

Supporting Information

Computational Study of $B(C_6F_5)_3$ -Catalyzed Selective Deoxygenation of 1,2-Diols: Cyclic and Non-Cyclic Pathways

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1. Initial formation of O-Si bond vs. O-B bond

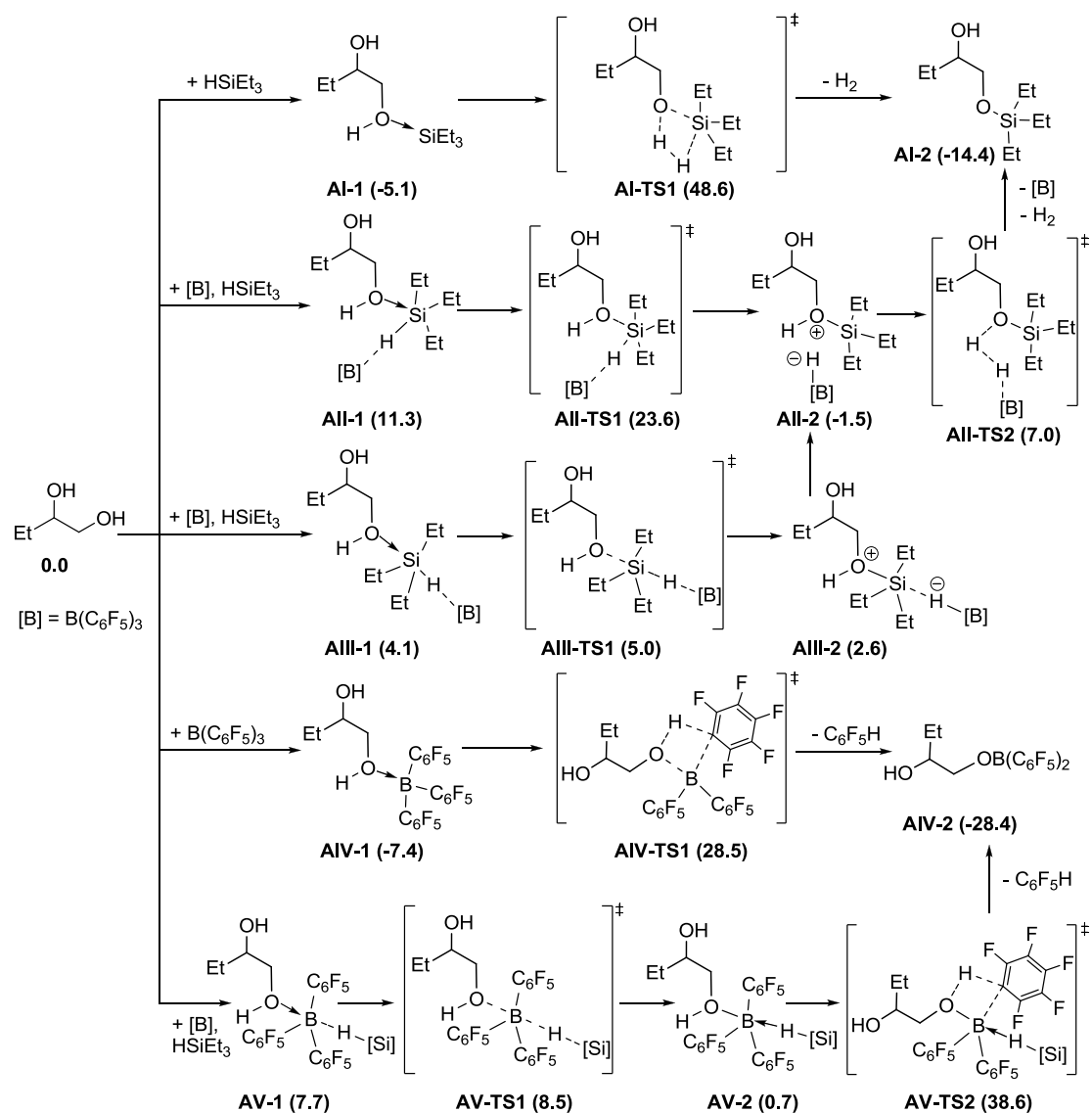


Figure S1. Plausible mechanisms for O-Si and O-B bond formation in the reactions of butane-1,2-diol with silane and $B(C_6F_5)_3$, respectively; free energies are given in kcal/mol.

2. First deoxygenation reaction of siloxane

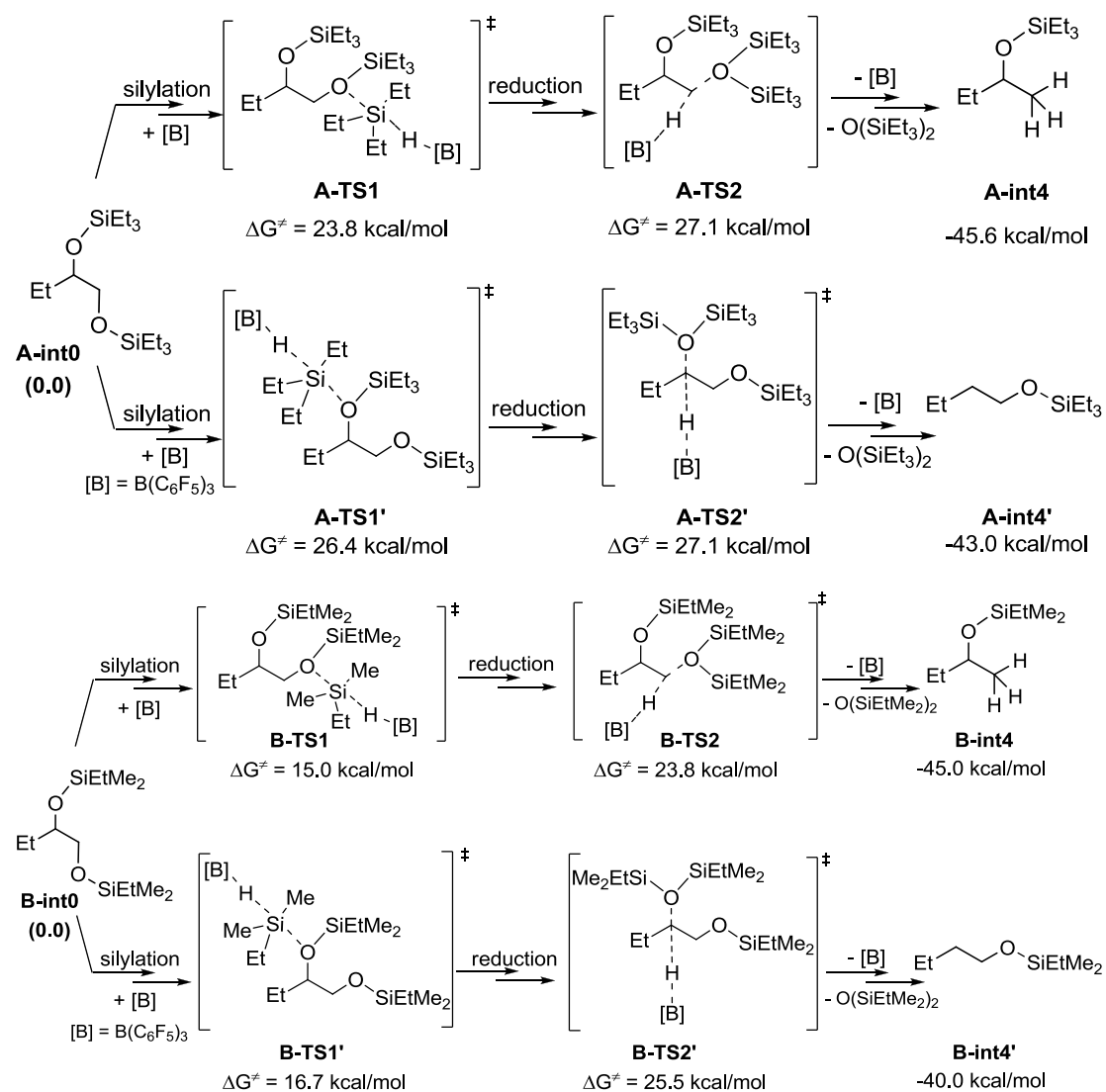
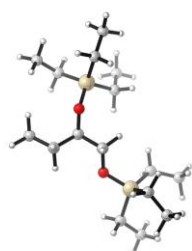
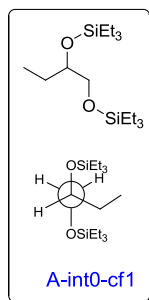
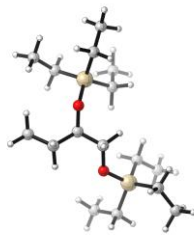


Figure S2. First deoxygenation of siloxane **A/B-int0** to afford 2-alkanols and 1-alkanols.

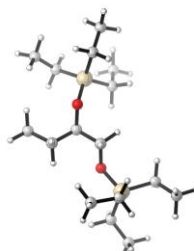
3. Conformational Studies on Siloxane Intermediates



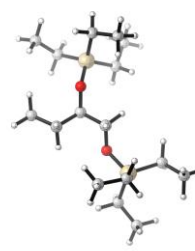
A-int0-cf1a
3.8(2.6)



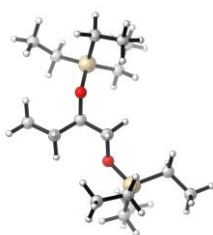
A-int0-cf1b
3.8(2.0)



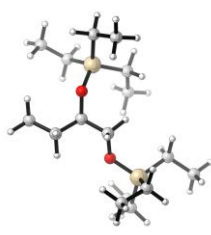
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1.9(1.3)



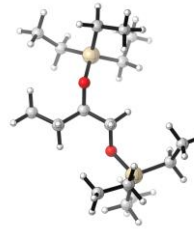
A-int0-cf1d
0.8(0.6)



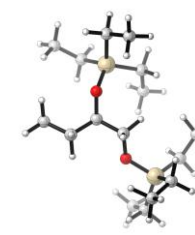
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0.0(0.0)



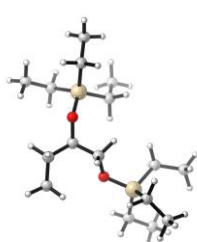
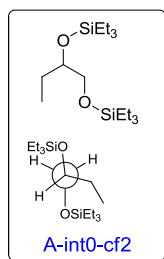
A-int0-cf1f
0.0(0.0)



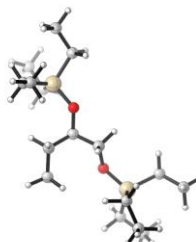
A-int0-cf1g
0.5(0.4)



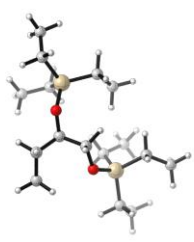
A-int0-cf1h
1.6(0.3)



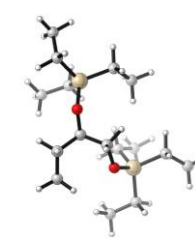
A-int0-cf2a
4.4(1.4)



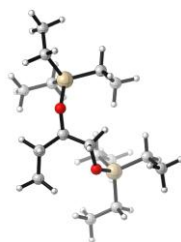
A-int0-cf2b
5.7(4.6)



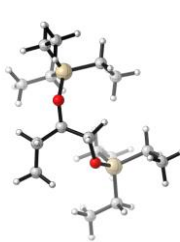
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5.7(3.7)



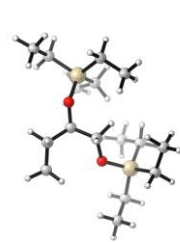
A-int0-cf2d
3.9(3.0)



A-int0-cf2e
3.3(2.1)



A-int0-cf2f
3.4(2.3)



A-int0-cf2g
3.4(2.5)

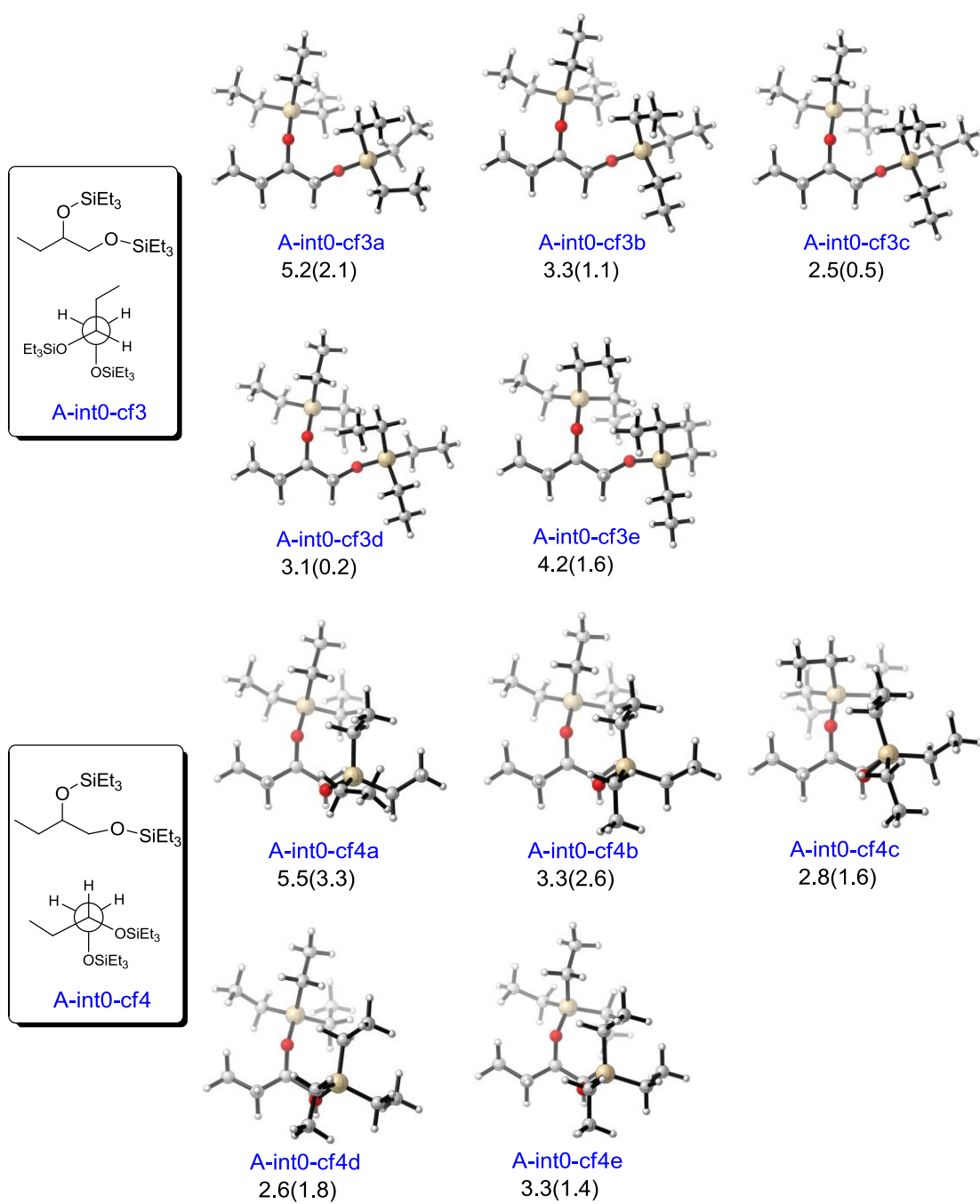
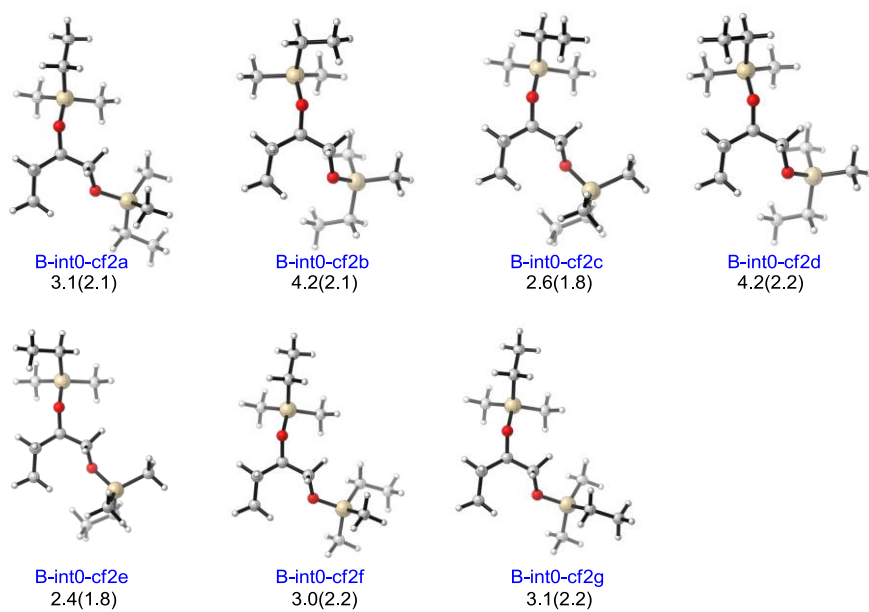
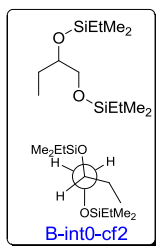
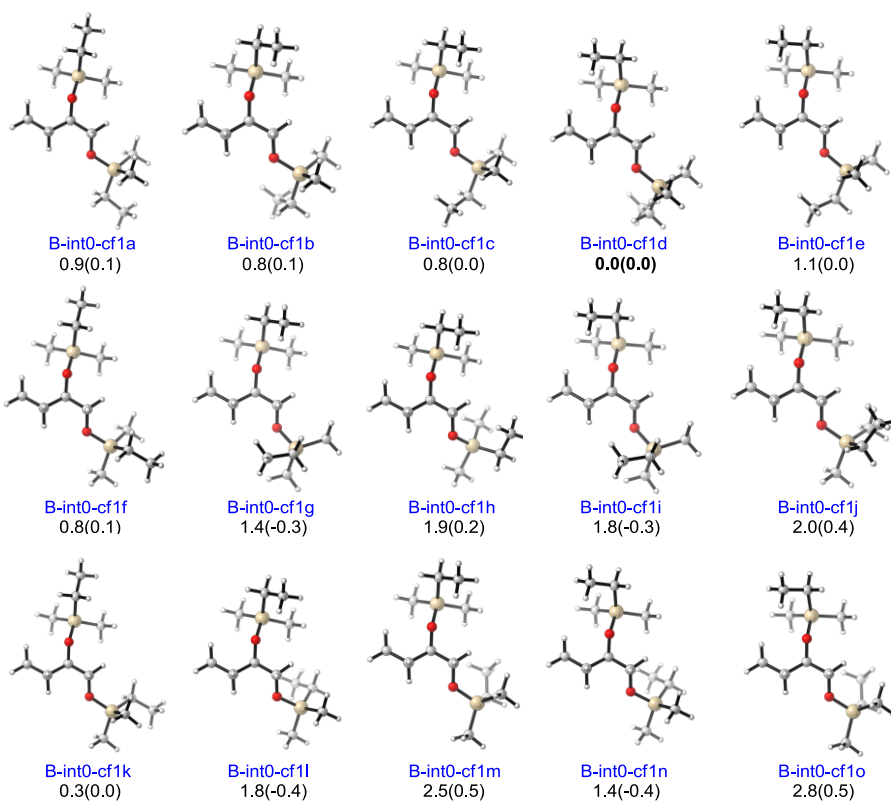
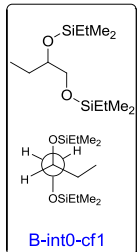
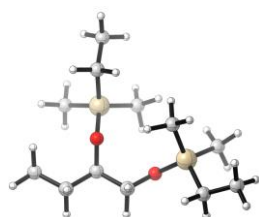
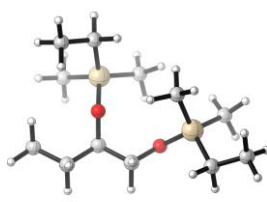


Figure S3. Possible conformations for siloxane **A-int0**; free energies (electronic energies) are given in kcal/mol.

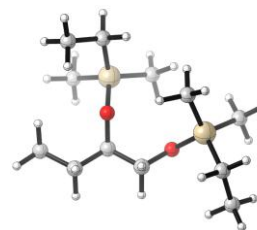




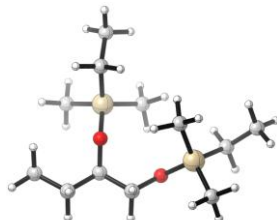
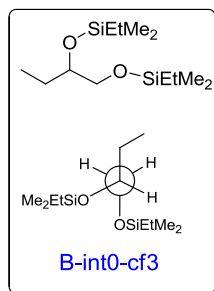
B-int0-cf3a
3.1(-0.1)



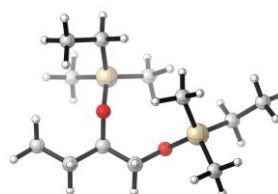
B-int0-cf3b
3.6(0.0)



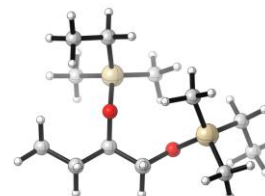
B-int0-cf3c
2.8(-0.4)



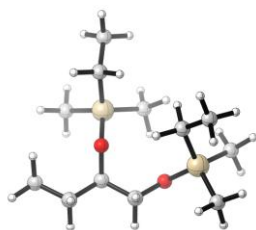
B-int0-cf3d
3.1(-0.2)



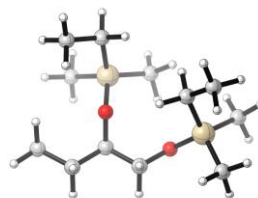
B-int0-cf3e
3.2(-0.2)



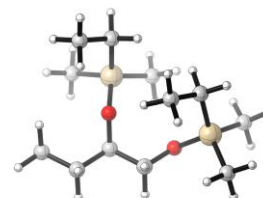
B-int0-cf3f
3.1(-0.2)



B-int0-cf3g
2.8(-0.3)



B-int0-cf3h
3.1(-0.2)



B-int0-cf3i
2.7(-0.6)

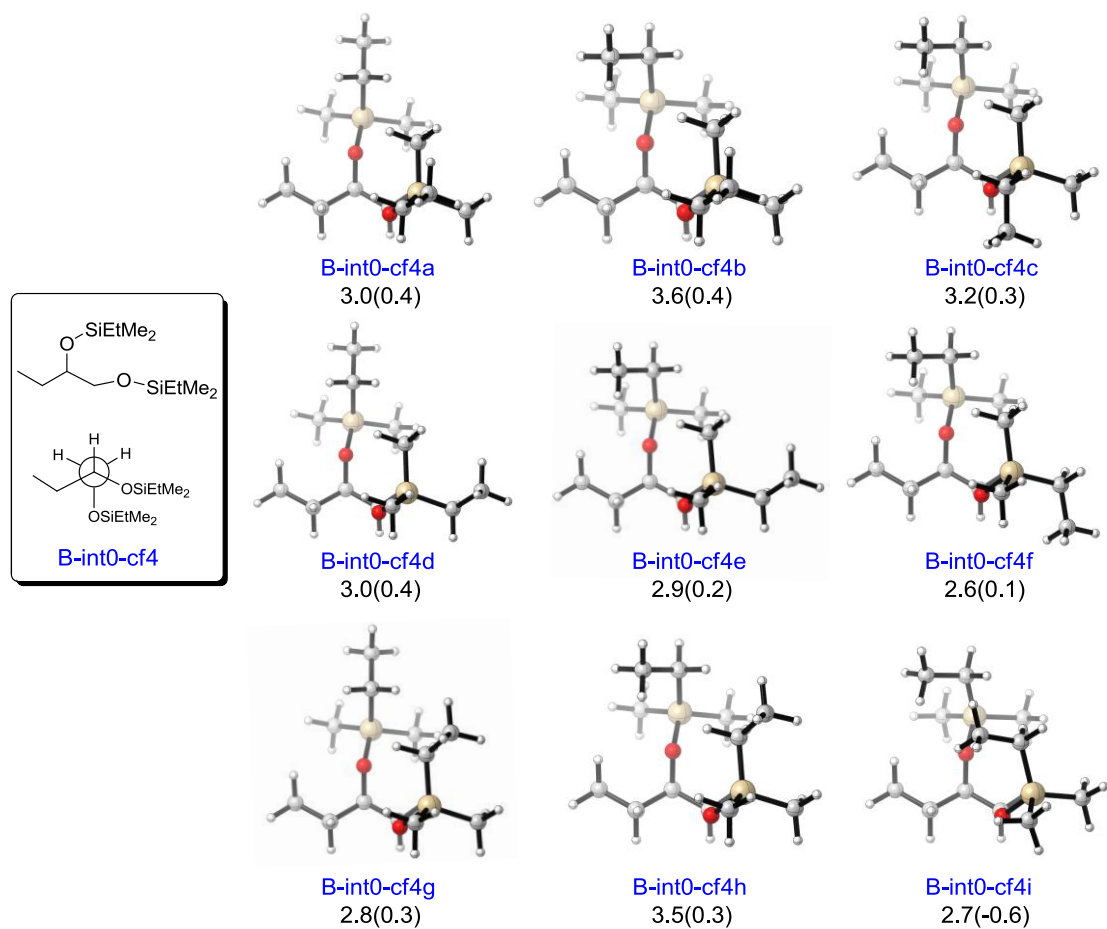


Figure S4. Possible conformations for siloxane **B-int0**; free energies (electronic energies) are given in kcal/mol.

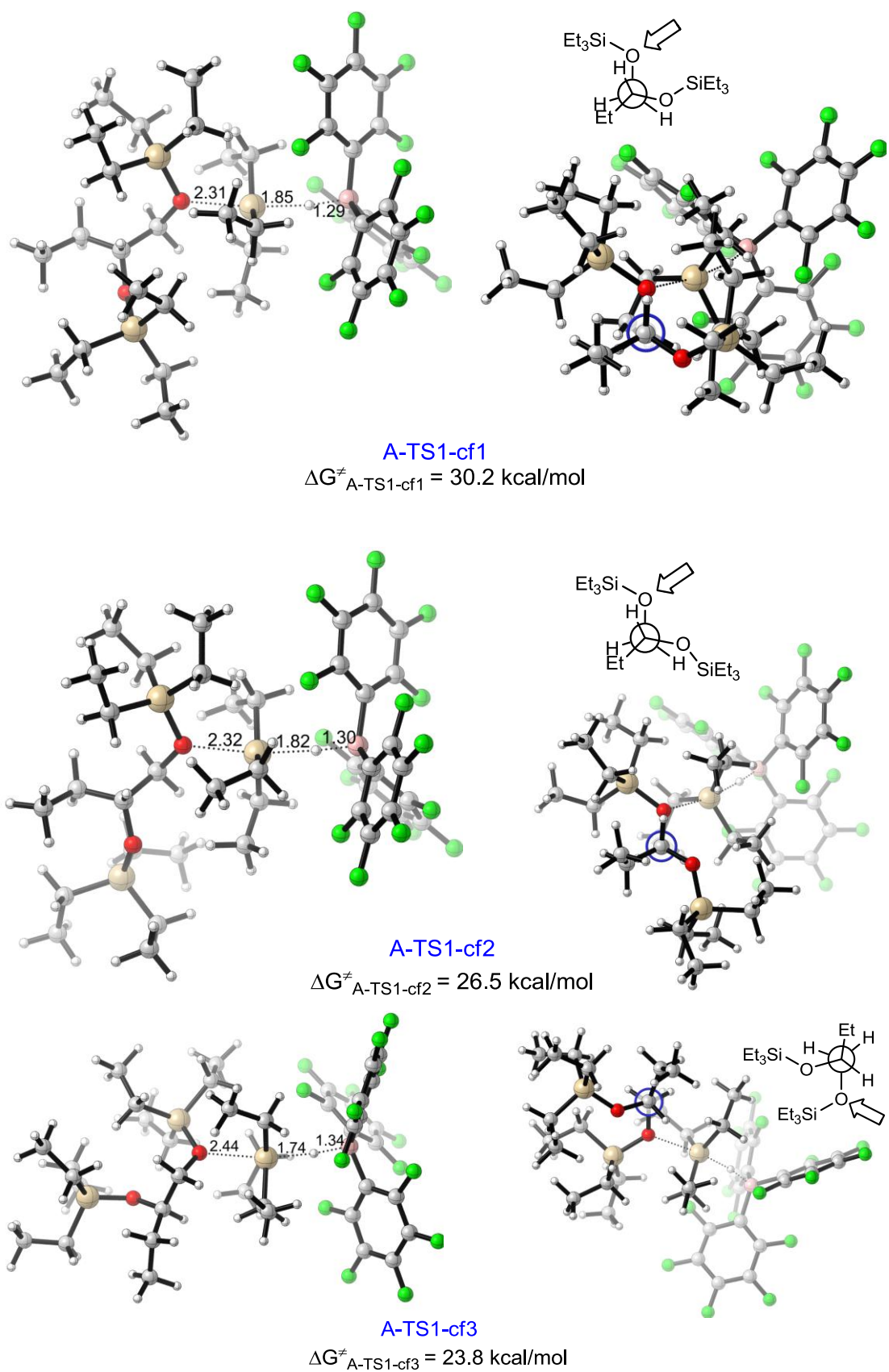


Figure S5. Possible conformations of **A-TS1**.

4. Natural bond orbital analysis

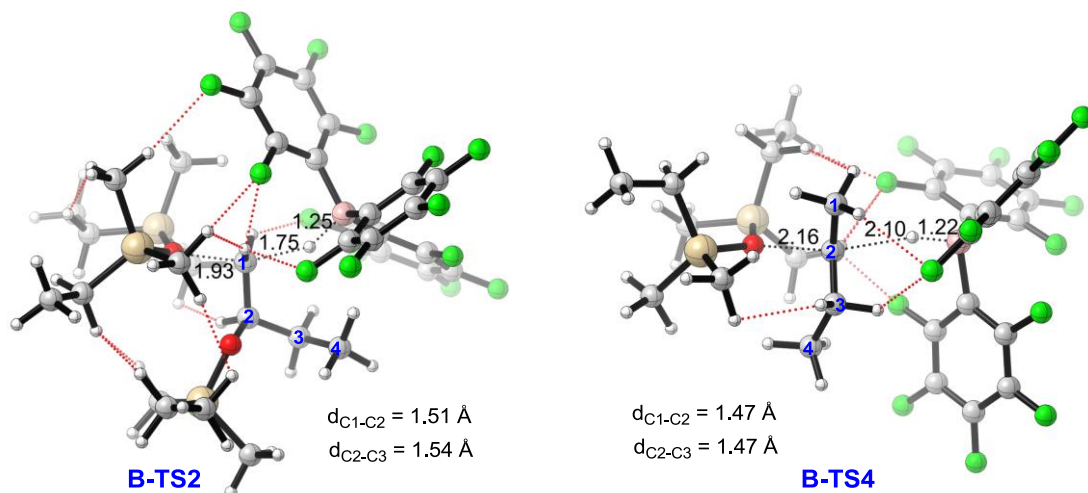


Table S1. Second-Order Perturbation Theory Analysis.

	Donor NBO	Acceptor NBO	E(2) (kcal/mol)
B-TS2	BD C2-H2a	LP* C1	8.12
B-TS4	BD C1-H1a	LP* C2	30.38
	BD C3-H3a	LP* C2	11.55

E(2) denotes the stabilization energy; BD denotes bonding orbital; BD* denotes antibonding orbital; LP denotes lone-pair; LP* denotes unfilled valence lone-pair.

Table S2. Energy table for the reaction of butane-1,2-diol and Et₃SiH. Listed are the zero-point vibrational energy (ZPVE), enthalpy correction (H_{corr}), and Gibbs free energy correction (G_{corr}) determined on the gas-phase geometries. Single-point solvent (SMD) corrected SCF energies and Gibbs free energies relative to **A-int0** are also presented. ZPVE, H_{corr}, G_{corr} and SCF_{SMD} are in Hartrees and ΔG is in kcal/mol.

	ZPVE	H _{corr}	G _{corr}	SCF _{SMD}	ΔG
A-int0	0.521833	0.553312	0.457509	-1361.997938	0.0
A-int1	0.894490	0.966136	0.787314	-4097.962484	22.1
A-TS1	0.894993	0.965594	0.789966	-4097.963702	23.8
A-int2	0.895769	0.967496	0.786647	-4097.984327	8.0
A-int3	0.896978	0.968103	0.792304	-4097.995277	5.5
A-TS2	0.892314	0.963580	0.786800	-4097.955387	27.1
A-int4	0.327450	0.346099	0.282854	-760.2069069	-45.6

Table S3. Energy table for the reaction of butane-1,2-diol and EtMe₂SiH. Listed are the zero-point vibrational energy (ZPVE), enthalpy correction (H_{corr}), and Gibbs free energy correction (G_{corr}) determined on the gas-phase geometries. Single-point solvent (SMD) corrected SCF energies and Gibbs free energies relative to **B-int0** are also presented. ZPVE, H_{corr}, G_{corr} and SCF_{SMD} are in Hartrees and ΔG is in kcal/mol.

	ZPVE	H _{corr}	G _{corr}	SCF _{SMD}	ΔG
B-int0	0.404917	0.431448	0.345328	-1204.795079	0.0
B-int1	0.717668	0.782485	0.616077	-3862.168756	13.1
B-TS1	0.719128	0.782677	0.620044	-3862.169622	15.0
B-int2	0.719675	0.784023	0.618507	-3862.176204	10.0
B-int3	0.719690	0.783082	0.622467	-3862.189942	3.8
B-TS2	0.716050	0.780346	0.616149	-3862.151741	23.8
B-int4	0.268684	0.285073	0.226368	-681.6054279	-45.0
B-int5	0.579674	0.635508	0.487313	-3338.972792	-34.0
B-TS3	0.582548	0.636345	0.495429	-3338.972975	-29.1
B-int6	0.583293	0.638006	0.493405	-3338.987870	-39.7
B-int7	0.582520	0.637349	0.493038	-3338.992713	-43.0
B-TS4	0.577809	0.633177	0.487129	-3338.964529	-29.0
butane	0.132705	0.139430	0.104672	-158.4089174	-87.3

Table S4. Energy table for the reaction of butane-1,2-diol and Ph₂SiH₂/Et₃SiH. Listed are the zero-point vibrational energy (ZPVE), enthalpy correction (H_{corr}), and Gibbs free energy correction (G_{corr}) determined on the gas-phase geometries. Single-point solvent (SMD) corrected SCF energies and Gibbs free energies relative to **C-int0** are also presented. ZPVE, H_{corr}, G_{corr} and SCF_{SMD} are in Hartrees and ΔG is in kcal/mol.

	ZPVE	H _{corr}	G _{corr}	SCF _{SMD}	ΔG
C-int0	0.307052	0.325624	0.259086	-1060.470751	0.0
C-int1	0.676240	0.736709	0.577831	-3796.449596	7.0
C-TS1	0.677641	0.736746	0.582246	-3796.450406	9.3
C-int2	0.678481	0.738562	0.579768	-3796.463022	-0.2
C-int3	0.677363	0.738054	0.577444	-3796.463732	-2.1
C-TS2	0.674234	0.734482	0.575905	-3796.435343	14.8
C-int4	0.516528	0.548567	0.450477	-1588.279291	-46.5
C-int5	0.884993	0.958958	0.769431	-4324.252400	-35.8
C-TS3	0.887714	0.959694	0.779082	-4324.240179	-22.0
C-int6	0.888087	0.961229	0.774917	-4324.262405	-38.6
C-int7	0.890043	0.962305	0.781785	-4324.261547	-33.8
C-TS4	0.885772	0.958279	0.777863	-4324.240379	-22.9
butane	0.132705	0.139430	0.104672	-158.4089174	-64.1

Cartesian Coordinates (in Å)

A-int0				A-int1			
H	-4.247990	1.627099	-1.282237	C	4.420868	3.119131	0.649970
C	0.367615	2.451979	0.049317	C	4.012151	1.747042	0.109658
C	0.615037	0.962954	-0.131478	H	3.602698	3.523078	1.254858
H	-0.611492	2.684931	-0.377538	H	5.274684	3.005268	1.328280
H	0.318859	2.649619	1.125928	C	3.218165	0.936425	1.127787
C	-0.546218	0.126115	0.389623	H	3.354121	1.908569	-0.753179
H	0.726915	0.749314	-1.206330	H	3.879567	0.583353	1.927252
H	-0.286368	-0.936763	0.308228	H	2.469946	1.588406	1.584141
H	-0.689158	0.360984	1.454907	O	5.105824	0.986385	-0.374601
O	1.777964	0.580726	0.587374	O	2.520877	-0.150533	0.534954
O	-1.703763	0.417621	-0.364194	Si	6.724965	0.914813	0.062494
Si	2.999858	-0.371108	-0.046396	Si	-0.152502	0.299058	0.283565
Si	-3.223273	-0.117301	0.090508	C	7.717987	2.358700	-0.619350
C	3.994532	-0.933358	1.436267	C	9.225431	2.125986	-0.423648
C	3.206159	-1.889596	2.342535	H	7.422835	3.285686	-0.117221
H	4.295257	-0.043755	1.999447	H	7.493563	2.496296	-1.682103
H	4.922703	-1.406061	1.095407	H	9.812721	2.970206	-0.789688
H	3.771309	-2.159133	3.237142	H	9.473954	1.990819	0.633220
H	2.268235	-1.430749	2.664798	H	9.563958	1.234213	-0.957723
H	2.957707	-2.816688	1.818486	C	6.973389	0.864739	1.942871
C	2.266001	-1.861951	-0.932207	C	7.944674	-0.230425	2.414749
C	3.341503	-2.861303	-1.386810	H	6.011740	0.734898	2.448622
H	1.671678	-1.534095	-1.792127	H	7.346172	1.844647	2.263412
H	1.567145	-2.361244	-0.252428	H	8.070080	-0.211036	3.499186
H	2.902354	-3.727116	-1.886507	H	7.585845	-1.226111	2.139814
H	4.045120	-2.402792	-2.086033				
H	3.920516	-3.232122	-0.536300				
C	4.045046	0.653943	-1.226699				
C	5.017756	1.598175	-0.503376				
H	3.367925	1.229541	-1.868811				
H	4.602379	-0.009834	-1.896205				
H	5.539317	2.255837	-1.201950				
H	4.498049	2.230372	0.221132				
H	5.773637	1.032338	0.046550				
C	-3.622917	0.584472	1.788535				
C	-3.373369	2.098231	1.869232				
H	-3.026844	0.063834	2.546510				
H	-4.668682	0.360864	2.026745				
H	-3.594874	2.493845	2.862597				
H	-2.331884	2.336333	1.637646				
H	-3.995631	2.639321	1.151880				
C	-4.381753	0.542108	-1.222730				
C	-4.139077	-0.093186	-2.599858				

H	8.933847	-0.108487	1.966336	H	2.821158	-1.742008	-2.162404
C	7.323017	-0.667004	-0.747240	H	4.776924	-2.897977	-3.084391
C	7.276606	-0.606726	-2.280739	H	5.598812	-2.901535	-1.534359
H	6.708954	-1.496645	-0.381682	H	4.164342	-3.897463	-1.771388
H	8.343367	-0.880835	-0.411399	C	4.572997	-1.957759	1.504824
H	7.574098	-1.556499	-2.730647	C	5.137745	-3.387511	1.509690
H	6.271377	-0.369543	-2.637362	H	4.140694	-1.738737	2.490447
H	7.950911	0.164184	-2.663734	H	5.380616	-1.237295	1.364786
C	0.243834	-0.508521	-1.370212	H	5.836117	-3.534425	2.336373
C	1.107398	0.375363	-2.282089	H	4.344270	-4.132159	1.618022
H	-0.708001	-0.679023	-1.874818	H	5.671995	-3.613920	0.584998
H	0.693926	-1.492959	-1.228952	B	-3.145246	0.065541	-0.075565
H	1.256603	-0.113871	-3.247347	C	-3.167125	-1.072491	-1.216340
H	0.620119	1.332850	-2.474478	C	-3.657078	-0.395381	1.381755
H	2.089348	0.561820	-1.848526	C	-3.576849	1.537677	-0.569147
C	-0.290335	-0.408011	2.026348	C	-2.408558	-2.227708	-1.075282
C	0.898597	-0.539395	2.984788	C	-3.921125	-1.003346	-2.379673
H	-0.834523	-1.354240	1.965180	C	-2.355391	-3.239394	-2.011549
H	-0.995342	0.302236	2.474453	C	-3.909363	-2.002471	-3.345416
H	0.531927	-0.827984	3.972323	C	-3.120254	-3.123399	-3.162800
H	1.609941	-1.295824	2.660240	F	-1.642654	-2.376153	0.022128
H	1.438872	0.400750	3.100424	F	-4.717105	0.041531	-2.623846
C	0.181292	2.146405	0.238513	F	-1.579802	-4.305327	-1.829513
C	-0.026510	2.911569	1.550650	F	-4.651358	-1.890489	-4.442067
H	-0.442163	2.576435	-0.550841	F	-3.093429	-4.080920	-4.079756
H	1.208777	2.261396	-0.123955	C	-3.500479	0.457076	2.468725
H	0.283125	3.953509	1.445806	C	-4.260701	-1.611910	1.679344
H	-1.075116	2.905069	1.846952	C	-3.871553	0.146497	3.761640
H	0.544577	2.477444	2.375835	C	-4.658249	-1.964325	2.963176
C	4.741338	4.096337	-0.480997	C	-4.460891	-1.083315	4.010013
H	3.826659	4.369201	-1.012324	F	-2.929422	1.658448	2.279577
H	5.423624	3.648699	-1.205063	F	-4.505359	-2.520968	0.730876
H	5.197557	5.013192	-0.104101	F	-3.665952	1.001761	4.758775
Si	3.200279	-1.690479	0.245734	F	-5.231241	-3.141722	3.191544
C	1.840802	-2.953849	0.627583	F	-4.831250	-1.409958	5.240561
C	1.677199	-4.098651	-0.383570	C	-2.866177	2.143376	-1.596175
H	0.885688	-2.432945	0.729923	C	-4.632661	2.283330	-0.063482
H	2.043951	-3.374657	1.619215	C	-3.132014	3.410852	-2.078555
H	0.806612	-4.711211	-0.143301	C	-4.945344	3.554209	-0.525159
H	1.538363	-3.724982	-1.402222	C	-4.188867	4.123115	-1.534993
H	2.551434	-4.753820	-0.392225	F	-1.843795	1.478931	-2.168672
C	3.733153	-1.754607	-1.555334	F	-5.413470	1.797321	0.905779
C	4.614676	-2.930563	-2.004540	F	-2.389614	3.945832	-3.044227
H	4.242857	-0.806487	-1.754409	F	-5.964612	4.230684	-0.005977

F	-4.472057	5.340877	-1.978621	C	-0.226364	-0.400368	1.983651
H	-1.814611	0.283393	0.135823	C	0.931412	-0.587945	2.968109
A-TS1				H	-0.821288	-1.315062	1.918026
C	4.326285	3.102993	0.556724	H	-0.902104	0.351856	2.405244
C	3.940715	1.714273	0.041081	H	0.530811	-0.865597	3.945534
H	3.489032	3.517988	1.126986	H	1.615644	-1.375830	2.657973
H	5.161221	3.012702	1.261652	H	1.509218	0.327416	3.103000
C	3.125921	0.927437	1.061870	C	0.243721	2.134230	0.144377
H	3.305084	1.849301	-0.842124	C	-0.007333	2.920260	1.436823
H	3.776807	0.549756	1.856285	H	-0.415246	2.503761	-0.645899
H	2.396218	1.592946	1.524259	H	1.254975	2.310959	-0.235132
O	5.050643	0.948800	-0.395859	H	0.266269	3.970098	1.312507
O	2.394098	-0.148356	0.469227	H	-1.059951	2.882374	1.715398
Si	6.658805	0.902352	0.088816	H	0.563129	2.526294	2.283125
Si	-0.000694	0.272469	0.234845	C	4.671573	4.051490	-0.591123
C	7.656808	2.348204	-0.580725	H	3.769461	4.304633	-1.152863
C	9.160035	2.130141	-0.339948	H	5.375043	3.589351	-1.284965
H	7.339922	3.277953	-0.097371	H	5.112501	4.980634	-0.226574
H	7.462613	2.472990	-1.650894	Si	3.091869	-1.703070	0.193547
H	9.749175	2.980458	-0.688262	C	1.740196	-2.975702	0.561143
H	9.378951	1.996674	0.723726	C	1.594816	-4.114885	-0.459608
H	9.522751	1.242388	-0.864525	H	0.777192	-2.471453	0.664406
C	6.846341	0.876303	1.976512	H	1.946113	-3.402394	1.549342
C	7.798823	-0.215148	2.493175	H	0.728447	-4.736194	-0.227634
H	5.868863	0.754785	2.453299	H	1.456876	-3.736919	-1.476630
H	7.210795	1.859381	2.296772	H	2.475177	-4.761718	-0.466840
H	7.888679	-0.182917	3.580770	C	3.668319	-1.767828	-1.593102
H	7.446601	-1.213286	2.218579	C	4.588970	-2.932263	-1.992589
H	8.802425	-0.100562	2.076108	H	4.168423	-0.814339	-1.790175
C	7.299923	-0.681450	-0.682768	H	2.777608	-1.784577	-2.229604
C	7.272912	-0.647592	-2.217574	H	4.781557	-2.915638	-3.067650
H	6.702658	-1.520372	-0.310776	H	5.557652	-2.869899	-1.494768
H	8.320445	-0.864711	-0.329659	H	4.153756	-3.904798	-1.754011
H	7.600514	-1.596619	-2.647622	C	4.449046	-1.944518	1.474548
H	6.266639	-0.442109	-2.590693	C	5.008994	-3.376321	1.511584
H	7.932590	0.133932	-2.604443	H	4.013559	-1.705634	2.453581
C	0.255692	-0.529794	-1.448558	H	5.260435	-1.230848	1.323468
C	1.099945	0.339653	-2.392114	H	5.700757	-3.506097	2.346513
H	-0.727737	-0.652065	-1.901291	H	4.213558	-4.116896	1.630699
H	0.671886	-1.534472	-1.351686	H	5.549606	-3.623786	0.596354
H	1.205214	-0.151592	-3.362169	B	-3.050676	0.081029	-0.048869
H	0.618754	1.303551	-2.566249	C	-3.139511	-1.052258	-1.198676
H	2.101479	0.515094	-2.000003	C	-3.564032	-0.390014	1.411673
				C	-3.500635	1.556758	-0.530555

C	-2.391111	-2.217584	-1.095024	Si	0.643052	0.344355	0.294682
C	-3.936292	-0.969339	-2.331818	C	7.798521	2.338606	-0.614564
C	-2.383024	-3.223349	-2.038991	C	9.301023	2.123464	-0.363809
C	-3.971182	-1.961388	-3.304798	H	7.478994	3.274035	-0.144322
C	-3.187763	-3.091588	-3.160788	H	7.611287	2.450732	-1.687164
F	-1.590537	-2.387174	-0.024247	H	9.888865	2.974659	-0.711307
F	-4.731546	0.084320	-2.540606	H	9.515273	1.993519	0.701214
F	-1.612018	-4.299284	-1.891717	H	9.668831	1.236134	-0.885201
F	-4.752533	-1.833184	-4.372521	C	6.982424	0.880762	1.954553
F	-3.204490	-4.042813	-4.085567	C	7.921374	-0.219264	2.478461
C	-3.402965	0.451852	2.506510	H	6.004020	0.773275	2.433266
C	-4.168023	-1.607439	1.706126	H	7.357134	1.860909	2.271415
C	-3.766217	0.131745	3.799322	H	8.009980	-0.182183	3.565735
C	-4.557050	-1.970927	2.990032	H	7.558674	-1.214866	2.208229
C	-4.353197	-1.099864	4.043168	H	8.926608	-0.117967	2.062350
F	-2.837892	1.658169	2.327314	C	7.437516	-0.690619	-0.699557
F	-4.423184	-2.512207	0.755245	C	7.373164	-0.668951	-2.233815
F	-3.556661	0.981262	4.801362	H	6.863625	-1.536148	-0.305932
F	-5.128871	-3.150889	3.211400	H	8.468555	-0.857913	-0.370076
F	-4.715766	-1.436372	5.274143	H	7.692463	-1.620486	-2.664054
C	-2.829327	2.152491	-1.589523	H	6.357915	-0.467287	-2.584542
C	-4.530882	2.314442	0.009139	H	8.022163	0.110319	-2.642021
C	-3.103151	3.419601	-2.068538	C	0.383708	-0.369653	-1.413152
C	-4.849898	3.586740	-0.445258	C	1.118753	0.458464	-2.480639
C	-4.129804	4.145141	-1.486609	H	-0.687087	-0.320239	-1.615948
F	-1.839139	1.475749	-2.204964	H	0.651148	-1.428747	-1.468025
F	-5.283742	1.840918	1.006802	H	1.022063	-0.011138	-3.461518
F	-2.395970	3.942010	-3.067861	H	0.684801	1.457087	-2.555851
F	-5.842909	4.274103	0.110478	H	2.187105	0.563368	-2.273074
F	-4.419558	5.364088	-1.924750	C	-0.039589	-0.310686	1.914723
H	-1.737798	0.270466	0.121491	C	0.977400	-0.456126	3.055600
A-int2				H	-0.582430	-1.242986	1.755356
C	4.482417	3.137214	0.454730	H	-0.801638	0.416441	2.206112
C	4.091454	1.725720	0.008814	H	0.474160	-0.779580	3.968237
H	3.647193	3.584159	1.003237	H	1.748344	-1.196611	2.829062
H	5.318941	3.078470	1.161215	H	1.477165	0.489329	3.283934
C	3.298885	0.993368	1.083792	C	0.567032	2.218101	0.202992
H	3.433619	1.818465	-0.863682	C	0.256277	2.970436	1.505498
H	3.953502	0.535112	1.823335	H	-0.242346	2.404833	-0.511684
H	2.622759	1.673096	1.596739	H	1.464765	2.617170	-0.281608
O	5.187119	0.936412	-0.410532	H	0.229818	4.047124	1.328871
O	2.466531	-0.059210	0.503378	H	-0.719167	2.679149	1.896046
Si	6.804429	0.898266	0.066815	H	0.991512	2.788132	2.295516
				C	4.826291	4.022317	-0.742744

H	3.922810	4.247541	-1.313909	F	-2.758218	1.619341	2.334873
H	5.528208	3.524631	-1.412673	F	-4.692923	-2.398851	0.757941
H	5.268403	4.967963	-0.426324	F	-3.501373	0.985493	4.821527
Si	3.147692	-1.696256	0.187451	F	-5.430726	-2.996575	3.234615
C	1.773212	-2.915571	0.572780	F	-4.855724	-1.329056	5.298635
C	1.766773	-4.141898	-0.357332	C	-3.004326	2.222074	-1.512509
H	0.789822	-2.448184	0.522060	C	-4.898791	2.077013	-0.153173
H	1.892804	-3.239521	1.612441	C	-3.401411	3.453488	-2.002332
H	0.923292	-4.791323	-0.121520	C	-5.342888	3.307183	-0.617493
H	1.662290	-3.848950	-1.405159	C	-4.588167	4.001994	-1.546782
H	2.682296	-4.731118	-0.261873	F	-1.842958	1.730053	-2.005656
C	3.690733	-1.695506	-1.601632	F	-5.690331	1.457179	0.731123
C	4.632544	-2.842283	-2.009804	F	-2.659101	4.111505	-2.895361
H	4.181251	-0.734708	-1.785712	F	-6.488696	3.827746	-0.181618
H	2.796256	-1.721549	-2.231231	F	-4.998125	5.184869	-1.998776
H	4.853719	-2.785077	-3.077290	H	-1.912612	0.312749	0.141577
H	5.585858	-2.787933	-1.481986				
H	4.195605	-3.824115	-1.818532	A-int3			
C	4.515618	-1.909632	1.450410	C	-2.514896	1.126053	0.979248
C	5.005903	-3.367627	1.524314	C	-1.491741	0.032420	0.726793
H	4.123211	-1.618487	2.432496	H	-3.259711	0.755607	1.692768
H	5.351852	-1.241943	1.237510	H	-0.607689	0.404844	0.215511
H	5.769231	-3.479218	2.296403	H	-1.187819	-0.380121	1.683091
H	4.190224	-4.051451	1.770926	Si	-4.632829	2.267335	-0.386920
H	5.441191	-3.700755	0.580305	O	-3.154847	1.464340	-0.235126
B	-3.098347	0.083539	-0.034499	O	-2.002297	-1.093941	-0.078120
C	-3.173960	-1.098714	-1.157071	C	-1.748576	2.293117	1.628706
C	-3.667572	-0.363076	1.423800	H	-2.459962	2.943304	2.140421
C	-3.711490	1.493114	-0.569210	H	-1.108041	1.870702	2.412004
C	-2.300519	-2.173759	-1.088479	C	-0.901651	3.113076	0.655811
C	-4.036186	-1.129764	-2.244784	H	-1.530444	3.605421	-0.089007
C	-2.226742	-3.185390	-2.026356	H	-0.353903	3.884942	1.200316
C	-4.012759	-2.132038	-3.207040	H	-0.159100	2.509995	0.125285
C	-3.097923	-3.164790	-3.102375	B	2.094818	0.349213	0.051921
F	-1.428373	-2.260964	-0.057797	C	3.212576	1.290840	-0.652185
F	-4.958254	-0.175832	-2.415798	C	1.776410	0.745004	1.611470
F	-1.321031	-4.162921	-1.912177	C	2.506105	-1.213600	-0.200092
F	-4.860468	-2.109281	-4.233450	C	2.920827	2.155839	-1.693888
F	-3.053487	-4.124769	-4.022389	C	4.542249	1.245977	-0.262914
C	-3.418654	0.456135	2.516956	C	3.881951	2.936900	-2.317978
C	-4.364068	-1.525646	1.720098	C	5.534901	2.008975	-0.854057
C	-3.793639	0.161126	3.814363	C	5.197259	2.861549	-1.893237
C	-4.768061	-1.863495	3.005956	F	1.660233	2.285667	-2.146313
C	-4.480296	-1.016717	4.060453	F	4.902265	0.436187	0.743254

F	3.556421	3.758130	-3.317653	C	-6.017298	4.496152	0.706166
F	6.800356	1.936923	-0.443210	H	-3.881877	4.217632	0.921219
F	6.133059	3.604310	-2.479991	H	-4.836556	3.140662	1.922285
C	1.153636	-0.120652	2.501414	H	-6.119457	5.236168	1.501684
C	1.972819	2.022867	2.128170	H	-5.942339	5.039865	-0.238744
C	0.781554	0.204950	3.794157	H	-6.942953	3.915418	0.680118
C	1.616263	2.401017	3.416948	H	-0.078690	0.470452	-2.449330
C	1.023090	1.483428	4.266196	Si	-2.033476	-2.715768	0.725179
F	0.798874	-1.367945	2.105987	C	-3.509391	-3.570491	-0.044024
F	2.490234	2.996953	1.371020	H	-3.443197	-3.589402	-1.134814
F	0.156679	-0.690549	4.566845	H	-4.418792	-3.011826	0.201545
F	1.818308	3.648614	3.834808	C	-2.314835	-2.512864	2.562759
F	0.665336	1.828980	5.499030	H	-1.477569	-1.995927	3.039835
C	2.235172	-1.765559	-1.445539	H	-2.219532	-3.549779	2.914267
C	3.065848	-2.096146	0.715357	C	-0.387872	-3.556577	0.419236
C	2.411316	-3.103987	-1.756947	H	-0.457040	-4.173689	-0.481823
C	3.256101	-3.444855	0.449479	H	0.352584	-2.778413	0.209469
C	2.913836	-3.957174	-0.790468	C	-3.612793	-5.009418	0.495178
F	1.717298	-0.997120	-2.423509	H	-3.752067	-5.022208	1.579259
F	3.408064	-1.682485	1.938916	H	-4.459567	-5.534289	0.051128
F	2.052958	-3.582970	-2.952144	H	-2.712252	-5.586053	0.268172
F	3.723755	-4.268199	1.387812	C	-3.443995	3.996919	-2.318479
F	3.047182	-5.258196	-1.039610	H	-2.492234	3.467819	-2.229157
H	1.065276	0.516074	-0.557434	H	-3.479357	4.451161	-3.310562
Si	-2.052622	-0.876656	-1.903176	H	-3.440933	4.808260	-1.584800
C	-1.132650	-2.376701	-2.555589	C	-5.754371	-0.082202	0.819349
C	-3.877013	-0.895749	-2.327730	H	-6.551437	-0.829314	0.844961
C	-1.150145	0.676869	-2.400339	H	-4.815991	-0.600378	0.598175
H	-0.219195	-2.487367	-1.966993	H	-5.668036	0.334164	1.827444
H	-1.701799	-3.302164	-2.427136	C	-4.200548	-1.586757	-3.661303
H	-4.429718	-1.373958	-1.514081	H	-3.845134	-2.620510	-3.676826
H	-4.216368	0.141468	-2.352916	H	-5.277169	-1.604532	-3.840139
H	-1.291046	1.468655	-1.665124	H	-3.737105	-1.066546	-4.502818
C	-0.720556	-2.221585	-4.032569	C	-1.653777	1.175768	-3.769743
H	-1.581011	-2.100175	-4.693926	H	-2.710795	1.452582	-3.735258
H	-0.058320	-1.364362	-4.160812	H	-1.090090	2.061523	-4.068501
H	-0.168531	-3.104302	-4.356775	H	-1.528662	0.429634	-4.557732
C	-4.625622	3.044139	-2.089431	C	0.106713	-4.406703	1.603150
H	-5.574383	3.579689	-2.212903	H	-0.610837	-5.182767	1.883488
H	-4.635944	2.261380	-2.854913	H	1.042716	-4.905451	1.344198
C	-6.030434	1.012720	-0.220644	H	0.298915	-3.785114	2.479379
H	-6.952161	1.545871	0.036117	C	-3.660658	-1.952963	3.035973
H	-6.214391	0.554738	-1.197620	H	-3.769143	-2.074757	4.114811
C	-4.787045	3.601526	0.928830	H	-3.755896	-0.889098	2.819106

H	-4.502946	-2.460983	2.558734	C	0.461425	-2.810065	-2.586040
				C	1.705761	-4.053391	-0.977228
A-TS2				C	0.889915	-4.030772	-2.093893
C	-1.160784	1.312142	1.262778	F	0.327790	-0.503705	-2.428033
C	-0.849531	0.140781	0.363000	F	2.892805	-2.989463	0.684915
H	-2.023549	0.977855	1.852468	F	-0.323825	-2.766044	-3.663618
H	-0.784148	0.300330	-0.702757	F	2.116545	-5.221339	-0.489254
H	-0.463327	-0.774235	0.782908	F	0.519120	-5.161132	-2.683391
Si	-2.502343	3.714679	0.778777	H	0.894038	0.368067	0.162065
O	-1.507880	2.401789	0.453284	Si	-3.429492	-0.472750	-1.327555
O	-2.617600	-0.654745	0.203216	C	-3.114221	-2.081192	-2.247262
C	-0.046996	1.651581	2.279169	C	-5.256597	-0.171648	-0.988630
H	-0.536699	2.088461	3.153876	C	-2.673971	0.971812	-2.249508
H	0.404904	0.717288	2.618564	H	-2.078947	-2.365905	-2.030299
C	1.022340	2.621248	1.784810	H	-3.737806	-2.888313	-1.846053
H	0.587115	3.594458	1.556341	H	-5.526543	-0.589167	-0.016136
H	1.773894	2.758602	2.565438	H	-5.421055	0.906431	-0.903245
H	1.529099	2.269303	0.887850	H	-2.383308	1.748633	-1.537793
B	1.993511	-0.162041	-0.124683	C	-3.283741	-1.989077	-3.772286
C	2.639948	0.797791	-1.255789	H	-4.306538	-1.731466	-4.056051
C	2.759873	-0.215989	1.308106	H	-2.613477	-1.235592	-4.191823
C	1.640725	-1.613157	-0.793911	H	-3.034296	-2.939671	-4.245953
C	1.962380	1.855895	-1.838312	C	-1.998494	5.001962	-0.476575
C	3.905883	0.543452	-1.763097	H	-2.609812	5.899500	-0.329448
C	2.511245	2.651465	-2.832705	H	-2.265086	4.616832	-1.467824
C	4.492915	1.306884	-2.756291	C	-4.296066	3.214382	0.520042
C	3.786884	2.374534	-3.291398	H	-4.923447	4.106447	0.626963
F	0.706517	2.155235	-1.458409	H	-4.411506	2.893780	-0.522273
F	4.610301	-0.480965	-1.267171	C	-2.272469	4.278813	2.557740
F	1.823042	3.669509	-3.349855	C	-3.197569	5.453233	2.914563
F	5.716166	1.034624	-3.203981	H	-1.227261	4.560896	2.721379
F	4.331654	3.123058	-4.245337	H	-2.468578	3.438437	3.234384
C	2.196997	-0.955780	2.339524	H	-3.041616	5.789298	3.941195
C	3.896681	0.493408	1.673098	H	-3.021657	6.310486	2.259395
C	2.696757	-1.034262	3.622758	H	-4.250139	5.174380	2.816688
C	4.445965	0.444261	2.950072	H	-1.745947	0.649084	-2.732655
C	3.846575	-0.323784	3.930825	Si	-2.693649	-2.050384	1.233186
F	1.046215	-1.634672	2.108706	C	-4.457560	-2.684653	1.276942
F	4.520847	1.299983	0.809552	H	-4.837797	-2.861756	0.265874
F	2.081056	-1.758221	4.556726	H	-5.108755	-1.928022	1.726290
F	5.539410	1.143691	3.240691	C	-2.180926	-1.543254	2.965988
F	4.355878	-0.371317	5.156467	H	-1.216660	-1.025955	2.953868
C	0.828062	-1.650586	-1.924217	H	-1.974516	-2.481669	3.494954
C	2.077704	-2.862970	-0.365125	C	-1.510019	-3.333680	0.528037

H	-2.063645	-3.952977	-0.187343	H	1.843738	0.384677	-2.025807
H	-0.753716	-2.808493	-0.063781	H	1.482584	-1.315352	-1.829518
C	-4.526711	-3.987686	2.093096	H	3.971174	-0.944961	-1.655311
H	-4.157106	-3.843447	3.112372	H	3.723708	0.198798	-0.338231
H	-5.551630	-4.354701	2.165636	H	3.352844	-1.506879	-0.104036
H	-3.926272	-4.775886	1.632341	C	1.337794	1.499399	1.026980
C	-0.503572	5.350884	-0.441582	H	0.589526	1.798465	1.770544
H	0.100001	4.464386	-0.644691	C	0.621470	-1.477634	1.316566
H	-0.252979	6.105197	-1.189674	H	-0.235817	-1.329899	1.983620
H	-0.209537	5.746856	0.534932	H	1.504728	-1.447495	1.964787
C	-4.775377	2.112829	1.475711	C	-2.960773	-1.588148	-0.422098
H	-5.834781	1.882246	1.339620	H	-2.741420	-1.950397	0.587382
H	-4.219201	1.185020	1.308234	H	-2.134131	-1.876569	-1.072245
H	-4.636173	2.405310	2.520938	H	2.230675	1.230218	1.602279
C	-6.177439	-0.750715	-2.075167	H	-3.021355	2.474059	0.595102
H	-6.039795	-1.829843	-2.183214	H	-3.863588	-2.091924	-0.771565
H	-7.227339	-0.573923	-1.834566	C	1.653937	2.668782	0.082569
H	-5.984120	-0.295799	-3.049616	H	1.926747	3.573819	0.629719
C	-3.627847	1.558229	-3.305780	H	2.488097	2.420031	-0.578828
H	-4.552810	1.927443	-2.854404	H	0.798636	2.907917	-0.554893
H	-3.158098	2.396758	-3.822933	C	0.523156	-2.848644	0.631628
H	-3.903666	0.821534	-4.064118	H	1.411262	-3.051792	0.027591
C	-0.803409	-4.227320	1.561297	H	0.428182	-3.657945	1.358937
H	-1.515695	-4.783669	2.176093	H	-0.341554	-2.898915	-0.033415
H	-0.160045	-4.956128	1.063067				
H	-0.172529	-3.637922	2.228328	B-int0			
C	-3.226718	-0.741819	3.754566	C	-0.479282	2.169666	-0.504653
H	-2.854466	-0.479222	4.746526	C	-0.552245	0.712760	-0.076642
H	-3.505739	0.186730	3.250163	H	0.495577	2.562020	-0.205632
H	-4.143983	-1.319963	3.891588	H	-0.526502	2.198460	-1.598686
				C	0.590822	-0.116037	-0.646093
A-int4				H	-0.486778	0.662367	1.022059
C	-3.130750	-0.073537	-0.433540	H	0.443883	-1.165015	-0.355680
C	-1.929157	0.656924	0.154707	H	0.553376	-0.057176	-1.742191
H	-4.020535	0.216321	0.134389	O	-1.768406	0.146669	-0.537682
H	-3.272101	0.279557	-1.460377	O	1.814844	0.383530	-0.150744
C	-2.101449	2.168233	0.091197	Si	-2.812677	-0.727269	0.428850
H	-1.823205	0.349428	1.207739	Si	3.279243	-0.380685	-0.407097
H	-1.262306	2.680685	0.564846	C	-4.256700	-1.128531	-0.687869
H	-2.151791	2.482474	-0.953980	C	-4.881077	0.127971	-1.312981
O	-0.768424	0.273875	-0.573231	H	-5.008320	-1.686634	-0.118916
Si	0.722398	-0.028851	0.116595	H	-3.905153	-1.802991	-1.475520
C	1.869239	-0.436912	-1.303425	H	-5.699044	-0.122440	-1.991637
C	3.308152	-0.687030	-0.827119	H	-5.283982	0.793758	-0.545197

H	-4.131958	0.687941	-1.876681	H	5.087850	-0.053017	2.550429
C	-1.956638	-2.273064	1.056673	C	3.293410	-2.885742	0.329743
H	-1.071056	-2.023904	1.648926	H	3.642747	-3.689484	-0.321643
H	-1.639164	-2.910878	0.227965	H	2.417384	-2.436836	-0.144912
C	-3.355970	0.316141	1.889932	C	6.360079	-2.392338	0.515732
H	-2.511915	0.590768	2.528249	H	6.465443	-2.866322	-0.465267
H	-4.067508	-0.238465	2.508270	H	6.457649	-3.197453	1.253085
C	3.637229	-0.473083	-2.243228	C	3.542755	4.824408	0.188849
H	3.655437	0.524678	-2.688192	H	2.475371	5.054197	0.282681
H	2.884556	-1.064088	-2.771654	C	3.081406	2.692004	2.379148
C	4.532782	0.677935	0.487654	H	3.315889	1.679235	2.713731
C	4.248896	0.801923	1.991650	H	1.995826	2.809031	2.380892
H	4.532954	1.669229	0.022475	C	5.666585	2.650912	0.724660
H	5.532838	0.262370	0.321678	H	6.201292	3.065612	-0.133081
H	4.967667	1.459460	2.484895	H	5.817671	1.568532	0.722306
H	3.249068	1.206102	2.163229	C	4.275246	-2.099629	-2.846253
H	4.301849	-0.172052	2.484805	H	3.259091	-2.472482	-2.691612
C	3.210357	-2.109430	0.317836	H	4.922834	-2.549150	-2.091711
H	2.529034	-2.758054	-0.238698	H	2.958929	-3.338239	1.267611
H	2.876654	-2.086076	1.358273	H	4.055972	5.491684	0.890232
C	-1.610823	3.001009	0.090959	H	6.122794	3.066034	1.627695
H	-1.589909	2.962372	1.184152	H	4.617651	-2.449977	-3.821064
H	-2.579215	2.621686	-0.241995	B	-2.244197	-0.372627	0.089635
H	-2.623757	-2.858469	1.695144	C	-2.225023	-1.021808	-1.380482
H	-3.839968	1.239806	1.564473	C	-1.855897	-1.339898	1.308443
H	4.608754	-0.940315	-2.425209	C	-3.372172	0.734357	0.367723
H	4.199180	-2.575740	0.293556	C	-1.065213	-1.596280	-1.883810
H	-1.534129	4.047477	-0.208832	C	-3.321435	-1.062375	-2.231096
				C	-0.960466	-2.152847	-3.142379
				C	-3.267159	-1.624068	-3.500316
B-int1				C	-2.080855	-2.169071	-3.959291
C	4.311721	-0.576900	-2.773766	F	0.051385	-1.591509	-1.128771
C	3.766198	-0.014090	-1.463560	F	-4.500428	-0.563060	-1.852799
H	3.716483	-0.164425	-3.595693	F	0.192117	-2.658147	-3.575239
H	5.336762	-0.213570	-2.901717	F	-4.343837	-1.642830	-4.277654
C	3.683905	1.505577	-1.551232	F	-2.013207	-2.700248	-5.171854
H	2.758650	-0.420117	-1.294014	C	-1.445621	-0.784836	2.513763
H	4.705953	1.889165	-1.657352	C	-1.848688	-2.726699	1.257445
H	3.123436	1.795327	-2.445722	C	-1.021353	-1.528011	3.597417
O	4.594158	-0.330182	-0.363840	C	-1.443600	-3.513905	2.327402
O	3.043951	2.067092	-0.417679	C	-1.025050	-2.911493	3.500877
Si	4.651455	-1.636851	0.684003	F	-1.406341	0.553115	2.636712
Si	3.837576	3.044978	0.708852	F	-2.241325	-3.376134	0.157796
C	4.489209	-0.959497	2.424936	F	-0.599137	-0.937090	4.710991
H	3.453667	-0.723195	2.679512				

F	-1.454781	-4.839306	2.234738	H	5.191861	-0.197931	-2.918604
F	-0.627912	-3.651518	4.526968	C	3.424817	1.435133	-1.634138
C	-3.416387	1.881303	-0.412609	H	2.656367	-0.554033	-1.273914
C	-4.337525	0.648047	1.360203	H	4.415150	1.896464	-1.677875
C	-4.329097	2.901665	-0.226593	H	2.912729	1.652224	-2.571272
C	-5.282440	1.641847	1.573467	O	4.485031	-0.268619	-0.368041
C	-5.276089	2.774642	0.777873	O	2.663285	2.033110	-0.566488
F	-2.514433	2.039298	-1.400632	Si	4.689146	-1.534865	0.720773
F	-4.399870	-0.419844	2.160415	Si	3.449841	3.120668	0.527524
F	-4.303932	3.991680	-0.987744	C	4.546913	-0.791952	2.438987
F	-6.191088	1.517609	2.534602	H	3.508440	-0.651169	2.746558
F	-6.168081	3.735458	0.977034	H	5.054170	0.175455	2.495294
H	-1.160864	0.444307	0.060135	C	3.411827	-2.886563	0.471399
Si	0.248329	1.207957	-0.043097	H	3.763777	-3.662425	-0.211213
C	0.411120	1.300310	-1.910741	H	2.463107	-2.508482	0.081702
C	1.253410	0.092756	1.065774	C	6.444465	-2.164263	0.517499
C	-0.207581	2.854303	0.702889	H	6.565700	-2.651789	-0.454742
H	1.210953	0.646144	-2.261834	H	6.614139	-2.944014	1.269258
H	-0.514417	0.903803	-2.336584	C	3.169460	4.852469	-0.132251
H	2.313899	0.225822	0.855984	H	2.116758	5.137103	-0.048956
H	1.072267	0.374409	2.106843	C	2.737801	2.857449	2.229234
H	0.982489	-0.955838	0.937607	H	3.043187	1.889124	2.632792
H	0.623393	3.553623	0.575071	H	1.651216	2.928113	2.280621
H	-1.075782	3.279616	0.195653	C	5.281574	2.752978	0.566009
H	-0.431440	2.758455	1.766176	H	5.824508	3.166998	-0.286448
C	0.600640	2.743719	-2.404065	H	5.465059	1.677346	0.596038
H	1.445475	3.231181	-1.912715	C	4.281219	-2.158503	-2.770294
H	0.771178	2.763656	-3.482626	H	3.297949	-2.599932	-2.585119
H	-0.293656	3.336841	-2.203635	H	4.970604	-2.522408	-2.007346
C	4.010956	5.105616	-1.247204	H	3.199644	-3.361804	1.433387
H	3.505158	4.451019	-1.962765	H	3.717964	5.542440	0.519960
H	3.806801	6.135701	-1.545235	H	5.700961	3.203440	1.470565
H	5.086233	4.941560	-1.354813	H	4.638678	-2.523047	-3.734315
H	3.487678	3.389303	3.117531	B	-2.034675	-0.316358	0.120036
H	4.848743	-1.696134	3.149523	C	-2.112224	-1.182209	-1.245409
C	7.472641	-1.352067	0.715956	C	-1.697266	-1.171099	1.448112
H	8.464885	-1.793383	0.603314	C	-3.206139	0.783252	0.291747
H	7.379410	-0.542697	-0.012123	C	-0.986970	-1.826655	-1.741252
H	7.423349	-0.905951	1.713000	C	-3.260907	-1.352253	-2.006149
				C	-0.960039	-2.559113	-2.911280
				C	-3.286698	-2.089195	-3.183593
B-TS1				C	-2.130000	-2.693612	-3.641487
C	4.200104	-0.636249	-2.763684	F	0.182322	-1.727789	-1.072156
C	3.622561	-0.068670	-1.467494	F	-4.422809	-0.811319	-1.627894
H	3.565909	-0.309238	-3.594744				

F	0.168436	-3.123961	-3.340824	H	3.147468	3.630233	2.887151
F	-4.414544	-2.219493	-3.874845	H	5.020129	-1.453038	3.171180
F	-2.138113	-3.392623	-4.769765	C	7.483621	-1.043872	0.675090
C	-1.304507	-0.504081	2.600922	H	8.501993	-1.417412	0.551871
C	-1.731199	-2.554042	1.553631	H	7.322074	-0.258075	-0.067065
C	-0.930482	-1.133173	3.770919	H	7.420950	-0.581858	1.664043
C	-1.376395	-3.231215	2.714624				
C	-0.969440	-2.518214	3.827205	B-int2			
F	-1.240832	0.840823	2.590470	C	4.224045	-0.638811	-2.727516
F	-2.120845	-3.317483	0.526366	C	3.640955	-0.094935	-1.422060
F	-0.520642	-0.432965	4.826396	H	3.618833	-0.260108	-3.558058
F	-1.427788	-4.559316	2.765780	H	5.234628	-0.234682	-2.849247
F	-0.618965	-3.151670	4.940262	C	3.469649	1.413635	-1.566020
C	-3.329526	1.806459	-0.637286	H	2.665455	-0.571718	-1.255911
C	-4.141691	0.805381	1.316255	H	4.459796	1.871479	-1.566252
C	-4.279227	2.807900	-0.566102	H	2.973288	1.664514	-2.500740
C	-5.120387	1.784042	1.423816	O	4.482816	-0.323266	-0.315205
C	-5.188358	2.792680	0.479634	O	2.691468	2.014194	-0.489069
F	-2.477194	1.852914	-1.682176	Si	4.685899	-1.641161	0.718096
F	-4.150974	-0.140377	2.261776	Si	3.514724	3.082710	0.647546
F	-4.325975	3.774915	-1.479903	C	4.584673	-0.951660	2.460401
F	-5.995011	1.760339	2.425282	H	3.553776	-0.813453	2.793990
F	-6.115655	3.738384	0.572558	H	5.101401	0.009167	2.537876
H	-0.982189	0.431733	-0.030407	C	3.375494	-2.949919	0.434415
Si	0.574271	1.237664	-0.276999	H	3.701605	-3.714513	-0.272958
C	0.430945	1.048939	-2.144960	H	2.436450	-2.532396	0.061492
C	1.335968	0.100200	1.000178	C	6.428380	-2.282082	0.456413
C	-0.146470	2.857033	0.314200	H	6.520727	-2.754462	-0.526111
H	1.173509	0.359145	-2.549079	H	6.612866	-3.075004	1.190355
H	-0.537467	0.589981	-2.345640	C	3.286295	4.814571	-0.019739
H	2.418271	0.095551	0.907756	H	2.241386	5.127083	0.049844
H	1.081969	0.488649	1.989568	C	2.780796	2.792271	2.331571
H	0.952638	-0.916312	0.928348	H	3.033911	1.793418	2.694721
H	0.562824	3.682449	0.259730	H	1.700706	2.922615	2.393024
H	-0.994864	3.112771	-0.322771	C	5.324149	2.633594	0.676154
H	-0.511035	2.762231	1.338064	H	5.890017	3.044056	-0.162609
C	0.468579	2.416421	-2.848800	H	5.460555	1.550757	0.684120
H	1.275205	3.057206	-2.483782	C	4.243255	-2.162498	-2.788886
H	0.592988	2.294580	-3.927031	H	3.240554	-2.568527	-2.630636
H	-0.469322	2.949136	-2.687792	H	4.908256	-2.585417	-2.035260
C	3.644094	5.019374	-1.584367	H	3.150861	-3.447654	1.381883
H	3.112426	4.339289	-2.254980	H	3.843648	5.486480	0.643867
H	3.474295	6.034483	-1.946916	H	5.755032	3.045843	1.593666
H	4.712650	4.812099	-1.683433	H	4.595608	-2.503342	-3.763181

B	-2.010291	-0.253503	0.102977	H	0.619682	3.769149	0.369306
C	-2.094026	-1.135272	-1.263215	H	-0.870033	3.092462	-0.275915
C	-1.761127	-1.143587	1.437576	H	-0.396903	2.713513	1.376628
C	-3.204590	0.837876	0.244351	C	0.540455	2.474026	-2.835053
C	-0.962510	-1.749127	-1.781290	H	1.399322	3.094725	-2.563094
C	-3.253429	-1.355369	-1.995124	H	0.557958	2.333167	-3.917471
C	-0.939639	-2.496511	-2.942876	H	-0.358248	3.043153	-2.595721
C	-3.284517	-2.106696	-3.163075	C	3.789338	4.975496	-1.463128
C	-2.119977	-2.678396	-3.643930	H	3.248578	4.318909	-2.149319
F	0.222497	-1.619188	-1.139990	H	3.653463	5.998189	-1.817597
F	-4.425037	-0.854696	-1.589654	H	4.853094	4.740348	-1.546485
F	0.198113	-3.031480	-3.392167	H	3.237508	3.514411	3.015883
F	-4.424413	-2.284573	-3.825223	H	5.066798	-1.638797	3.161914
F	-2.131874	-3.392598	-4.764359	C	7.478746	-1.170628	0.604269
C	-1.368613	-0.504341	2.606137	H	8.491029	-1.547999	0.448056
C	-1.860475	-2.523719	1.534385	H	7.302522	-0.372337	-0.121027
C	-1.058584	-1.157463	3.782537	H	7.445889	-0.723964	1.601730
C	-1.567668	-3.224953	2.698699				
C	-1.161363	-2.539337	3.828143	B-int3			
F	-1.242789	0.837926	2.612500	C	2.171774	-1.523423	0.284188
F	-2.254531	-3.265295	0.491346	C	1.538093	-0.172995	0.005435
F	-0.650995	-0.482758	4.857533	H	2.524580	-1.536452	1.323974
F	-1.675039	-4.551332	2.736351	H	1.018576	-0.152933	-0.944387
F	-0.870119	-3.196064	4.946728	H	0.820824	0.108576	0.775747
C	-3.278863	1.882529	-0.664857	Si	4.590021	-2.669247	-0.227402
C	-4.193012	0.843261	1.218178	O	3.275411	-1.681380	-0.593311
C	-4.228188	2.886838	-0.621837	O	2.563835	0.895722	-0.053437
C	-5.170911	1.825423	1.299593	C	1.114739	-2.622435	0.105042
C	-5.188230	2.855297	0.375896	H	1.491141	-3.537083	0.567734
F	-2.374131	1.954783	-1.666200	H	0.221581	-2.333533	0.668676
F	-4.256201	-0.125336	2.139796	C	0.750088	-2.897274	-1.352879
F	-4.224953	3.874464	-1.516953	H	0.283458	-2.035971	-1.835250
F	-6.094497	1.786137	2.257032	H	1.634374	-3.182424	-1.928220
F	-6.115203	3.805658	0.444804	H	0.031126	-3.716238	-1.405151
H	-0.981628	0.445905	-0.005277	B	-1.941432	-0.181384	-0.066911
Si	0.833772	1.343968	-0.267032	C	-3.111023	-0.443833	-1.165648
C	0.520709	1.117680	-2.106824	C	-2.034691	-1.049902	1.314469
C	1.353819	0.089135	1.018226	C	-1.873781	1.437296	0.183155
C	-0.014980	2.882705	0.368663	C	-2.809348	-0.637418	-2.505030
H	1.201240	0.397740	-2.565516	C	-4.463722	-0.426677	-0.857612
H	-0.475589	0.690654	-2.213713	C	-3.776999	-0.817218	-3.483641
H	2.437853	-0.005210	1.026221	C	-5.462846	-0.605879	-1.798419
H	1.036209	0.456960	1.996906	C	-5.112836	-0.801023	-3.125530
H	0.899748	-0.887293	0.864449	F	-1.530921	-0.662476	-2.928935

F	-4.845268	-0.247037	0.413243	H	1.238112	0.518425	-2.992441
F	-3.435166	-1.003385	-4.759908	H	5.547452	1.904287	-1.240147
F	-6.749076	-0.592618	-1.451151	Si	2.805613	1.823876	1.457474
F	-6.056555	-0.971667	-4.048701	C	4.508841	2.578491	1.319907
C	-1.293700	-0.708022	2.438253	H	4.580714	3.257756	0.467404
C	-2.693391	-2.269233	1.426642	H	5.239054	1.780521	1.150892
C	-1.190749	-1.481007	3.581131	C	2.753716	0.615967	2.868104
C	-2.633174	-3.075745	2.556109	H	1.804722	0.082794	2.947816
C	-1.873986	-2.682741	3.644007	H	3.578982	-0.098224	2.830383
F	-0.562862	0.438229	2.453678	H	2.861093	1.194930	3.791043
F	-3.413090	-2.753941	0.408173	C	1.416655	3.047663	1.527199
F	-0.426671	-1.088155	4.604121	H	1.545130	3.695045	2.399590
F	-3.286519	-4.234605	2.597249	H	1.374181	3.680628	0.637812
F	-1.793101	-3.449831	4.727989	H	0.457137	2.534163	1.640584
C	-1.116845	2.261025	-0.635848	C	4.860635	3.340338	2.612290
C	-2.600992	2.106639	1.162638	H	4.874157	2.675479	3.478339
C	-1.086434	3.641723	-0.525550	H	5.848164	3.796504	2.534974
C	-2.591904	3.485557	1.316849	H	4.145303	4.140931	2.814315
C	-1.827429	4.262527	0.461869	H	4.909783	-5.075400	0.190124
F	-0.309823	1.733718	-1.587205	C	4.866618	-3.022518	-3.030448
F	-3.341197	1.420754	2.036687	H	4.030196	-2.337282	-3.187277
F	-0.289065	4.376887	-1.313042	H	5.498484	-2.993171	-3.920471
F	-3.300602	4.071842	2.278310	H	4.449924	-4.030237	-2.956644
F	-1.784562	5.584694	0.603244	C	5.582531	0.723325	-3.055360
H	-0.916548	-0.526063	-0.585660	H	6.664556	0.580720	-3.030569
Si	3.190817	1.336592	-1.688788	H	5.135657	-0.183809	-3.467877
C	2.757891	3.132816	-1.906439	H	5.378992	1.540469	-3.753056
C	5.034900	1.030310	-1.650286	H	3.142894	3.451372	-2.881052
C	2.306843	0.296991	-2.944752				
H	1.674903	3.270109	-1.924147	B-TS2			
H	3.184418	3.802313	-1.157879	C	1.504383	-0.935584	1.529571
H	5.235376	0.194523	-0.974782	C	1.089437	-0.024063	0.403344
H	2.445442	-0.769001	-2.758743	H	2.181314	-0.327319	2.139783
H	2.734403	0.535536	-3.923975	H	1.036241	-0.413790	-0.598679
C	5.653538	-2.652456	-1.764107	H	0.652790	0.939281	0.621670
H	6.472183	-3.364835	-1.611488	Si	3.412237	-2.886994	1.758271
H	6.129546	-1.674648	-1.883802	O	2.210479	-2.013705	0.971698
C	5.481008	-1.950481	1.259705	O	2.803145	0.779782	0.036237
H	4.895219	-2.063701	2.176036	C	0.378511	-1.399762	2.472664
H	6.430646	-2.468197	1.420584	H	0.874497	-1.706635	3.399705
H	5.703548	-0.888079	1.124477	H	-0.239188	-0.536714	2.731043
C	4.037613	-4.415899	0.156478	C	-0.475951	-2.556718	1.964460
H	3.357215	-4.801622	-0.606865	H	-1.084990	-2.280857	1.105278
H	3.536688	-4.489703	1.124638	H	0.152388	-3.399150	1.672845

H	-1.149390	-2.887084	2.757942	H	3.485770	-1.701655	-2.843151
B	-1.753592	0.000992	-0.099464	C	4.349338	-3.694840	0.356639
C	-2.270346	-1.119869	-1.145481	H	5.246602	-4.186919	0.746909
C	-2.533721	0.112854	1.318645	H	4.700989	-2.912576	-0.323856
C	-1.564761	1.417999	-0.894819	C	4.430862	-1.673064	2.767029
C	-1.472024	-2.131385	-1.652904	H	3.909550	-1.381875	3.683872
C	-3.555049	-1.050749	-1.666270	H	5.383297	-2.119099	3.064659
C	-1.914581	-3.042330	-2.601044	H	4.649981	-0.762412	2.201786
C	-4.041048	-1.937630	-2.609513	C	2.683079	-4.192699	2.882740
C	-3.209089	-2.944052	-3.078689	H	2.030776	-4.873582	2.331465
F	-0.194814	-2.269776	-1.244868	H	2.101184	-3.760444	3.700199
F	-4.377025	-0.085747	-1.237392	H	1.884921	-1.027594	-2.571658
F	-1.107811	-3.999693	-3.057463	H	5.928698	0.755666	-0.549820
F	-5.283809	-1.839671	-3.074356	Si	2.911491	2.336505	0.774350
F	-3.653252	-3.806277	-3.987494	C	4.697192	2.903264	0.720977
C	-2.086851	1.040859	2.251129	H	5.065852	2.942720	-0.307576
C	-3.564306	-0.701434	1.765640	H	5.309251	2.158305	1.241536
C	-2.609293	1.193821	3.518999	C	2.375706	2.185575	2.558333
C	-4.128243	-0.585076	3.031395	H	1.345113	1.842727	2.677595
C	-3.651979	0.368260	3.911938	H	3.037726	1.537175	3.138423
F	-1.038683	1.838606	1.933660	H	2.422314	3.182774	3.006483
F	-4.058891	-1.676906	0.996734	C	1.750603	3.477579	-0.139710
F	-2.115169	2.097244	4.364127	H	1.858091	4.499759	0.233832
F	-5.116251	-1.392333	3.407671	H	1.942808	3.490259	-1.215431
F	-4.175652	0.484544	5.127192	H	0.706494	3.187568	0.019163
C	-0.672278	1.498482	-1.958216	C	4.877842	4.279830	1.384346
C	-2.254975	2.599110	-0.638216	H	4.574240	4.262527	2.433311
C	-0.437653	2.645848	-2.694933	H	5.921812	4.595069	1.352406
C	-2.049494	3.775017	-1.348602	H	4.288446	5.048121	0.878698
C	-1.128016	3.802512	-2.380453	H	3.485280	-4.789200	3.327741
F	0.041873	0.411102	-2.320630	C	3.481505	-4.706485	-0.412033
F	-3.175773	2.662219	0.326223	H	2.538603	-4.259504	-0.738713
F	0.470153	2.660090	-3.674019	H	3.996350	-5.081810	-1.298389
F	-2.731313	4.875748	-1.047814	H	3.236660	-5.567196	0.214204
F	-0.903885	4.922415	-3.057525	C	6.221116	-0.896820	-1.914613
H	-0.613982	-0.377359	0.255876	H	7.256446	-1.052806	-1.606970
Si	3.665258	0.215266	-1.360369	H	5.795410	-1.876350	-2.143495
C	3.630311	1.587448	-2.630395	H	6.239956	-0.320891	-2.843753
C	5.419220	-0.173682	-0.819182	H	4.168771	1.257727	-3.524093
C	2.825108	-1.281371	-2.078313				
H	2.601736	1.794964	-2.937720	B-int4			
H	4.087432	2.522430	-2.300168	C	2.726911	-0.110877	-0.563965
H	5.395392	-0.784253	0.088544	C	1.552783	-0.627807	0.258585
H	2.622924	-2.049619	-1.332395	H	3.656948	-0.411320	-0.070827

H	2.698448	-0.610392	-1.537814	H	-7.043611	2.030003	1.869583
C	1.605376	-2.134750	0.460308	H	-7.615097	2.435230	0.251761
H	1.580472	-0.131620	1.242876	C	-4.221194	1.693795	1.142061
H	0.756353	-2.472431	1.057863	H	-3.160070	1.833194	0.926696
H	1.561342	-2.632384	-0.511123	H	-4.299929	1.193511	2.111614
O	0.347452	-0.289394	-0.416761	C	-5.237777	1.703183	-1.773482
Si	-0.972406	0.398350	0.336008	H	-4.258043	2.050316	-2.107555
C	-2.299590	0.461071	-0.978959	H	-5.875191	2.583274	-1.649825
C	-2.649217	-0.923381	-1.543621	C	-5.144646	-4.300422	0.438996
H	-1.946100	1.115028	-1.783173	H	-4.796831	-4.866285	-0.427171
H	-3.192592	0.941710	-0.564480	H	-6.234512	-4.231411	0.380166
H	-3.388311	-0.857550	-2.344769	H	-4.664350	2.688429	1.245922
H	-1.758422	-1.411269	-1.944590	H	-5.666390	1.091901	-2.572667
H	-3.062559	-1.573414	-0.768273	H	-5.175419	-3.442986	-2.209559
C	-1.496344	-0.667890	1.789067	H	-4.896223	-4.877396	1.330549
H	-0.697331	-0.749594	2.531702	B	1.722815	0.160988	0.136561
H	-1.757036	-1.678999	1.466783	C	1.704301	1.677537	-0.384194
C	-0.536927	2.115382	0.950660	C	1.807718	-0.054326	1.723788
H	0.291570	2.090870	1.663862	C	2.466727	-0.909873	-0.796876
H	-1.391434	2.574906	1.455007	C	0.696683	2.542720	0.020895
C	2.687902	1.402274	-0.748825	C	2.653084	2.222406	-1.237325
H	2.695774	1.914289	0.218022	C	0.597444	3.855784	-0.395007
H	1.779839	1.694832	-1.278311	C	2.601116	3.540499	-1.670271
H	-2.368088	-0.239347	2.291101	C	1.567658	4.359078	-1.248668
H	-0.244494	2.765460	0.122502	F	-0.267041	2.085799	0.842652
H	2.527596	-2.429691	0.966386	F	3.679964	1.488624	-1.673910
H	3.546747	1.755027	-1.32227	F	-0.407832	4.628577	0.004183
				F	3.532896	4.023142	-2.484663
				F	1.502163	5.617412	-1.661078
B-int5				C	1.436920	-1.275127	2.272609
C	-4.510690	-2.912862	0.497916	C	2.210114	0.910810	2.637159
C	-4.967383	-1.983087	-0.622388	C	1.426902	-1.538587	3.627996
H	-3.419037	-2.991021	0.465173	C	2.230044	0.684737	4.007097
H	-4.757184	-2.429049	1.448903	C	1.833137	-0.543860	4.504496
C	-4.657442	-2.501622	-2.017969	F	1.033359	-2.264640	1.456213
H	-6.055077	-1.862832	-0.535469	F	2.610447	2.118752	2.230904
H	-4.982312	-1.777716	-2.768200	F	1.028039	-2.717956	4.094336
H	-3.583328	-2.662697	-2.140758	F	2.625123	1.638004	4.843915
O	-4.329591	-0.715711	-0.436851	F	1.838243	-0.769398	5.810856
Si	-5.143605	0.734281	-0.173936	C	2.046599	-1.083849	-2.108603
C	-6.885063	0.380160	0.445815	C	3.513520	-1.724920	-0.391054
C	-7.574290	1.638248	0.999094	C	2.590375	-2.014937	-2.972239
H	-6.842011	-0.388466	1.226292	C	4.101060	-2.661884	-1.229554
H	-7.489044	-0.039407	-0.365835	C	3.635050	-2.808931	-2.524994
H	-8.600247	1.428036	1.306513				

F	1.028493	-0.337227	-2.576773	C	-5.147800	1.638759	-1.791368
F	4.007030	-1.634802	0.846695	H	-4.286671	2.114668	-2.262511
F	2.120659	-2.159781	-4.207732	H	-5.900207	2.411756	-1.609644
F	5.103579	-3.420823	-0.801099	C	-5.056010	-4.132608	0.250731
F	4.181022	-3.707451	-3.332858	H	-4.678733	-4.739152	-0.574340
H	0.430898	-0.200649	-0.091396	H	-6.120050	-3.948651	0.076916
Si	-1.083066	-0.623466	-0.358244	H	-4.312363	2.871247	0.994503
C	-1.608005	0.745582	-1.528121	H	-5.573991	0.928206	-2.505581
C	-1.685934	-0.682010	1.403004	H	-4.948579	-3.260106	-2.350676
C	-0.836518	-2.300262	-1.141849	H	-4.965263	-4.722527	1.163022
H	-2.299416	1.413784	-1.010293	B	1.430351	0.100165	0.131025
H	-0.713798	1.337300	-1.744797	C	1.572466	1.647765	-0.320900
H	-2.775291	-0.722144	1.410591	C	1.595723	-0.165086	1.718794
H	-1.300055	-1.579464	1.892134	C	2.229693	-0.936201	-0.821148
H	-1.356275	0.195803	1.962209	C	0.613821	2.572468	0.067094
H	-1.688668	-2.951470	-0.938516	C	2.603701	2.164081	-1.092559
H	-0.702412	-2.230428	-2.222308	C	0.625857	3.905157	-0.292857
H	0.047978	-2.773365	-0.708454	C	2.667076	3.499717	-1.470595
C	-2.207361	0.247724	-2.849996	C	1.671734	4.374080	-1.072617
H	-3.112167	-0.335357	-2.676921	F	-0.420106	2.162264	0.831875
H	-2.467324	1.091108	-3.493484	F	3.609973	1.386518	-1.504839
H	-1.491709	-0.368719	-3.397175	F	-0.348003	4.729490	0.090398
				F	3.676372	3.946482	-2.212147
				F	1.715257	5.650954	-1.434295
B-TS3				C	1.271156	-1.414286	2.231519
C	-4.284789	-2.821063	0.382962	C	2.027526	0.758363	2.660387
C	-4.547663	-1.862940	-0.775350	C	1.331757	-1.743539	3.570909
H	-3.216097	-3.020056	0.478001	C	2.113304	0.470437	4.017505
H	-4.580923	-2.310249	1.304437	C	1.761349	-0.785193	4.476055
C	-4.297375	-2.402173	-2.173475	F	0.841667	-2.377136	1.392420
H	-5.609114	-1.602266	-0.732789	F	2.396270	1.993954	2.303262
H	-4.547790	-1.641306	-2.914284	F	0.975053	-2.953055	3.998660
H	-3.267630	-2.714526	-2.332021	F	2.532120	1.393250	4.879297
O	-3.796505	-0.628589	-0.552046	F	1.830426	-1.071974	5.770884
Si	-4.729546	0.791344	-0.180509	C	1.845429	-1.078478	-2.146440
C	-6.328854	0.277529	0.671186	C	3.306440	-1.723121	-0.436396
C	-7.003781	1.479112	1.356710	C	2.441954	-1.948633	-3.039663
H	-6.130868	-0.502869	1.414117	C	3.944859	-2.603174	-1.299464
H	-7.025523	-0.152872	-0.054593	C	3.509101	-2.718870	-2.608029
H	-7.965895	1.194338	1.785131	F	0.814608	-0.346854	-2.614735
H	-6.387510	1.877810	2.164363	F	3.792536	-1.659883	0.807699
H	-7.190502	2.292954	0.650769	F	2.002143	-2.054147	-4.292415
C	-3.807479	1.899603	1.007513	F	4.972835	-3.336705	-0.882271
H	-2.755875	2.080177	0.791299	F	4.106626	-3.561952	-3.442176
H	-3.876694	1.514633	2.027860				

H	0.195333	-0.175997	-0.094841	H	-6.595918	-3.610168	0.363210
Si	-1.572489	-0.527988	-0.396571	H	-4.311552	2.964375	1.208974
C	-1.643578	0.915673	-1.605119	H	-5.736706	1.113634	-2.321842
C	-1.771320	-0.563813	1.466313	H	-5.461301	-3.003195	-2.246804
C	-1.099036	-2.167230	-1.165512	H	-5.457922	-4.514706	1.362858
H	-2.242072	1.736783	-1.207773	B	1.471548	0.060723	0.085296
H	-0.630348	1.305891	-1.701378	C	1.631282	1.650575	-0.228861
H	-2.816175	-0.578098	1.769193	C	1.800562	-0.346699	1.624470
H	-1.307574	-1.489035	1.817366	C	2.250392	-0.879542	-0.993498
H	-1.264759	0.273032	1.947398	C	0.632296	2.542186	0.128706
H	-1.732235	-2.998121	-0.863105	C	2.719799	2.228541	-0.868852
H	-1.081510	-2.110578	-2.254892	C	0.658340	3.897207	-0.150098
H	-0.087900	-2.398372	-0.823506	C	2.799294	3.582638	-1.161253
C	-2.137449	0.506711	-2.999898	C	1.758304	4.423508	-0.804175
H	-3.122646	0.041364	-2.965148	F	-0.464468	2.097853	0.787753
H	-2.204796	1.383458	-3.648186	F	3.771306	1.482284	-1.223548
H	-1.443139	-0.189777	-3.471016	F	-0.360756	4.687938	0.197033
				F	3.864462	4.086168	-1.780709
				F	1.814902	5.722510	-1.085324
B-int6				C	1.361712	-1.575930	2.095261
C	-4.630139	-2.694069	0.539014	C	2.472652	0.429804	2.556632
C	-4.841520	-1.751585	-0.636591	C	1.535155	-2.015461	3.395083
H	-3.586399	-3.013617	0.578814	C	2.677880	0.028680	3.870116
H	-4.823293	-2.141233	1.462636	C	2.203906	-1.200423	4.293433
C	-4.618483	-2.350020	-2.013306	F	0.706417	-2.413329	1.261804
H	-5.869378	-1.387859	-0.601882	F	2.972948	1.625644	2.220118
H	-4.586978	-1.564725	-2.769707	F	1.061602	-3.198535	3.791001
H	-3.707042	-2.940093	-2.074875	F	3.326503	0.813463	4.728947
O	-4.007518	-0.537417	-0.439205	F	2.385893	-1.595466	5.551229
Si	-4.880783	0.961032	-0.004717	C	1.704816	-1.097975	-2.248793
C	-6.462809	0.468952	0.878575	C	3.455769	-1.529262	-0.761855
C	-7.061181	1.681334	1.617376	C	2.268739	-1.920449	-3.209784
H	-6.274649	-0.337294	1.594753	C	4.062813	-2.358024	-1.693461
H	-7.199233	0.091149	0.163101	C	3.462831	-2.558745	-2.925715
H	-8.020119	1.423454	2.068260	F	0.547411	-0.490124	-2.593996
H	-6.402794	2.028884	2.415074	F	4.104711	-1.361388	0.395773
H	-7.236083	2.521807	0.940347	F	1.676436	-2.101507	-4.392122
C	-3.845966	1.973763	1.164324	F	5.218220	-2.961408	-1.421578
H	-2.801590	2.121949	0.893038	F	4.030643	-3.354168	-3.828562
H	-3.876863	1.556078	2.173178	H	0.292523	-0.189662	-0.057648
C	-5.283362	1.809785	-1.610671	Si	-2.113217	-0.558645	-0.389047
H	-4.411160	2.262626	-2.083545	C	-1.835733	0.908355	-1.521394
H	-6.012071	2.602968	-1.418679	C	-1.881817	-0.566819	1.463960
C	-5.549284	-3.911980	0.459537	C	-1.501681	-2.142672	-1.154497
H	-5.298762	-4.548230	-0.390829				

H	-2.293217	1.820344	-1.132544	F	-4.471904	-1.803236	-3.856432
H	-0.762030	1.099423	-1.533229	F	-3.601670	-4.339828	-3.428053
H	-2.837826	-0.571762	1.990959	C	-0.770464	0.313307	2.306807
H	-1.343873	-1.480747	1.725428	C	-2.534998	-1.197068	2.065493
H	-1.285715	0.276915	1.810423	C	-0.750725	0.140845	3.678688
H	-1.929595	-3.046950	-0.722664	C	-2.562511	-1.398131	3.440360
H	-1.600009	-2.168971	-2.239519	C	-1.662514	-0.730059	4.252568
H	-0.433268	-2.158772	-0.915574	F	0.146895	1.168391	1.796247
C	-2.306033	0.626347	-2.957031	F	-3.431344	-1.884083	1.351268
H	-3.353411	0.316782	-3.000560	F	0.136737	0.784591	4.443274
H	-2.203872	1.521600	-3.573853	F	-3.443609	-2.232248	3.988659
H	-1.698764	-0.153240	-3.417722	F	-1.671031	-0.920899	5.569715
				H	-0.283515	-0.137820	-0.396507
B-int7				Si	5.120259	-1.202989	-0.039847
C	1.968396	-1.382376	1.292649	C	6.369377	-0.381548	1.080194
C	2.263469	-0.675631	-0.017406	C	4.743422	-2.877502	0.680358
H	2.305511	-2.418758	1.250408	C	5.638439	-1.351423	-1.829290
H	1.659629	0.232699	-0.060259	H	7.094059	0.236517	0.551532
O	3.696388	-0.136521	-0.056563	H	5.877668	0.236430	1.836357
C	2.503049	-0.681292	2.537436	H	3.995057	-3.461754	0.147309
H	3.597239	-0.670922	2.560841	H	5.690576	-3.425942	0.614658
H	2.150481	0.348822	2.595619	H	4.937935	-2.029281	-2.328510
B	-1.464559	-0.066542	-0.161607	H	5.540151	-0.389570	-2.340987
C	-1.917962	1.472880	-0.416998	H	4.475275	-2.829103	1.736859
C	-2.161967	-1.199933	-1.096420	Si	3.732207	1.612742	-0.522776
C	-1.630019	-0.349265	1.443169	C	5.518058	2.142618	-0.644644
C	-1.019613	2.472389	-0.737659	H	6.150498	1.516417	-1.275452
C	-3.221643	1.900094	-0.203242	H	5.991035	2.262788	0.330026
C	-1.366637	3.808386	-0.865573	C	2.899328	2.534539	0.848621
C	-3.621958	3.219226	-0.328153	H	1.835849	2.315162	0.936101
C	-2.681992	4.183434	-0.664528	H	3.387086	2.336902	1.806330
F	0.292124	2.189086	-0.930970	H	2.998456	3.604562	0.639172
F	-4.150214	1.003680	0.145252	C	2.912512	1.720291	-2.191474
F	-0.444520	4.728415	-1.173078	H	3.537872	1.204370	-2.929205
F	-4.886837	3.580769	-0.123476	H	1.942621	1.220177	-2.180051
F	-3.042359	5.458837	-0.784412	H	0.874768	-1.432541	1.325661
C	-1.747547	-2.516004	-0.933801	H	2.159475	-1.197544	3.435197
C	-3.086835	-1.008558	-2.111474	C	2.025321	-1.526783	-1.243855
C	-2.206505	-3.578732	-1.688159	H	2.236391	-0.983178	-2.165085
C	-3.582337	-2.044970	-2.894262	H	2.622141	-2.440573	-1.220246
C	-3.142111	-3.337868	-2.681487	H	0.973318	-1.817328	-1.242831
F	-0.826524	-2.806118	0.013302	C	2.702630	3.191351	-2.599646
F	-3.549036	0.213733	-2.407020	H	3.640211	3.752977	-2.622811
F	-1.758570	-4.818464	-1.480721	H	2.264918	3.249061	-3.596854

H	2.014170	3.689483	-1.915398	C	-2.899328	-1.382382	3.339545
H	5.489719	3.133860	-1.110158	C	-1.990792	-0.826473	4.225065
H	6.920557	-1.162476	1.610788	F	0.105020	1.002875	1.950526
C	7.076249	-1.879989	-1.969015	F	-3.688859	-1.707047	1.187154
H	7.195398	-2.854171	-1.488276	F	-0.080677	0.512999	4.573156
H	7.349039	-2.001294	-3.017895	F	-3.876751	-2.154606	3.805425
H	7.798856	-1.196638	-1.516643	F	-2.088934	-1.067449	5.528298
B-TS4				H	-0.305743	-0.224578	-0.275005
C	1.583135	-1.647603	1.151993	Si	5.029350	-1.434160	-0.099107
C	1.706737	-0.743613	0.001781	C	6.323026	-1.195779	1.232632
H	1.842911	-2.668303	0.870238	C	4.309760	-3.148132	0.111751
H	1.576477	0.313501	0.188055	C	5.764602	-1.265937	-1.816649
O	3.809547	-0.253496	0.060123	H	7.063010	-0.436530	0.976055
C	2.222084	-1.199490	2.462262	H	5.863417	-0.912007	2.183342
H	3.309771	-1.255175	2.404819	H	3.502468	-3.393466	-0.580682
H	1.942547	-0.174363	2.704593	H	5.121469	-3.857251	-0.079136
B	-1.497373	-0.027474	-0.132069	H	4.983124	-1.455445	-2.561762
C	-1.733233	1.550610	-0.414348	H	6.082723	-0.230387	-1.976842
C	-2.220442	-1.062978	-1.150395	H	3.967333	-3.330785	1.132507
C	-1.773320	-0.339824	1.443241	Si	3.987325	1.447619	-0.122291
C	-0.732490	2.397194	-0.851776	C	5.762008	1.934810	0.224492
C	-2.949616	2.161378	-0.141425	H	6.492732	1.453596	-0.428440
C	-0.900349	3.763424	-1.014857	H	6.041051	1.740190	1.262362
C	-3.170929	3.518646	-0.297526	C	2.902556	2.306725	1.129299
C	-2.132253	4.327202	-0.736426	H	1.839213	2.298623	0.885721
F	0.504719	1.914718	-1.132731	H	3.032521	1.882796	2.128144
F	-3.971126	1.413894	0.287599	H	3.209990	3.355846	1.178168
F	0.109468	4.535619	-1.425525	C	3.514450	1.871459	-1.880293
F	-4.355804	4.060305	-0.029394	H	4.288888	1.496578	-2.558972
F	-2.318934	5.634664	-0.886625	H	2.590715	1.350164	-2.144713
C	-1.862842	-2.402962	-1.087206	H	0.483185	-1.665084	1.270432
C	-3.156399	-0.759380	-2.128766	H	1.883415	-1.844102	3.274050
C	-2.375017	-3.389160	-1.908380	C	1.604220	-1.246502	-1.392318
C	-3.703679	-1.714928	-2.976114	H	1.211494	-0.481384	-2.058804
C	-3.311913	-3.036936	-2.866560	H	2.590387	-1.559352	-1.741990
F	-0.949187	-2.801063	-0.169449	H	0.953963	-2.124540	-1.403710
F	-3.584990	0.494884	-2.308774	C	3.311274	3.383192	-2.073640
F	-1.975844	-4.655997	-1.796994	H	4.211148	3.948794	-1.816496
F	-4.599189	-1.370141	-3.898014	H	3.062535	3.618301	-3.109628
F	-3.821836	-3.959807	-3.676072	H	2.490473	3.747068	-1.453493
C	-0.906232	0.211645	2.376667	H	5.845006	3.014021	0.062779
C	-2.778222	-1.134245	1.978196	H	6.854234	-2.137706	1.395181
C	-0.976835	-0.017223	3.739125	C	6.953177	-2.213148	-2.046802
				H	6.653560	-3.260051	-1.958719

H	7.380788	-2.080230	-3.041696	C	4.507310	-0.591840	-0.538666
H	7.749725	-2.033989	-1.320062	H	4.502997	-2.059015	1.031358
Butane				H	4.214281	0.914840	-2.043695
C	0.561711	0.517566	-0.000126	H	5.566333	-0.699550	-0.742517
C	-0.561713	-0.517562	-0.000131	O	-1.053097	-1.171500	-0.580233
H	0.451843	1.165161	0.876541	O	-0.357324	-0.906137	1.793430
H	-0.451833	-1.165272	0.876448	C	-2.861433	-2.734532	-0.256402
C	1.948766	-0.119888	0.000107	H	-3.217151	-3.520472	0.419049
H	2.086453	-0.749824	0.882741	H	-3.549626	-1.888302	-0.160564
H	2.086369	-0.750787	-0.881856	C	-2.837955	-3.235575	-1.696999
H	-0.452000	-1.165021	-0.876922	H	-2.183464	-4.105255	-1.795104
H	0.451994	1.165112	-0.876842	H	-3.835196	-3.523985	-2.032732
H	2.738531	0.633646	-0.000380	H	-2.460480	-2.453605	-2.356921
C	-1.948767	0.119887	0.000101	C-int1			
H	-2.738532	-0.633647	0.000356	C	-4.732860	-0.994567	2.677755
H	-2.086208	0.750358	0.882402	C	-3.512241	-0.070331	2.601100
H	-2.086602	0.750255	-0.882193	H	-4.398517	-2.041552	2.636067
C-int0				H	-3.774448	0.921249	2.990641
C	-1.494229	-2.278984	0.213623	H	-2.671705	-0.470246	3.168274
C	-1.473828	-1.781676	1.667746	Si	-4.552332	-0.096133	0.287488
H	-0.767804	-3.095602	0.097540	C	-5.070333	1.592254	-0.277349
H	-2.399846	-1.235912	1.889349	C	-6.119912	1.783057	-1.184520
H	-1.366494	-2.602494	2.378598	C	-4.414096	2.718604	0.235422
Si	-0.051294	-0.179209	0.318709	C	-6.501884	3.063168	-1.569158
C	-0.654669	1.565496	0.113844	H	-6.645353	0.925617	-1.594518
C	0.134906	2.658996	0.491432	C	-4.792405	3.999553	-0.150320
C	-1.938376	1.810292	-0.389114	H	-3.596771	2.587891	0.939539
C	-0.346300	3.958158	0.378576	C	-5.836068	4.170746	-1.053725
H	1.137939	2.493916	0.873621	H	-7.316227	3.197832	-2.270918
C	-2.421043	3.108940	-0.506628	H	-4.274138	4.862411	0.250655
H	-2.553594	0.973138	-0.702036	H	-6.130950	5.168320	-1.357032
C	-1.625556	4.182545	-0.120499	C	-4.392405	-1.328909	-1.086968
H	0.274729	4.794670	0.676427	C	-4.356272	-0.969943	-2.438364
H	-3.414731	3.284727	-0.901631	C	-4.261459	-2.683956	-0.750679
H	-2.000754	5.195240	-0.211871	C	-4.166820	-1.932309	-3.424884
C	1.771249	-0.311055	-0.010042	H	-4.464996	0.071346	-2.724113
C	2.551137	-1.217881	0.718027	C	-4.063672	-3.646356	-1.731974
C	2.390904	0.456290	-1.004462	H	-4.319342	-2.989083	0.290092
C	3.909718	-1.357134	0.457173	C	-4.010703	-3.267776	-3.070695
H	2.086959	-1.805300	1.503037	H	-4.137622	-1.640443	-4.467942
C	3.748045	0.316020	-1.270269	H	-3.955293	-4.688601	-1.457145
H	1.808111	1.174623	-1.573455	H	-3.855197	-4.016545	-3.838375
				O	-5.502243	-0.724889	1.504314

O	-3.141246	0.047089	1.218715	C	-0.516402	1.911336	0.944457
C	-5.575326	-0.774857	3.918903	C	-0.327065	-1.166140	1.887901
H	-4.934813	-0.894916	4.799692	C	-1.007844	-0.404360	-1.174646
H	-5.926600	0.261544	3.907223	H	0.380511	2.429202	0.591025
C	-6.760362	-1.733152	3.984010	H	-1.336646	2.292294	0.326876
H	-6.420369	-2.770556	4.034467	H	0.715497	-1.416300	2.101605
H	-7.376437	-1.537738	4.862592	H	-0.674523	-0.650668	2.788248
H	-7.380557	-1.621592	3.093940	H	-1.738369	-1.205153	-1.016828
B	2.571818	0.025741	-0.143840	H	-0.188824	-0.858074	-1.740257
C	3.059617	1.370059	0.587342	C	-0.770842	2.237309	2.420806
C	2.985482	-1.360262	0.555243	H	-1.698091	1.781478	2.771294
C	2.496991	0.043178	-1.748415	H	0.037989	1.883708	3.062266
C	2.699127	1.588649	1.910082	H	-0.858066	3.316287	2.566308
C	3.791666	2.387690	-0.005697	C	-1.632295	0.745015	-1.978287
C	3.000890	2.739644	2.611461	H	-0.931612	1.567946	-2.127294
C	4.130777	3.555568	0.664227	H	-1.949751	0.394090	-2.961987
C	3.730221	3.733898	1.977202	H	-2.511648	1.161256	-1.478054
F	1.985098	0.647662	2.555102	C	-1.135993	-2.443282	1.625334
F	4.202708	2.284288	-1.272247	H	-1.114685	-3.101866	2.496676
F	2.598714	2.902577	3.869188	H	-2.177237	-2.211561	1.394001
F	4.832937	4.505757	0.056074	H	-0.727880	-3.000417	0.779543
F	4.040221	4.848819	2.625327				
C	2.245759	-2.506834	0.295524	C-TS1			
C	4.025581	-1.517211	1.459795	C	-4.132527	1.410244	2.527357
C	2.478484	-3.728242	0.895598	C	-3.139944	1.959061	1.495630
C	4.305699	-2.729359	2.077673	H	-3.588139	0.921825	3.344604
C	3.526804	-3.838115	1.797135	H	-3.618354	2.741305	0.895676
F	1.214759	-2.434540	-0.564490	H	-2.241836	2.362355	1.954515
F	4.817399	-0.490180	1.779578	Si	-4.270903	0.016367	0.363590
F	1.713335	-4.782690	0.626974	C	-5.103529	0.854885	-1.068936
F	5.313753	-2.833429	2.937242	C	-6.363820	0.419316	-1.498801
F	3.778926	-4.998995	2.386723	C	-4.510976	1.939927	-1.726404
C	1.804005	1.068128	-2.380603	C	-7.014617	1.054340	-2.550108
C	3.009495	-0.932953	-2.591187	H	-6.840795	-0.426480	-1.012078
C	1.587305	1.128077	-3.742969	C	-5.157806	2.574242	-2.780577
C	2.829006	-0.906014	-3.968208	H	-3.527047	2.283587	-1.419405
C	2.110864	0.125756	-4.545948	C	-6.411123	2.131888	-3.190542
F	1.273284	2.052228	-1.634347	H	-7.989229	0.707868	-2.872019
F	3.708622	-1.962980	-2.106879	H	-4.684418	3.408513	-3.284023
F	0.883276	2.118423	-4.283358	H	-6.916281	2.624537	-4.012754
F	3.337794	-1.864466	-4.735429	C	-4.210720	-1.818609	0.187535
F	1.923566	0.157620	-5.858564	C	-4.306737	-2.429040	-1.069614
H	1.251127	0.073957	0.150020	C	-4.079679	-2.628319	1.323949
Si	-0.332829	0.096217	0.500090	C	-4.228257	-3.810954	-1.191976

H	-4.438958	-1.820748	-1.958546	C	2.212871	-2.785137	-3.628390
C	-3.998930	-4.009673	1.201524	F	1.216851	0.516347	-2.635528
H	-4.050904	-2.174237	2.308349	F	3.662653	-2.815262	-0.349509
C	-4.062993	-4.598963	-0.057408	F	0.978998	-1.112660	-4.739000
H	-4.296177	-4.273076	-2.169353	F	3.443774	-4.403945	-2.459386
H	-3.889568	-4.626169	2.085354	F	2.102325	-3.594963	-4.674945
H	-3.994840	-5.676100	-0.153389	H	1.140667	0.160313	0.037592
O	-4.894943	0.405569	1.852649	Si	-0.600223	0.489390	0.276374
O	-2.780814	0.863704	0.614418	C	-0.461933	2.126074	-0.641591
C	-5.045892	2.487251	3.081797	C	-0.412986	0.316382	2.140321
H	-4.425584	3.286689	3.502405	C	-1.043641	-1.017099	-0.745520
H	-5.609209	2.914992	2.246098	H	0.504344	2.092244	-1.147634
C	-5.999983	1.939868	4.138477	H	-1.202239	2.075261	-1.447838
H	-5.448025	1.546581	4.995563	H	0.650676	0.216159	2.358414
H	-6.672745	2.718376	4.499765	H	-0.700614	1.254078	2.623858
H	-6.599927	1.130990	3.719907	H	-1.688559	-1.659772	-0.138566
B	2.407552	-0.060307	-0.121900	H	-0.130369	-1.593758	-0.901852
C	2.971747	1.427860	-0.397300	C	-0.586263	3.460902	0.113012
C	2.828578	-0.710406	1.295817	H	-1.626730	3.748785	0.265037
C	2.431421	-1.070416	-1.384990	H	-0.092263	3.440147	1.086513
C	2.602875	2.451414	0.464717	H	-0.118601	4.260611	-0.465310
C	3.753809	1.818951	-1.473386	C	-1.694852	-0.705389	-2.099967
C	2.935656	3.778912	0.279779	H	-1.017213	-0.144706	-2.746046
C	4.126603	3.139153	-1.693355	H	-1.959179	-1.629666	-2.618272
C	3.711414	4.125028	-0.815784	H	-2.608810	-0.111372	-2.003244
F	1.842438	2.158574	1.537732	C	-1.187343	-0.863472	2.743277
F	4.185521	0.924870	-2.368367	H	-1.023372	-0.921576	3.821700
F	2.511324	4.718147	1.124069	H	-2.261374	-0.767133	2.574222
F	4.875065	3.466103	-2.742960	H	-0.869324	-1.812921	2.308575
F	4.050215	5.392697	-1.020799				
C	2.091139	-1.778540	1.790283	C-int2			
C	3.846886	-0.265683	2.125166	C	-4.495426	1.259270	2.485564
C	2.301132	-2.361475	3.023844	C	-3.451488	1.866921	1.544140
C	4.104932	-0.828667	3.369610	H	-3.996811	0.768177	3.328200
C	3.326497	-1.878024	3.823059	H	-3.892263	2.655739	0.929162
F	1.081878	-2.270336	1.047806	H	-2.578226	2.248878	2.067340
F	4.641583	0.745173	1.759269	Si	-4.503407	-0.120789	0.278804
F	1.532647	-3.361334	3.452523	C	-5.256812	0.737624	-1.175859
F	5.092592	-0.365413	4.130557	C	-6.469782	0.263370	-1.693141
F	3.556382	-2.418987	5.013839	C	-4.666987	1.862167	-1.767312
C	1.783089	-0.702205	-2.556925	C	-7.079111	0.900522	-2.767475
C	2.991115	-2.340173	-1.403508	H	-6.942098	-0.613079	-1.258906
C	1.647446	-1.519791	-3.661544	C	-5.273780	2.497538	-2.843775
C	2.892474	-3.193976	-2.495541	H	-3.714807	2.234921	-1.399601

C	-6.480783	2.017277	-3.341649	F	4.878618	0.296353	1.679785
H	-8.016438	0.524540	-3.158864	F	1.338767	-3.487009	3.280439
H	-4.803533	3.361236	-3.297712	F	5.332847	-1.085494	3.916869
H	-6.952831	2.511268	-4.182366	F	3.580415	-2.982405	4.747925
C	-4.292561	-1.932641	0.089375	C	1.837760	-0.445204	-2.551588
C	-4.308597	-2.532566	-1.177005	C	3.382210	-1.949584	-1.645499
C	-4.087967	-2.733575	1.221408	C	1.818166	-1.127769	-3.754611
C	-4.085131	-3.896826	-1.310433	C	3.405729	-2.661450	-2.837335
H	-4.485644	-1.930678	-2.062272	C	2.614812	-2.251700	-3.897114
C	-3.859629	-4.096529	1.085661	F	1.051197	0.649216	-2.468632
H	-4.111747	-2.288997	2.210033	F	4.177709	-2.400455	-0.668546
C	-3.848872	-4.674138	-0.180606	F	1.041476	-0.724203	-4.762705
H	-4.090592	-4.352957	-2.292712	F	4.178580	-3.737551	-2.973969
H	-3.690281	-4.707648	1.963502	F	2.619238	-2.930409	-5.041971
H	-3.663151	-5.736290	-0.286392	H	1.233983	0.182652	0.043219
O	-5.179820	0.250010	1.740796	Si	-1.168849	0.567439	0.334966
O	-3.028076	0.795778	0.636251	C	-0.732437	2.182701	-0.494721
C	-5.474193	2.301393	2.994411	C	-0.658748	0.271887	2.108087
H	-4.906298	3.106598	3.473604	C	-1.202283	-0.904289	-0.807014
H	-5.988688	2.732463	2.129444	H	0.315875	2.059308	-0.782370
C	-6.483236	1.705774	3.970816	H	-1.277119	2.219165	-1.445774
H	-5.981562	1.308866	4.856398	H	0.420636	0.113468	2.102602
H	-7.198692	2.460078	4.299033	H	-0.798014	1.181648	2.701836
H	-7.032417	0.891950	3.496166	H	-1.706000	-1.737981	-0.307922
B	2.427920	0.005026	-0.065066	H	-0.162822	-1.223651	-0.916357
C	3.053655	1.503064	-0.123972	C	-0.897828	3.502956	0.273880
C	2.845536	-0.837322	1.259511	H	-1.942209	3.816034	0.338601
C	2.590908	-0.827253	-1.451126	H	-0.488537	3.440135	1.284011
C	2.509538	2.495123	0.677780	H	-0.357197	4.302839	-0.235493
C	4.073009	1.923171	-0.965507	C	-1.806165	-0.631453	-2.193179
C	2.896914	3.823097	0.638653	H	-1.178971	0.058292	-2.758962
C	4.505395	3.240350	-1.031385	H	-1.877936	-1.558363	-2.766353
C	3.909110	4.198414	-0.228383	H	-2.810445	-0.198884	-2.149423
F	1.528151	2.182816	1.552498	C	-1.369446	-0.923131	2.758619
F	4.696903	1.048378	-1.762232	H	-0.995203	-1.091364	3.770383
F	2.303417	4.735728	1.412662	H	-2.449468	-0.765680	2.828829
F	5.485380	3.597427	-1.859204	H	-1.199904	-1.840522	2.191413
F	4.305641	5.467338	-0.287588				
C	2.002214	-1.839997	1.715592	C-int3			
C	3.973881	-0.622266	2.036599	C	1.161249	-0.870111	-1.177148
C	2.213582	-2.562276	2.876432	C	1.261339	-0.273779	0.231406
C	4.236946	-1.330713	3.201135	H	0.440955	-1.689592	-1.154415
C	3.348074	-2.303242	3.627294	H	0.604187	0.573171	0.394412
F	0.885827	-2.139605	1.017590	Si	3.697884	-0.916904	-0.531332

C	5.000799	0.007804	-1.448255	F	-4.079572	5.374477	0.424712
C	6.337587	-0.030828	-1.028404	C	-2.276551	-2.236594	-1.571919
C	4.664867	0.775733	-2.571897	C	-3.378845	-0.426896	-2.559121
C	7.311716	0.692549	-1.705965	C	-2.482085	-3.022589	-2.691377
H	6.618100	-0.626808	-0.165343	C	-3.608928	-1.177447	-3.706220
C	5.636825	1.510514	-3.240250	C	-3.160776	-2.483719	-3.773165
H	3.642092	0.786357	-2.934803	F	-1.585344	-2.801255	-0.561478
C	6.958893	1.468304	-2.805732	F	-3.830962	0.834666	-2.589374
H	8.342689	0.654208	-1.376059	F	-2.030238	-4.275511	-2.747196
H	5.367684	2.103624	-4.105666	F	-4.254368	-0.649032	-4.745186
H	7.717330	2.035787	-3.331817	F	-3.371828	-3.214247	-4.865450
C	4.365950	-2.111369	0.705641	C	-1.951621	-0.515212	2.422415
C	3.976331	-2.061172	2.049311	C	-3.734335	-1.714162	1.497459
C	5.261866	-3.110569	0.299153	C	-2.174036	-1.066732	3.670742
C	4.467465	-2.985168	2.964567	C	-4.001809	-2.289835	2.732992
H	3.284392	-1.297102	2.387932	C	-3.216124	-1.965751	3.826288
C	5.749196	-4.036064	1.212793	F	-0.919182	0.358608	2.330361
H	5.580379	-3.170839	-0.737416	F	-4.522782	-2.081430	0.482906
C	5.351981	-3.972307	2.545257	F	-1.397491	-0.749959	4.711943
H	4.156537	-2.936858	4.001019	F	-5.003003	-3.155263	2.880784
H	6.435898	-4.807688	0.887035	F	-3.456942	-2.513991	5.015207
H	5.731824	-4.695336	3.257024	H	-1.088473	-0.111553	-0.123183
O	2.458122	-1.434449	-1.469051	Si	2.914385	1.866092	1.029751
O	2.664802	0.205958	0.373608	C	2.455991	3.026320	-0.352545
C	0.777286	0.137011	-2.248481	C	1.761393	1.985640	2.485062
H	-0.158319	0.613007	-1.943296	C	4.727719	1.883053	1.510909
H	1.541812	0.921908	-2.287440	H	3.270089	3.075288	-1.083140
C	0.610438	-0.526753	-3.611292	H	1.579508	2.627492	-0.869799
H	-0.206953	-1.252432	-3.575648	H	2.009774	2.942088	2.963684
H	0.367994	0.210106	-4.377824	H	0.730350	2.090538	2.135900
H	1.520665	-1.052467	-3.906493	H	5.131964	0.864301	1.483207
B	-2.285102	-0.099409	-0.111926	H	4.778209	2.181052	2.563995
C	-2.767110	1.453931	-0.035838	C	2.112287	4.427925	0.187216
C	-2.712591	-0.921898	-1.447740	H	1.224755	4.390022	0.821155
C	-2.699477	-0.814259	1.293733	H	2.931833	4.860009	0.768623
C	-1.899465	2.523690	0.064772	H	1.893886	5.113209	-0.632507
C	-4.114321	1.785430	0.039177	C	5.591647	2.827289	0.658497
C	-2.307877	3.839976	0.218887	H	5.256336	3.862450	0.755956
C	-4.575732	3.081615	0.185314	H	6.636887	2.787630	0.970124
C	-3.659726	4.120619	0.278175	H	5.552737	2.566042	-0.400999
F	-0.553143	2.335765	0.022400	C	1.863493	0.849300	3.512298
F	-5.025586	0.811469	-0.038773	H	1.238364	1.057470	4.381225
F	-1.411226	4.828254	0.314732	H	1.502319	-0.092599	3.094983
F	-5.877932	3.349892	0.243890	H	2.890465	0.705966	3.861537

H	1.111031	-1.025000	1.007746	C	-4.136737	1.509378	-0.252006
				C	-2.667232	3.818352	-0.377302
C-TS2				C	-4.793353	2.724647	-0.312462
C	0.936269	-0.706667	-1.252231	C	-4.047298	3.893264	-0.373120
C	0.788185	0.041900	0.079503	F	-0.702745	2.590073	-0.334339
H	0.251373	-1.553773	-1.213430	F	-4.887244	0.403148	-0.199399
H	0.529373	1.086666	0.109677	F	-1.935014	4.931352	-0.430232
Si	3.456008	-0.800924	-0.389573	F	-6.121193	2.791084	-0.311041
C	4.887876	-0.121699	-1.344154	F	-4.655373	5.073192	-0.426429
C	6.204798	-0.285933	-0.896715	C	-2.031370	-2.467982	-1.195545
C	4.659543	0.618517	-2.511843	C	-3.014086	-0.809402	-2.524202
C	7.265217	0.286281	-1.590616	C	-2.213169	-3.418949	-2.183024
H	6.402590	-0.864330	0.000766	C	-3.222182	-1.730700	-3.542438
C	5.717491	1.199260	-3.201329	C	-2.823811	-3.044098	-3.369757
H	3.647450	0.731015	-2.889254	F	-1.402718	-2.871748	-0.077845
C	7.020084	1.033363	-2.738232	F	-3.401264	0.445186	-2.787201
H	8.280259	0.151688	-1.236879	F	-1.806567	-4.673886	-2.012397
H	5.529852	1.771168	-4.102063	F	-3.792384	-1.359477	-4.685750
H	7.845761	1.482224	-3.277607	F	-3.012627	-3.935313	-4.335744
C	3.969210	-2.059312	0.865397	C	-1.841148	0.015128	2.465651
C	3.640692	-1.906216	2.217053	C	-3.328708	-1.649062	1.756219
C	4.693748	-3.193541	0.473147	C	-2.031751	-0.321950	3.793209
C	4.022440	-2.861489	3.153541	C	-3.559216	-2.017131	3.074768
H	3.082787	-1.033877	2.541355	C	-2.904186	-1.353545	4.098850
C	5.072088	-4.149888	1.406502	F	-0.992795	1.036482	2.214398
H	4.963682	-3.333312	-0.569595	F	-3.993166	-2.332396	0.821472
C	4.736269	-3.982718	2.747246	F	-1.390579	0.325464	4.767198
H	3.760605	-2.731973	4.196742	F	-4.401078	-3.004119	3.367540
H	5.626389	-5.025439	1.090908	F	-3.110702	-1.701971	5.364371
H	5.031301	-4.729116	3.475109	H	-0.869316	-0.001855	-0.099951
O	2.240446	-1.262074	-1.400109	Si	2.936223	2.049113	0.902874
O	2.583519	0.420642	0.404628	C	2.583440	3.152899	-0.566474
C	0.598351	0.174337	-2.445290	C	1.769208	2.410473	2.313346
H	-0.373829	0.644184	-2.267771	C	4.737673	2.059588	1.446501
H	1.339456	0.979822	-2.505723	H	3.411222	3.087883	-1.280597
C	0.564013	-0.638155	-3.734772	H	1.692623	2.780387	-1.082672
H	-0.194077	-1.423759	-3.660793	H	2.081804	3.375788	2.730334
H	0.313839	-0.009633	-4.590025	H	0.757070	2.569552	1.929680
H	1.528073	-1.115150	-3.918942	H	5.087195	1.025954	1.556772
B	-2.121999	-0.108373	-0.098942	H	4.774193	2.486754	2.454810
C	-2.752144	1.381037	-0.259100	C	2.338442	4.613808	-0.148207
C	-2.427966	-1.139238	-1.308123	H	1.425568	4.697826	0.445407
C	-2.454511	-0.631474	1.402043	H	3.164089	5.015221	0.446510
C	-2.057665	2.573436	-0.322379	H	2.220876	5.257496	-1.021069

C	5.679034	2.840741	0.515510	C	4.172963	0.182047	2.602877
H	5.394912	3.894452	0.461658	H	3.073420	-1.267958	3.744811
H	6.710061	2.794046	0.871371	H	5.029020	1.638904	1.273031
H	5.663324	2.442967	-0.501195	H	5.020091	0.187344	3.278924
C	1.755126	1.345640	3.418638	Si	-2.252153	-0.719425	0.744799
H	1.101467	1.638608	4.240991	C	-3.257150	-0.904660	-0.829682
H	1.377022	0.392684	3.041172	C	-4.757134	-1.096020	-0.558123
H	2.756112	1.175257	3.826641	H	-2.869027	-1.748741	-1.409254
H	0.666983	-0.531804	0.991779	H	-3.095293	-0.012293	-1.444813
C-int4				H	-5.330565	-1.166519	-1.484619
C	2.603736	-2.077714	-2.720755	H	-4.941253	-2.010493	0.012421
C	1.382684	-1.971452	-1.818475	H	-5.167820	-0.262129	0.017634
H	2.887581	-3.132758	-2.789634	C	-2.611370	0.925169	1.574475
H	2.313193	-1.752989	-3.725375	C	-1.668399	1.212666	2.752468
C	0.210949	-2.809754	-2.302317	H	-3.652894	0.941820	1.914042
H	1.671063	-2.302240	-0.808483	H	-2.520921	1.715938	0.820231
H	-0.628032	-2.714133	-1.610495	H	-1.826082	2.213306	3.160963
H	-0.106106	-2.462940	-3.288786	H	-1.818695	0.495795	3.563969
O	0.981418	-0.598141	-1.767898	H	-0.619512	1.142039	2.449176
Si	0.554910	0.117846	-0.344593	C	-2.548969	-2.172811	1.889736
C	3.775897	-1.244006	-2.213194	C	-2.188219	-3.507978	1.221670
H	4.038579	-1.521187	-1.187855	H	-3.594369	-2.177142	2.216915
H	3.514833	-0.184757	-2.213238	H	-1.946681	-2.031991	2.793744
H	0.490302	-3.863676	-2.371941	H	-2.323869	-4.353717	1.899055
O	-0.625295	-0.773735	0.372617	H	-2.809580	-3.689816	0.339828
C	-0.069390	1.816368	-0.780135	H	-1.145543	-3.504469	0.893310
C	0.082633	2.895686	0.098074	H	4.659101	-1.379404	-2.839922
C	-0.816847	2.007891	-1.949375	C-int5			
C	-0.508995	4.125391	-0.172805	C	-4.510690	-2.912862	0.497916
H	0.668655	2.774592	1.004567	C	-4.967383	-1.983087	-0.622388
C	-1.411779	3.234791	-2.222367	H	-3.419037	-2.991021	0.465173
H	-0.923742	1.187799	-2.652737	H	-4.757184	-2.429049	1.448903
C	-1.262291	4.292515	-1.330191	C	-4.657442	-2.501622	-2.017969
H	-0.382947	4.951689	0.516940	H	-6.055077	-1.862832	-0.535469
H	-1.988115	3.368572	-3.130382	H	-4.982312	-1.777716	-2.768200
H	-1.726700	5.248830	-1.541027	H	-3.583328	-2.662697	-2.140758
C	1.983408	0.167146	0.852571	O	-4.329591	-0.715711	-0.436851
C	1.992148	-0.640010	1.995538	Si	-5.143605	0.734281	-0.173936
C	3.092142	0.988203	0.608395	C	-6.885063	0.380160	0.445815
C	3.079410	-0.635879	2.864480	C	-7.574290	1.638248	0.999094
H	1.134409	-1.273228	2.201312	H	-6.842011	-0.388466	1.226292
C	4.178767	0.998028	1.474785	H	-7.489044	-0.039407	-0.365835
H	3.104754	1.629368	-0.268849	H	-8.600247	1.428036	1.306513

H	-7.043611	2.030003	1.869583	F	1.028493	-0.337227	-2.576773
H	-7.615097	2.435230	0.251761	F	4.007030	-1.634802	0.846695
C	-4.221194	1.693795	1.142061	F	2.120659	-2.159781	-4.207732
H	-3.160070	1.833194	0.926696	F	5.103579	-3.420823	-0.801099
H	-4.299929	1.193511	2.111614	F	4.181022	-3.707451	-3.332858
C	-5.237777	1.703183	-1.773482	H	0.430898	-0.200649	-0.091396
H	-4.258043	2.050316	-2.107555	Si	-1.083066	-0.623466	-0.358244
H	-5.875191	2.583274	-1.649825	C	-1.608005	0.745582	-1.528121
C	-5.144646	-4.300422	0.438996	C	-1.685934	-0.682010	1.403004
H	-4.796831	-4.866285	-0.427171	C	-0.836518	-2.300262	-1.141849
H	-6.234512	-4.231411	0.380166	H	-2.299416	1.413784	-1.010293
H	-4.664350	2.688429	1.245922	H	-0.713798	1.337300	-1.744797
H	-5.666390	1.091901	-2.572667	H	-2.775291	-0.722144	1.410591
H	-5.175419	-3.442986	-2.209559	H	-1.300055	-1.579464	1.892134
H	-4.896223	-4.877396	1.330549	H	-1.356275	0.195803	1.962209
B	1.722815	0.160988	0.136561	H	-1.688668	-2.951470	-0.938516
C	1.704301	1.677537	-0.384194	H	-0.702412	-2.230428	-2.222308
C	1.807718	-0.054326	1.723788	H	0.047978	-2.773365	-0.708454
C	2.466727	-0.909873	-0.796876	C	-2.207361	0.247724	-2.849996
C	0.696683	2.542720	0.020895	H	-3.112167	-0.335357	-2.676921
C	2.653084	2.222406	-1.237325	H	-2.467324	1.091108	-3.493484
C	0.597444	3.855784	-0.395007	H	-1.491709	-0.368719	-3.397175
C	2.601116	3.540499	-1.670271				
C	1.567658	4.359078	-1.248668	C-TS3			
F	-0.267041	2.085799	0.842652	C	-4.284789	-2.821063	0.382962
F	3.679964	1.488624	-1.673910	C	-4.547663	-1.862940	-0.775350
F	-0.407832	4.628577	0.004183	H	-3.216097	-3.020056	0.478001
F	3.532896	4.023142	-2.484663	H	-4.580923	-2.310249	1.304437
F	1.502163	5.617412	-1.661078	C	-4.297375	-2.402173	-2.173475
C	1.436920	-1.275127	2.272609	H	-5.609114	-1.602266	-0.732789
C	2.210114	0.910810	2.637159	H	-4.547790	-1.641306	-2.914284
C	1.426902	-1.538587	3.627996	H	-3.267630	-2.714526	-2.332021
C	2.230044	0.684737	4.007097	O	-3.796505	-0.628589	-0.552046
C	1.833137	-0.543860	4.504496	Si	-4.729546	0.791344	-0.180509
F	1.033359	-2.264640	1.456213	C	-6.328854	0.277529	0.671186
F	2.610447	2.118752	2.230904	C	-7.003781	1.479112	1.356710
F	1.028039	-2.717956	4.094336	H	-6.130868	-0.502869	1.414117
F	2.625123	1.638004	4.843915	H	-7.025523	-0.152872	-0.054593
F	1.838243	-0.769398	5.810856	H	-7.965895	1.194338	1.785131
C	2.046599	-1.083849	-2.108603	H	-6.387510	1.877810	2.164363
C	3.513520	-1.724920	-0.391054	H	-7.190502	2.292954	0.650769
C	2.590375	-2.014937	-2.972239	C	-3.807479	1.899603	1.007513
C	4.101060	-2.661884	-1.229554	H	-2.755875	2.080177	0.791299
C	3.635050	-2.808931	-2.524994	H	-3.876694	1.514633	2.027860

C	-5.147800	1.638759	-1.791368	H	0.195333	-0.175997	-0.094841
H	-4.286671	2.114668	-2.262511	Si	-1.572489	-0.527988	-0.396571
H	-5.900207	2.411756	-1.609644	C	-1.643578	0.915673	-1.605119
C	-5.056010	-4.132608	0.250731	C	-1.771320	-0.563813	1.466313
H	-4.678733	-4.739152	-0.574340	C	-1.099036	-2.167230	-1.165512
H	-6.120050	-3.948651	0.076916	H	-2.242072	1.736783	-1.207773
H	-4.312363	2.871247	0.994503	H	-0.630348	1.305891	-1.701378
H	-5.573991	0.928206	-2.505581	H	-2.816175	-0.578098	1.769193
H	-4.948579	-3.260106	-2.350676	H	-1.307574	-1.489035	1.817366
H	-4.965263	-4.722527	1.163022	H	-1.264759	0.273032	1.947398
B	1.430351	0.100165	0.131025	H	-1.732235	-2.998121	-0.863105
C	1.572466	1.647765	-0.320900	H	-1.081510	-2.110578	-2.254892
C	1.595723	-0.165086	1.718794	H	-0.087900	-2.398372	-0.823506
C	2.229693	-0.936201	-0.821148	C	-2.137449	0.506711	-2.999898
C	0.613821	2.572468	0.067094	H	-3.122646	0.041364	-2.965148
C	2.603701	2.164081	-1.092559	H	-2.204796	1.383458	-3.648186
C	0.625857	3.905157	-0.292857	H	-1.443139	-0.189777	-3.471016
C	2.667076	3.499717	-1.470595				
C	1.671734	4.374080	-1.072617	C-int6			
F	-0.420106	2.162264	0.831875	C	-4.630139	-2.694069	0.539014
F	3.609973	1.386518	-1.504839	C	-4.841520	-1.751585	-0.636591
F	-0.348003	4.729490	0.090398	H	-3.586399	-3.013617	0.578814
F	3.676372	3.946482	-2.212147	H	-4.823293	-2.141233	1.462636
F	1.715257	5.650954	-1.434295	C	-4.618483	-2.350020	-2.013306
C	1.271156	-1.414286	2.231519	H	-5.869378	-1.387859	-0.601882
C	2.027526	0.758363	2.660387	H	-4.586978	-1.564725	-2.769707
C	1.331757	-1.743539	3.570909	H	-3.707042	-2.940093	-2.074875
C	2.113304	0.470437	4.017505	O	-4.007518	-0.537417	-0.439205
C	1.761349	-0.785193	4.476055	Si	-4.880783	0.961032	-0.004717
F	0.841667	-2.377136	1.392420	C	-6.462809	0.468952	0.878575
F	2.396270	1.993954	2.303262	C	-7.061181	1.681334	1.617376
F	0.975053	-2.953055	3.998660	H	-6.274649	-0.337294	1.594753
F	2.532120	1.393250	4.879297	H	-7.199233	0.091149	0.163101
F	1.830426	-1.071974	5.770884	H	-8.020119	1.423454	2.068260
C	1.845429	-1.078478	-2.146440	H	-6.402794	2.028884	2.415074
C	3.306440	-1.723121	-0.436396	H	-7.236083	2.521807	0.940347
C	2.441954	-1.948633	-3.039663	C	-3.845966	1.973763	1.164324
C	3.944859	-2.603174	-1.299464	H	-2.801590	2.121949	0.893038
C	3.509101	-2.718870	-2.608029	H	-3.876863	1.556078	2.173178
F	0.814608	-0.346854	-2.614735	C	-5.283362	1.809785	-1.610671
F	3.792536	-1.659883	0.807699	H	-4.411160	2.262626	-2.083545
F	2.002143	-2.054147	-4.292415	H	-6.012071	2.602968	-1.418679
F	4.972835	-3.336705	-0.882271	C	-5.549284	-3.911980	0.459537
F	4.106626	-3.561952	-3.442176	H	-5.298762	-4.548230	-0.390829

H	-6.595918	-3.610168	0.363210	H	-2.293217	1.820344	-1.132544
H	-4.311552	2.964375	1.208974	H	-0.762030	1.099423	-1.533229
H	-5.736706	1.113634	-2.321842	H	-2.837826	-0.571762	1.990959
H	-5.461301	-3.003195	-2.246804	H	-1.343873	-1.480747	1.725428
H	-5.457922	-4.514706	1.362858	H	-1.285715	0.276915	1.810423
B	1.471548	0.060723	0.085296	H	-1.929595	-3.046950	-0.722664
C	1.631282	1.650575	-0.228861	H	-1.600009	-2.168971	-2.239519
C	1.800562	-0.346699	1.624470	H	-0.433268	-2.158772	-0.915574
C	2.250392	-0.879542	-0.993498	C	-2.306033	0.626347	-2.957031
C	0.632296	2.542186	0.128706	H	-3.353411	0.316782	-3.000560
C	2.719799	2.228541	-0.868852	H	-2.203872	1.521600	-3.573853
C	0.658340	3.897207	-0.150098	H	-1.698764	-0.153240	-3.417722
C	2.799294	3.582638	-1.161253				
C	1.758304	4.423508	-0.804175	C-int7			
F	-0.464468	2.097853	0.787753	C	0.110594	-2.577794	-0.818994
F	3.771306	1.482284	-1.223548	C	0.787970	-1.247152	-1.076346
F	-0.360756	4.687938	0.197033	H	-0.952576	-2.321375	-0.833006
F	3.864462	4.086168	-1.780709	H	0.253849	-3.261976	-1.654704
F	1.814902	5.722510	-1.085324	C	0.593646	-0.705844	-2.470616
C	1.361712	-1.575930	2.095261	H	0.439867	-0.528880	-0.333188
C	2.472652	0.429804	2.556632	H	1.049226	0.279560	-2.568856
C	1.535155	-2.015461	3.395083	H	1.015163	-1.380548	-3.219904
C	2.677880	0.028680	3.870116	O	2.314715	-1.287576	-0.804754
C	2.203906	-1.200423	4.293433	Si	2.887912	0.162568	0.098689
F	0.706417	-2.413329	1.261804	C	0.446107	-3.231869	0.513546
F	2.972948	1.625644	2.220118	H	0.330015	-2.519449	1.331933
F	1.061602	-3.198535	3.791001	H	1.468596	-3.618724	0.536047
F	3.326503	0.813463	4.728947	H	-0.477983	-0.612624	-2.656601
F	2.385893	-1.595466	5.551229	O	1.897359	1.351033	-0.339612
C	1.704816	-1.097975	-2.248793	C	4.596397	0.548948	-0.514675
C	3.455769	-1.529262	-0.761855	C	5.747825	0.108366	0.148358
C	2.268739	-1.920449	-3.209784	C	4.744203	1.333140	-1.665987
C	4.062813	-2.358024	-1.693461	C	7.011437	0.397093	-0.356580
C	3.462831	-2.558745	-2.925715	H	5.658343	-0.452856	1.073764
F	0.547411	-0.490124	-2.593996	C	6.003967	1.631234	-2.169071
F	4.104711	-1.361388	0.395773	H	3.864138	1.708172	-2.179084
F	1.676436	-2.101507	-4.392122	C	7.138105	1.149915	-1.520338
F	5.218220	-2.961408	-1.421578	H	7.895662	0.047398	0.162522
F	4.030643	-3.354168	-3.828562	H	6.103426	2.236219	-3.062400
H	0.292523	-0.189662	-0.057648	H	8.122378	1.376283	-1.912887
Si	-2.113217	-0.558645	-0.389047	C	2.900752	-0.232457	1.903555
C	-1.835733	0.908355	-1.521394	C	3.232990	0.842221	2.742851
C	-1.881817	-0.566819	1.463960	C	2.729023	-1.495480	2.477939
C	-1.501681	-2.142672	-1.154497	C	3.377456	0.658825	4.111598

H	3.381700	1.835540	2.326853	H	1.305712	-5.075958	-1.106091
C	2.864158	-1.680279	3.849731	C	4.381385	-3.212591	-0.075921
H	2.489484	-2.344892	1.853981	C	5.664440	-3.909902	-0.562626
C	3.190405	-0.603425	4.665219	H	3.754125	-3.921805	0.473318
H	3.624968	1.500926	4.746224	H	4.638165	-2.423006	0.633906
H	2.706253	-2.661292	4.281116	H	6.186103	-4.389080	0.266891
H	3.288224	-0.745203	5.734689	H	5.450142	-4.684589	-1.305043
Si	1.475823	2.978862	-0.578498	H	6.349948	-3.192224	-1.019257
C	0.717811	3.054885	-2.287756	B	-2.523153	-0.213782	-0.113839
C	0.367320	4.484015	-2.734185	C	-2.037429	-0.869923	1.303466
H	-0.183358	2.430948	-2.291898	C	-2.835483	1.387426	-0.024976
H	1.405800	2.601271	-3.012527	C	-3.786973	-0.963454	-0.803931
H	-0.173740	4.479325	-3.681384	C	-1.023356	-0.242650	2.014388
H	-0.274380	4.986203	-2.005549	C	-2.482058	-2.052560	1.879906
H	1.267809	5.089329	-2.865328	C	-0.522377	-0.675707	3.227316
C	3.055572	4.004238	-0.455029	C	-1.978439	-2.557840	3.074325
C	2.794415	5.487506	-0.139710	C	-0.997014	-1.863123	3.759370
H	3.620063	3.925306	-1.389983	F	-0.463686	0.874251	1.512202
H	3.706356	3.572544	0.315764	F	-3.420200	-2.802402	1.285662
H	3.726579	6.055149	-0.109308	F	0.399332	0.034292	3.878536
H	2.151332	5.952163	-0.890324	F	-2.426905	-3.713778	3.563744
H	2.300744	5.609822	0.826108	F	-0.506807	-2.330279	4.907149
C	0.264657	3.544619	0.718766	C	-2.717290	2.131972	-1.192030
C	0.754071	3.465933	2.171893	C	-3.156246	2.121344	1.107976
H	-0.648954	2.958492	0.601913	C	-2.862984	3.508326	-1.246027
H	-0.005913	4.578996	0.469426	C	-3.305930	3.502198	1.102174
H	0.966511	2.435737	2.460121	C	-3.152028	4.201238	-0.082553
H	1.661322	4.057829	2.328673	F	-2.415767	1.519400	-2.351397
H	-0.008459	3.842223	2.857654	F	-3.291444	1.516884	2.294701
H	-0.226545	-4.070747	0.703091	F	-2.712132	4.171394	-2.395860
Si	3.423616	-2.524892	-1.527337	F	-3.567429	4.166135	2.228330
C	4.552438	-1.721187	-2.787277	F	-3.260091	5.528863	-0.103072
C	3.842498	-0.974452	-3.923682	C	-3.706868	-1.654339	-1.999610
H	5.099850	-2.574167	-3.209300	C	-5.051706	-0.900351	-0.236190
H	5.309501	-1.093305	-2.318465	C	-4.801465	-2.251341	-2.609142
H	4.565533	-0.568188	-4.633358	C	-6.172374	-1.479324	-0.804009
H	3.169961	-1.634713	-4.478213	C	-6.042540	-2.159493	-2.005947
H	3.246052	-0.141109	-3.547206	F	-2.524614	-1.795287	-2.635988
C	2.552445	-3.896226	-2.480496	F	-5.209059	-0.267168	0.933776
C	2.171746	-5.194504	-1.755471	F	-4.670800	-2.910867	-3.762086
H	3.329508	-4.139890	-3.217815	F	-7.366740	-1.398157	-0.219181
H	1.722309	-3.521169	-3.081978	F	-7.106224	-2.725118	-2.572527
H	1.929935	-5.972362	-2.481563	H	-1.588893	-0.288451	-0.865879
H	2.997862	-5.565610	-1.143840				

C-TS4

C	-0.190458	-2.578384	-0.864103	H	0.018335	5.108417	-1.856893
C	0.259470	-1.199355	-1.111302	H	1.584496	5.138583	-2.677373
H	-1.281577	-2.435102	-0.801322	C	3.214059	3.879231	-0.289875
H	-0.033514	-3.207359	-1.740268	C	2.990044	5.350197	0.103167
C	0.335965	-0.618820	-2.460298	H	3.789080	3.836643	-1.220200
H	0.306118	-0.525737	-0.262489	H	3.844604	3.387811	0.461017
H	0.833729	0.347761	-2.445163	H	3.938494	5.885995	0.177625
H	0.811302	-1.306533	-3.160303	H	2.373609	5.875201	-0.629862
O	2.450528	-1.325866	-0.829074	H	2.485520	5.436153	1.067119
Si	2.954291	0.049114	0.042005	C	0.389059	3.463721	0.805866
C	0.291249	-3.213420	0.435521	C	0.840845	3.314596	2.265781
H	0.194370	-2.514778	1.267322	H	-0.539985	2.912681	0.647565
H	1.337101	-3.510539	0.356118	H	0.155661	4.515043	0.591444
H	-0.701503	-0.478246	-2.790692	H	1.036570	2.271104	2.514755
O	1.928146	1.252220	-0.353652	H	1.751562	3.885724	2.469326
C	4.676993	0.523222	-0.492814	H	0.067334	3.672063	2.949757
C	5.805794	0.055312	0.190197	H	-0.303124	-4.100032	0.660283
C	4.871082	1.314996	-1.631562	Si	3.434011	-2.542168	-1.550153
C	7.087918	0.335425	-0.272961	C	4.576528	-1.760676	-2.817907
H	5.682996	-0.526591	1.099191	C	3.807585	-0.931052	-3.856711
C	6.148162	1.605029	-2.094541	H	5.086046	-2.590879	-3.321129
H	4.012636	1.703003	-2.171388	H	5.362388	-1.165512	-2.349429
C	7.258423	1.103981	-1.419801	H	4.484125	-0.437181	-4.557104
H	7.951956	-0.037069	0.264248	H	3.128998	-1.559154	-4.442069
H	6.280162	2.217692	-2.978604	H	3.204203	-0.153480	-3.379731
H	8.256091	1.323514	-1.781332	C	2.445300	-3.810765	-2.549758
C	2.949694	-0.337413	1.860173	C	2.025777	-5.133654	-1.891173
C	3.291757	0.697674	2.742495	H	3.152122	-4.051600	-3.354496
C	2.729538	-1.611290	2.393727	H	1.601305	-3.354137	-3.073065
C	3.396812	0.469330	4.108363	H	1.697303	-5.850436	-2.646188
H	3.484600	1.696620	2.359489	H	2.859510	-5.589147	-1.351429
C	2.825208	-1.844479	3.762480	H	1.207100	-5.015122	-1.181947
H	2.492876	-2.434896	1.733265	C	4.390243	-3.409623	-0.190075
C	3.160313	-0.803267	4.619225	C	5.560080	-4.226193	-0.764845
H	3.655789	1.283203	4.774840	H	3.717597	-4.063713	0.376292
H	2.635989	-2.835056	4.158829	H	4.768267	-2.674154	0.526673
H	3.230040	-0.980448	5.685720	H	6.067457	-4.797201	0.014415
Si	1.608739	2.907721	-0.492216	H	5.224217	-4.937105	-1.525964
C	0.877607	3.126616	-2.206154	H	6.298658	-3.570388	-1.231540
C	0.640292	4.594681	-2.595014	B	-2.587692	-0.177100	-0.079165
H	-0.070192	2.577387	-2.251039	C	-2.134136	-0.849037	1.335570
H	1.539693	2.652575	-2.942345	C	-2.805987	1.435294	-0.021971
H	0.124786	4.671958	-3.553426	C	-3.860370	-0.876643	-0.801431
				C	-1.085719	-0.266737	2.035638

C	-2.626100	-2.012188	1.913017	C	6.927533	1.885235	2.530557
C	-0.583366	-0.728012	3.237318	H	8.409833	0.482869	1.855218
C	-2.128344	-2.543005	3.098759	H	5.258171	3.157634	2.994972
C	-1.104827	-1.896076	3.770097	H	7.561559	2.303522	3.303189
F	-0.481851	0.819012	1.519568	C	4.193354	-1.804114	-0.610556
F	-3.606138	-2.713246	1.327203	C	4.326897	-2.389372	0.656024
F	0.382182	-0.068235	3.870975	C	4.035108	-2.638972	-1.724118
F	-2.625016	-3.675043	3.593986	C	4.250412	-3.767630	0.810434
F	-0.621936	-2.390216	4.906861	H	4.489457	-1.763600	1.527665
C	-2.600166	2.156515	-1.190269	C	3.959082	-4.018001	-1.570806
C	-3.117305	2.196905	1.094906	H	3.985087	-2.208491	-2.718359
C	-2.659448	3.537724	-1.263302	C	4.054858	-4.580296	-0.302206
C	-3.184145	3.583800	1.069645	H	4.345417	-4.208408	1.795329
C	-2.946845	4.258326	-0.116093	H	3.829348	-4.652972	-2.438653
F	-2.287322	1.509185	-2.330548	H	3.989522	-5.655076	-0.181415
F	-3.321168	1.610382	2.279531	O	4.830154	0.383456	-2.351051
F	-2.420864	4.175482	-2.410860	O	2.782504	0.890061	-1.027763
F	-3.440869	4.274766	2.178780	B	-2.312553	-0.102903	0.277696
F	-2.969010	5.588444	-0.151044	C	-2.964188	1.373077	0.403421
C	-3.800786	-1.519642	-2.023511	C	-2.846069	-0.986627	-0.970736
C	-5.123619	-0.797531	-0.231000	C	-2.146156	-0.922960	1.665696
C	-4.909833	-2.059762	-2.658767	C	-2.861580	2.231164	-0.682905
C	-6.259100	-1.320232	-0.822527	C	-3.569003	1.920634	1.525186
C	-6.147812	-1.955488	-2.051441	C	-3.276436	3.548286	-0.675212
F	-2.617624	-1.667503	-2.664683	C	-4.013826	3.236218	1.576786
F	-5.260878	-0.201671	0.959037	C	-3.861645	4.056837	0.473846
F	-4.794819	-2.673935	-3.836372	F	-2.304340	1.777610	-1.822918
F	-7.450407	-1.225680	-0.237155	F	-3.752433	1.195387	2.633728
F	-7.226140	-2.464998	-2.639333	F	-3.104062	4.328829	-1.741281
H	-1.642273	-0.297896	-0.825706	F	-4.581828	3.715905	2.680112
				F	-4.270097	5.320515	0.514042
				C	-2.086011	-2.064576	-1.403643
C-TS1'				C	-3.995470	-0.749188	-1.709362
C	3.922507	1.185380	-3.095569	C	-2.393614	-2.842980	-2.502245
C	3.014903	1.891264	-2.079419	C	-4.354529	-1.511356	-2.814245
H	3.339976	0.551031	-3.769252	C	-3.547904	-2.560795	-3.216177
H	2.045780	2.127141	-2.516098	F	-0.958314	-2.376232	-0.736124
Si	4.280358	0.029875	-0.823663	F	-4.826010	0.248286	-1.387575
C	5.284716	0.801651	0.536237	F	-1.598750	-3.843286	-2.880977
C	6.586430	0.320824	0.733199	F	-5.466274	-1.239468	-3.492546
C	4.822345	1.830358	1.365059	F	-3.874567	-3.291998	-4.276109
C	7.404370	0.862001	1.718451	C	-1.393066	-0.368036	2.692500
H	6.967124	-0.486365	0.113861	C	-2.625360	-2.199639	1.923231
C	5.634224	2.367344	2.356620	C	-1.085509	-1.014897	3.872628
H	3.812568	2.208304	1.242852				

C	-2.353914	-2.886944	3.100782	Si	-3.624809	0.907003	-0.836525
C	-1.575506	-2.295526	4.078308	C	-4.828189	-0.208824	-1.698468
F	-0.892845	0.872618	2.538301	C	-6.204936	-0.127978	-1.455392
F	-3.384016	-2.847737	1.032916	C	-4.360153	-1.180295	-2.593498
F	-0.322239	-0.433169	4.796730	C	-7.088283	-1.003218	-2.077634
F	-2.834639	-4.112355	3.294149	H	-6.590347	0.625384	-0.774719
F	-1.299726	-2.945251	5.203599	C	-5.240421	-2.060863	-3.211620
H	-1.102813	0.168764	-0.055428	H	-3.299950	-1.247722	-2.818025
Si	0.682749	0.517866	-0.510278	C	-6.604895	-1.972149	-2.951004
C	0.473712	2.275318	0.125821	H	-8.151328	-0.930264	-1.882157
C	0.273597	0.089599	-2.293392	H	-4.865321	-2.808893	-3.899527
C	1.192109	-0.840892	0.669464	H	-7.292444	-2.656119	-3.434248
H	-0.358419	2.230132	0.831373	C	-4.428266	2.405752	-0.107997
H	1.357311	2.506335	0.731855	C	-4.249290	2.717458	1.245187
H	-0.804525	-0.070855	-2.347422	C	-5.225691	3.249489	-0.893028
H	0.448887	0.965040	-2.925917	C	-4.844562	3.845661	1.799498
H	1.770330	-1.574845	0.100552	H	-3.640053	2.070149	1.868783
H	0.284120	-1.367078	0.963461	C	-5.816842	4.379397	-0.341801
C	0.203319	3.399694	-0.891252	H	-5.385921	3.023911	-1.943183
H	1.113307	3.743558	-1.381102	C	-5.625577	4.676920	1.004527
H	-0.496114	3.096982	-1.670913	H	-4.698825	4.076105	2.847940
H	-0.229551	4.265578	-0.385746	H	-6.426139	5.027912	-0.959569
C	1.950633	-0.389791	1.923521	H	-6.087809	5.557698	1.434094
H	1.371250	0.328910	2.505683	O	-2.344302	1.270513	-1.835359
H	2.158956	-1.246074	2.569536	O	-2.757785	0.111264	0.372052
H	2.908609	0.079926	1.692717	B	2.226317	0.132907	-0.244343
C	1.016570	-1.133985	-2.844083	C	2.705046	-1.149441	-1.116287
H	0.730398	-1.326061	-3.880531	C	2.835990	1.568153	-0.693635
H	2.097476	-0.990564	-2.817399	C	2.426581	-0.287191	1.321621
H	0.793156	-2.032374	-2.266179	C	1.846770	-2.047417	-1.720467
H	4.486855	1.905854	-3.688062	C	4.053984	-1.468362	-1.202248
C	3.651269	3.152324	-1.505232	C	2.273521	-3.190217	-2.380895
C	3.633155	4.304998	-2.509368	C	4.530800	-2.589814	-1.856276
H	4.680538	2.938445	-1.202135	C	3.627793	-3.459962	-2.450679
H	3.105542	3.437015	-0.602829	F	0.511033	-1.845183	-1.688644
H	4.036704	5.209337	-2.053562	F	4.950391	-0.653203	-0.633980
H	4.238151	4.087151	-3.391305	F	1.396358	-4.022549	-2.942154
H	2.617354	4.526582	-2.846644	F	5.833904	-2.848979	-1.920411
				F	4.062821	-4.547004	-3.079869
C-TS2'				C	2.743594	2.690030	0.124747
C	-1.146312	0.553860	-1.599425	C	3.417787	1.810725	-1.934454
C	-0.816005	0.579276	-0.117859	C	3.205522	3.947376	-0.222861
H	-0.338349	1.051187	-2.140409	C	3.898502	3.052735	-2.324391
H	-0.540385	-0.329433	0.392717	C	3.793391	4.129656	-1.462797

F	2.170157	2.590001	1.339250	H	-1.447871	1.527092	2.535721
F	3.542101	0.831966	-2.839326	H	0.285355	1.193709	2.347406
F	3.081570	4.976454	0.612667				
F	4.450894	3.219342	-3.523270	C-int4'			
F	4.240469	5.326844	-1.824220	C	-1.243289	-0.636345	2.817133
C	1.599986	-1.259607	1.868532	C	-2.333330	-1.530553	2.241301
C	3.409948	0.183165	2.183405	H	-1.537704	-0.262790	3.801257
C	1.664037	-1.695935	3.179073	H	-2.005610	-1.906302	1.264535
C	3.518976	-0.228853	3.505680	Si	-0.484045	0.468106	0.444314
C	2.634876	-1.166517	4.012464	C	0.188575	2.169979	0.111455
F	0.645582	-1.838626	1.100014	C	0.524754	2.542867	-1.195505
F	4.313123	1.072948	1.768325	C	0.474976	3.056993	1.154895
F	0.803459	-2.608422	3.638122	C	1.156661	3.754189	-1.452170
F	4.467570	0.267037	4.293937	H	0.288777	1.878687	-2.023183
F	2.724184	-1.563417	5.276770	C	1.098517	4.274557	0.901131
H	1.000990	0.259170	-0.423064	H	0.208936	2.780999	2.169642
Si	-2.994234	-1.371248	1.238080	C	1.448311	4.618421	-0.400682
C	-2.250302	-2.704359	0.150830	H	1.418308	4.027156	-2.467815
C	-2.134923	-1.135057	2.886169	H	1.316027	4.953255	1.717630
C	-4.849781	-1.573020	1.503952	H	1.941212	5.563362	-0.597820
H	-2.981999	-2.949242	-0.627854	C	-1.837992	0.048067	-0.777208
H	-1.377361	-2.295914	-0.368330	C	-1.816184	-1.142135	-1.512079
H	-1.062780	-0.973970	2.736727	C	-2.907661	0.929945	-0.977689
H	-2.528297	-0.206409	3.316122	C	-2.831702	-1.448048	-2.413772
H	-5.346039	-0.628326	1.251732	H	-0.994871	-1.837676	-1.371255
H	-5.018200	-1.707405	2.577486	C	-3.929482	0.626275	-1.870114
C	-1.819126	-3.979742	0.893485	H	-2.941451	1.867574	-0.429458
H	-0.993196	-3.765989	1.574401	C	-3.891062	-0.564656	-2.590175
H	-2.636248	-4.413566	1.476555	H	-2.797789	-2.374352	-2.975516
H	-1.477242	-4.739270	0.188537	H	-4.752634	1.317448	-2.008458
C	-5.496926	-2.731474	0.730117	H	-4.685278	-0.801643	-3.288511
H	-5.054651	-3.689702	1.014220	O	-1.004743	0.509925	2.007791
H	-6.568649	-2.788919	0.930912	O	0.667314	-0.686206	0.295575
H	-5.370289	-2.617237	-0.348360	H	-2.443702	-2.408613	2.887101
C	-2.348905	-2.279735	3.891485	Si	2.142092	-1.298323	-0.168475
H	-1.900925	-2.031154	4.854838	C	2.959495	-2.012532	1.364537
H	-3.410626	-2.474025	4.063158	C	1.780184	-2.605629	-1.469640
H	-1.888490	-3.206977	3.552747	C	3.219228	0.058733	-0.892669
H	-1.219569	-0.475714	-1.950253	H	2.805640	-1.289780	2.174045
C	-0.688396	1.902514	0.547133	H	2.419484	-2.917299	1.664859
C	-0.527540	1.863137	2.058911	H	0.975269	-3.245043	-1.089704
H	-1.531029	2.530139	0.241445	H	1.369361	-2.091035	-2.346467
H	0.186696	2.370586	0.078404	H	2.683364	0.516841	-1.731984
H	-0.284229	2.857344	2.432652	H	4.106694	-0.416401	-1.328982

C	4.459776	-2.313420	1.218266
H	4.651101	-3.060367	0.445435
H	5.020263	-1.416096	0.944940
H	4.883448	-2.692505	2.150716
C	3.646099	1.145428	0.106208
H	4.185158	0.718513	0.956298
H	4.301121	1.882690	-0.363237
H	2.781992	1.683629	0.500271
C	2.976863	-3.474220	-1.883423
H	2.725879	-4.130025	-2.719722
H	3.832412	-2.866295	-2.190135
H	3.303638	-4.110439	-1.057974
H	-0.309948	-1.199080	2.928222
C	-3.675968	-0.814584	2.092149
C	-4.634948	-1.572865	1.178915
H	-3.503292	0.184810	1.685408
H	-4.120770	-0.676389	3.083418
H	-5.601473	-1.070058	1.106894
H	-4.218171	-1.643917	0.169950
H	-4.809540	-2.588378	1.545740