-0.53712	-1.31623
H	-3.00002	-1.89174	-0.18680
C	-5.31392	-0.72647	-0.48781
H	-5.39555	-1.81862	-0.42135
H	-5.24398	-0.45947	-1.54971

C	-6.54471	-0.08697	0.11722
H	-6.60799	-0.35887	1.17513
H	-6.45649	1.00123	0.04569
O	-4.19446	-0.26222	0.22166
O	-7.66320	-0.56509	-0.60853
Si	0.97957	-0.06940	1.02032
C	0.97341	-0.56939	2.80710
H	0.08103	-0.19876	3.31293
H	0.99595	-1.65594	2.90669
H	1.84594	-0.16171	3.31844
H	-8.45745	-0.17550	-0.24780

gas_water.log Energy: -47964.2313678

O	0.00000	0.11619	-0.00000
H	0.76011	-0.46477	-0.00000
H	-0.76011	-0.46477	0.00000

soln_hydroxyl_radical.log Energy: -47530.5536898

O	0.00000	0.00000	0.10797
H	-0.00000	-0.00000	-0.86374

soln_H_radical.log Energy: -314.0653976

H	0.00000	0.00000	0.00000

soln_TriSil-1n-aH-OH.log Energy: -1032633.6543212

C	0.54126	-0.30723	2.35910
H	0.83660	-1.00861	3.13302
O	1.44865	-0.63636	-0.34876
O	1.48631	1.77273	0.68862
Si	1.34651	-2.23224	-0.80528
Si	0.82409	2.55527	-0.62835
C	2.94820	-2.67650	-1.64644
H	3.78682	-2.54213	-0.95923
H	2.94408	-3.71735	-1.97710
H	3.12109	-2.04390	-2.51944
C	-0.09738	-2.36214	-1.97464
H	-0.17919	-3.37328	-2.37976
H	-1.03471	-2.12601	-1.46610
H	0.01872	-1.67191	-2.81279
C	1.08639	-3.31161	0.69387

H	1.90338	-3.20088	1.41043
H	0.15142	-3.06968	1.20226
H	1.04601	-4.36165	0.39398
C	-0.83723	1.82826	-1.06875
H	-1.51433	1.82901	-0.21253
H	-1.29762	2.42523	-1.86010
H	-0.73975	0.80485	-1.43364
C	1.99303	2.40636	-2.07318
H	2.10830	1.36338	-2.37347
H	1.61622	2.96651	-2.93204
H	2.97973	2.79996	-1.82062
C	0.63038	4.33480	-0.11382
H	-0.04303	4.42163	0.74142
H	1.59204	4.77053	0.16452
H	0.21480	4.92783	-0.93146
C	-0.89476	0.11189	2.33742
H	-1.36604	-0.01556	3.31312
H	-0.97245	1.16844	2.06273
C	-1.68211	-0.67658	1.29378
H	-1.17367	-0.62413	0.32807
H	-1.75891	-1.73147	1.57819
C	-3.65916	-0.62617	0.03794
H	-3.78080	-1.71205	0.12188
H	-3.08577	-0.41415	-0.87192
C	-5.01070	0.04677	-0.03564
H	-5.58274	-0.16722	0.87073
H	-4.87795	1.12858	-0.11708
O	-2.97886	-0.11657	1.16776
O	-5.67799	-0.46506	-1.18346
Si	1.73998	0.18710	1.04878
C	3.49276	-0.08869	1.57968
H	3.74776	0.51659	2.45128
H	3.64673	-1.13844	1.84034
H	4.18180	0.16415	0.77158
H	-6.52555	-0.02302	-1.25748

soln_TriSil-1n-bH-OH.log Energy: -1032634.4099682

C	-0.12931	-1.20290	1.57505
H	-0.22522	-2.29312	1.65820
H	-0.95882	-0.75939	2.12762

O	-1.95324	-1.29091	-0.62799
O	-0.17314	0.71696	-0.63508
Si	-3.50205	-0.77562	-0.30070
Si	-0.05662	2.23142	0.04276
C	-4.63496	-2.05441	-1.04065
H	-4.45859	-3.03664	-0.59760
H	-5.67982	-1.78836	-0.86619
H	-4.48303	-2.13499	-2.11891
C	-3.78588	0.88735	-1.09351
H	-4.84461	1.15215	-1.03919
H	-3.22184	1.67175	-0.58854
H	-3.49403	0.87786	-2.14534
C	-3.75979	-0.66524	1.54302
H	-3.53871	-1.61719	2.02966
H	-3.12955	0.10402	1.99260
H	-4.80085	-0.41123	1.75716
C	1.73107	2.60700	0.41358
H	2.36644	2.38700	-0.44694
H	1.84356	3.66716	0.65395
H	2.09543	2.02786	1.26233
C	-1.07394	2.32338	1.60305
H	-0.73040	1.60596	2.35006
H	-0.98673	3.32327	2.03560
H	-2.13067	2.13666	1.40593
C	-0.70063	3.42572	-1.23420
H	-0.09795	3.38075	-2.14388
H	-1.73524	3.20412	-1.50192
H	-0.66011	4.44940	-0.85521
C	1.17209	-0.73955	2.10003
H	1.21898	0.19602	2.64352
C	2.45393	-1.35236	1.68104
H	3.13808	-1.47259	2.52975
H	2.28620	-2.34069	1.23841
C	4.23961	-1.09210	0.14457
H	3.99391	-2.05997	-0.30834
H	5.00465	-1.25777	0.91190
C	4.75154	-0.14038	-0.91298
H	3.97835	0.01293	-1.67057
H	4.98773	0.82493	-0.45782
O	3.08619	-0.50707	0.70911

O	5.91478	-0.72094	-1.49203
Si	-0.40924	-0.86181	-0.26280
C	0.70149	-1.88515	-1.33548
H	1.74835	-1.62189	-1.18099
H	0.57757	-2.94771	-1.11916
H	0.46062	-1.72249	-2.38805
H	6.23908	-0.12623	-2.17094

soln_TriSil-1n-cH-OH.log Energy: -1032633.9623343

C	-0.41781	-0.76703	0.17559
H	-0.43764	-1.84799	0.34651
H	-0.27688	-0.62833	-0.89885
O	2.45218	-0.54006	0.34006
O	1.02037	1.58380	1.01083
Si	2.95670	-1.90596	-0.46702
Si	1.26169	2.64774	-0.25218
C	2.43639	-3.41159	0.50341
H	1.34936	-3.46881	0.59248
H	2.77909	-4.32273	0.00766
H	2.86102	-3.39511	1.50915
C	4.81065	-1.78992	-0.58037
H	5.21984	-2.65364	-1.10891
H	5.11076	-0.89022	-1.12158
H	5.26227	-1.75616	0.41301
C	2.19883	-1.92977	-2.17001
H	1.11395	-2.03709	-2.12317
H	2.42962	-1.01091	-2.71287
H	2.59484	-2.76905	-2.74683
C	0.34365	4.20502	0.19137
H	0.70907	4.62119	1.13234
H	0.47218	4.96244	-0.58493
H	-0.72517	4.00864	0.29814
C	0.59374	1.92077	-1.83595
H	-0.47011	1.69045	-1.75154
H	0.71957	2.63773	-2.65091
H	1.12314	1.00622	-2.11142
C	3.08915	2.97114	-0.42033
H	3.50711	3.35884	0.51083
H	3.62273	2.05399	-0.67710
H	3.27890	3.70494	-1.20702

C	-1.75118	-0.14661	0.60376
H	-1.90431	-0.26642	1.68132
H	-1.72337	0.93818	0.42527
C	-2.89863	-0.74655	-0.12181
H	-2.81447	-1.02690	-1.16883
C	-5.21682	-0.82329	-0.48110
H	-5.24704	-1.91339	-0.41142
H	-5.09034	-0.53949	-1.52929
C	-6.48576	-0.22322	0.07940
H	-6.59196	-0.50004	1.13115
H	-6.44300	0.86649	0.00803
O	-4.13094	-0.32153	0.28754
O	-7.56679	-0.73669	-0.68820
Si	1.05802	-0.06120	1.07494
C	1.07368	-0.56446	2.85804
H	0.17387	-0.21931	3.37085
H	1.11413	-1.65269	2.94073
H	1.94135	-0.15074	3.37497
H	-8.38216	-0.37920	-0.33190

soln_TriSil-1n-dH-OH.log Energy: -1032636.3320297

C	-0.41585	-1.40169	-0.00629
H	-0.33298	-2.49200	-0.02719
H	-0.28329	-1.06409	-1.03865
O	2.40045	-1.40637	0.50111
O	1.09976	0.90427	0.82218
Si	3.60935	-0.92755	-0.54065
Si	0.49203	2.22287	0.01792
C	4.68472	-2.42438	-0.80617
H	4.12079	-3.23524	-1.27167
H	5.52619	-2.18123	-1.45873
H	5.08728	-2.78945	0.14086
C	4.58530	0.45465	0.24114
H	5.38094	0.78895	-0.42875
H	3.94498	1.31049	0.45985
H	5.04715	0.12656	1.17467
C	2.86575	-0.36512	-2.15632
H	2.14687	-1.09360	-2.53660
H	2.36019	0.59504	-2.05182
H	3.65089	-0.24431	-2.90658

C	-0.64974	3.12204	1.18374
H	-0.12617	3.42803	2.09158
H	-1.05867	4.01752	0.71039
H	-1.48647	2.48200	1.47253
C	-0.44736	1.73094	-1.51890
H	-1.37456	1.20692	-1.28267
H	-0.71153	2.63694	-2.07077
H	0.14478	1.09860	-2.18177
C	1.95133	3.28612	-0.44232
H	2.52606	3.56697	0.44245
H	2.61904	2.76250	-1.12947
H	1.61556	4.20337	-0.93162
C	-1.79681	-0.99514	0.51731
H	-1.99302	-1.48660	1.47233
H	-1.84583	0.08160	0.70014
C	-2.88356	-1.36555	-0.46459
H	-2.73523	-0.84818	-1.41646
H	-2.89095	-2.44264	-0.65048
C	-5.21919	-1.23053	-0.71799
C	-6.51387	-0.72881	-0.23561
H	-7.31512	-1.22830	-0.78306
H	-6.62813	-0.94484	0.83010
O	-4.15168	-0.97995	0.07811
O	-6.60976	0.70167	-0.43817
Si	0.99108	-0.72351	1.00878
C	0.78413	-1.09278	2.81334
H	-0.12981	-0.63606	3.19789
H	0.72460	-2.16886	2.98773
H	1.62639	-0.70076	3.38663
H	-7.45929	0.98577	-0.09137
H	-5.02440	-1.43608	-1.76397

soln_TriSil-1n-eH-OH.log Energy: -1032634.6042953

C	-0.35770	-1.07946	0.34773
H	-0.34128	-2.15228	0.56492
H	-0.18788	-0.98515	-0.72711
O	2.47559	-1.03798	0.81105
O	1.16972	1.30744	0.95291
Si	3.31706	-1.42083	-0.57226
Si	0.78068	2.43732	-0.20245

C	4.65060	-2.61027	-0.04900
H	4.22010	-3.51435	0.38631
H	5.25963	-2.90513	-0.90631
H	5.31045	-2.15647	0.69325
C	4.06358	0.12711	-1.29374
H	4.75610	-0.13183	-2.09841
H	3.29582	0.77744	-1.71482
H	4.61732	0.68998	-0.54019
C	2.18554	-2.21602	-1.82395
H	1.63349	-3.05230	-1.39115
H	1.46636	-1.49963	-2.22487
H	2.77643	-2.59846	-2.65998
C	-0.61270	3.48727	0.45420
H	-0.33001	3.96614	1.39397
H	-0.86325	4.27411	-0.26126
H	-1.51260	2.89545	0.63114
C	0.26070	1.60219	-1.78837
H	-0.70319	1.10220	-1.67640
H	0.15887	2.35096	-2.57772
H	0.99354	0.86396	-2.11959
C	2.28913	3.49754	-0.47094
H	2.58609	3.98542	0.45994
H	3.13582	2.91176	-0.83160
H	2.07919	4.27785	-1.20610
C	-1.72403	-0.49452	0.71186
H	-1.93631	-0.65534	1.77140
H	-1.73439	0.58514	0.54588
C	-2.82815	-1.11787	-0.11398
H	-2.64297	-0.94644	-1.18149
H	-2.86284	-2.20165	0.04960
C	-5.14782	-1.06984	-0.51109
H	-5.12684	-2.16853	-0.43831
H	-5.03346	-0.81072	-1.57043
C	-6.42127	-0.51506	-0.00008
H	-6.74568	-0.68299	1.01974
O	-4.07329	-0.54003	0.25005
O	-7.40145	-0.35470	-0.94623
Si	1.07315	-0.30605	1.25979
C	0.90738	-0.50564	3.09529
H	0.00600	-0.00811	3.45799

H	0.84528	-1.56087	3.36790
H	1.76518	-0.07030	3.61150
H	-8.23355	-0.15657	-0.50893

soln_TriSil-1n-fH-OH.log Energy: -1032625.4744592

C	-0.37482	-1.06591	0.33391
H	-0.37049	-2.13807	0.55470
H	-0.19331	-0.97677	-0.73948
O	2.45192	-1.05817	0.83195
O	1.17778	1.30614	0.93628
Si	3.30528	-1.44896	-0.54212
Si	0.79976	2.43671	-0.22189
C	4.62486	-2.64649	-0.00235
H	4.18338	-3.54617	0.43107
H	5.24044	-2.94822	-0.85255
H	5.28034	-2.19537	0.74538
C	4.06862	0.09290	-1.25888
H	4.76857	-0.17168	-2.05522
H	3.30877	0.74584	-1.69017
H	4.61677	0.65499	-0.50071
C	2.18095	-2.23828	-1.80399
H	1.61726	-3.06876	-1.37505
H	1.47219	-1.51701	-2.21472
H	2.77770	-2.62789	-2.63251
C	-0.58870	3.49794	0.42730
H	-0.30615	3.97609	1.36748
H	-0.82979	4.28569	-0.29043
H	-1.49427	2.91404	0.60140
C	0.28139	1.60206	-1.80853
H	-0.68590	1.10785	-1.70037
H	0.18790	2.34983	-2.59985
H	1.01178	0.85905	-2.13445
C	2.31595	3.48685	-0.48638
H	2.61501	3.97108	0.44572
H	3.15923	2.89627	-0.84720
H	2.11206	4.26989	-1.22035
C	-1.73890	-0.46719	0.68321
H	-1.96483	-0.62743	1.73993
H	-1.73687	0.61267	0.51858
C	-2.83979	-1.07743	-0.15621

H	-2.64262	-0.90574	-1.22124
H	-2.88973	-2.16061	0.00574
C	-5.15584	-1.00683	-0.56251
H	-5.25424	-2.08567	-0.40057
H	-4.99174	-0.83117	-1.63119
C	-6.42120	-0.30259	-0.11474
H	-6.59749	-0.42920	0.96819
H	-6.34210	0.79264	-0.23183
O	-4.08308	-0.48742	0.19498
O	-7.55251	-0.70863	-0.76673
Si	1.05449	-0.30280	1.25710
C	0.86318	-0.48345	3.09203
H	-0.03477	0.03130	3.43890
H	0.78129	-1.53501	3.37341
H	1.72116	-0.05658	3.61495

soln_TriSil-1n-gH-OH.log Energy: -1032627.2350061

C	-0.33440	-1.04412	0.36486
H	-0.34070	-2.11315	0.59947
H	-0.15039	-0.96905	-0.70937
O	2.49464	-1.02565	0.84617
O	1.18962	1.33439	0.98025
Si	3.33550	-1.48467	-0.51573
Si	0.87731	2.44179	-0.22218
C	4.62389	-2.69724	0.06357
H	4.15936	-3.57164	0.52381
H	5.23278	-3.04059	-0.77559
H	5.28948	-2.23958	0.79825
C	4.13866	0.01429	-1.27800
H	4.82212	-0.29294	-2.07338
H	3.39753	0.68268	-1.71845
H	4.71274	0.57548	-0.53851
C	2.18913	-2.28652	-1.74901
H	1.60606	-3.08778	-1.29136
H	1.49750	-1.56265	-2.18341
H	2.77485	-2.71896	-2.56402
C	-0.50316	3.54849	0.36211
H	-0.23675	4.04441	1.29769
H	-0.70973	4.32216	-0.38116
H	-1.42365	2.98482	0.52525

C	0.38094	1.57610	-1.79901
H	-0.60309	1.11302	-1.70503
H	0.33176	2.30371	-2.61279
H	1.09765	0.80355	-2.08377
C	2.43053	3.43938	-0.47074
H	2.71181	3.95001	0.45270
H	3.26672	2.80963	-0.77831
H	2.27683	4.19873	-1.24085
C	-1.69026	-0.42450	0.70889
H	-1.90838	-0.55793	1.77150
H	-1.67832	0.65143	0.51983
C	-2.80360	-1.04265	-0.10816
H	-2.61329	-0.89466	-1.17817
H	-2.85995	-2.12207	0.07610
C	-5.12094	-0.95911	-0.50037
H	-5.21370	-2.03746	-0.32884
H	-4.96115	-0.79567	-1.57219
C	-6.37969	-0.25310	-0.04961
H	-6.53628	-0.42364	1.01837
H	-6.28198	0.82217	-0.21998
O	-4.03816	-0.43582	0.24163
O	-7.46136	-0.78494	-0.80608
Si	1.09960	-0.27772	1.27929
C	0.91860	-0.46870	3.09705
H	0.50606	0.30847	3.73102
H	1.15591	-1.39403	3.61142
H	-8.27169	-0.37764	-0.49482

soln_TriSil-1n-neutral.log Energy: -1033051.4127575

C	-0.38061	-0.82014	0.17989
H	-0.36710	-1.90319	0.33991
H	-0.23472	-0.66574	-0.89186
O	2.48376	-0.51994	0.39005
O	0.98301	1.56721	1.02537
Si	3.02987	-1.83060	-0.47777
Si	1.21680	2.63334	-0.23685
C	2.52291	-3.39434	0.40345
H	1.43592	-3.47748	0.46804
H	2.89418	-4.27245	-0.12987
H	2.92791	-3.41943	1.41715

C	4.88299	-1.67231	-0.54776
H	5.31982	-2.49828	-1.11330
H	5.17385	-0.73920	-1.03485
H	5.31559	-1.68241	0.45456
C	2.31036	-1.77884	-2.19680
H	1.22679	-1.90627	-2.18370
H	2.53825	-0.82912	-2.68510
H	2.73547	-2.58005	-2.80623
C	0.33332	4.20225	0.23532
H	0.72576	4.60671	1.17053
H	0.45711	4.96229	-0.53917
H	-0.73594	4.02248	0.36435
C	0.50411	1.92525	-1.80967
H	-0.55585	1.68919	-1.69642
H	0.60316	2.65310	-2.61866
H	1.02874	1.01674	-2.11259
C	3.04511	2.92940	-0.44473
H	3.49111	3.30065	0.48012
H	3.55759	2.00667	-0.72359
H	3.22772	3.66856	-1.22811
C	-1.73430	-0.24538	0.60396
H	-1.90427	-0.41306	1.67042
H	-1.74916	0.83521	0.44295
C	-2.86886	-0.87007	-0.17881
H	-2.72929	-0.69393	-1.25224
H	-2.89335	-1.95434	-0.01745
C	-5.20276	-0.83216	-0.46748
H	-5.26021	-1.91685	-0.32232
H	-5.09737	-0.63577	-1.54050
C	-6.45646	-0.17209	0.06031
H	-6.56036	-0.37749	1.12863
H	-6.39262	0.90975	-0.08184
O	-4.10032	-0.30050	0.23861
O	-7.55797	-0.70909	-0.66321
Si	1.06432	-0.07622	1.09709
C	1.06918	-0.57354	2.88189
H	0.15206	-0.25625	3.38168
H	1.14318	-1.65996	2.96694
H	1.91631	-0.13207	3.40987
H	-8.36201	-0.31870	-0.31602

soln_water.log Energy: -47971.9724922

O	0.00000	0.11747	-0.00000
H	0.75906	-0.47000	0.00000
H	-0.75906	-0.46975	-0.00000

TriSil-1n-reduced-a.log Energy: -1032633.3761589

C	0.18460	-1.20355	0.22336
H	0.01318	-1.64932	-0.75372
O	-1.41446	1.17064	0.51034
O	-2.61176	-1.16297	0.79070
Si	-0.36782	2.29004	-0.14332
Si	-3.63091	-1.13809	-0.53247
C	1.10025	2.48480	0.99192
H	1.62633	1.54104	1.14525
H	1.81266	3.20050	0.57527
H	0.78206	2.85657	1.96828
C	-1.32170	3.88446	-0.25926
H	-0.70728	4.67003	-0.70475
H	-2.21069	3.75873	-0.88089
H	-1.64113	4.22441	0.72782
C	0.15959	1.73261	-1.84337
H	0.58957	0.72991	-1.82353
H	-0.69200	1.72397	-2.52693
H	0.90953	2.41503	-2.25059
C	-4.69509	-2.65959	-0.40295
H	-5.27631	-2.65414	0.52135
H	-5.39477	-2.70917	-1.24021
H	-4.08635	-3.56579	-0.41772
C	-2.61402	-1.17049	-2.09630
H	-2.00884	-2.07692	-2.15705
H	-3.26932	-1.14373	-2.97012
H	-1.94618	-0.30843	-2.15286
C	-4.67679	0.40363	-0.47588
H	-5.21681	0.47609	0.47032
H	-4.06274	1.29876	-0.58787
H	-5.41245	0.39352	-1.28351
C	1.57742	-1.33472	0.74207
H	1.71818	-0.76832	1.66497
H	1.77928	-2.38691	0.98252

C	2.61076	-0.88912	-0.28127
H	2.49947	-1.46457	-1.20742
H	2.47764	0.17020	-0.52514
C	4.92047	-0.64171	-0.62123
H	4.79248	0.42575	-0.83317
H	4.87024	-1.18762	-1.57001
C	6.25627	-0.88044	0.04552
H	6.29875	-0.33588	0.99216
H	6.38276	-1.94643	0.25078
O	3.90748	-1.09034	0.25667
O	7.26434	-0.41754	-0.84552
Si	-1.20512	-0.36212	1.08929
C	-0.91682	-0.28858	2.91717
H	-0.79639	-1.28642	3.34254
H	-0.01353	0.28501	3.13555
H	-1.75548	0.19943	3.41724
H	8.11760	-0.56497	-0.43373

TriSil-1n-reduced-b.log Energy: -1032633.4894369

C	-0.14871	-0.83711	1.57318
H	-0.33457	-1.91546	1.63952
H	-0.94285	-0.32689	2.11994
O	-1.93053	-0.36911	-0.65751
O	0.26186	1.10320	-0.54613
Si	-3.28746	-1.23637	-0.23292
Si	-0.27402	2.61612	-0.08616
C	-2.84391	-3.04343	-0.10421
H	-2.09451	-3.21678	0.67097
H	-3.72786	-3.63328	0.14920
H	-2.44990	-3.41810	-1.05103
C	-4.53584	-0.95186	-1.58330
H	-5.46674	-1.47950	-1.36445
H	-4.76605	0.11099	-1.68191
H	-4.16210	-1.31021	-2.54445
C	-3.93054	-0.59712	1.39547
H	-3.21555	-0.76522	2.20259
H	-4.13772	0.47346	1.33915
H	-4.86074	-1.10566	1.66006
C	1.24255	3.68283	0.07273
H	1.78987	3.72836	-0.87096

H	0.97111	4.70235	0.35502
H	1.91491	3.28750	0.83689
C	-1.17730	2.50633	1.54311
H	-0.52839	2.12859	2.33537
H	-1.52372	3.49992	1.83764
H	-2.05126	1.85524	1.47388
C	-1.41793	3.26072	-1.40783
H	-0.91503	3.30285	-2.37599
H	-2.29418	2.61688	-1.50687
H	-1.76323	4.26751	-1.16221
C	1.18234	-0.48695	2.11205
H	1.31689	0.47614	2.58991
C	2.40121	-1.24158	1.74171
H	3.06138	-1.38685	2.60541
H	2.13896	-2.22894	1.34532
C	4.21927	-1.25676	0.22942
H	3.87153	-2.21374	-0.17703
H	4.94625	-1.46599	1.02266
C	4.85898	-0.43332	-0.86506
H	4.12522	-0.23701	-1.65124
H	5.19769	0.52309	-0.45883
O	3.12893	-0.51624	0.73779
O	5.95810	-1.17747	-1.37839
Si	-0.33411	-0.39978	-0.25843
C	0.56406	-1.61097	-1.33313
H	1.63372	-1.61244	-1.11885
H	0.17831	-2.61861	-1.16495
H	0.42528	-1.36578	-2.38784
H	6.36967	-0.65973	-2.07282

TriSil-1n-reduced-c.log Energy: -1032633.9472866

C	-0.41537	-0.77485	0.18585
H	-0.42888	-1.85529	0.36288
H	-0.28112	-0.64130	-0.88978
O	2.45366	-0.53202	0.33373
O	1.01270	1.58377	1.01210
Si	2.96072	-1.89542	-0.47595
Si	1.24981	2.64702	-0.25235
C	2.44884	-3.40385	0.49473
H	1.36233	-3.46498	0.58750

H	2.79298	-4.31322	-0.00328
H	2.87689	-3.38707	1.49901
C	4.81390	-1.77275	-0.59484
H	5.22445	-2.63455	-1.12546
H	5.10918	-0.87153	-1.13621
H	5.26854	-1.73828	0.39714
C	2.19813	-1.92080	-2.17676
H	1.11375	-2.03185	-2.12706
H	2.42418	-1.00080	-2.71965
H	2.59547	-2.75834	-2.75521
C	0.32989	4.20305	0.19172
H	0.69672	4.62080	1.13145
H	0.45553	4.95989	-0.58563
H	-0.73837	4.00510	0.30099
C	0.57963	1.91641	-1.83340
H	-0.48317	1.68265	-1.74535
H	0.70055	2.63270	-2.64967
H	1.11107	1.00320	-2.10931
C	3.07619	2.97439	-0.42494
H	3.49566	3.36280	0.50526
H	3.61128	2.05866	-0.68349
H	3.26212	3.70895	-1.21184
C	-1.74956	-0.16016	0.61965
H	-1.87405	-0.26413	1.70773
H	-1.74965	0.91662	0.42255
C	-2.89960	-0.78531	-0.08000
H	-2.91730	-1.85180	-0.28874
C	-5.21961	-0.88160	-0.42011
H	-5.26234	-1.90542	-0.03920
H	-5.11085	-0.91309	-1.50695
C	-6.46938	-0.12347	-0.03570
H	-6.56100	-0.08905	1.05275
H	-6.41205	0.90027	-0.41357
O	-4.11186	-0.20055	0.15525
O	-7.57097	-0.81278	-0.61265
Si	1.06139	-0.06088	1.07724
C	1.09310	-0.56305	2.86057
H	0.19613	-0.22151	3.38066
H	1.13910	-1.65104	2.94355
H	1.96329	-0.14524	3.37000

H	-8.37261	-0.33863	-0.38440

TriSil-1n-reduced-d.log Energy: -1032636.3334353

C	-0.46050	-0.89100	0.14449
H	-0.48672	-1.97227	0.31068
H	-0.20878	-0.74657	-0.90945
O	2.36921	-0.72707	0.71425
O	0.89732	1.47276	1.04901
Si	3.00218	-1.74964	-0.43531
Si	1.20916	2.53852	-0.19332
C	2.30764	-3.46064	-0.17974
H	1.22903	-3.47626	-0.34771
H	2.76561	-4.16638	-0.87661
H	2.50026	-3.81494	0.83491
C	4.84570	-1.72762	-0.17839
H	5.34313	-2.38446	-0.89526
H	5.24189	-0.71889	-0.31352
H	5.10701	-2.06407	0.82684
C	2.58665	-1.13832	-2.14751
H	1.51442	-1.18312	-2.34432
H	2.92120	-0.11005	-2.29542
H	3.08790	-1.76396	-2.89045
C	0.58195	4.19606	0.37690
H	1.08116	4.50804	1.29645
H	0.76612	4.95904	-0.38259
H	-0.49273	4.16233	0.56722
C	0.31389	2.00242	-1.74008
H	-0.75440	1.87342	-1.55498
H	0.43225	2.76384	-2.51498
H	0.71011	1.06457	-2.13173
C	3.04807	2.59537	-0.49503
H	3.58104	2.90273	0.40706
H	3.42903	1.61844	-0.79727
H	3.28467	3.30998	-1.28677
C	-1.83617	-0.28474	0.43390
H	-2.13165	-0.48514	1.46630
H	-1.80504	0.80014	0.31237
C	-2.88377	-0.84841	-0.49801
H	-2.62908	-0.63345	-1.53918
H	-2.97289	-1.93120	-0.37687

C	-5.18351	-0.66921	-0.96116
C	-6.50723	-0.13877	-0.60582
H	-6.44209	0.93482	-0.40929
H	-7.19108	-0.30213	-1.44060
O	-4.14747	-0.24377	-0.19848
O	-7.02123	-0.80190	0.57469
Si	0.90014	-0.16725	1.19672
C	0.66409	-0.55596	2.99278
H	-0.27915	-0.14673	3.35937
H	0.64982	-1.63590	3.15254
H	1.47313	-0.13386	3.59185
H	-7.87783	-0.41462	0.77263
H	-5.05063	-1.59141	-1.51427

TriSil-1n-reduced-e.log Energy: -1032636.2360835

C	-0.33845	-0.96119	0.16725
H	-0.21664	-2.03762	0.32682
H	-0.21180	-0.79315	-0.90494
O	2.47227	-0.32669	0.32081
O	0.75306	1.54658	1.05784
Si	3.16242	-1.59518	-0.50789
Si	0.79435	2.66823	-0.17657
C	2.86448	-3.17471	0.43845
H	1.79725	-3.38761	0.52985
H	3.33066	-4.01950	-0.07385
H	3.28813	-3.11456	1.44294
C	4.98121	-1.21731	-0.62153
H	5.50627	-2.00779	-1.16216
H	5.14996	-0.27731	-1.15104
H	5.42682	-1.13324	0.37157
C	2.41189	-1.69819	-2.21128
H	1.35337	-1.95949	-2.16822
H	2.50884	-0.74641	-2.73764
H	2.92262	-2.46233	-2.80226
C	-0.37600	4.03087	0.31076
H	-0.07970	4.48170	1.26001
H	-0.38899	4.81735	-0.44691
H	-1.39298	3.64792	0.41805
C	0.25054	1.87827	-1.77773
H	-0.76180	1.47666	-1.70153

H	0.25762	2.62471	-2.57573
H	0.92105	1.06823	-2.07255
C	2.53819	3.30402	-0.34130
H	2.88862	3.73903	0.59681
H	3.21852	2.49560	-0.61646
H	2.59718	4.07406	-1.11380
C	-1.74114	-0.52258	0.59523
H	-1.89083	-0.70491	1.66240
H	-1.86186	0.55148	0.43442
C	-2.81199	-1.25436	-0.18532
H	-2.68122	-1.07672	-1.26005
H	-2.73669	-2.33532	-0.01500
C	-5.14733	-1.45719	-0.49591
H	-5.09874	-2.53153	-0.29425
H	-4.99352	-1.29967	-1.57005
C	-6.46065	-0.94242	-0.08724
H	-6.97036	-1.27006	0.80860
O	-4.09240	-0.79451	0.22048
O	-6.80760	0.28101	-0.59450
Si	1.03008	-0.07648	1.07705
C	1.13698	-0.61770	2.84605
H	0.20060	-0.42238	3.37219
H	1.33790	-1.68989	2.89923
H	1.93873	-0.09425	3.36990
H	-7.62396	0.57874	-0.18432

TriSil-1n-reduced-f.log Energy: -1032625.2590227

C	-0.41831	-0.83915	0.17807
H	-0.39629	-1.92148	0.34193
H	-0.26709	-0.68693	-0.89325
O	2.44156	-0.50700	0.40023
O	0.91497	1.56273	1.03040
Si	3.00754	-1.80267	-0.47703
Si	1.14393	2.63120	-0.23075
C	2.50900	-3.38064	0.38316
H	1.42240	-3.47550	0.43670
H	2.89429	-4.24934	-0.15559
H	2.90484	-3.41201	1.40030
C	4.85952	-1.62503	-0.53013
H	5.30923	-2.44011	-1.10135

H	5.14466	-0.68358	-1.00444
H	5.28426	-1.64197	0.47544
C	2.30279	-1.74015	-2.20183
H	1.22052	-1.87869	-2.20056
H	2.52579	-0.78341	-2.67850
H	2.74173	-2.53088	-2.81517
C	0.25074	4.19444	0.24206
H	0.63975	4.60013	1.17817
H	0.37108	4.95602	-0.53144
H	-0.81763	4.00843	0.36967
C	0.43630	1.91947	-1.80419
H	-0.62142	1.67384	-1.69021
H	0.52831	2.64910	-2.61239
H	0.96862	1.01595	-2.10853
C	2.97051	2.93852	-0.43736
H	3.41388	3.31094	0.48829
H	3.48870	2.01940	-0.71754
H	3.14891	3.68013	-1.21940
C	-1.77974	-0.27481	0.59121
H	-1.95475	-0.43814	1.65750
H	-1.80380	0.80460	0.42376
C	-2.90293	-0.91474	-0.19529
H	-2.75644	-0.74713	-1.26900
H	-2.92231	-1.99743	-0.02403
C	-5.23514	-0.89681	-0.50189
H	-5.30105	-1.97702	-0.33256
H	-5.12218	-0.72174	-1.57728
C	-6.49589	-0.22049	-0.00123
H	-6.62327	-0.34946	1.08825
H	-6.44654	0.87604	-0.12218
O	-4.14269	-0.34954	0.20614
O	-7.64445	-0.65273	-0.60453
Si	1.01451	-0.07976	1.10160
C	1.01802	-0.57836	2.88598
H	0.09446	-0.27401	3.38197
H	1.10642	-1.66376	2.97038
H	1.85672	-0.12595	3.41813

TriSil-1n-reduced-g.log Energy: -1032627.9634692

C	-0.70154	-1.04322	-0.42698

H	-0.72650	-2.13092	-0.54831
H	-0.64823	-0.62346	-1.43544
O	2.10997	-0.93184	-0.56132
O	0.88649	0.98136	0.88547
Si	3.72884	-1.24754	-0.28997
Si	0.92671	2.40049	0.01058
C	4.32444	-0.28886	1.19515
H	3.80673	-0.60328	2.10401
H	5.39324	-0.46079	1.34391
H	4.16990	0.78334	1.06625
C	4.63333	-0.71474	-1.82656
H	5.70163	-0.92277	-1.73467
H	4.26049	-1.24565	-2.70474
H	4.51154	0.35665	-1.99871
C	3.92440	-3.07597	0.01010
H	3.36485	-3.38032	0.89754
H	3.55878	-3.65681	-0.83899
H	4.97440	-3.33204	0.16864
C	0.13173	3.69882	1.08079
H	0.66147	3.80166	2.02993
H	0.14380	4.66957	0.58046
H	-0.90756	3.44265	1.29642
C	-0.01799	2.19515	-1.58528
H	-1.05177	1.89583	-1.40237
H	-0.03238	3.14386	-2.12731
H	0.44692	1.44941	-2.23297
C	2.70169	2.83292	-0.35629
H	3.27824	2.95884	0.56194
H	3.17806	2.05551	-0.95688
H	2.75292	3.76927	-0.91713
C	-1.97098	-0.56378	0.27928
H	-2.03680	-1.00193	1.27875
H	-1.94348	0.52097	0.40757
C	-3.21344	-0.93061	-0.50251
H	-3.17656	-0.48372	-1.50340
H	-3.28150	-2.01826	-0.62364
C	-5.56075	-0.78256	-0.48578
H	-5.65965	-1.86974	-0.58205
H	-5.56303	-0.34871	-1.49211
C	-6.71264	-0.22765	0.32126

H	-6.69728	-0.65391	1.32759
H	-6.61923	0.85825	0.40178
O	-4.36093	-0.45724	0.18608
O	-7.91453	-0.57947	-0.35433
Si	0.86815	-0.60995	0.47367
C	1.04638	-1.55541	2.03898
H	1.22676	-1.08564	2.99933
H	0.95856	-2.63637	2.07194
H	-8.65178	-0.22046	0.14244

methyl_radical.log Energy: -24995.5223725

C	-0.00001	0.00003	-0.00028
H	-0.96685	0.48112	0.00057
H	0.90024	0.59651	0.00057
H	0.06664	-1.07784	0.00057

PDMS_a.log Energy: -839548.0387342

C	0.24571	1.83278	1.61069
H	1.28377	2.13315	1.76880
H	0.01335	1.02684	2.30817
O	0.82164	-0.08274	-0.46028
O	-1.60911	0.92990	-0.40992
Si	2.33835	-0.62166	-0.02754
Si	-2.47653	-0.45202	-0.04406
C	3.55457	0.77656	-0.24059
H	3.32128	1.60914	0.42686
H	4.56991	0.44245	-0.01540
H	3.54055	1.14952	-1.26694
C	2.73339	-2.03947	-1.16586
H	3.71216	-2.46289	-0.93025
H	1.98999	-2.83329	-1.06733
H	2.74756	-1.71365	-2.20774
C	2.29271	-1.19464	1.74550
H	2.06880	-0.36962	2.42380
H	1.53435	-1.96781	1.88523
H	3.25887	-1.61523	2.03437
C	-4.26950	0.04635	-0.02077
H	-4.57775	0.44512	-0.98935
H	-4.90279	-0.81422	0.20587
H	-4.45409	0.81026	0.73707

C	-1.94501	-1.09620	1.62468
H	-2.11136	-0.35375	2.40743
H	-2.52014	-1.98926	1.88036
H	-0.88698	-1.36681	1.62826
C	-2.16442	-1.73363	-1.36021
H	-2.41445	-1.34775	-2.35053
H	-1.11684	-2.03935	-1.36733
H	-2.77564	-2.62107	-1.18043
Si	-0.02696	1.29622	-0.14501
C	0.46048	2.61671	-1.32313
H	0.02665	2.71989	-2.31208
H	1.24795	3.32793	-1.09689
H	-0.39077	2.68683	1.85030

PDMS_b.log Energy: -839548.4265287

C	0.21053	1.71396	1.73171
H	1.25507	1.96756	1.92419
H	-0.06130	0.87232	2.37034
O	0.81340	-0.00655	-0.50686
O	-1.65274	0.93185	-0.30317
Si	2.28634	-0.63926	-0.05670
Si	-2.44326	-0.52304	-0.08786
C	3.55551	0.72790	-0.04997
H	3.29751	1.50561	0.67212
H	4.53864	0.33510	0.21950
H	3.63653	1.19087	-1.03551
C	2.70707	-1.93647	-1.32284
H	3.66051	-2.41307	-1.08480
H	1.93988	-2.71301	-1.35157
H	2.78720	-1.49971	-2.32021
C	2.13656	-1.40310	1.63706
H	1.87056	-0.65786	2.38853
H	1.37578	-2.18619	1.64665
H	3.08664	-1.85477	1.93260
C	-4.26017	-0.12891	-0.18589
H	-4.51500	0.29949	-1.15716
H	-4.86018	-1.03021	-0.04562
H	-4.53960	0.58901	0.58831
C	-1.99392	-1.25207	1.56715
H	-2.25672	-0.57319	2.38047

H	-2.53255	-2.18981	1.72245
H	-0.92485	-1.46475	1.62980
C	-1.94229	-1.68726	-1.42717
H	-2.02690	-1.43981	-2.48084
H	-1.52169	-2.66764	-1.22861
Si	-0.06533	1.31559	-0.06218
C	0.36182	2.74559	-1.15952
H	-0.24919	3.61866	-0.92253
H	1.41053	3.02108	-1.02810
H	0.20538	2.49273	-2.20973
H	-0.40076	2.57144	2.02127

PDMS_c.log Energy: -839548.4172228

C	0.20927	1.77195	1.68782
H	1.25246	2.04052	1.86762
H	-0.05122	0.94663	2.35171
O	0.80243	-0.02250	-0.49255
O	-1.65191	0.94006	-0.33773
Si	2.27550	-0.65049	-0.03863
Si	-2.48060	-0.47708	-0.05434
C	3.55928	0.70023	-0.12176
H	3.32267	1.51357	0.56783
H	4.54361	0.31034	0.14749
H	3.62539	1.11575	-1.12928
C	2.65195	-2.01396	-1.24768
H	3.60250	-2.49438	-1.00589
H	1.87199	-2.77792	-1.22300
H	2.71781	-1.62744	-2.26660
C	2.15106	-1.32876	1.69325
H	1.91607	-0.54341	2.41355
H	1.37705	-2.09605	1.75830
H	3.09970	-1.78338	1.98896
C	-4.26768	-0.03871	-0.08117
H	-5.04658	-0.79129	-0.15162
H	-4.63038	0.98021	0.00405
C	-1.98174	-1.17198	1.60647
H	-2.17636	-0.46349	2.41302
H	-2.54267	-2.08588	1.81459
H	-0.91803	-1.42123	1.61444
C	-2.09555	-1.72340	-1.38666

H	-2.26857	-1.30838	-2.38103
H	-1.05353	-2.04247	-1.32396
H	-2.72889	-2.60623	-1.27334
Si	-0.06461	1.32052	-0.09340
C	0.37944	2.71291	-1.23164
H	-0.22102	3.59987	-1.02072
H	1.43137	2.97936	-1.10735
H	0.22055	2.43161	-2.27420
H	-0.40824	2.63214	1.95510

PDMS_cation.log Energy: -814793.0299409

O	0.86378	0.04936	0.17878
O	-1.60748	1.04095	0.03565
Si	2.47325	-0.53026	-0.01176
Si	-2.57189	-0.39894	-0.00040
C	3.47895	0.88681	-0.65688
H	3.48298	1.72295	0.04467
H	4.51284	0.56646	-0.80350
H	3.09806	1.23879	-1.61741
C	2.31025	-1.92119	-1.22120
H	3.28723	-2.36829	-1.41667
H	1.65295	-2.69987	-0.83092
H	1.90369	-1.56619	-2.16961
C	2.98906	-1.07762	1.67820
H	2.98820	-0.23915	2.37663
H	2.31906	-1.84919	2.06067
H	3.99946	-1.49066	1.64546
C	-4.29681	0.22012	-0.24464
H	-4.38502	0.77065	-1.18255
H	-4.99336	-0.62026	-0.27728
H	-4.59607	0.87691	0.57368
C	-2.30733	-1.22903	1.63419
H	-2.59846	-0.57611	2.45855
H	-2.90984	-2.13810	1.69267
H	-1.26067	-1.50968	1.76523
C	-1.94174	-1.40130	-1.42708
H	-1.98553	-0.82976	-2.35588
H	-0.91094	-1.72145	-1.26366
H	-2.55585	-2.29575	-1.55221
Si	-0.06166	1.30430	0.06669

C	0.58991	2.98801	-0.01689
H	-0.22061	3.70971	-0.09018
H	1.18706	3.18232	0.87595
H	1.24498	3.06795	-0.88671

PDMS_neutral_B3LYP.log Energy: -840106.3264225

C	0.13362	1.84933	1.68315
H	1.13766	2.23181	1.87743
H	-0.07142	1.05666	2.40392
O	0.93974	-0.09362	-0.30161
O	-1.57611	0.77558	-0.37857
Si	2.50359	-0.61158	-0.02295
Si	-2.61652	-0.48972	-0.04653
C	3.71607	0.72013	-0.54160
H	3.59942	1.62596	0.05641
H	4.74208	0.36784	-0.41121
H	3.58676	0.98785	-1.59192
C	2.73581	-2.15337	-1.05705
H	3.74052	-2.56101	-0.92607
H	2.02103	-2.92844	-0.77337
H	2.59714	-1.93938	-2.11869
C	2.70858	-1.00496	1.79749
H	2.59609	-0.11269	2.41576
H	1.97114	-1.73961	2.12689
H	3.70098	-1.41978	1.98905
C	-4.34424	0.16709	-0.33959
H	-4.46150	0.51828	-1.36684
H	-5.09070	-0.61084	-0.16516
H	-4.56746	1.00087	0.32915
C	-2.41560	-1.03981	1.73402
H	-2.60527	-0.21880	2.42784
H	-3.12465	-1.83917	1.96252
H	-1.41216	-1.42332	1.92698
C	-2.24796	-1.90727	-1.21403
H	-2.32986	-1.58886	-2.25530
H	-1.24092	-2.29820	-1.05959
H	-2.95304	-2.72721	-1.05916
Si	-0.01873	1.23449	-0.07258
C	0.41003	2.55719	-1.31314
H	-0.27379	3.40411	-1.22733

H	1.42427	2.92963	-1.15990
H	0.34174	2.17124	-2.33204
H	-0.57187	2.66268	1.86545

PDMS_neutral_m062x.log Energy: -839886.7862170

C	0.24612	1.74106	1.69044
H	1.29301	1.99104	1.87418
H	-0.03436	0.92541	2.35799
O	0.79797	-0.09109	-0.46495
O	-1.62489	0.94869	-0.34443
Si	2.31071	-0.64404	-0.03627
Si	-2.46197	-0.46745	-0.05341
C	3.53520	0.75363	-0.19809
H	3.29686	1.57501	0.48071
H	4.54142	0.40412	0.04180
H	3.54729	1.14362	-1.21739
C	2.71482	-2.02560	-1.21430
H	3.69010	-2.45814	-0.98484
H	1.96815	-2.81881	-1.14645
H	2.73671	-1.66493	-2.24387
C	2.26353	-1.27371	1.71739
H	2.00767	-0.48031	2.42105
H	1.53266	-2.07708	1.82386
H	3.24157	-1.67025	1.99835
C	-4.26286	-0.00760	0.03024
H	-4.59156	0.44480	-0.90689
H	-4.87727	-0.89094	0.21280
H	-4.44536	0.70503	0.83609
C	-1.88625	-1.20168	1.56224
H	-2.07864	-0.52361	2.39523
H	-2.41676	-2.13585	1.75803
H	-0.81669	-1.42159	1.53671
C	-2.15337	-1.65851	-1.45262
H	-2.41563	-1.20668	-2.41081
H	-1.10436	-1.95551	-1.48978
H	-2.75799	-2.55880	-1.32712
Si	-0.03077	1.28616	-0.08921
C	0.46100	2.65857	-1.23109
H	-0.15089	3.54494	-1.05633
H	1.50565	2.93263	-1.07398

H	0.33870	2.35784	-2.27266
H	-0.35571	2.61488	1.94757

PDMS_neutral_wb97xd.log Energy: -839972.4310437

C	0.24384	1.75435	1.69210
H	1.28746	2.01923	1.87496
H	-0.01980	0.92647	2.35149
O	0.84315	-0.02414	-0.49972
O	-1.61496	0.93546	-0.34123
Si	2.31563	-0.64873	-0.03968
Si	-2.45507	-0.47864	-0.05267
C	3.59031	0.71275	-0.07977
H	3.33826	1.51175	0.62099
H	4.57352	0.32468	0.19617
H	3.66775	1.14704	-1.07854
C	2.72041	-1.98487	-1.27010
H	3.66961	-2.46484	-1.02215
H	1.94474	-2.75355	-1.27462
H	2.80121	-1.57688	-2.27954
C	2.17482	-1.36209	1.67683
H	1.91744	-0.59398	2.40803
H	1.41096	-2.14126	1.71512
H	3.12520	-1.80893	1.97871
C	-4.26065	-0.02567	-0.05100
H	-4.55732	0.40475	-1.00962
H	-4.87669	-0.91012	0.12581
H	-4.48190	0.70174	0.73254
C	-1.94642	-1.18237	1.59883
H	-2.14826	-0.47984	2.40953
H	-2.50363	-2.10012	1.80149
H	-0.88226	-1.42690	1.61420
C	-2.08477	-1.70102	-1.41064
H	-2.30946	-1.27743	-2.39161
H	-1.03332	-1.99333	-1.39807
H	-2.68908	-2.60271	-1.28684
Si	-0.02952	1.31376	-0.09247
C	0.41753	2.71505	-1.21927
H	-0.18412	3.60015	-1.00388
H	1.46889	2.98127	-1.08967
H	0.26226	2.44144	-2.26445

H	-0.37183	2.61470	1.96317

PDMS_ox_B3LYP.log Energy: -839947.6322083

C	0.15229	2.05843	1.70825
H	1.19411	2.35879	1.70626
H	-0.10647	1.20382	2.32560
O	0.94260	-0.07299	-0.12090
O	-1.60036	0.80218	-0.25190
Si	2.54758	-0.64404	-0.00511
Si	-2.64823	-0.53351	-0.02534
C	3.67199	0.62376	-0.78245
H	3.64817	1.56883	-0.23745
H	4.70221	0.26064	-0.77274
H	3.39572	0.81712	-1.82023
C	2.54353	-2.25982	-0.93287
H	3.53458	-2.71715	-0.89547
H	1.83149	-2.96140	-0.49567
H	2.28034	-2.11146	-1.98127
C	2.88358	-0.86726	1.81528
H	2.80534	0.08057	2.35011
H	2.18094	-1.57262	2.26155
H	3.89311	-1.25601	1.96551
C	-4.33964	0.11495	-0.45610
H	-4.37612	0.46200	-1.49008
H	-5.08875	-0.67079	-0.33842
H	-4.61874	0.94567	0.19426
C	-2.51361	-1.03188	1.76809
H	-2.77853	-0.20417	2.42774
H	-3.19645	-1.85879	1.97558
H	-1.50367	-1.36193	2.01593
C	-2.08455	-1.88387	-1.18192
H	-2.09958	-1.54360	-2.21873
H	-1.07340	-2.21775	-0.94463
H	-2.75140	-2.74529	-1.10211
Si	-0.04644	1.17871	-0.19129
C	0.43204	2.61281	-1.27389
H	-0.27181	3.43017	-1.13507
H	1.44391	2.93602	-1.04272
H	0.38103	2.24689	-2.30258
H	-0.57840	2.85799	1.65506

PDMS_ox_m062x.log Energy: -839721.3631309

C	0.68944	2.46930	1.23336
H	1.70951	2.65315	0.89980
H	0.69425	2.18261	2.28808
O	0.81908	-0.24291	0.05183
O	-1.59883	0.82392	0.44493
Si	2.47830	-0.63557	-0.02449
Si	-2.61184	-0.48902	0.03051
C	3.24173	0.50350	-1.27537
H	3.18150	1.54404	-0.94917
H	4.29638	0.25632	-1.40996
H	2.74564	0.41274	-2.24305
C	2.51597	-2.41153	-0.54426
H	3.54483	-2.76568	-0.62330
H	1.99537	-3.03548	0.18363
H	2.03548	-2.53916	-1.51530
C	3.16046	-0.36158	1.67865
H	3.07571	0.68686	1.97039
H	2.62796	-0.96928	2.41160
H	4.21625	-0.63630	1.71221
C	-4.33095	0.11961	0.34854
H	-4.55207	0.99277	-0.26660
H	-5.05811	-0.65817	0.11023
H	-4.45693	0.39338	1.39684
C	-2.13430	-1.90696	1.12670
H	-2.22025	-1.63104	2.17858
H	-2.79120	-2.75937	0.94447
H	-1.10799	-2.22197	0.93263
C	-2.29858	-0.85403	-1.76276
H	-2.50474	0.02050	-2.38192
H	-1.26389	-1.16232	-1.92654
H	-2.94693	-1.66606	-2.09704
Si	-0.03632	1.07553	0.29502
C	0.02779	2.00439	-1.69909
H	-0.81427	2.67753	-1.58355
H	1.02068	2.43774	-1.69992
H	-0.12453	1.08559	-2.25705
H	0.08397	3.36408	1.10171

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PDMS_ox_wb97xd.log Energy: -839810.8068999

C	0.22598	1.79824	1.77573
H	1.26417	2.11300	1.74611
H	0.00340	0.84693	2.24954
O	0.84895	-0.11042	-0.36150
O	-1.61892	0.90383	-0.31694
Si	2.42349	-0.65880	-0.01613
Si	-2.55321	-0.50225	-0.03677
C	3.56657	0.78980	-0.21614
H	3.30777	1.59439	0.47562
H	4.59505	0.48732	-0.00750
H	3.52886	1.18288	-1.23360
C	2.74068	-2.00881	-1.24345
H	3.73169	-2.43926	-1.08540
H	2.00363	-2.80701	-1.13961
H	2.69512	-1.62732	-2.26479
C	2.36704	-1.27378	1.73287
H	2.13504	-0.46367	2.42648
H	1.61274	-2.05415	1.84756
H	3.33453	-1.69326	2.01735
C	-4.30686	0.09272	-0.00703
H	-4.57785	0.55614	-0.95723
H	-4.98642	-0.74396	0.16774
H	-4.45734	0.82359	0.78933
C	-2.00548	-1.20023	1.59500
H	-2.16100	-0.48232	2.40224
H	-2.58149	-2.09862	1.82714
H	-0.94871	-1.47544	1.57366
C	-2.21214	-1.66429	-1.44234
H	-2.44613	-1.19811	-2.40097
H	-1.16482	-1.97058	-1.45264
H	-2.82651	-2.56186	-1.34356
Si	-0.05460	1.19309	-0.28323
C	0.51366	2.72916	-1.10833
H	-0.13109	3.56366	-0.83966
H	1.54415	2.94444	-0.83231
H	0.45505	2.55295	-2.18563
H	-0.52627	2.57766	1.83550

PDMS_reduced_B3lYP.log Energy: -840118.7993781

C	0.02964	1.69374	1.70538
H	0.98707	2.16793	1.93800
H	-0.10989	0.86089	2.39743
O	1.04844	-0.12753	-0.30671
O	-1.51199	0.58572	-0.48586
Si	2.63722	-0.56561	-0.02752
Si	-2.72472	-0.47928	-0.05717
C	3.78842	0.77336	-0.66135
H	3.66373	1.70738	-0.10806
H	4.82989	0.45685	-0.54896
H	3.61325	0.97935	-1.72011
C	2.91835	-2.16104	-0.96591
H	3.94587	-2.51330	-0.83162
H	2.24429	-2.94643	-0.61220
H	2.74447	-2.02505	-2.03686
C	2.91361	-0.83508	1.80753
H	2.79708	0.09077	2.37633
H	2.20711	-1.56897	2.20635
H	3.92579	-1.21302	1.98520
C	-4.23761	0.06563	-1.01816
H	-4.05024	0.03704	-2.09421
H	-5.08851	-0.58748	-0.80825
H	-4.52390	1.08636	-0.75234
C	-3.06361	-0.38273	1.78483
H	-3.28612	0.64093	2.09752
H	-3.92554	-1.00713	2.03851
H	-2.21277	-0.74091	2.36911
C	-2.23705	-2.22343	-0.54045
H	-1.99573	-2.28657	-1.60552
H	-1.36349	-2.56513	0.02239
H	-3.05707	-2.92003	-0.33813
Si	-0.00645	1.12532	-0.07404
C	0.39198	2.51889	-1.24837
H	-0.34074	3.32470	-1.15313
H	1.37990	2.93835	-1.04703
H	0.37690	2.16814	-2.28310
H	-0.75999	2.42750	1.89047

PDMS_reduced_wb97xd.log Energy: -839968.8028153

C	0.19642	1.72918	1.69564

H	1.22309	2.05716	1.88503
H	-0.02094	0.88726	2.35738
O	0.85923	-0.09220	-0.43764
O	-1.60070	0.88170	-0.39316
Si	2.38423	-0.62794	-0.03577
Si	-2.52091	-0.46891	-0.05428
C	3.61645	0.74416	-0.32366
H	3.41626	1.59943	0.32747
H	4.63109	0.39301	-0.11373
H	3.58368	1.08909	-1.36031
C	2.73633	-2.07781	-1.14884
H	3.72405	-2.49685	-0.93728
H	1.99435	-2.86706	-1.00051
H	2.71051	-1.77953	-2.19989
C	2.41308	-1.15765	1.75267
H	2.26029	-0.30912	2.42387
H	1.63016	-1.89518	1.95333
H	3.37767	-1.61339	1.99694
C	-4.29866	0.05728	-0.23214
H	-4.50000	0.41493	-1.24465
H	-4.96836	-0.78267	-0.03100
H	-4.54215	0.85954	0.46789
C	-2.17599	-1.05153	1.68524
H	-2.37642	-0.26315	2.41585
H	-2.81005	-1.90948	1.92701
H	-1.13368	-1.36338	1.79827
C	-2.12357	-1.82033	-1.27679
H	-2.23016	-1.46245	-2.30434
H	-1.10167	-2.18332	-1.14706
H	-2.80275	-2.66679	-1.14003
Si	-0.02405	1.25809	-0.09011
C	0.45581	2.64001	-1.22948
H	-0.16855	3.52100	-1.05707
H	1.49767	2.92747	-1.06720
H	0.34214	2.33635	-2.27342
H	-0.47354	2.55380	1.95615

PDMS_red_m062x.log Energy: -839897.6668045

C	0.07008	1.46232	1.71734
H	1.04198	1.89877	1.96220

H	-0.06878	0.57442	2.33572
O	1.03346	-0.18002	-0.44134
O	-1.51947	0.60961	-0.54265
Si	2.60691	-0.55528	-0.04981
Si	-2.71445	-0.44768	-0.06996
C	3.67829	0.94644	-0.34374
H	3.38832	1.77334	0.30852
H	4.72541	0.70898	-0.13978
H	3.60151	1.28554	-1.37915
C	3.15088	-1.95729	-1.14885
H	4.19528	-2.21428	-0.94771
H	2.53519	-2.84374	-0.97782
H	3.05764	-1.68390	-2.20276
C	2.73836	-1.05915	1.74281
H	2.45015	-0.24591	2.41154
H	2.09667	-1.91785	1.95293
H	3.77070	-1.33868	1.97325
C	-4.32290	0.36902	-0.53954
H	-4.35824	0.56345	-1.61312
H	-5.17076	-0.26883	-0.28273
H	-4.44277	1.32009	-0.01743
C	-2.66362	-0.72805	1.77456
H	-2.71389	0.21436	2.32372
H	-3.51954	-1.34055	2.07034
H	-1.75379	-1.25493	2.07117
C	-2.54434	-2.06704	-0.98051
H	-2.49337	-1.90209	-2.06031
H	-1.63462	-2.59394	-0.68255
H	-3.40530	-2.70891	-0.76942
Si	0.00011	1.05630	-0.09689
C	0.43193	2.54212	-1.12181
H	-0.27643	3.35368	-0.94070
H	1.43371	2.90410	-0.88462
H	0.40245	2.29195	-2.18444
H	-0.70144	2.19121	1.97685

hydroxide_anion.log Energy: -47659.5421295

O	0.00000	0.00000	0.10645
H	-0.00000	-0.00000	-0.85159

hydroxyl_radical.log Energy: -47530.5536898

O	0.00000	0.00000	0.10797
H	-0.00000	-0.00000	-0.86374

PEG_3n_neutral_b3lyp.log Energy: -337679.7018048

C	4.14432	-0.51726	-0.00007
H	4.11088	-1.15334	-0.88731
H	4.11093	-1.15320	0.88726
C	2.96647	0.43529	-0.00011
H	2.99777	1.07534	-0.88765
H	2.99781	1.07545	0.88735
O	5.33611	0.28071	-0.00018
O	1.77312	-0.34342	-0.00003
C	0.59903	0.46410	-0.00002
H	0.58303	1.10429	0.88753
H	0.58299	1.10426	-0.88759
C	-0.59903	-0.46410	0.00002
H	-0.58303	-1.10428	-0.88753
H	-0.58298	-1.10426	0.88758
O	-1.77312	0.34342	0.00005
C	-2.96647	-0.43529	0.00008
H	-2.99776	-1.07540	0.88758
H	-2.99782	-1.07540	-0.88742
C	-4.14432	0.51726	0.00012
H	-4.11088	1.15327	0.88740
H	-4.11093	1.15328	-0.88717
O	-5.33611	-0.28071	0.00015
H	6.09259	-0.31490	-0.00012
H	-6.09259	0.31490	0.00017

PEG_3n_neutral_m062x.log Energy: -337532.4159524

C	4.12032	-0.51657	-0.00011
H	4.08353	-1.15158	-0.88765
H	4.08357	-1.15157	0.88744
C	2.94263	0.42972	-0.00009
H	2.97330	1.06905	-0.88818
H	2.97335	1.06905	0.88800
O	5.29634	0.28393	-0.00014
O	1.76056	-0.34865	-0.00005
C	0.59927	0.46012	-0.00003

H	0.58442	1.09942	0.88817
H	0.58437	1.09939	-0.88825
C	-0.59927	-0.46012	0.00002
H	-0.58442	-1.09942	-0.88818
H	-0.58437	-1.09939	0.88824
O	-1.76056	0.34865	0.00003
C	-2.94263	-0.42972	0.00011
H	-2.97330	-1.06900	0.88823
H	-2.97335	-1.06910	-0.88795
C	-4.12032	0.51657	0.00009
H	-4.08352	1.15163	0.88759
H	-4.08358	1.15152	-0.88750
O	-5.29634	-0.28393	0.00017
H	6.05869	-0.30172	-0.00014
H	-6.05869	0.30172	0.00015

PEG_3n_neutral_wb97xd.log Energy: -337569.5516967

C	4.12272	-0.51431	0.00033
H	4.08514	-1.15181	-0.88657
H	4.08554	-1.15014	0.88845
C	2.94516	0.43380	-0.00030
H	2.97731	1.07396	-0.88872
H	2.97745	1.07533	0.88711
O	5.30364	0.27873	-0.00068
O	1.76226	-0.34149	0.00038
C	0.59845	0.46187	0.00023
H	0.58061	1.10283	0.88816
H	0.58068	1.10260	-0.88786
C	-0.59845	-0.46187	0.00027
H	-0.58069	-1.10265	-0.88778
H	-0.58059	-1.10277	0.88824
O	-1.76226	0.34149	0.00039
C	-2.94516	-0.43380	-0.00029
H	-2.97744	-1.07534	0.88712
H	-2.97731	-1.07396	-0.88871
C	-4.12273	0.51431	0.00036
H	-4.08556	1.15010	0.88850
H	-4.08512	1.15185	-0.88652
O	-5.30364	-0.27873	-0.00072
H	6.05888	-0.31182	0.00002

H	-6.05888	0.31182	0.00005

PEG_3n_oxidized_b3lyp.log Energy: -337530.0236572

C	3.96148	-0.02275	-0.16202
H	4.24507	0.87865	0.38489
H	4.17083	0.12535	-1.22252
C	2.48500	-0.30117	0.03872
H	2.26253	-0.46763	1.09584
H	2.14316	-1.15256	-0.54741
O	4.65799	-1.16592	0.33906
O	1.76881	0.88087	-0.37375
C	0.47613	0.74731	-0.72296
H	0.13400	1.63508	-1.24292
H	0.22254	-0.20615	-1.18383
C	-0.47617	0.74760	0.72289
H	-0.22253	-0.20566	1.18415
H	-0.13403	1.63559	1.24248
O	-1.76885	0.88098	0.37365
C	-2.48498	-0.30128	-0.03835
H	-2.14337	-1.15233	0.54839
H	-2.26222	-0.46837	-1.09530
C	-3.96151	-0.02266	0.16176
H	-4.17122	0.12599	1.22211
H	-4.24486	0.87847	-0.38572
O	-4.65791	-1.16605	-0.33898
H	5.58774	-1.07383	0.10408
H	-5.58772	-1.07384	-0.10430

PEG_3n_oxidized_m062x.log Energy: -337376.0093082

C	-3.95899	0.38487	-0.28962
H	-3.85539	0.42932	-1.37515
H	-4.17288	1.38567	0.08881
C	-2.67700	-0.12938	0.32116
H	-2.44595	-1.13050	-0.04983
H	-2.72060	-0.14057	1.40989
O	-4.96858	-0.53543	0.09334
O	-1.62715	0.75765	-0.09137
C	-0.44253	0.59298	0.48475
H	0.19046	1.46613	0.35047
H	-0.45159	0.12552	1.46608

C	0.44260	-0.59308	-0.48509
H	-0.19043	-1.46621	-0.35089
H	0.45174	-0.12555	-1.46639
O	1.62720	-0.75791	0.09105
C	2.67702	0.12931	-0.32113
H	2.44584	1.13029	0.05019
H	2.72069	0.14089	-1.40986
C	3.95903	-0.38493	0.28960
H	3.85527	-0.42991	1.37509
H	4.17323	-1.38551	-0.08925
O	4.96842	0.53581	-0.09279
H	-5.80971	-0.22044	-0.25039
H	5.80951	0.22118	0.25135

PEG_3n_oxidized_wb97xd.log Energy: -337417.2597488

C	3.70309	0.18286	0.24752
H	4.04393	-0.84495	0.10415
H	3.86285	0.46604	1.28994
C	2.23344	0.28302	-0.09166
H	2.05993	0.01081	-1.13523
H	1.84045	1.28156	0.09833
O	4.37439	1.07151	-0.63138
O	1.54160	-0.66226	0.73699
C	0.22715	-0.52367	0.85635
H	-0.15900	-1.10479	1.68665
H	-0.15419	0.49018	0.74100
C	-0.53079	-1.34837	-0.51509
H	-0.13833	-0.76527	-1.34795
H	-0.15854	-2.36029	-0.40053
O	-1.84399	-1.29210	-0.34070
C	-2.53261	-0.09891	-0.75218
H	-3.22136	-0.39842	-1.54087
H	-1.81897	0.62637	-1.14179
C	-3.28217	0.44076	0.44835
H	-3.96383	-0.32336	0.82778
H	-2.57439	0.70448	1.23774
O	-3.99251	1.58192	-0.00363
H	5.30794	1.06166	-0.41145
H	-4.47105	1.94928	0.74217

PEG_3n_reduced_b3lyp.log Energy: -337685.3365863

C	-4.14441	0.50584	-0.00532
H	-4.08690	1.16806	-0.87387
H	-4.13050	1.12415	0.89672
C	-2.97215	-0.44924	-0.00132
H	-2.97851	-1.07349	-0.90007
H	-3.00876	-1.10512	0.87389
O	-5.35554	-0.26975	-0.05478
O	-1.77518	0.33839	0.03232
C	-0.59720	-0.46564	0.03528
H	-0.58112	-1.10659	0.92250
H	-0.57740	-1.10624	-0.85203
C	0.59720	0.46564	0.03534
H	0.57744	1.10629	-0.85194
H	0.58107	1.10654	0.92259
O	1.77518	-0.33839	0.03240
C	2.97215	0.44924	-0.00113
H	3.00872	1.10506	0.87413
H	2.97856	1.07355	-0.89984
C	4.14441	-0.50584	-0.00513
H	4.13045	-1.12421	0.89687
H	4.08695	-1.16800	-0.87373
O	5.35554	0.26975	-0.05447
H	-6.10520	0.36693	-0.06284
H	6.10521	-0.36693	-0.06254

PEG_3n_reduced_m062x.log Energy: -337526.4602286

C	4.11599	-0.50647	0.00522
H	4.09296	-1.13230	-0.89169
H	4.05948	-1.16189	0.87927
C	2.94403	0.44448	0.00009
H	2.97995	1.09440	-0.87991
H	2.95675	1.07334	0.89586
O	5.30822	0.27222	0.04113
O	1.76154	-0.33969	-0.02417
C	0.59636	0.46331	-0.02793
H	0.57576	1.10357	0.85959
H	0.57995	1.10259	-0.91626
C	-0.59636	-0.46331	-0.02788
H	-0.57999	-1.10264	-0.91617

H	-0.57571	-1.10352	0.85968
O	-1.76154	0.33969	-0.02411
C	-2.94403	-0.44448	0.00027
H	-2.95670	-1.07328	0.89610
H	-2.98000	-1.09446	-0.87968
C	-4.11599	0.50647	0.00541
H	-4.05943	1.16195	0.87940
H	-4.09301	1.13223	-0.89156
O	-5.30821	-0.27222	0.04144
H	6.05774	-0.35209	0.04986
H	-6.05774	0.35209	0.05017

PEG_3n_reduced_wb97xd.log Energy: -337560.0588884

C	-4.12752	-0.51468	0.00017
H	-4.09548	-1.15168	0.88763
H	-4.09533	-1.15217	-0.88694
C	-2.94228	0.42445	0.00001
H	-2.96827	1.06638	0.88854
H	-2.96821	1.06599	-0.88881
O	-5.30292	0.28872	-0.00015
O	-1.76291	-0.35742	0.00021
C	-0.60441	0.45633	0.00019
H	-0.58857	1.09788	-0.89306
H	-0.58853	1.09788	0.89343
C	0.60441	-0.45633	0.00015
H	0.58858	-1.09789	0.89338
H	0.58852	-1.09786	-0.89311
O	1.76291	0.35742	0.00013
C	2.94228	-0.42445	-0.00019
H	2.96816	-1.06594	-0.88904
H	2.96832	-1.06644	0.88830
C	4.12752	0.51468	-0.00003
H	4.09528	1.15223	-0.88709
H	4.09553	1.15162	0.88748
O	5.30292	-0.28872	-0.00047
H	-6.06243	-0.29625	0.00002
H	6.06243	0.29625	-0.00026

PEG_1n_neutral_wb97xd.log Energy: -144501.8611893

C	-0.57482	-0.49071	-0.00000

H	-0.51747	-1.12666	0.88733
H	-0.51749	-1.12664	-0.88735
C	0.57482	0.49071	0.00000
H	0.51749	1.12663	0.88735
H	0.51747	1.12666	-0.88733
O	-1.78090	0.26283	0.00002
O	1.78090	-0.26283	-0.00003
H	-2.51643	-0.35216	0.00004
H	2.51643	0.35216	-0.00003

PEG_1n_wB97XD_ox.log Energy: -144347.4131421

C	0.72454	0.56672	-0.03389
H	0.52284	1.09705	0.89247
H	0.53886	1.07575	-0.97269
C	-0.72449	-0.56644	-0.03384
H	-0.52246	-1.09677	0.89250
H	-0.53848	-1.07566	-0.97251
O	1.81295	-0.18540	-0.06739
O	-1.81306	0.18519	-0.06740
H	2.08631	-0.44501	0.82247
H	-2.08655	0.44470	0.82244

PEG_2n_neutral_wb97xd.log Energy: -241035.7008760

C	-2.36314	0.50816	0.00001
H	-2.33402	1.14534	-0.88746
H	-2.33402	1.14530	0.88751
C	-1.17330	-0.42453	-0.00001
H	-1.19763	-1.06583	-0.88789
H	-1.19762	-1.06586	0.88784
O	-3.53311	-0.30013	-0.00001
O	0.00000	0.36506	-0.00000
C	1.17330	-0.42453	0.00001
H	1.19763	-1.06583	0.88788
H	1.19762	-1.06586	-0.88784
C	2.36314	0.50816	-0.00001
H	2.33402	1.14530	-0.88751
H	2.33402	1.14534	0.88746
O	3.53311	-0.30013	0.00001
H	-4.29636	0.28000	0.00001
H	4.29636	0.28000	-0.00001

PEG_2n_wB97XD_ox.log Energy: -240882.3674633

C	2.15485	0.49739	0.41640
H	2.06997	0.22647	1.46225
H	1.61626	1.38074	0.07976
C	1.16574	-0.78257	-0.35337
H	1.73885	-1.66021	-0.07470
H	1.19830	-0.46455	-1.39348
O	3.40030	0.36596	-0.03443
O	-0.02135	-0.77174	0.22738
C	-0.99982	0.15892	-0.26202
H	-0.74407	1.14577	0.13032
H	-0.96695	0.17372	-1.35096
C	-2.34246	-0.29609	0.26269
H	-2.58487	-1.28006	-0.14419
H	-2.30443	-0.36385	1.35219
O	-3.28533	0.67660	-0.15667
H	3.50912	0.80522	-0.88790
H	-4.15091	0.40439	0.15426

PEG_3n_neutral_wb97xd.log Energy: -337569.5516967

C	-4.12272	-0.51431	-0.00033
H	-4.08514	-1.15181	0.88657
H	-4.08554	-1.15014	-0.88845
C	-2.94516	0.43380	0.00030
H	-2.97731	1.07396	0.88872
H	-2.97745	1.07533	-0.88711
O	-5.30364	0.27873	0.00068
O	-1.76226	-0.34149	-0.00038
C	-0.59845	0.46187	-0.00023
H	-0.58061	1.10283	-0.88816
H	-0.58068	1.10260	0.88786
C	0.59845	-0.46187	-0.00027
H	0.58069	-1.10265	0.88778
H	0.58059	-1.10277	-0.88824
O	1.76226	0.34149	-0.00039
C	2.94516	-0.43380	0.00029
H	2.97744	-1.07534	-0.88712
H	2.97731	-1.07396	0.88871
C	4.12273	0.51431	-0.00036

H	4.08556	1.15010	-0.88850
H	4.08512	1.15185	0.88652
O	5.30364	-0.27873	0.00072
H	-6.05888	-0.31182	-0.00002
H	6.05888	0.31182	-0.00005

PEG_3n_wB97XD_ox.log Energy: -337417.2597488

C	3.70309	0.18286	0.24752
H	4.04393	-0.84495	0.10415
H	3.86285	0.46604	1.28994
C	2.23344	0.28302	-0.09166
H	2.05993	0.01081	-1.13523
H	1.84045	1.28156	0.09833
O	4.37439	1.07151	-0.63138
O	1.54160	-0.66226	0.73699
C	0.22715	-0.52367	0.85635
H	-0.15900	-1.10479	1.68665
H	-0.15419	0.49018	0.74100
C	-0.53079	-1.34837	-0.51509
H	-0.13833	-0.76527	-1.34795
H	-0.15854	-2.36029	-0.40053
O	-1.84399	-1.29210	-0.34070
C	-2.53261	-0.09891	-0.75218
H	-3.22136	-0.39842	-1.54087
H	-1.81897	0.62637	-1.14179
C	-3.28217	0.44076	0.44835
H	-3.96383	-0.32336	0.82778
H	-2.57439	0.70448	1.23774
O	-3.99251	1.58192	-0.00363
H	5.30794	1.06166	-0.41145
H	-4.47105	1.94928	0.74217

PEG_4n_neutral_wb97xd.log Energy: -434103.4102332

C	-5.89774	0.47797	0.00043
H	-5.87255	1.11564	-0.88672
H	-5.87251	1.11436	0.88851
C	-4.70289	-0.44808	-0.00026
H	-4.72351	-1.08873	-0.88866
H	-4.72348	-1.09000	0.88723
O	-7.06362	-0.33746	-0.00014

O	-3.53401	0.34833	0.00029
C	-2.35684	-0.43518	-0.00006
H	-2.32835	-1.07591	0.88775
H	-2.32847	-1.07531	-0.88830
C	-1.17413	0.50659	0.00019
H	-1.20056	1.14703	-0.88784
H	-1.20063	1.14667	0.88847
O	0.00000	-0.28175	0.00008
C	1.17413	0.50659	-0.00010
H	1.20057	1.14708	0.88789
H	1.20062	1.14662	-0.88842
C	2.35684	-0.43518	0.00017
H	2.32850	-1.07524	0.88846
H	2.32832	-1.07597	-0.88758
C	4.70289	-0.44808	0.00024
H	4.72356	-1.08871	0.88865
H	4.72344	-1.09002	-0.88723
C	5.89774	0.47797	-0.00053
H	5.87260	1.11565	0.88662
H	5.87246	1.11435	-0.88861
H	7.82996	0.23849	-0.00024
O	7.06362	-0.33746	-0.00003
O	3.53401	0.34833	-0.00027
H	-7.82996	0.23849	0.00009

PEG_4n_wB97XD_ox.log Energy: -433939.7929104

C	-5.84385	-0.44984	0.38212
H	-5.74144	-0.53418	1.46680
H	-5.80874	-1.45271	-0.05070
C	-4.71379	0.38537	-0.17491
H	-4.72565	1.38603	0.26871
H	-4.81393	0.48449	-1.26047
O	-7.05908	0.20396	0.04010
O	-3.49882	-0.27271	0.14313
C	-2.37547	0.44221	-0.31478
H	-2.42511	0.60201	-1.39575
H	-2.29050	1.41106	0.18535
C	-1.18019	-0.41785	0.02084
H	-1.15069	-0.64584	1.10600
H	-1.13452	-1.38447	-0.49127

O	0.00013	0.29563	-0.20368
C	1.19541	-0.42162	-0.32035
H	1.28108	-0.59958	-1.41166
H	1.11027	-1.39486	0.16544
C	2.35062	0.44200	0.14532
H	2.31249	1.41725	-0.34742
H	2.28345	0.58409	1.22785
C	4.68748	0.38285	0.27418
H	4.75387	1.39256	-0.14320
H	4.65692	0.45810	1.36578
C	5.87425	-0.44514	-0.16274
H	5.89115	-0.51976	-1.25289
H	5.79532	-1.45184	0.25484
H	7.80239	-0.32243	0.06901
O	7.04278	0.20839	0.31561
O	3.51772	-0.26337	-0.20125
H	-7.78501	-0.31289	0.39414

PEG_5n_neutral_wb97xd.log Energy: -530637.2603209

C	7.65740	-0.50346	-0.06525
H	7.64986	-1.13379	0.82750
H	7.60093	-1.14701	-0.94678
C	6.47225	0.43480	-0.03935
H	6.52292	1.08140	0.84348
H	6.47509	1.07035	-0.93166
C	4.12674	0.44415	0.02691
H	4.12443	1.08189	0.91731
H	4.08386	1.08776	-0.85822
C	2.93654	-0.48795	0.04924
H	2.97370	-1.12869	0.93667
H	2.94265	-1.12838	-0.83917
O	8.83110	0.29937	-0.10369
O	5.29628	-0.35022	-0.00282
O	1.76806	0.30865	0.06931
C	0.58959	-0.47315	0.07818
H	0.55563	-1.11616	-0.80773
H	0.56424	-1.11065	0.96835
C	-0.58959	0.47315	0.07816
H	-0.56423	1.11070	0.96830
H	-0.55564	1.11612	-0.80778

O	-1.76806	-0.30864	0.06935
C	-2.93654	0.48795	0.04925
H	-2.94266	1.12834	-0.83920
H	-2.97369	1.12874	0.93665
C	-4.12674	-0.44415	0.02697
H	-4.08387	-1.08780	-0.85812
H	-4.12442	-1.08184	0.91740
C	-6.47225	-0.43480	-0.03927
H	-6.47510	-1.07039	-0.93155
H	-6.52291	-1.08137	0.84359
C	-7.65740	0.50345	-0.06520
H	-7.60094	1.14697	-0.94676
H	-7.64986	1.13382	0.82752
H	-9.59132	0.28470	-0.11182
O	-8.83110	-0.29938	-0.10360
O	-5.29628	0.35022	-0.00279
H	9.59132	-0.28471	-0.11188

PEG_5n_wB97XD_ox.log Energy: -530484.6044960

C	6.36813	1.82760	-0.03891
H	5.79986	2.51882	-0.66662
H	6.30506	2.16633	0.99800
C	5.78874	0.43644	-0.15793
H	5.86269	0.08189	-1.19137
H	6.33687	-0.25848	0.48680
C	3.80056	-0.75941	0.19553
H	3.84901	-1.18165	-0.81300
H	4.28163	-1.45532	0.88992
C	2.36196	-0.53389	0.59647
H	1.85046	0.11443	-0.11672
H	2.28470	-0.10636	1.59626
O	7.72375	1.76054	-0.46429
O	4.43087	0.50225	0.23859
O	1.71890	-1.81830	0.61224
C	0.40413	-1.82718	0.80034
H	0.05643	-2.79915	1.13276
H	-0.00209	-0.95416	1.30978
C	-0.35913	-1.71745	-0.78306
H	0.05336	-0.78407	-1.16422
H	-0.01626	-2.63313	-1.25163

O	-1.67490	-1.72995	-0.60207
C	-2.31205	-0.47679	-0.31448
H	-1.95101	0.27530	-1.01532
H	-2.05257	-0.18433	0.70507
C	-3.80196	-0.69813	-0.43883
H	-4.06285	-0.96116	-1.46850
H	-4.11505	-1.51328	0.22110
C	-5.83221	0.43922	-0.13919
H	-6.14337	0.22962	-1.16795
H	-6.20341	-0.36435	0.50551
C	-6.38595	1.77074	0.31421
H	-6.00615	2.56741	-0.33022
H	-6.06950	1.97176	1.34078
H	-8.16664	2.53611	0.50077
O	-7.80361	1.69024	0.23176
O	-4.42023	0.51274	-0.06165
H	8.11722	2.62661	-0.34280

PEG_6n_neutral_wb97xd.log Energy: -627171.1189001

C	9.42659	0.45062	-0.14353
H	9.43823	1.10641	0.73062
H	9.36782	1.06913	-1.04266
C	8.22977	-0.47060	-0.07607
H	8.28388	-1.09273	0.82398
H	8.21264	-1.13098	-0.94999
C	5.88584	-0.44800	0.02139
H	5.88886	-1.06159	0.92860
H	5.82230	-1.11459	-0.84528
C	4.70699	0.49860	0.03593
H	4.76508	1.16277	0.90479
H	4.70641	1.11445	-0.86972
C	2.36015	0.51010	0.10389
H	2.35452	1.16839	0.97913
H	2.31885	1.13240	-0.79636
C	1.17292	-0.42525	0.14342
H	1.20575	-1.04135	1.04829
H	1.18970	-1.08977	-0.72698
O	10.58903	-0.36893	-0.17251
O	7.06447	0.33044	-0.04649
O	3.53042	-0.28392	0.09572

O	-0.00001	0.36489	0.13150
C	-1.17295	-0.42524	0.14320
H	-1.18958	-1.08976	-0.72720
H	-1.20594	-1.04134	1.04807
C	-2.36016	0.51012	0.10347
H	-2.35468	1.16841	0.97871
H	-2.31871	1.13241	-0.79678
O	-3.53044	-0.28389	0.09510
C	-4.70699	0.49863	0.03516
H	-4.70627	1.11451	-0.87047
H	-4.76522	1.16277	0.90403
C	-5.88585	-0.44797	0.02041
H	-5.82220	-1.11449	-0.84630
H	-5.88897	-1.06162	0.92758
C	-8.22974	-0.47060	-0.07741
H	-8.21253	-1.13077	-0.95148
H	-8.28390	-1.09293	0.82249
C	-9.42659	0.45061	-0.14474
H	-9.36773	1.06940	-1.04368
H	-9.43836	1.10614	0.72960
H	-11.35716	0.20398	-0.20217
O	-10.58899	-0.36898	-0.17412
O	-7.06446	0.33047	-0.04755
H	11.35718	0.20406	-0.20074

PEG_6n_wB97XD_ox.log Energy: -627007.5357018

C	-9.38828	-0.14412	0.55902
H	-9.27728	0.01732	1.63426
H	-9.44249	-1.21933	0.37145
C	-8.20236	0.44404	-0.17113
H	-8.14925	1.52394	0.00466
H	-8.30124	0.27476	-1.24881
C	-5.86628	0.29067	-0.31859
H	-5.76759	1.37099	-0.16904
H	-5.91164	0.09318	-1.39476
C	-4.68523	-0.42732	0.29380
H	-4.63328	-0.22640	1.36826
H	-4.77563	-1.50748	0.14362
C	-2.35007	-0.54182	0.16042
H	-2.27306	-0.39640	1.24182

H	-2.31949	-1.61176	-0.06188
C	-1.19799	0.16745	-0.52348
H	-1.11540	1.23494	-0.31514
H	-1.28801	0.04363	-1.62184
O	-10.55265	0.51090	0.07009
O	-7.03446	-0.18764	0.31736
O	-3.51723	0.05722	-0.34840
O	0.00083	-0.48845	-0.22419
C	1.17531	0.26851	-0.18315
H	1.12281	1.07999	-0.91669
H	1.14419	0.75209	0.81438
C	2.37876	-0.63643	-0.30398
H	2.30963	-1.45054	0.42301
H	2.42329	-1.06021	-1.31138
O	3.49602	0.18202	-0.04979
C	4.71548	-0.52972	-0.17801
H	4.81429	-0.92585	-1.19337
H	4.73726	-1.36644	0.52712
C	5.83702	0.43889	0.12048
H	5.81011	1.27544	-0.58577
H	5.72942	0.83886	1.13422
C	8.17619	0.55878	0.25198
H	8.19901	1.39322	-0.45738
H	8.12117	0.97006	1.26574
C	9.41992	-0.28692	0.09943
H	9.46226	-0.70236	-0.91051
H	9.39710	-1.11234	0.81535
H	11.33549	0.03567	0.24373
O	10.53790	0.55874	0.34192
O	7.05566	-0.26672	-0.00136
H	-11.31518	0.13456	0.51310

PEG_7n_wB97XD_ox.log Energy: -723552.4716793

C	10.14229	1.74870	-0.20682
H	10.58738	0.77754	0.02372
H	10.09530	1.86128	-1.29293
C	8.74885	1.82283	0.37505
H	8.78767	1.70856	1.46379
H	8.29515	2.79333	0.14641
C	6.65491	0.76318	0.27657

H	6.64135	0.62735	1.36310
H	6.15558	1.70877	0.03996
C	5.94475	-0.38466	-0.40415
H	6.42949	-1.33338	-0.15204
H	5.97814	-0.25627	-1.49085
C	3.85656	-1.43295	-0.54594
H	4.24986	-2.40794	-0.24192
H	3.89587	-1.36446	-1.63739
C	2.42861	-1.27685	-0.07256
H	2.36357	-1.35440	1.01457
H	1.99488	-0.33446	-0.40461
C	0.38533	-2.20413	-0.82787
H	0.06850	-1.18380	-1.04429
H	-0.02212	-2.99192	-1.45172
C	-0.44150	-2.49893	0.70325
H	-0.09427	-1.65985	1.30560
H	-0.06737	-3.48281	0.96464
O	10.90295	2.80050	0.37485
O	7.98610	0.77940	-0.19933
O	4.60100	-0.38913	0.04310
O	1.68620	-2.37123	-0.63023
O	-1.74544	-2.52893	0.45513
C	-2.43568	-1.27291	0.39651
H	-2.14293	-0.66466	1.25195
H	-2.15176	-0.76821	-0.52956
C	-3.91558	-1.57970	0.39866
H	-4.16009	-2.24453	-0.43564
H	-4.20134	-2.07119	1.33372
O	-4.58247	-0.34376	0.26111
C	-5.98950	-0.49870	0.22566
H	-6.34259	-0.95752	1.15481
H	-6.27585	-1.14405	-0.61104
C	-6.59541	0.87597	0.05576
H	-6.31522	1.51863	0.89705
H	-6.23007	1.33730	-0.86792
C	-8.66756	1.96123	-0.13576
H	-8.43768	2.61238	0.71461
H	-8.34270	2.46491	-1.05271
C	-10.15245	1.68300	-0.19198
H	-10.46670	1.17182	0.72141

H	-10.37627	1.03904	-1.04620
H	-11.75955	2.77252	-0.34404
O	-10.81486	2.93544	-0.31989
O	-7.99986	0.72196	0.00380
H	11.79301	2.75554	0.02084

PEG_8n_neutral_wb97xd.log Energy: -820238.8198762

C	-12.95636	0.36872	-0.28713
H	-12.89596	0.93471	-1.22011
H	-12.98335	1.07376	0.54743
C	-11.75029	-0.53332	-0.15572
H	-11.80723	-1.10399	0.77762
H	-11.71678	-1.24183	-0.99059
C	-9.40795	-0.47884	-0.03818
H	-9.32633	-1.18869	-0.86820
H	-9.41549	-1.04463	0.89955
C	-8.23955	0.48058	-0.05780
H	-8.23159	1.04739	-0.99487
H	-8.31794	1.18929	0.77346
C	-5.89448	0.52219	0.05382
H	-5.83731	1.09532	-0.87765
H	-5.91681	1.22665	0.89204
C	-4.69974	-0.39657	0.17394
H	-4.68464	-1.10451	-0.66156
H	-4.75353	-0.96623	1.10776
C	-2.35595	-0.37233	0.24962
H	-2.30699	-1.08603	-0.57964
H	-2.34646	-0.93462	1.18938
C	-1.17447	0.56934	0.19157
H	-1.19242	1.13826	-0.74405
H	-1.21056	1.27689	1.02673
C	1.17446	0.56936	0.19153
H	1.19239	1.13825	-0.74411
H	1.21055	1.27694	1.02667
C	2.35596	-0.37228	0.24961
H	2.30699	-1.08604	-0.57961
H	2.34650	-0.93452	1.18941
O	-10.59412	0.28135	-0.16009
O	-7.05605	-0.28448	0.06126
O	-3.53420	0.40434	0.15584

O	0.00000	-0.21526	0.26417
O	3.53419	0.40439	0.15575
C	4.69974	-0.39651	0.17392
H	4.75355	-0.96608	1.10779
H	4.68464	-1.10452	-0.66152
C	5.89447	0.52225	0.05371
H	5.83730	1.09530	-0.87781
H	5.91680	1.22680	0.89187
O	7.05605	-0.28441	0.06123
C	8.23955	0.48065	-0.05787
H	8.31794	1.18940	0.77335
H	8.23160	1.04740	-0.99497
C	9.40794	-0.47879	-0.03820
H	9.41546	-1.04455	0.89955
H	9.32633	-1.18867	-0.86820
C	11.75027	-0.53333	-0.15570
H	11.80717	-1.10400	0.77764
H	11.71677	-1.24184	-0.99057
C	12.95639	0.36866	-0.28708
H	12.98339	1.07369	0.54749
H	12.89603	0.93467	-1.22004
H	14.88393	0.09658	-0.34289
O	14.10936	-0.46471	-0.27827
O	10.59413	0.28137	-0.16011
O	-14.10937	-0.46460	-0.27834
H	-14.88391	0.09673	-0.34308

PEG_8n_wB97XD_ox.log Energy: -820075.2817407

C	11.50151	-2.80376	0.02646
H	11.21261	-3.37284	-0.86071
H	11.19430	-3.36229	0.91418
C	10.82209	-1.45334	0.01168
H	11.10738	-0.87799	0.89913
H	11.12448	-0.88831	-0.87675
C	8.69651	-0.45882	-0.01042
H	8.95227	0.12927	-0.89822
H	8.93753	0.13477	0.87785
C	7.22506	-0.80615	-0.02113
H	6.98229	-1.39672	-0.91082
H	6.96995	-1.39631	0.86538

C	5.10028	0.18825	-0.03432
H	4.80936	-0.37567	-0.92680
H	4.80080	-0.38446	0.84968
C	4.42732	1.54176	-0.03002
H	4.72108	2.11606	-0.91414
H	4.71381	2.10550	0.86323
C	2.30489	2.53128	-0.01785
H	2.53178	3.13846	-0.89879
H	2.53314	3.11060	0.88138
C	0.84876	2.13846	-0.02130
H	0.55699	1.56434	-0.91582
H	0.57019	1.50930	0.83948
C	-1.33228	3.20657	0.03054
H	-1.63093	3.81056	0.90588
H	-1.64471	3.84080	-0.81888
C	-1.95030	1.83612	0.01011
H	-1.63279	1.25694	0.88576
H	-1.64695	1.28807	-0.89007
O	9.42442	-1.67107	-0.00042
O	6.49709	0.40673	-0.02629
O	3.02694	1.32180	-0.03683
O	0.05682	3.29212	0.02023
O	-3.34101	2.04284	0.02482
C	-4.05411	0.81608	0.00948
H	-3.80035	0.24736	-0.89014
H	-3.78958	0.21903	0.88737
C	-5.52924	1.14533	0.02359
H	-5.78080	1.71740	0.92276
H	-5.79127	1.74593	-0.85372
O	-6.23409	-0.07982	0.00799
C	-7.63613	0.10885	0.02013
H	-7.94772	0.68681	-0.85623
H	-7.93661	0.65585	0.91995
C	-8.27960	-1.25915	0.00001
H	-7.97724	-1.80415	-0.90055
H	-7.96380	-1.83704	0.87510
C	-10.37501	-2.31170	-0.01504
H	-10.11562	-2.86954	-0.92146
H	-10.10032	-2.92005	0.85355
C	-11.85738	-2.01548	0.00577

H	-12.12456	-1.40269	-0.85884
H	-12.11305	-1.46605	0.91518
H	-13.47975	-3.09498	-0.01019
O	-12.53645	-3.26506	-0.03468
O	-9.68214	-1.07892	0.01395
O	12.90539	-2.57246	0.03968
H	13.34826	-3.42294	0.05266

PEG_1n_wB97XD_reduced.log Energy: -144494.0589769

C	-0.58007	-0.48655	0.00342
H	-0.52413	-1.12614	0.89008
H	-0.52922	-1.13256	-0.87879
C	0.58007	0.48655	-0.00342
H	0.52922	1.13256	0.87879
H	0.52413	1.12614	-0.89008
O	-1.78863	0.26559	0.00361
O	1.78863	-0.26559	-0.00361
H	-2.52031	-0.36398	-0.02580
H	2.52031	0.36398	0.02580

PEG_1n_wB97XD_reduced_a.log Energy: -144075.6985476

C	-0.52556	-0.51157	-0.00012
H	-0.48363	-1.14699	0.88781
H	-0.48398	-1.14668	-0.88831
C	0.65714	0.43606	-0.00022
H	0.63119	1.12147	0.86579
H	0.63075	1.12309	-0.86479
O	-1.70396	0.28345	0.00013
O	1.87622	-0.18271	0.00006
H	-2.46193	-0.30379	0.00005

PEG_1n_wB97XD_reduced_b.log Energy: -144086.6352068

C	-0.66095	0.52295	-0.30186
H	-0.60808	0.40704	-1.38805
H	-1.13299	1.48015	-0.07341
C	0.68937	0.50594	0.27376
H	0.92501	0.93173	1.23975
O	-1.46094	-0.55257	0.24679
O	1.53821	-0.45101	-0.21359
H	-2.32322	-0.51363	-0.17461

H	2.35066	-0.44998	0.29936

PEG_2n_wB97XD_reduced.log Energy: -241043.7204270

C	2.36399	0.51170	0.00009
H	2.33207	1.14863	0.88760
H	2.33188	1.14887	-0.88724
C	1.17851	-0.42658	0.00006
H	1.20736	-1.06846	0.88763
H	1.20746	-1.06848	-0.88750
O	3.53961	-0.29010	-0.00014
O	0.00259	0.35738	-0.00002
C	-1.17297	-0.43921	0.00005
H	-1.18451	-1.08216	-0.88697
H	-1.18453	-1.08200	0.88719
C	-2.36351	0.48875	-0.00004
H	-2.32476	1.13714	0.88271
H	-2.32472	1.13700	-0.88290
O	-3.55071	-0.28790	-0.00001
H	4.29914	0.29488	-0.00002
H	-4.32739	0.39149	-0.00015

PEG_3n_wB97XD_reduced.log Energy: -337560.0588884

C	4.12752	-0.51468	-0.00017
H	4.09548	-1.15168	-0.88763
H	4.09533	-1.15217	0.88694
C	2.94228	0.42445	-0.00001
H	2.96827	1.06638	-0.88854
H	2.96821	1.06599	0.88881
O	5.30292	0.28872	0.00015
O	1.76291	-0.35742	-0.00021
C	0.60441	0.45633	-0.00019
H	0.58857	1.09788	0.89306
H	0.58853	1.09788	-0.89343
C	-0.60441	-0.45633	-0.00015
H	-0.58858	-1.09789	-0.89338
H	-0.58852	-1.09786	0.89311
O	-1.76291	0.35742	-0.00013
C	-2.94228	-0.42445	0.00019
H	-2.96816	-1.06594	0.88904
H	-2.96832	-1.06644	-0.88830

C	-4.12752	0.51468	0.00003
H	-4.09528	1.15223	0.88709
H	-4.09553	1.15162	-0.88748
O	-5.30292	-0.28872	0.00047
H	6.06243	-0.29625	-0.00002
H	-6.06243	0.29625	0.00026

PEG_4n_wB97XD_reduced.log Energy: -434099.2112053

C	-5.88162	0.50002	-0.10613
H	-5.79635	1.14000	-0.98781
H	-5.89921	1.13381	0.78409
C	-4.69980	-0.44051	-0.04096
H	-4.67124	-1.07184	-0.93568
H	-4.78477	-1.09136	0.83640
O	-7.05718	-0.29861	-0.17722
O	-3.52565	0.34232	0.04273
C	-2.35697	-0.45604	0.08817
H	-2.37295	-1.10486	0.97001
H	-2.29072	-1.08607	-0.80991
C	-1.17040	0.47576	0.11985
H	-1.13422	1.04745	-0.82276
H	-1.24181	1.17222	0.96309
O	-0.00000	-0.31334	0.23450
C	1.17040	0.47576	0.11985
H	1.24181	1.17223	0.96308
H	1.13421	1.04744	-0.82276
C	2.35697	-0.45604	0.08818
H	2.37296	-1.10483	0.97004
H	2.29072	-1.08611	-0.80987
C	4.69980	-0.44051	-0.04095
H	4.78477	-1.09131	0.83646
H	4.67124	-1.07189	-0.93563
C	5.88162	0.50002	-0.10616
H	5.89919	1.13387	0.78402
H	5.79635	1.13994	-0.98788
H	7.81340	0.28884	-0.22520
O	7.05718	-0.29860	-0.17719
O	3.52564	0.34232	0.04271
H	-7.81340	0.28884	-0.22512

PEG_5n_wB97XD_reduced.log Energy: -530633.1269462

C	7.64297	0.50562	-0.16853
H	7.55415	1.12063	-1.06750
H	7.66047	1.16383	0.70374
C	6.46402	-0.43617	-0.07468
H	6.43932	-1.09758	-0.94754
H	6.54783	-1.05641	0.82449
C	4.12112	-0.45001	0.06780
H	4.05263	-1.11919	-0.79684
H	4.14819	-1.06143	0.97611
C	2.92957	0.47951	0.09564
H	2.89031	1.06723	-0.82863
H	3.00517	1.16910	0.94374
O	8.82020	-0.29164	-0.21979
O	5.28730	0.34614	-0.02065
O	1.76549	-0.31513	0.21340
C	0.58877	0.47006	0.15769
H	0.54988	1.16522	1.00278
H	0.56379	1.04093	-0.79145
C	-0.58878	-0.46946	0.15790
H	-0.56444	-1.04001	-0.79152
H	-0.54935	-1.16482	1.00281
O	-1.76557	0.31555	0.21445
C	-2.92954	-0.47923	0.09627
H	-3.00533	-1.16883	0.94436
H	-2.88980	-1.06689	-0.82805
C	-4.12117	0.45013	0.06790
H	-4.14847	1.06199	0.97591
H	-4.05260	1.11889	-0.79707
C	-6.46406	0.43593	-0.07490
H	-6.54808	1.05656	0.82398
H	-6.43932	1.09697	-0.94805
C	-7.64287	-0.50604	-0.16850
H	-7.66036	-1.16392	0.70402
H	-7.55388	-1.12140	-1.06722
H	-9.57533	-0.29713	-0.27647
O	-8.82022	0.29102	-0.22020
O	-5.28725	-0.34621	-0.02035
H	9.57542	0.29638	-0.27593

PEG_6n_wB97XD_reduced.log Energy: -627165.8970330

C	-9.43891	0.42004	0.10926
H	-9.44675	1.08076	-0.76116
H	-9.39480	1.03370	1.01246
C	-8.23385	-0.49095	0.04930
H	-8.27380	-1.10887	-0.85443
H	-8.22044	-1.15581	0.91991
C	-5.88908	-0.44886	-0.02236
H	-5.87827	-1.05947	-0.93157
H	-5.82958	-1.11804	0.84265
C	-4.71681	0.50609	-0.02174
H	-4.77134	1.17325	-0.88851
H	-4.73078	1.12014	0.88499
C	-2.36955	0.54472	-0.06932
H	-2.35616	1.21306	-0.93858
H	-2.33424	1.17600	0.82671
C	-1.17866	-0.39218	-0.10161
H	-1.21511	-1.01446	-1.00240
H	-1.19992	-1.05250	0.77216
O	-10.59492	-0.40924	0.12113
O	-7.07506	0.31964	0.03592
O	-3.53384	-0.26686	-0.07157
O	0.00000	0.39340	-0.09411
C	1.17866	-0.39218	-0.10160
H	1.19992	-1.05250	0.77216
H	1.21511	-1.01446	-1.00240
C	2.36955	0.54472	-0.06931
H	2.35616	1.21306	-0.93857
H	2.33424	1.17600	0.82671
O	3.53384	-0.26686	-0.07156
C	4.71681	0.50609	-0.02173
H	4.73078	1.12013	0.88500
H	4.77134	1.17326	-0.88850
C	5.88908	-0.44886	-0.02236
H	5.82958	-1.11805	0.84265
H	5.87827	-1.05947	-0.93157
C	8.23385	-0.49095	0.04930
H	8.22045	-1.15581	0.91991
H	8.27379	-1.10887	-0.85443
C	9.43891	0.42004	0.10925

H	9.39480	1.03370	1.01246
H	9.44675	1.08076	-0.76117
H	11.36799	0.15710	0.14899
O	10.59492	-0.40924	0.12113
O	7.07506	0.31964	0.03592
H	-11.36799	0.15710	0.14900

PEG_7n_wb97xd_reduced.log Energy: -723713.0702154

C	11.17043	-0.53096	-0.24729
H	11.17825	-1.16498	0.64670
H	11.05154	-1.19079	-1.11425
C	10.00475	0.42544	-0.17918
H	10.09035	1.08010	0.69499
H	9.96824	1.05496	-1.07502
C	7.65682	0.45743	-0.02900
H	7.69169	1.11476	0.84655
H	7.58300	1.08257	-0.92548
C	6.46370	-0.46690	0.05921
H	6.53045	-1.08543	0.96052
H	6.43645	-1.12966	-0.81225
C	4.12084	-0.44928	0.17363
H	4.12568	-1.05765	1.08430
H	4.05907	-1.12091	-0.68921
C	2.93985	0.49470	0.18084
H	2.99186	1.16158	1.04800
H	2.94327	1.10781	-0.72662
C	0.59274	0.50298	0.21897
H	0.57247	1.16891	1.08818
H	0.56497	1.11740	-0.68719
C	-0.59423	-0.43312	0.24649
H	-0.58014	-1.03792	1.15940
H	-0.55881	-1.10826	-0.61509
O	12.37452	0.21293	-0.34439
O	8.81688	-0.34734	-0.08633
O	5.29716	0.33225	0.10058
O	1.76404	-0.28942	0.23586
O	-1.76697	0.35610	0.19983
C	-2.93973	-0.43428	0.18942
H	-2.93575	-1.10505	-0.67632
H	-2.99424	-1.04374	1.09771

C	-4.12528	0.50111	0.11533
H	-4.13803	1.16706	0.98467
H	-4.06391	1.11543	-0.78923
O	-5.29601	-0.29185	0.08879
C	-6.46987	0.49218	0.00174
H	-6.45212	1.10063	-0.90871
H	-6.54189	1.16355	0.86398
C	-7.65049	-0.45196	-0.02538
H	-7.57480	-1.12502	-0.88601
H	-7.66962	-1.05882	0.88613
C	-9.99304	-0.46877	-0.15601
H	-9.96489	-1.13906	-1.02204
H	-10.06280	-1.08036	0.75013
C	-11.18541	0.45568	-0.25207
H	-11.11097	1.06330	-1.15744
H	-11.20748	1.12178	0.61402
H	-13.11593	0.21566	-0.33347
O	-12.35046	-0.35987	-0.28869
O	-8.82578	0.32904	-0.11777
H	13.13043	-0.48790	-0.39017

PEG_8n_wb97xd_reduced.log Energy: -820246.9225044

C	-12.93400	0.48694	-0.34346
H	-12.81184	1.12713	-1.22461
H	-12.95338	1.14161	0.53536
C	-11.76296	-0.46007	-0.24369
H	-11.85052	-1.09310	0.64608
H	-11.71632	-1.11165	-1.12313
C	-9.41610	-0.47297	-0.07426
H	-9.33225	-1.12309	-0.95186
H	-9.45297	-1.10515	0.81956
C	-8.22949	0.46124	-0.00413
H	-8.19726	1.09592	-0.89608
H	-8.30922	1.10792	0.87610
C	-5.88794	0.46231	0.13443
H	-5.81669	1.09946	-0.75347
H	-5.91010	1.10632	1.02000
C	-4.70222	-0.47355	0.19803
H	-4.68735	-1.12254	-0.68403
H	-4.76523	-1.10543	1.09029

C	-2.35685	-0.46774	0.28368
H	-2.30914	-1.12352	-0.59214
H	-2.35097	-1.09247	1.18316
C	-1.17382	0.47374	0.29051
H	-1.19350	1.10691	-0.60286
H	-1.20835	1.12128	1.17306
C	1.17304	0.47962	0.28002
H	1.18271	1.11133	-0.61457
H	1.21120	1.12885	1.16118
C	2.36038	-0.45632	0.26615
H	2.31022	-1.11302	-0.60884
H	2.36279	-1.08036	1.16613
O	-10.58069	0.32244	-0.16235
O	-7.05865	-0.32872	0.07495
O	-3.53143	0.31879	0.24100
O	0.00169	-0.31255	0.30554
O	3.53147	0.33509	0.21578
C	4.70495	-0.45298	0.17010
H	4.77272	-1.08390	1.06270
H	4.69003	-1.10282	-0.71134
C	5.88765	0.48653	0.10308
H	5.81448	1.12124	-0.78639
H	5.90876	1.13255	0.98718
O	7.06010	-0.30224	0.04514
C	8.23056	0.48786	-0.03215
H	8.30789	1.13702	0.84648
H	8.20256	1.11958	-0.92636
C	9.41459	-0.45035	-0.09382
H	9.44348	-1.08109	0.80108
H	9.33514	-1.10060	-0.97149
C	11.75675	-0.45188	-0.23877
H	11.83540	-1.08453	0.65206
H	11.72700	-1.10144	-1.12040
C	12.94297	0.48189	-0.31976
H	12.96509	1.12832	0.56115
H	12.85994	1.10952	-1.21060
H	14.87407	0.25725	-0.42332
O	14.11324	-0.32463	-0.38077
O	10.58553	0.33840	-0.17437
O	-14.13254	-0.26672	-0.43290

H -14.89313 0.42791 -0.49193

PEG_4n_wB97XD_ox.log Energy: -433939.7929104

C	-5.84385	0.44984	-0.38212
H	-5.74144	0.53418	-1.46680
H	-5.80874	1.45271	0.05070
C	-4.71379	-0.38537	0.17491
H	-4.72565	-1.38603	-0.26871
H	-4.81393	-0.48449	1.26047
O	-7.05908	-0.20396	-0.04010
O	-3.49882	0.27271	-0.14313
C	-2.37547	-0.44221	0.31478
H	-2.42511	-0.60201	1.39575
H	-2.29050	-1.41106	-0.18535
C	-1.18019	0.41785	-0.02084
H	-1.15069	0.64584	-1.10600
H	-1.13452	1.38447	0.49127
O	0.00013	-0.29563	0.20368
C	1.19541	0.42162	0.32035
H	1.28108	0.59958	1.41166
H	1.11027	1.39486	-0.16544
C	2.35062	-0.44200	-0.14532
H	2.31249	-1.41725	0.34742
H	2.28345	-0.58409	-1.22785
C	4.68748	-0.38285	-0.27418
H	4.75387	-1.39256	0.14320
H	4.65692	-0.45810	-1.36578
C	5.87425	0.44514	0.16274
H	5.89115	0.51976	1.25289
H	5.79532	1.45184	-0.25484
H	7.80239	0.32243	-0.06901
O	7.04278	-0.20839	-0.31561
O	3.51772	0.26337	0.20125
H	-7.78501	0.31289	-0.39414

PEG_5n_wB97XD_ox.log Energy: -530484.6044960

C	6.36813	1.82760	-0.03891
H	5.79986	2.51882	-0.66662
H	6.30506	2.16633	0.99800
C	5.78874	0.43644	-0.15793

H	5.86269	0.08189	-1.19137
H	6.33687	-0.25848	0.48680
C	3.80056	-0.75941	0.19553
H	3.84901	-1.18165	-0.81300
H	4.28163	-1.45532	0.88992
C	2.36196	-0.53389	0.59647
H	1.85046	0.11443	-0.11672
H	2.28470	-0.10636	1.59626
O	7.72375	1.76054	-0.46429
O	4.43087	0.50225	0.23859
O	1.71890	-1.81830	0.61224
C	0.40413	-1.82718	0.80034
H	0.05643	-2.79915	1.13276
H	-0.00209	-0.95416	1.30978
C	-0.35913	-1.71745	-0.78306
H	0.05336	-0.78407	-1.16422
H	-0.01626	-2.63313	-1.25163
O	-1.67490	-1.72995	-0.60207
C	-2.31205	-0.47679	-0.31448
H	-1.95101	0.27530	-1.01532
H	-2.05257	-0.18433	0.70507
C	-3.80196	-0.69813	-0.43883
H	-4.06285	-0.96116	-1.46850
H	-4.11505	-1.51328	0.22110
C	-5.83221	0.43922	-0.13919
H	-6.14337	0.22962	-1.16795
H	-6.20341	-0.36435	0.50551
C	-6.38595	1.77074	0.31421
H	-6.00615	2.56741	-0.33022
H	-6.06950	1.97176	1.34078
H	-8.16664	2.53611	0.50077
O	-7.80361	1.69024	0.23176
O	-4.42023	0.51274	-0.06165
H	8.11722	2.62661	-0.34280

PEG_6n_wB97XD_ox.log Energy: -627007.5357018

C	-9.38828	0.14412	-0.55902
H	-9.27728	-0.01732	-1.63426
H	-9.44249	1.21933	-0.37145
C	-8.20236	-0.44404	0.17113

H	-8.14925	-1.52394	-0.00466
H	-8.30124	-0.27476	1.24881
C	-5.86628	-0.29067	0.31859
H	-5.76759	-1.37099	0.16904
H	-5.91164	-0.09318	1.39476
C	-4.68523	0.42732	-0.29380
H	-4.63328	0.22640	-1.36826
H	-4.77563	1.50748	-0.14362
C	-2.35007	0.54182	-0.16042
H	-2.27306	0.39640	-1.24182
H	-2.31949	1.61176	0.06188
C	-1.19799	-0.16745	0.52348
H	-1.11540	-1.23494	0.31514
H	-1.28801	-0.04363	1.62184
O	-10.55265	-0.51090	-0.07009
O	-7.03446	0.18764	-0.31736
O	-3.51723	-0.05722	0.34840
O	0.00083	0.48845	0.22419
C	1.17531	-0.26851	0.18315
H	1.12281	-1.07999	0.91669
H	1.14419	-0.75209	-0.81438
C	2.37876	0.63643	0.30398
H	2.30963	1.45054	-0.42301
H	2.42329	1.06021	1.31138
O	3.49602	-0.18202	0.04979
C	4.71548	0.52972	0.17801
H	4.81429	0.92585	1.19337
H	4.73726	1.36644	-0.52712
C	5.83702	-0.43889	-0.12048
H	5.81011	-1.27544	0.58577
H	5.72942	-0.83886	-1.13422
C	8.17619	-0.55878	-0.25198
H	8.19901	-1.39322	0.45738
H	8.12117	-0.97006	-1.26574
C	9.41992	0.28692	-0.09943
H	9.46226	0.70236	0.91051
H	9.39710	1.11234	-0.81535
H	11.33549	-0.03567	-0.24373
O	10.53790	-0.55874	-0.34192
O	7.05566	0.26672	0.00136

H	-11.31518	-0.13456	-0.51310