Supporting Information

1,5-X Insertions of Free Alkylidene Carbenes: A Theoretical Study

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S1. Benchmark Calculations

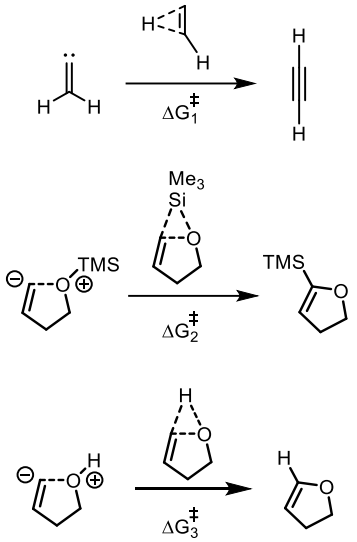
To assess the performance of different functionals (B3LYP[1], B3LYP-D3(BJ)[1,2], M06-2X[3], PBE0-D3(BJ)[2,4], ωB97X-D[5], BMK-D3(BJ)[2,6], BP86[7]) on the structures of the alkylidene carbene, benchmark calculations were carried out by optimizing the alkylidene carbene with 6-31+G(d,p) basis set (**Table S1**). The results from the method beyond CCSD(T)[8] were utilized as reference. M06-2X performs best on the geometry optimization of the simplest alkylidene carbene among these functionals.

Table S1. Structures of alkylidene carbene optimized with different computational methods.

Method[a]	C=C(Å)	C-H(Å)	H-C-H (°)
B3LYP	1.30219	1.0908	118.84
B3LYP-D3(BJ)	1.3022	1.0908	119.01
M06-2X	**1.2988**	**1.0894**	**119.61**
PBE0-D3(BJ)	1.3004	1.0904	119.05
ωB97X-D	1.2997	1.0896	119.32
BMK-D3(BJ)	1.3019	1.0934	119.20
BP86	1.3113	1.1001	118.18
Beyond CCSD(T)[8]	**1.2982**	**1.0844**	**120.05**

[a]Computed with 6-31+G(d,p) basis set.

Table S2. Three represented reactions of alkylidene carbene computed by different computational methods.



Method[a]	$\Delta G_1^{\ddagger}$ (kcal/mol)	$\Delta G_2^{\ddagger}$ (kcal/mol)	$\Delta G_3^{\ddagger}$ (kcal/mol)	RMSD
CCSD(T)	**1.3**	**0.65**	**11.6**	**0.0**

B3LYP-D3(BJ)	2.2	0.71	11.5	0.5
B3LYP	2.1	0.74	11.3	0.5
M06-2X	0.1	0.72	11.9	0.7
BP86	-1.3	0.42	5.7	3.7
PBE0-D3(BJ)	-0.2	0.36	4.8	4.0
BMK-D3(BJ)	1.7	0.57	12.1	0.4
ωB97X-D	**1.6**	**0.63**	**11.7**	**0.2**
Experimental estimation[10]	1.3-2	/	/	/

[a]Computed with maug-cc-PVTZ basis set based on the optimized structures at M06-2X/6-31+G(d,p).

To assess the performance of different functionals (B3LYP[1], B3LYP-D3(BJ)[1,2], M06-2X[3], PBE0-D3(BJ)[2,4], ωB97X-D[5], BMK-D3(BJ)[2,6], BP86[7]) on the 1,2 migrations and 1,5 insertions of the alkylidene carbenes, benchmark calculations were carried out by performing gas-phase single-point energy calculations (with the maug-cc-PVTZ basis set) on the optimized geometries computed at the M06-2X/6-31+G(d,p) level. Three reactions including 1,2-H migration, 1,5 O-H insertion, 1,5 O-Si insertion were selected. The results from CCSD(T)[9] based on M06-2X/6-31+G(d,p) geometries in the gas phase were utilized as reference. The smallest root-mean-square deviation (RMSD) was obtained with ωB97X-D, which also gives a comparable activation free energy of 1,2-H migration with the experimental estimation[10].

S2. Mechanisms of Reaction 2c and 2d.

Mechanism of 1,5 O-allyl insertion in reaction 2c.

It's well-known that allyl group has high migratory aptitudes in the Steven rearrangement through 2,3 sigmatropic rearrangement, however, in reaction **2c**, the authors only isolated the major product dihydrofuran and no insertion product was observed, checked by 1H NMR and TLC. This result led us to study the mechanism of 1,5 O-allyl insertion and answer the question why the 1,5 O-allyl insertions could not happen even though the oxonium ylide may form.

The free energy surface of reaction **2c** is shown in Figure **S1**. The alkylidene carbene **19** could easily form the oxonium ylide **20** with a decrease of free energy of 11.2 kcal/mol. **19** could also undergo 1,2 migrations to give corresponding alkyne through **TS25**, requiring an activation free energy of 4.8 kcal/mol. Consistent with the above discussion, the predicted Gibbs free energy of activation for 2,3 sigmatropic rearrangements via **TS26** is lower than that for 1,2 allyl rearrangement of oxonium ylide via **TS27** by 9.9 kcal/mol. However, the energy difference of 2.9 kcal/mol between **TS26** and **TS25** indicates that 2,3 sigmatropic rearrangement could not happen.

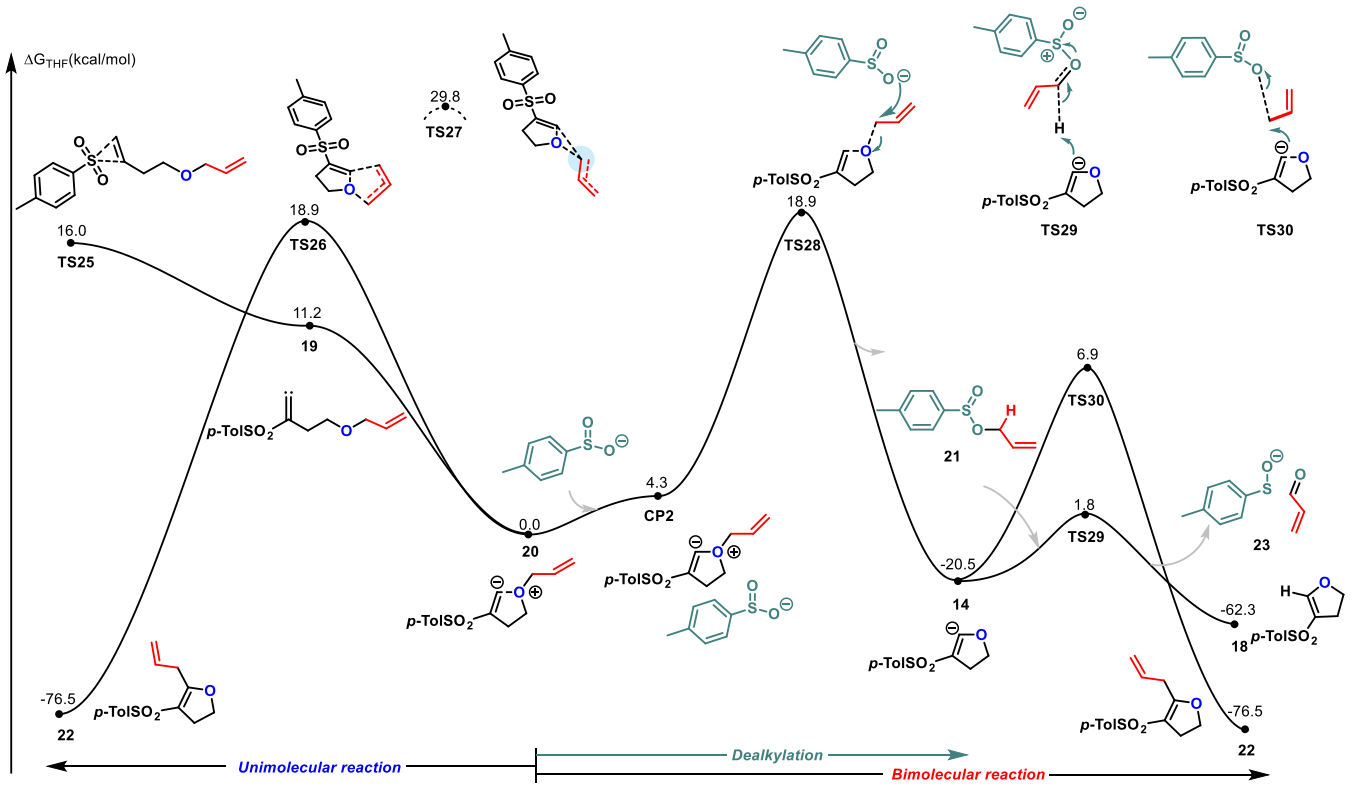


Figure S1. Computed reaction pathways for 1,5 O-allyl insertions in **reaction 2c**.

The dealkylation process, which is similar to reaction **2a**, was also studied. The nucleophiles *p*-TolSO_2Na could attack the carbon atom of allyl group via **TS28**, requiring an activation free energy of 18.9 kcal/mol. Then the anion **14** could attract the hydrogen atom and the carbon atom to give **18** and **22**, respectively. Our calculation showed that the protonation is much favored over the alkylation. The predicated Gibbs free energies of activation for the protonation (**TS29**) and alkylation (**TS30**) are 22.3 kcal/mol and 27.4 kcal/mol, respectively. The protonation gives the sulfenate anion and acrolein **23** (this is a volatile species and we speculate it could escape from the reaction system and was not detected by the experimentalists). The generated sulfenate anion is a highly reactive species that could easily be oxidized by air or act as a nucleophile[11] to further interact with **20**. Therefore, unlike reaction **2a**, the bimolecular reaction in **reaction 2c** could only afford **18** rather than the desired **22**, answering why the 1,5 O-allyl insertion failed**.**

The overestimation of entropy in bimolecular reactions.

A key problem for this free energy surface in **Figure S1** is that bimolecular reactions seem to have higher free energies of transition state (**TS28** vs. **TS25**) and the alkyne formation as an intramolecular process was then become favored, disagreeing with the experimental results. However, the continuum dielectric models do not consider properly the changes of solvation entropy in bimolecular reactions, which led to incorrect results.[12] Though there has been no accurate method to calculate entropy in solution, previous experiments provide us some information. According to Wertz and Abraham[13], various molecules lose a constant fraction (~0.5) of their entropy when they are dissolved in water. For other unrelated systems, authors also found the reaction entropy in solution was overestimated by nearly 50%.[14] If we follow the approach of Lau and others[15] who assigned the solvation entropy of each species as half of its gas-phase entropy, the activation free energy of dealkylation (**TS28**) should decrease by 6.0 kcal/mol, which is favored over **TS25**. With this entropy correction, the energy difference of 2.9 kcal/mol between **TS25** and **TS28** is relatively small. Thus, the dealkylation could take place in reaction **2c** and give the proton-trapping product with yield of 36%.

Mechanism of 1,5 O-benzyl insertion in reaction 2d.

In order to answer the question why benzyl group could undergo 1,2 Stevens rearrangement via homolytic pathways in general oxonium ylide but failed in **reaction 2d**. We carried out DFT calculations to study the mechanisms of **reaction 2d** shown in **Figure S2**. This energy surface is similar to that from **reaction 2c**. Both the dealkylation (**TS33**) and 1,2 migration (**TS31**) are favored over 1,5 O-benzyl

insertion via concerted transition state **TS32** by 9.7 and 14.1 kcal/mol. Surprisingly, the expected homolytic pathway via diradical species **26** with a computed $\langle S^2 \rangle$ of 0.32 was highly endergonic by 39.2 kcal/mol. Our calculation indicated that 1,2 migration giving corresponding alkynes could take place, which is observed experimentally. Similarly, the overestimation of entropy by 50% for bimolecular reactions may cause the increase of activation free energy for the bimolecular reaction (**TS33**) by 6.7 kcal/mol. Thus, the dealkylation may also take place, giving dealkylation product. This is consistent with experimental observation in **reaction 2d**.

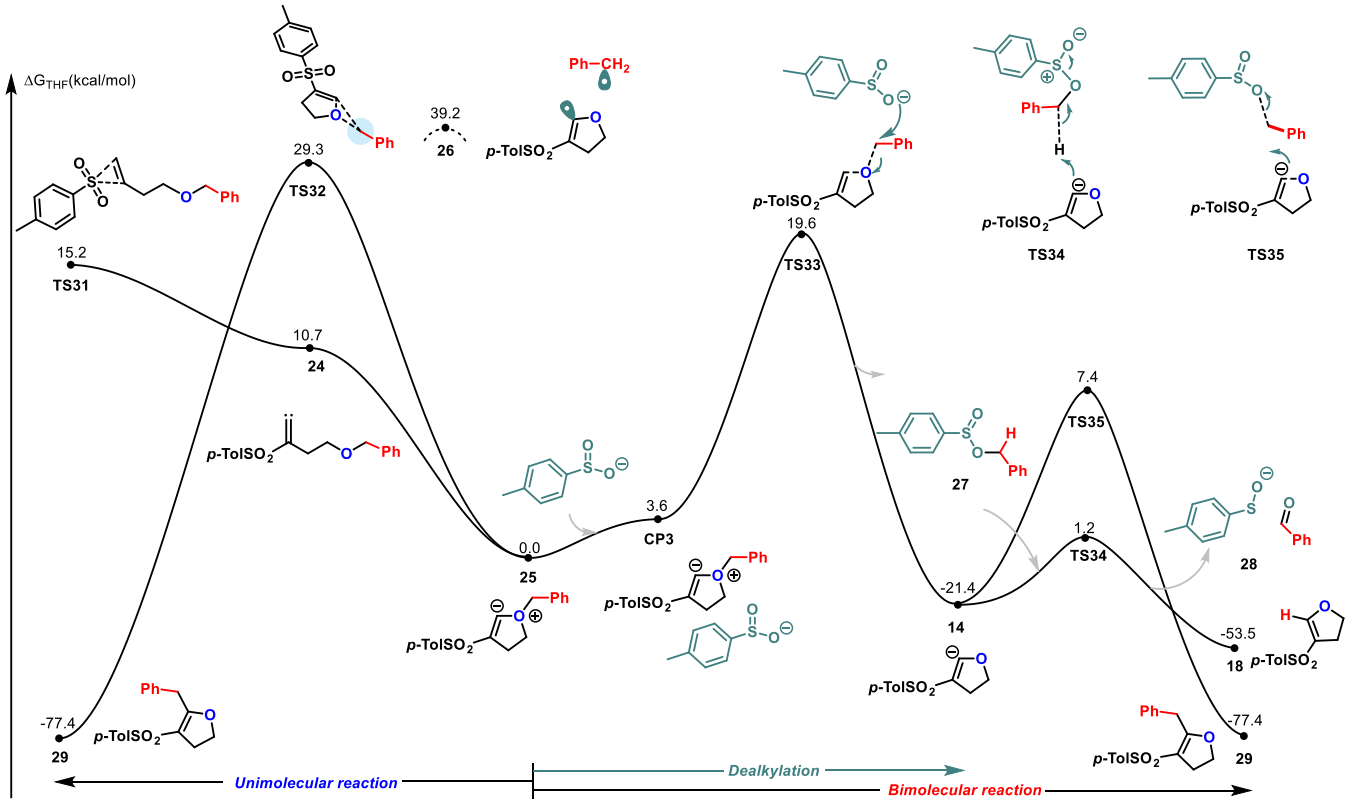


Figure S2. Computed reaction pathways for 1,5 O-benzyl insertions in **reaction 2d**.

S3. IBO Analysis of 1,5 S-H/O-H Insertion

Figure S3a shows the corresponding electron flow of 1,5 S-H insertion. One localized IBO was transformed from a S-H σ-bond into a part of the C-S bond while the other IBO was transformed from carbenic carbene into a part of C-H bond. This scenario is consistent with the expected concerted pathway previously described for C-H insertion of alkylidene carbene. While for 1,5 O-H insertion, the localized IBO was transformed from a O-H σ-bond into a part of the lone pair of oxygen atom and the other IBO was transformed from the lone pair of carbon into a part of C-H bond. Thus, 1,5 S-H insertion proceeds through a concerted pathway, while the 1,5 O-H insertion could be considered as a 1,2-proton transfer via ylide compared with 1,5 S-H insertion.

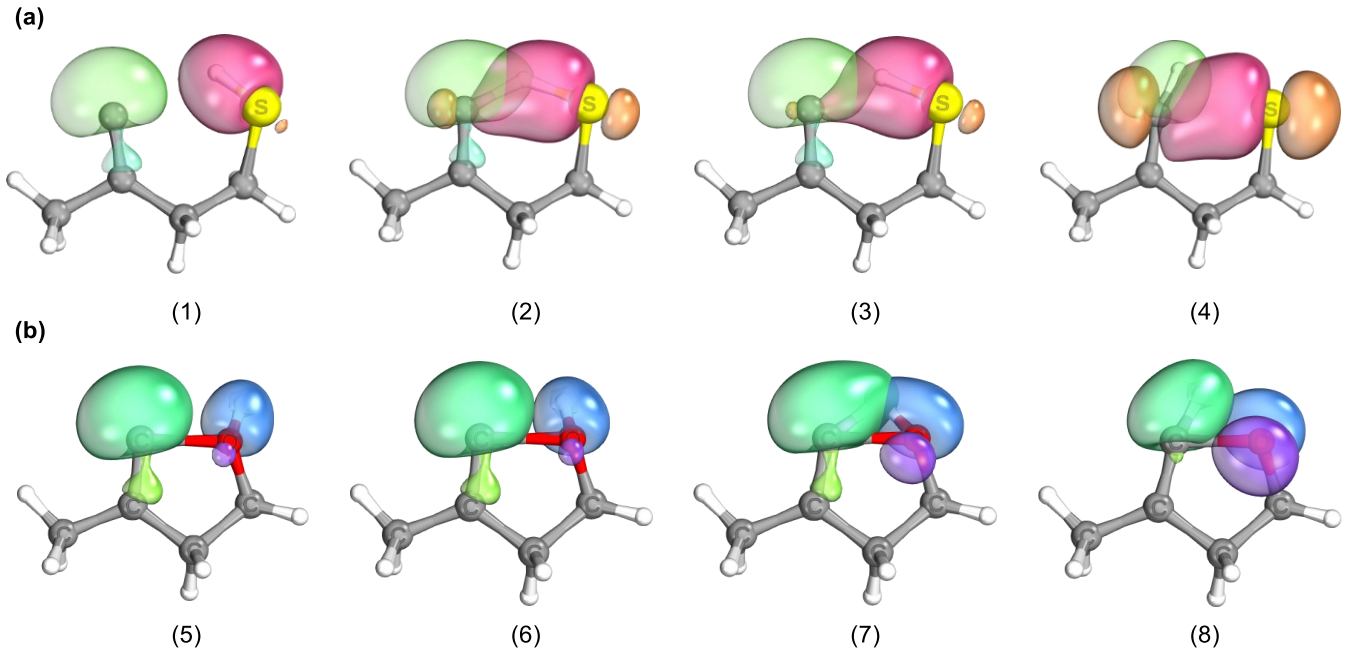
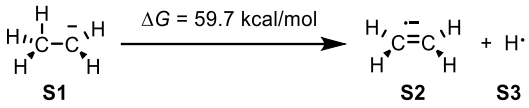


Figure S3. (a) Changes of carbene IBO (green) and S-H (pink) along IRC (b) Changes of carbene IBO (green) and O-H (blue) along IRC.

S4. 1,2-Proton Shift of Ethyl Anion via Diradical Mechanism

In ref. 22a in the main text, the authors did not compute the 1,2-proton shift of ethyl anion via a diradical mechanism, which was found in Stevens rearrangement, see ref. 8a and also part e) in the main text. We found that the dissociation of ethyl anion into ethylene anion radical and hydrogen atom is highly endergonic by 59.7 kcal/mol in terms of Gibbs free energy.



	G (in gas phase)[a] (hartree)
S1	-79.102063
S2	-78.493649
S3	-0.513322

[a] Computed at (U)ωB97X-D/6-311+G(d,p)

Scheme S1. 1,2-Proton Shift of Ethyl Anion via Diradical Mechanism.

S5. Reference

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S6. Computed Energies of the Stationary Points

Table S3. Computed Energies for the Stationary Points.

Thermal corrections to Gibbs energies (TCGs), single-point energies (SPEs) in gas phase and solvent.

	SPEs (in gas phase)[a] (hartree)	**TCGs (in gas phase)[a] (hartree)**	**SPEs (under SMD model)[b] (hartree)**
THF	-232.352215	0.089256	-232.469143
***p*-TolSO$_2^-$**	-819.414971	0.089092	-819.730594
1	-678.933209	0.174808	-679.178968
2	-678.944164	0.181666	-679.190825
3	-679.015716	0.184254	-679.2581
4	-678.856947	0.17807	-679.060308
5	-269.791347	0.077321	-269.991568
5'	-408.873789	0.076579	-409.080207
6	-679.013241	0.175773	-679.257819
7	-270.313288	0.085199	-270.445848
8	-270.315567	0.089948	-270.452287
8'	-270.237959	0.080313	-270.28044
9	-270.43037	0.092672	-270.558245
10	-270.393363	0.086926	-270.524823
11	-1280.93776	0.253759	-1281.393156
12	-1280.958622	0.260914	-1281.416626
13	-231.468659	0.079289	-231.669166
14	-1049.29208	0.155895	-1049.700983
15	-1051.128837	0.193544	-1051.477589
16	-1281.065839	0.261545	-1281.52289
17	-231.130327	0.066867	-231.237527
18	-1049.889203	0.170486	-1050.246897
19	-1166.410688	0.217949	-1166.817182
20	-1166.430552	0.225014	-1166.842071
21	-936.601052	0.157185	-936.903329
22	-1166.556622	0.225536	-1166.964425
23	-936.074157	0.138464	-936.41985
24	-1320.015649	0.262351	-1320.474465
25	-1320.036479	0.270545	-1320.499752
26	-1320.007653	0.263432	-1320.430195
27	-1090.210587	0.203142	-1090.562926
28	-1089.678774	0.187878	-1090.067446
29	-1320.163131	0.2707	-1320.62331

30	-593.274769	0.080662	-593.428552
30'	-593.271671	0.078465	-593.426279
31	-593.286867	0.083984	-593.449676
32	-593.354542	0.081187	-593.508062
33	-593.402341	0.088613	-593.553162
34	-368.334724	0.177312	-368.52058
35	-368.378165	0.186112	-368.572406
36	-368.414502	0.17831	-368.600094
37	-368.457823	0.184574	-368.641042
38	-790.964963	0.299319	-791.296862
39	-791.008113	0.309066	-791.344301
40	-791.044526	0.300277	-791.375313
41	-790.962254	0.297914	-791.30221
42	-791.101181	0.3062	-791.431576
S-Me	-309.596582	0.111342	-309.745709
S-tBu	-427.495989	0.190216	-427.706043
S-allyl	-386.959863	0.140591	-387.141725
S-benzyl	-540.564875	0.18233	-540.799011
S-THF	-501.487259	0.175771	-501.718122
S-THP	-540.786886	0.204674	-541.038032
S-dioxane	-576.683869	0.179423	-576.943522
S'-Me	-309.605328	0.117366	-309.75805
S'-tBu	-427.506328	0.197118	-427.717846
S'-allyl	-386.968595	0.147236	-387.152013
S'-benzyl	-540.575816	0.192169	-540.810847
S'-THF	-501.497674	0.183125	-501.726838
S'-THP	-540.791325	0.210759	-541.044092
S'-dioxane	-576.686698	0.186581	-576.948569
IN1	-277.266793	0.072468	-277.415794
IN2	-277.339124	0.080028	-277.48038
IN3	-375.255679	0.163461	-375.455658
IN4	-375.354923	0.170295	-375.555054
CP1	-2100.426979	0.376531	-2101.166169
CP2	-1985.894382	0.339043	-1986.587762
CP3	-2139.502014	0.384846	-2140.246849
TS1	-678.941475	0.183432	-679.184411
TS2	-678.917998	0.173983	-679.167722
TS3	-270.293752	0.085744	-270.423493
TS4	-270.298008	0.085026	-270.434546
TS5	-309.541324	0.114834	-309.691352
TS6	-427.444499	0.193693	-427.659317
TS7	-386.913832	0.144818	-387.0968

TS7'	-386.938376	0.148637	-387.117967
TS8	-540.514349	0.188297	-540.750538
TS8'	-540.529295	0.189518	-540.768444
TS9	-501.449006	0.178906	-501.688535
TS10	-540.7399	0.207091	-541.004536
TS11	-576.647336	0.18243	-576.921007
TS12	-309.581313	0.111176	-309.734424
TS13	-427.480786	0.189919	-427.69484
TS14	-386.944556	0.140358	-387.130413
TS15	-540.549437	0.181706	-540.787677
TS16	-501.472005	0.175427	-501.706806
TS17	-540.768506	0.204822	-541.023796
TS18	-576.669054	0.181748	-576.93187
TS19	-1280.93135	0.254459	-1281.386079
TS20	-1280.930222	0.257351	-1281.397151
TS21	-2100.397163	0.365944	-2101.144705
TS21'	-2100.391192	0.368489	-2101.146483
TS22	-1281.608877	0.262689	-1282.118252
TS23	-2100.403284	0.361304	-2101.145655
TS24	-2100.414618	0.371111	-2101.155738
TS25	-1166.403372	0.217958	-1166.809566
TS26	-1166.400034	0.221833	-1166.808844
TS27	-1166.379782	0.223056	-1166.792671
TS28	-1985.863001	0.332092	-1986.557576
TS29	-1985.891758	0.32853	-1986.581228
TS30	-1985.890121	0.334307	-1986.57892
TS31	-1320.008296	0.261707	-1320.466758
TS32	-1319.980676	0.265637	-1320.448109
TS33	-2139.471341	0.380921	-2140.21743
TS34	-2139.503349	0.373625	-2140.242366
TS35	-2139.500063	0.380689	-2140.23953
TS36	-593.259141	0.078777	-593.416103
TS37	-593.271494	0.080565	-593.425111
TS38	-368.319451	0.176229	-368.509055
TS39	-368.332224	0.179729	-368.517131
TS39'	-368.273283	0.172939	-368.458566
TS40	-790.942551	0.299802	-791.277328
TS41	-790.954586	0.303152	-791.291344
TS42	-790.928798	0.304649	-791.263171
TS-R1	-678.926857	0.176485	-679.172767
TS-R2	-270.305252	0.086475	-270.439667
TS-R3	-1280.932934	0.255431	-1281.388098

TS-R4	-593.265387	0.080231	-593.420378
TS-R5	-593.271118	0.080673	-593.425513
TS-R6	-368.327761	0.178606	-368.51399
TS-R7	-790.962208	0.301821	-791.293359
TS-R-Me	-309.590944	0.113048	-309.740273
TS-R-tBu	-427.490254	0.192061	-427.700333
TS-R-allyl	-386.954252	0.142558	-387.136314
TS-R-benzyl	-540.559168	0.186354	-540.793576
TS-R-THF	-501.481804	0.177885	-501.712599
TS-R-THP	-540.78151	0.206698	-541.032534
TS-R-dioxane	-576.677778	0.182807	-576.937769

[a] Computed at (U)M06-2X/6-31+G(d,p)

[b] *Computed at* SMD(THF/Et_2O)/(U)ωB97X-D/maug-cc-PVTZ//(U)M06-2X/6-31+G(d,p)

S7. Cartesian Coordinates for the Stationary Points

1

C	4.545758	-0.576112	0.000203
H	4.610717	-1.205882	-0.891362
H	4.610455	-1.205892	0.891780
H	5.393683	0.112557	0.000331
C	3.207495	0.155667	0.000007
C	1.927905	-0.642448	-0.000216
H	1.914088	-1.294180	0.881687
H	1.914369	-1.294138	-0.882154
C	0.677754	0.224447	-0.000414
H	0.678447	0.872127	0.889190
O	-0.446550	-0.626938	-0.000742
C	3.340459	1.452581	0.000052
Si	-2.014491	-0.028100	0.000030
C	-3.110609	-1.539986	-0.002739
H	-2.920912	-2.155958	0.881246
H	-4.168764	-1.259732	-0.002476
H	-2.920549	-2.152993	-0.888702
C	-2.286719	1.022429	-1.532024
H	-1.657338	1.918389	-1.527401
H	-2.064381	0.455907	-2.441758
H	-3.328801	1.354761	-1.588710
C	-2.287333	1.017091	1.535617
H	-1.658216	1.913245	1.534209
H	-3.329530	1.348922	1.593184
H	-2.065049	0.447512	2.443447
H	0.678806	0.872249	-0.889919

2

C	3.571644	0.947015	0.114371
H	4.261007	0.698177	-0.701996
H	4.053772	0.643573	1.051515
H	3.439010	2.031012	0.129858
C	2.249295	0.261800	-0.067062
C	2.181530	-1.252203	-0.153438
H	2.777425	-1.740804	0.625103
H	2.546895	-1.611274	-1.124638
C	0.700502	-1.538944	0.030625
H	0.305484	-2.361324	-0.569244
O	0.075337	-0.307169	-0.420083
C	1.102827	0.941444	-0.219419
Si	-1.536097	0.181884	0.026809
C	-2.047557	1.489749	-1.188938
H	-1.930153	1.126424	-2.214057
H	-3.096645	1.765705	-1.039163
H	-1.418783	2.374042	-1.066143
C	-1.504701	0.746377	1.803036
H	-1.057695	-0.012392	2.453642
H	-0.913589	1.660685	1.892800
H	-2.521283	0.938340	2.162465
C	-2.538786	-1.390683	-0.166419
H	-2.232593	-2.165358	0.544022
H	-3.598046	-1.180290	0.015579
H	-2.450777	-1.796985	-1.179059
H	0.450101	-1.685884	1.088112

3

C	-1.471219	2.246547	-0.041267
H	-1.960156	2.663715	0.847750
H	-2.019313	2.623660	-0.912509
H	-0.454571	2.639396	-0.084391
C	-1.496510	0.752809	-0.001437
C	-2.800853	-0.013856	0.114776
H	-3.550684	0.311764	-0.613636
H	-3.234890	0.116917	1.115771
C	-2.328157	-1.448172	-0.143840
H	-2.781131	-2.200328	0.504105
O	-0.912565	-1.442391	0.102884
C	-0.479801	-0.122323	0.023461
Si	1.404085	-0.028001	-0.000814
C	1.992235	-0.934748	-1.538795
H	1.659702	-0.426091	-2.448826
H	3.085213	-0.997329	-1.562270
H	1.590198	-1.952211	-1.552317
C	2.019443	-0.914928	1.537603
H	1.704250	-0.393737	2.446713
H	1.615000	-1.930820	1.572889
H	3.112553	-0.978916	1.541486
C	2.033703	1.745156	-0.018544
H	1.702683	2.306907	0.860211
H	3.129199	1.730848	-0.009451
H	1.717964	2.284801	-0.916528
H	-2.485733	-1.730338	-1.192414

4

C	1.398654	2.314213	0.168580

H	2.212672	2.859163	0.659660
H	0.494314	2.456132	0.775117
H	1.227243	2.763397	-0.812182
C	1.718366	0.863832	0.048624
C	2.033533	-0.044093	1.234905
H	1.286337	0.063426	2.030009
H	3.020172	0.180163	1.659641
C	1.966098	-1.442346	0.588597
H	2.774193	-2.116834	0.870778
O	2.073808	-1.223185	-0.852530
C	1.804735	0.077613	-1.017181
Si	-1.668404	-0.054120	0.147785
C	-1.734865	1.344469	-1.119463
H	-0.823294	1.357390	-1.725012
H	-2.589225	1.202134	-1.793015
H	-1.842511	2.322769	-0.641593
C	-3.285070	-0.104209	1.129231
H	-3.274849	-0.903033	1.876315
H	-3.465695	0.841708	1.647924
H	-4.130732	-0.285168	0.453582
C	-1.407156	-1.701450	-0.739533
H	-1.434120	-2.540802	-0.037293
H	-2.203107	-1.859104	-1.478346
H	-0.447402	-1.726189	-1.265848
H	0.997426	-1.920168	0.768948

5'

Si	0.000003	0.000016	0.000006
C	1.829206	0.107817	0.000047
H	2.310532	-0.871725	0.001841

H	2.164934	0.673623	-0.878410
H	2.165033	0.677133	0.876150
C	-1.007965	1.530082	-0.000048
H	-1.665938	1.537906	0.878348
H	-0.400459	2.436788	-0.001799
H	-1.668913	1.536237	-0.876178
C	-0.821199	-1.637927	-0.000009
H	-1.910173	-1.564922	-0.000423
H	-0.497320	-2.212713	-0.877058
H	-0.497987	-2.212380	0.877507

5

C	-2.206201	-0.013053	0.043423
H	-2.608886	0.464020	-0.868641
H	-2.595523	0.574919	0.892250
H	-2.630528	-1.021089	0.109064
C	-0.712606	-0.104070	0.028801
C	0.147582	1.139881	-0.130624
H	-0.093064	1.950010	0.575041
H	0.077208	1.572408	-1.147352
C	1.522024	0.531556	0.148663
H	2.335081	0.932806	-0.470927
O	1.390890	-0.869220	-0.101403
C	0.016197	-1.253844	-0.005088
H	1.786617	0.677865	1.210743

6

C	5.384033	0.638365	0.000375
H	5.300601	1.719497	-0.137701

H	6.002204	0.239566	-0.808147
H	5.900519	0.455428	0.946211
C	2.974623	-0.519107	0.000006
C	1.641447	-1.127925	-0.000091
H	1.513788	-1.765079	0.881343
H	1.514597	-1.766702	-0.880465
C	0.537334	-0.071982	-0.001557
H	0.643096	0.566707	0.886990
O	-0.708664	-0.734672	-0.001624
C	4.060992	0.011065	0.000225
Si	-2.160894	0.101533	0.000093
C	-3.484489	-1.216295	-0.002541
H	-3.394956	-1.854452	0.881517
H	-4.484596	-0.771191	-0.002497
H	-3.393912	-1.851994	-0.888258
C	-2.268674	1.184808	-1.530573
H	-1.503561	1.968089	-1.527308
H	-2.143108	0.591427	-2.441663
H	-3.244382	1.679744	-1.582372
C	-2.268754	1.178390	1.535278
H	-1.504004	1.962024	1.535208
H	-3.244677	1.672648	1.589449
H	-2.142692	0.581154	2.443779
H	0.643845	0.565130	-0.891130

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C	-2.392439	-0.630350	-0.000265
H	-2.414476	-1.263583	0.890928
H	-2.414918	-1.262373	-0.892286
H	-3.284800	-0.000316	0.000431

C	-1.106919	0.190041	0.000094
C	0.222683	-0.520706	0.000179
H	0.278517	-1.170884	-0.881198
H	0.279054	-1.169596	0.882480
C	1.412219	0.424913	-0.000738
H	1.375577	1.065844	-0.892290
O	2.574234	-0.384592	0.000705
H	3.357563	0.174813	-0.001671
C	-1.326454	1.475201	0.000542
H	1.375060	1.068239	0.889093

8

C	-2.254755	0.022295	-0.027964
H	-2.582005	0.617531	-0.887922
H	-2.612237	0.524970	0.878406
H	-2.731043	-0.958523	-0.087854
C	-0.756876	-0.115500	-0.006991
C	0.103346	1.121362	0.145450
H	0.022437	1.523459	1.164425
H	-0.202283	1.918141	-0.541681
C	1.509335	0.637747	-0.175918
H	1.751627	0.768328	-1.231135
O	1.485214	-0.801770	0.016363
H	1.758450	-1.061101	0.907865
C	-0.198823	-1.331098	-0.063226
H	2.299967	1.072521	0.438887

8‘

C	-2.266340	-0.060023	-0.040209

H	-2.650015	0.532714	-0.877854
H	-2.645105	0.394689	0.882437
H	-2.678902	-1.068016	-0.117127
C	-0.774955	-0.094136	-0.043007
C	0.119137	1.137262	0.089417
H	0.061034	1.560862	1.101603
H	-0.152942	1.926254	-0.619097
C	1.509984	0.550050	-0.223026
H	1.792405	0.717520	-1.266973
O	1.383150	-0.893022	-0.040169
H	0.983382	-0.278685	2.514632
C	0.065113	-1.121517	-0.072387
H	2.307308	0.889024	0.439001

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C	-2.227288	-0.016940	0.041925
H	-2.586494	-0.579005	0.911219
H	-2.619355	-0.517825	-0.851167
H	-2.659757	0.986059	0.084902
C	-0.735460	0.038506	0.010660
C	0.155582	-1.181832	-0.111579
H	0.060481	-1.634411	-1.107927
H	-0.077040	-1.957370	0.625262
C	1.543352	-0.562885	0.129283
H	1.863818	-0.709339	1.167308
O	1.395863	0.854027	-0.082994
C	0.053476	1.112988	-0.008112
H	-0.208861	2.163854	0.004953
H	2.322333	-0.923212	-0.543663

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C	3.281860	-0.287681	0.000086
H	3.692926	-0.248310	1.012142
H	3.853817	0.401168	-0.626963
H	3.427373	-1.299472	-0.387135
C	0.693519	0.379280	0.000015
C	-0.731271	0.722814	0.000030
H	-0.976797	1.325525	-0.880776
H	-0.976720	1.325503	0.880874
C	-1.612268	-0.522323	0.000061
H	-1.392607	-1.126388	-0.889974
O	-2.956177	-0.073915	-0.000138
H	-3.548678	-0.832313	0.000229
C	1.861971	0.069873	0.000214
H	-1.392768	-1.126169	0.890274

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C	-0.325122	-1.739497	-0.498792
C	0.751078	-1.085637	0.331467
H	0.845688	-1.646791	1.266659
H	0.433303	-0.066172	0.582709
C	2.086665	-1.033941	-0.394585
O	2.999120	-0.408649	0.484023
C	-0.281426	-2.225146	-1.712124
C	4.307114	-0.325837	-0.034703
O	4.353078	0.453502	-1.201370
C	5.159913	0.413964	0.982697
H	4.658176	-1.329910	-0.306248
C	4.597154	1.826944	-0.861633

C	4.804395	1.870072	0.659770
H	6.215554	0.211177	0.779079
H	4.924796	0.115822	2.005150
H	5.489965	2.145321	-1.409537
H	3.748846	2.434121	-1.190203
H	5.584692	2.576090	0.950493
H	3.877878	2.146829	1.168287
H	2.430176	-2.051566	-0.637069
H	2.006170	-0.465494	-1.329474
S	-1.963821	-1.876143	0.257976
O	-2.787922	-2.735170	-0.578304
O	-1.728730	-2.173180	1.664611
C	-2.566207	-0.207264	0.142031
C	-3.112347	0.226774	-1.064794
C	-2.478819	0.625532	1.251163
C	-3.578755	1.531078	-1.151113
H	-3.172457	-0.453027	-1.909851
C	-2.954192	1.931545	1.142863
H	-2.062211	0.246787	2.179257
C	-3.507453	2.399428	-0.051521
H	-4.011132	1.884737	-2.083163
H	-2.898539	2.592967	2.002587
C	-4.035662	3.805514	-0.165533
H	-5.124416	3.799189	-0.277672
H	-3.790228	4.395350	0.719885
H	-3.617512	4.309665	-1.041339

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C	-0.524355	0.711781	0.246946
C	-0.618972	1.198359	1.675123

H	-0.547841	2.286163	1.741732
H	0.163509	0.756692	2.303675
C	-2.002680	0.695706	2.047808
O	-2.184033	-0.449928	1.139081
C	-1.360067	-0.252064	-0.176327
C	-3.592990	-0.877710	0.956538
O	-4.336581	0.127647	0.406374
C	-3.642960	-2.073393	0.019724
H	-3.927835	-1.057752	1.980606
C	-4.329911	0.010800	-1.037053
C	-3.978693	-1.453859	-1.351415
H	-4.440922	-2.734206	0.368685
H	-2.700177	-2.620303	0.022823
H	-5.326079	0.308609	-1.367747
H	-3.580632	0.697022	-1.437955
H	-4.815246	-1.973208	-1.823102
H	-3.109227	-1.494236	-2.006916
H	-2.109964	0.318541	3.065940
H	-2.785435	1.417613	1.803102
S	0.723767	1.344663	-0.816130
O	0.383314	1.047910	-2.203765
O	0.985869	2.719889	-0.377266
C	2.173528	0.386709	-0.399723
C	2.329902	-0.878102	-0.964183
C	3.112591	0.909606	0.480059
C	3.450794	-1.627001	-0.630362
H	1.581102	-1.251881	-1.656432
C	4.232706	0.143318	0.803478
H	2.969765	1.907604	0.882847
C	4.416866	-1.127738	0.255189
H	3.587459	-2.613140	-1.066925

H	4.977544	0.544599	1.485338
C	5.638471	-1.947282	0.583775
H	6.311006	-2.000135	-0.278495
H	6.194632	-1.513573	1.417794
H	5.364142	-2.971956	0.850257

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C	-1.081650	-0.517105	-0.047520
O	-0.050261	-1.223667	-0.059138
C	-0.841489	0.929220	0.099699
H	-2.034804	-1.041929	-0.124894
C	1.180681	-0.385382	0.107555
C	0.679605	1.038201	-0.133101
H	-1.469356	1.513163	-0.580024
H	1.513255	-0.597650	1.124735
H	1.892131	-0.775860	-0.617087
H	1.150761	1.746507	0.547786
H	0.884149	1.353534	-1.157335
H	-1.156935	1.201961	1.120123

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C	-1.975669	-0.056353	-0.077152
C	-2.444834	-0.448516	1.310475
H	-2.957341	0.354737	1.846356
H	-1.620974	-0.808784	1.946939
C	-3.391050	-1.577188	0.897622
O	-2.964274	-1.993215	-0.420131
C	-2.191593	-1.025114	-1.037023
H	-3.374447	-2.451160	1.556073

H	-4.422861	-1.208345	0.815134
S	-0.874149	1.231542	-0.302715
O	-0.899171	1.763332	-1.671080
O	-0.998343	2.171634	0.832536
C	0.779100	0.521828	-0.119769
C	1.215467	-0.413559	-1.060207
C	1.594643	0.902124	0.935672
C	2.486927	-0.957179	-0.935216
H	0.539175	-0.711817	-1.858282
C	2.872697	0.345534	1.049456
H	1.221472	1.632277	1.647317
C	3.334445	-0.584965	0.119790
H	2.833339	-1.688074	-1.663385
H	3.517594	0.642160	1.874123
C	4.709737	-1.194938	0.239933
H	5.300703	-1.018152	-0.665032
H	5.255916	-0.772486	1.087894
H	4.648891	-2.279071	0.384212

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C	-2.437299	-1.097101	-0.359812
O	-3.167578	-0.031721	-0.870417
C	-3.109300	-1.475795	0.948378
H	-2.386933	-1.874778	-1.126244
C	-3.778796	0.704945	0.211666
C	-3.465183	-0.085148	1.490487
H	-2.450220	-2.051089	1.599824
H	-4.006692	-2.062448	0.726912
H	-3.351499	1.709980	0.222500
H	-4.850180	0.752500	-0.003452

H	-2.598693	0.348131	1.995718
H	-4.306733	-0.102252	2.185432
C	1.835522	-0.905578	-0.852869
C	3.160646	-1.127020	-0.501038
C	3.860381	-0.204215	0.289896
C	3.197976	0.946675	0.720570
C	1.867071	1.184419	0.374910
C	1.198739	0.248774	-0.400190
H	1.296775	-1.627959	-1.460259
H	3.664912	-2.027600	-0.842407
H	3.729148	1.670289	1.332932
H	1.338810	2.075918	0.699642
C	5.300926	-0.458810	0.653518
H	5.928833	-0.493156	-0.242232
H	5.688240	0.324831	1.308224
H	5.410211	-1.417791	1.168899
S	-0.496187	0.593388	-0.898376
O	-1.087315	-0.702897	-0.022022
O	-0.863992	1.846408	-0.188133

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C	0.694574	-1.299704	0.303748
C	0.607425	-2.042083	1.614580
H	0.787416	-3.111756	1.472620
H	-0.369219	-1.927716	2.094746
C	1.725302	-1.334247	2.407154
H	1.324027	-0.647301	3.157203
O	2.467504	-0.535291	1.454736
C	1.760771	-0.483328	0.299976
C	2.275578	0.488425	-0.724176

O	1.926580	1.802149	-0.269113
C	3.809898	0.465967	-0.851393
H	1.774228	0.289973	-1.672273
C	3.101350	2.599564	-0.118821
C	4.244884	1.609578	0.071289
H	4.087305	0.679848	-1.887517
H	4.234546	-0.500387	-0.572706
H	3.248249	3.206028	-1.023647
H	2.945043	3.265709	0.732787
H	5.215442	2.030524	-0.201165
H	4.280297	1.266171	1.108063
H	2.430473	-2.018594	2.879653
S	-0.518326	-1.478023	-0.942647
O	0.017589	-0.980979	-2.210126
O	-1.043239	-2.839915	-0.838209
C	-1.814116	-0.366426	-0.421069
C	-1.566582	1.007044	-0.414223
C	-3.043037	-0.887984	-0.040836
C	-2.585160	1.864363	-0.022291
H	-0.590769	1.396091	-0.697831
C	-4.055098	-0.008483	0.346084
H	-3.195992	-1.962391	-0.059779
C	-3.842365	1.370956	0.358629
H	-2.406609	2.936410	-0.010182
H	-5.023269	-0.403672	0.640707
C	-4.936690	2.324829	0.763085
H	-4.588240	3.015006	1.536897
H	-5.260318	2.926061	-0.092454
H	-5.807268	1.789825	1.148500

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C	-1.195216	-0.107363	0.013050
O	-0.347136	-1.171442	-0.099851
C	-0.600247	1.083603	0.060481
H	-2.246181	-0.365348	0.031553
C	0.982978	-0.654146	0.103960
C	0.891335	0.872236	-0.088197
H	-1.101611	2.038640	0.121113
H	1.278347	-0.905592	1.129026
H	1.648047	-1.157365	-0.598666
H	1.485057	1.405922	0.658659
H	1.240331	1.189298	-1.078634

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C	-1.863199	-0.092696	0.013300
C	-2.030866	-1.165142	1.059773
H	-2.261599	-0.754782	2.045610
H	-1.128886	-1.782797	1.144939
C	-3.225792	-1.938377	0.456801
O	-3.370362	-1.485049	-0.914509
C	-2.621983	-0.374586	-1.051032
H	-3.088059	-3.019072	0.430047
H	-4.160936	-1.699526	0.970324
S	-0.797810	1.284065	0.111832
O	-1.001070	2.077250	-1.100534
O	-0.946261	1.870027	1.443371
C	0.833628	0.568415	0.033997
C	1.413328	0.328873	-1.210422
C	1.489076	0.240472	1.215485
C	2.672769	-0.255359	-1.262112

H	0.883439	0.614593	-2.114108
C	2.750904	-0.347570	1.143805
H	1.020882	0.464822	2.169038
C	3.357666	-0.601697	-0.089040
H	3.138975	-0.440999	-2.226203
H	3.274741	-0.604029	2.060438
C	4.733798	-1.210754	-0.166464
H	5.472729	-0.455088	-0.452098
H	5.036966	-1.630253	0.795197
H	4.769906	-2.006417	-0.915579
H	-2.707635	0.161202	-1.988092

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C	0.429213	-0.015980	0.031755
C	1.856393	0.478213	0.033704
H	2.027419	1.045349	-0.887332
H	1.985013	1.159475	0.881500
C	2.851644	-0.667881	0.131928
H	2.726251	-1.357398	-0.718238
O	4.135938	-0.097678	0.121026
C	-0.062764	-1.224641	0.075662
C	5.164404	-1.065332	0.214259
H	5.014860	-1.666236	1.127019
H	5.130156	-1.747736	-0.649002
C	6.483434	-0.359769	0.273138
H	6.564305	0.422424	1.025712
C	7.514731	-0.655420	-0.513628
H	8.465106	-0.140500	-0.420968
H	7.440846	-1.425738	-1.277365
H	2.688974	-1.238477	1.060362

O	-0.632495	1.953287	-1.336014
O	-0.673883	2.057760	1.196335
C	-2.360749	0.447825	-0.033060
C	-2.925324	0.064592	-1.245334
C	-2.958072	0.151766	1.191042
C	-4.120906	-0.647173	-1.222719
H	-2.435472	0.325647	-2.177968
C	-4.150315	-0.560003	1.188120
H	-2.492021	0.480283	2.114478
C	-4.745065	-0.968861	-0.013313
H	-4.576688	-0.955964	-2.158775
H	-4.631597	-0.802256	2.131633
S	-0.811460	1.304816	-0.043616
C	-6.044944	-1.729393	0.010058
H	-6.311351	-2.092141	-0.984607
H	-6.858083	-1.089778	0.367453
H	-5.980912	-2.588607	0.683503

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C	0.950165	0.357370	0.151143
C	1.241273	0.107287	1.614957
H	0.471600	-0.524362	2.074189
H	1.310963	1.039039	2.180544
C	2.580298	-0.603733	1.522876
H	3.420480	0.095961	1.534789
O	2.525369	-1.199869	0.182707
C	1.609120	-0.347855	-0.785346
C	3.786286	-1.610441	-0.415855
H	3.478051	-2.100487	-1.340086
H	4.231362	-2.336854	0.270252

C	4.687657	-0.444887	-0.674430
H	4.285666	0.326035	-1.328636
C	5.916593	-0.360594	-0.169057
H	6.568481	0.474164	-0.403589
H	6.316330	-1.132407	0.485313
H	2.734260	-1.417732	2.233151
O	-0.370965	2.494363	0.768962
O	-0.158067	1.878768	-1.694850
C	-1.817005	0.524868	-0.173830
C	-2.599337	0.616885	0.969972
C	-2.168216	-0.312555	-1.231588
C	-3.760702	-0.151800	1.055286
H	-2.306723	1.296404	1.764465
C	-3.327127	-1.070554	-1.128697
H	-1.538054	-0.353738	-2.115332
C	-4.138761	-1.000612	0.013087
H	-4.384831	-0.082825	1.942087
H	-3.615354	-1.724428	-1.947895
S	-0.318238	1.489417	-0.298758
C	-5.402749	-1.817790	0.093394
H	-5.849160	-1.761625	1.088631
H	-6.142122	-1.458224	-0.629343
H	-5.204810	-2.869216	-0.134430

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C	-3.094963	0.065070	0.036369
H	-3.352234	1.009808	0.531669
H	-3.445620	0.097442	-1.003557
C	-3.696014	-1.093120	0.767090
H	-3.343539	-1.241096	1.785686

C	-4.617248	-1.895416	0.239626
H	-5.053873	-2.708416	0.809971
H	-4.968281	-1.760517	-0.780420
C	1.105492	-0.761343	-0.921466
C	2.369205	-1.287069	-0.685459
C	3.284580	-0.621422	0.142468
C	2.902744	0.585963	0.730682
C	1.637303	1.128410	0.505528
C	0.751853	0.440931	-0.311168
H	0.396335	-1.285911	-1.555583
H	2.654694	-2.228550	-1.147795
H	3.603577	1.111809	1.373188
H	1.324832	2.065402	0.957065
C	4.651128	-1.209526	0.384304
H	5.187234	-1.352814	-0.558702
H	5.254288	-0.560597	1.022819
H	4.573248	-2.186855	0.870494
S	-0.853948	1.175216	-0.636399
O	-1.666723	-0.100542	0.071866
O	-0.949773	2.365788	0.246847

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C	-1.101472	0.747411	0.141793
C	-0.946278	2.240888	-0.009762
H	-0.001040	2.495762	-0.505456
H	-0.985797	2.765348	0.947493
C	-2.174958	2.541318	-0.888208
H	-3.010064	2.920494	-0.291837
O	-2.595570	1.275155	-1.447734
C	-2.016960	0.284534	-0.730746

C	-4.939633	-1.530447	-0.450240
H	-5.244086	-1.365991	-1.480921
H	-5.717046	-1.779576	0.264562
C	-3.665608	-1.432260	-0.078738
H	-3.366197	-1.595838	0.954702
C	-2.539840	-1.086764	-1.024960
H	-1.732187	-1.812805	-0.908887
H	-2.896109	-1.090321	-2.059084
H	-1.978515	3.218495	-1.719171
O	-0.037554	0.555864	2.492669
O	-0.678571	-1.571858	1.242659
C	1.472707	-0.245955	0.514451
C	2.394635	0.738938	0.852405
C	1.783928	-1.246874	-0.403359
C	3.650273	0.722127	0.248111
H	2.131389	1.488827	1.592126
C	3.041833	-1.249389	-0.994166
H	1.052074	-2.016332	-0.629907
C	3.990506	-0.267483	-0.678322
H	4.379532	1.484490	0.507918
H	3.298342	-2.029147	-1.706488
S	-0.152750	-0.204232	1.248416
C	5.360184	-0.304199	-1.305569
H	5.300292	-0.553947	-2.368171
H	5.867869	0.657744	-1.206293
H	5.983216	-1.063841	-0.822150

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C	-2.344476	-1.181560	-0.928484
H	-1.894285	-0.172209	-0.861512

C	-3.091509	-1.630701	0.265005
H	-3.510022	-2.635391	0.222653
C	-3.239344	-0.810742	1.312373
H	-3.800089	-1.126798	2.189638
H	-2.790833	0.190235	1.287802
C	1.825677	1.185669	-0.880850
C	2.868883	0.284825	-0.731136
C	2.819566	-0.744839	0.222970
C	1.678104	-0.825021	1.021985
C	0.619217	0.073052	0.886815
C	0.673470	1.094707	-0.073212
H	1.890329	1.971470	-1.631234
H	3.747062	0.375333	-1.370222
H	1.611064	-1.613596	1.770893
H	-0.266112	0.015084	1.513808
C	3.956247	-1.728125	0.357946
H	4.913799	-1.220065	0.523963
H	3.788048	-2.404529	1.201694
H	4.067657	-2.344431	-0.542581
S	-0.663286	2.215964	-0.261439
O	-2.239420	-1.868374	-1.930051
O	-1.727962	1.769110	0.824756

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C	0.869642	-0.083855	0.000748
C	-0.570302	0.371045	-0.001146
H	-0.736070	0.996107	0.882782
H	-0.736393	0.987414	-0.891064
C	-1.533543	-0.805951	0.004947
H	-1.374011	-1.427138	0.900435

O	-2.834175	-0.273469	0.000336
C	1.394669	-1.279362	0.000290
C	-3.829098	-1.270579	0.005655
H	-3.712828	-1.918426	-0.878421
H	-3.714030	-1.907672	0.897672
H	-1.372227	-1.437970	-0.882673
O	1.894867	1.966088	1.273579
O	1.894268	1.972783	-1.261167
C	3.645747	0.459676	0.001743
C	4.237686	0.136392	1.219312
C	4.236477	0.140680	-1.218969
C	5.453415	-0.538878	1.204519
H	3.754130	0.418802	2.149006
C	5.451021	-0.533909	-1.208149
H	3.751371	0.426772	-2.146719
C	6.070747	-0.886284	-0.002313
H	5.932930	-0.796860	2.144234
H	5.929887	-0.788634	-2.149386
S	2.073345	1.273140	0.004341
C	7.371150	-1.645953	-0.010555
H	7.185748	-2.714076	-0.164827
H	7.903629	-1.531909	0.936048
H	8.022944	-1.302899	-0.817814
C	-5.201557	-0.643968	0.000988
C	-6.324061	-1.477210	0.003243
C	-5.376527	0.738875	-0.005247
C	-7.605991	-0.936494	-0.000612
H	-6.192846	-2.557411	0.008055
C	-6.662862	1.280710	-0.009138
H	-4.504478	1.383089	-0.007032
C	-7.778856	0.448319	-0.006831

H	-8.469816	-1.594019	0.001187
H	-6.789940	2.358927	-0.013995
H	-8.777746	0.872947	-0.009844

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C	0.005962	0.178100	0.296984
C	-0.240195	-0.397570	1.674715
H	0.575247	-1.063529	1.981221
H	-0.354763	0.383880	2.428969
C	-1.536727	-1.154119	1.440085
H	-2.415208	-0.526702	1.612080
O	-1.475407	-1.436869	0.000705
C	-0.630532	-0.352233	-0.762479
C	-2.701861	-1.858389	-0.666150
H	-2.396011	-1.946430	-1.708197
H	-2.938838	-2.843961	-0.256409
H	-1.628192	-2.112052	1.955203
O	1.233639	2.200244	1.345319
O	0.969892	2.128341	-1.188403
C	2.750645	0.576409	-0.040105
C	3.571337	0.473422	1.075325
C	3.105604	0.004934	-1.261257
C	4.776031	-0.221988	0.963364
H	3.273073	0.949964	2.004038
C	4.307438	-0.684324	-1.353569
H	2.444081	0.111953	-2.116082
C	5.158524	-0.806724	-0.245318
H	5.430177	-0.302602	1.827236
H	4.598722	-1.131165	-2.300803
S	1.197750	1.451844	0.083784

C	6.465933	-1.545638	-0.374588
H	6.966978	-1.637698	0.591533
H	7.141471	-1.020927	-1.057532
H	6.309154	-2.551311	-0.775772
C	-3.833768	-0.889049	-0.473049
C	-3.773456	0.389457	-1.040178
C	-4.949318	-1.259412	0.280881
C	-4.821575	1.284226	-0.843361
H	-2.897859	0.677415	-1.615704
C	-6.002818	-0.365435	0.467873
H	-4.996749	-2.253053	0.721030
C	-5.936403	0.908223	-0.092514
H	-4.768325	2.276774	-1.278581
H	-6.868640	-0.661905	1.051118
H	-6.752229	1.608785	0.055192

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C	-0.355570	0.487446	-0.316557
C	-0.529002	1.758287	0.492570
H	0.430177	2.246819	0.698184
H	-1.035005	1.559092	1.441987
C	-1.422767	2.590575	-0.462524
H	-2.448162	2.670638	-0.097387
O	-1.490420	1.849665	-1.734535
C	-0.924529	0.686035	-1.504264
C	-3.979630	1.278906	1.898714
H	-4.541563	2.175373	1.661701
H	-3.640622	1.144078	2.919074
C	-3.745881	0.285641	0.919560
C	-3.038826	-0.905096	1.236695

C	-4.193650	0.450501	-0.417821
C	-2.796843	-1.868053	0.272259
H	-2.658849	-1.043489	2.245024
C	-3.940150	-0.516309	-1.378474
H	-4.736430	1.354441	-0.684885
C	-3.237804	-1.678976	-1.042436
H	-2.224868	-2.753621	0.529006
H	-4.278957	-0.362519	-2.398565
H	-3.018320	-2.424581	-1.799276
H	-1.022280	3.575508	-0.700313
S	0.479130	-0.949898	0.201911
O	0.255562	-1.992302	-0.798218
O	0.157379	-1.168489	1.613772
C	2.200310	-0.484742	0.133068
C	2.821259	0.003153	1.276622
C	2.887468	-0.604221	-1.073889
C	4.159614	0.388030	1.203556
H	2.264919	0.057621	2.207290
C	4.220554	-0.218117	-1.126878
H	2.378571	-1.007175	-1.944461
C	4.874142	0.283419	0.007811
H	4.656937	0.766255	2.092365
H	4.769695	-0.312243	-2.060195
C	6.325793	0.680648	-0.069284
H	6.651465	1.174315	0.848788
H	6.959048	-0.198779	-0.223376
H	6.501054	1.362882	-0.906056

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C	-0.968516	-0.598652	0.185730

H	-0.621405	-1.576953	0.530032
H	-0.442711	-0.339995	-0.740197
C	2.391180	-0.218221	1.251588
C	3.527591	-0.931329	0.890869
C	4.095917	-0.786957	-0.383151
C	3.493796	0.087340	-1.290495
C	2.352721	0.811757	-0.943617
C	1.808762	0.644169	0.322525
H	1.948906	-0.341030	2.237029
H	3.984177	-1.612553	1.604445
H	3.922095	0.205626	-2.282080
H	1.871832	1.491789	-1.640945
C	5.341228	-1.553401	-0.747984
H	5.559241	-1.470543	-1.814851
H	5.236009	-2.613659	-0.501183
H	6.205976	-1.171063	-0.196209
S	0.356964	1.611822	0.792413
O	-0.624223	0.355652	1.216419
O	-0.120734	2.196029	-0.491838
C	-2.455727	-0.590469	-0.039725
C	-3.069815	0.557453	-0.551550
C	-3.227375	-1.716301	0.243389
C	-4.442436	0.570871	-0.777428
H	-2.459136	1.431917	-0.766072
C	-4.603674	-1.704296	0.013192
H	-2.752048	-2.606911	0.646965
C	-5.211843	-0.560367	-0.496529
H	-4.915142	1.463514	-1.175189
H	-5.197673	-2.585097	0.236196
H	-6.282744	-0.547223	-0.674080

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C	1.365357	1.223019	-0.799047
H	1.613020	1.635636	-1.807555
C	-2.661474	-1.573703	0.232751
C	-3.987806	-1.205425	0.460027
C	-4.404648	0.116467	0.299895
C	-3.443652	1.063875	-0.078363
C	-2.111789	0.721489	-0.284352
C	-1.711763	-0.613575	-0.131582
H	-2.364369	-2.615637	0.329592
H	-4.712497	-1.965265	0.747938
H	-3.743645	2.104558	-0.193948
H	-1.349116	1.463882	-0.513438
C	-5.842767	0.520782	0.516480
H	-6.306049	0.865651	-0.415107
H	-5.921393	1.338788	1.241032
H	-6.435435	-0.318597	0.892733
S	-0.032488	-1.124690	-0.354666
O	0.667886	1.937371	-0.009895
O	0.564732	-0.042366	-1.428660
C	2.621033	0.566510	-0.205923
C	2.896866	0.729975	1.150121
C	3.505601	-0.171670	-0.995344
C	4.039465	0.161170	1.713780
H	2.184116	1.312058	1.728189
C	4.651624	-0.738600	-0.439888
H	3.273322	-0.310437	-2.049270
C	4.922237	-0.572805	0.920398
H	4.244694	0.288611	2.774186
H	5.332377	-1.314400	-1.062523

H	5.814136	-1.014905	1.357542

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C	0.110897	0.892614	0.461927
C	-0.214301	2.313195	0.857770
H	-1.202652	2.613671	0.487026
H	-0.192039	2.461317	1.939484
C	0.933864	3.050041	0.145718
H	1.755270	3.268785	0.834571
O	1.447349	2.133238	-0.847874
C	1.022515	0.888160	-0.529590
C	1.670040	-0.204335	-1.316433
H	1.075699	-1.113901	-1.226281
H	1.692177	0.114873	-2.363589
C	3.082593	-0.452206	-0.817478
C	4.172530	0.190077	-1.406900
C	3.293295	-1.313763	0.262796
C	5.463380	-0.030125	-0.928312
H	4.008174	0.866838	-2.241467
C	4.583636	-1.534039	0.739873
H	2.438558	-1.803759	0.723220
C	5.671017	-0.893829	0.145580
H	6.305472	0.471332	-1.395379
H	4.739749	-2.207808	1.576641
H	6.675889	-1.068304	0.517423
S	-0.710661	-0.479414	1.154817
O	-0.038636	-1.706406	0.717305
O	-0.904212	-0.194158	2.576036
C	-2.323940	-0.451918	0.393312
C	-2.516145	-1.102523	-0.823782

C	-3.356626	0.240379	1.015830
C	-3.767576	-1.047050	-1.424911
H	-1.697168	-1.654493	-1.275139
C	-4.604761	0.287070	0.397046
H	-3.181883	0.713679	1.977199
C	-4.827192	-0.352815	-0.825162
H	-3.931205	-1.556011	-2.371180
H	-5.420008	0.821661	0.876665
C	-6.185017	-0.328002	-1.478181
H	-6.101049	-0.153812	-2.554229
H	-6.696320	-1.285912	-1.337583
H	-6.816128	0.454621	-1.051532
H	0.632774	3.960878	-0.371277

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C	2.845911	-0.734528	-0.000130
H	2.823979	-1.366590	-0.892207
H	2.824208	-1.366735	0.891851
H	3.780807	-0.169253	-0.000200
C	1.623035	0.176219	0.000101
C	0.245546	-0.436146	0.000285
H	0.155680	-1.083154	0.882084
H	0.155783	-1.083860	-0.881010
C	-0.872929	0.603024	-0.000182
H	-0.798415	1.232528	0.889427
H	-3.256346	0.807962	0.000766
C	1.940630	1.441408	0.000038
H	-0.798187	1.231963	-0.890169
S	-2.473792	-0.281420	-0.000076

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C	-2.735692	-0.067623	0.036102
H	-3.107983	0.360909	-0.899049
H	-3.005341	0.591019	0.866403
H	-3.221919	-1.034030	0.186854
C	-1.214617	-0.188511	-0.041475
C	-0.388317	1.050930	-0.288145
H	-0.941259	1.922503	0.084871
H	-0.267759	1.182345	-1.370336
C	0.979253	0.999776	0.386662
H	1.557231	1.889276	0.123478
H	1.426506	-1.326829	0.674532
C	-0.844472	-1.435700	0.092874
H	0.874129	0.978636	1.473739
S	1.994342	-0.419816	-0.141038

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C	-2.497684	-0.253557	-0.020582
H	-2.922002	0.265126	-0.888897
H	-2.920677	0.216931	0.876176
H	-2.811734	-1.297600	-0.049802
C	-0.994421	-0.161855	-0.016618
C	-0.418027	1.247551	0.128287
H	-0.624621	1.615290	1.142737
H	-0.900216	1.945208	-0.565850
C	1.086642	1.192086	-0.133991
H	1.344722	1.487316	-1.152387
H	1.787650	-0.686591	1.272538
C	-0.236902	-1.279993	-0.050638

H	1.702763	1.757971	0.565975
S	1.481654	-0.610565	-0.039952

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C	-3.227872	-0.628938	0.106283
H	-3.457716	-1.194780	-0.800132
H	-4.044653	0.074859	0.285598
H	-3.192405	-1.328392	0.945451
C	-0.912739	0.681229	-0.158323
C	0.367745	1.385310	-0.286889
H	0.251847	2.412138	0.080383
H	0.648814	1.444787	-1.343749
C	1.493542	0.705480	0.501373
H	2.410050	1.293683	0.411933
H	0.697557	-1.470614	0.016123
C	-1.955357	0.081866	-0.033135
H	1.232565	0.644385	1.560295
S	1.928876	-0.951609	-0.120735

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C	2.504573	-0.253940	0.049264
H	2.935151	0.299553	0.891301
H	2.958493	0.147398	-0.864878
H	2.794620	-1.302843	0.143497
C	1.015510	-0.098416	0.008682
C	0.385689	1.261927	-0.206221
H	0.453751	1.520543	-1.273501
H	0.901028	2.050450	0.353049
C	-1.076905	1.146217	0.234928

H	-1.171784	1.334706	1.307813
C	0.120915	-1.090099	0.052661
H	-1.746276	1.815058	-0.306931
S	-1.573351	-0.594496	-0.076098
H	0.349948	-2.147054	0.131331

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C	3.099870	-0.643410	-0.120802
H	3.282517	-1.124933	0.848955
H	3.848702	0.151392	-0.228820
H	3.260687	-1.381791	-0.908878
C	1.705142	-0.097157	-0.202958
C	1.255240	0.928988	0.825486
H	1.124649	0.474870	1.818419
C	-0.062720	1.427209	0.242140
H	-0.854811	1.613253	0.970552
C	0.797506	-0.492237	-1.116851
N	-0.465717	0.337650	-0.722594
C	-1.579561	-0.563690	-0.261430
H	-1.580049	-1.358514	-1.013465
H	-0.792947	0.759327	-1.591542
H	1.970068	1.751896	0.941053
C	-1.259079	-1.174574	1.094482
H	-1.279795	-0.424090	1.891780
H	-2.013349	-1.929362	1.330727
H	-0.278402	-1.655069	1.074217
C	-2.912194	0.175466	-0.276072
H	-3.122615	0.607884	-1.259970
H	-3.719898	-0.522616	-0.041283
H	-2.940909	0.977079	0.469166

H	0.090945	2.333559	-0.346727

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C	-3.099742	-0.643322	0.120640
H	-3.281987	-1.125528	-0.848854
H	-3.848548	0.151618	0.227785
H	-3.260938	-1.381172	0.909135
C	-1.705043	-0.097118	0.202974
C	-1.255262	0.929188	-0.825362
H	-1.124965	0.475417	-1.818479
C	0.062751	1.427256	-0.242112
H	0.854909	1.613129	-0.970486
C	-0.797414	-0.492403	1.116771
N	0.465802	0.337711	0.722593
C	1.579633	-0.563628	0.261570
H	1.580461	-1.358080	1.013997
H	0.792682	0.759322	1.591699
H	-1.970192	1.752089	-0.940568
C	1.258760	-1.175217	-1.093919
H	1.279805	-0.425268	-1.891708
H	2.012621	-1.930555	-1.329690
H	0.277870	-1.655293	-1.073250
C	2.912153	0.175768	0.275450
H	3.122974	0.608448	1.259144
H	3.719890	-0.522199	0.040420
H	2.940327	0.977208	-0.469991
H	-0.090533	2.333745	0.346619

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C	2.373051	-0.434043	0.183308
C	1.023065	-0.955673	0.415130
H	0.921310	-1.929009	-0.082014
C	-0.062044	-0.004021	-0.097041
H	0.041480	0.952136	0.424508
C	3.475985	0.017673	-0.017877
N	-1.378560	-0.560018	0.180845
C	-2.495525	0.203151	-0.379480
H	-2.322830	0.414367	-1.452482
H	-1.417898	-1.508615	-0.187164
C	-2.649502	1.536008	0.349330
H	-3.529488	2.070222	-0.021100
H	-2.771932	1.355629	1.422324
H	-1.783291	2.186989	0.204874
C	-3.766292	-0.629572	-0.248167
H	-4.623453	-0.098023	-0.670439
H	-3.670986	-1.585639	-0.774446
H	-3.967378	-0.837217	0.807639
H	0.862684	-1.126980	1.484902
H	0.101214	0.192122	-1.171737
C	4.816906	0.556060	-0.254743
H	5.290819	0.846481	0.686499
H	5.453408	-0.187820	-0.740984
H	4.772385	1.437986	-0.899056

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C	3.228250	-0.706834	-0.096622
H	3.674446	-0.715495	0.904580
H	3.885062	-0.101303	-0.734174
H	3.237154	-1.730718	-0.480249

C	1.842292	-0.151088	-0.068253
C	1.517590	1.267232	0.355487
H	1.976199	1.562116	1.304853
C	-0.018858	1.237436	0.431383
H	-0.326713	0.980330	1.458143
C	0.717100	-0.695673	-0.548765
N	-0.397236	0.161044	-0.499234
C	-1.713573	-0.459739	-0.333407
H	-1.789251	-1.196654	-1.143965
C	-2.809217	0.581903	-0.537756
H	-2.667288	1.107184	-1.485865
H	-3.793325	0.104850	-0.540676
H	-2.801208	1.319497	0.272306
C	-1.891339	-1.201572	0.998420
H	-2.828077	-1.767094	0.991721
H	-1.067582	-1.901173	1.171099
H	-1.931559	-0.507277	1.843716
H	1.862882	1.976312	-0.411562
H	-0.487567	2.184275	0.153174
H	0.604014	-1.672150	-1.011380

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C	3.209110	3.901837	1.224003
H	3.537819	3.272861	2.055955
H	2.413909	4.568398	1.570145
H	4.053541	4.512727	0.896800
C	2.671056	3.015975	0.106851
C	1.489112	2.117426	0.372970
H	1.681559	1.527721	1.277947
C	1.189312	1.162393	-0.780794

H	1.152735	1.714178	-1.739112
C	3.326529	3.144770	-1.013829
N	-0.049102	0.429747	-0.541255
C	-1.223677	1.189359	-0.957265
H	-1.080473	2.230386	-0.645619
H	0.620689	2.752868	0.591458
H	2.012262	0.445050	-0.856159
C	-0.038418	-0.898244	-1.149851
H	-1.047488	-1.314479	-1.044633
H	0.176444	-0.843611	-2.233966
C	0.950712	-1.824370	-0.479725
C	0.978175	-1.923513	0.915360
C	1.833110	-2.601772	-1.230050
C	1.867737	-2.789425	1.544826
H	0.297103	-1.307450	1.496273
C	2.724835	-3.472649	-0.602219
H	1.826637	-2.522235	-2.314502
C	2.744129	-3.568056	0.786756
H	1.878782	-2.859369	2.628375
H	3.407686	-4.069172	-1.199232
H	3.439458	-4.241629	1.277781
H	-1.324800	1.202815	-2.059185
C	-2.498492	0.663718	-0.335408
C	-2.547909	0.401172	1.037597
C	-3.641321	0.450159	-1.106092
C	-3.721084	-0.060226	1.627321
H	-1.650948	0.554577	1.632053
C	-4.820201	-0.010189	-0.517765
H	-3.608182	0.641412	-2.176040
C	-4.862318	-0.266556	0.850188
H	-3.747497	-0.261018	2.694054

H	-5.701321	-0.174203	-1.130387
H	-5.776585	-0.628911	1.309531

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C	-1.891491	3.937775	-0.146490
H	-1.250314	4.812060	0.026264
H	-2.712869	3.994629	0.579000
H	-2.309858	4.012577	-1.152536
C	-1.120215	2.659583	-0.000469
C	-0.420510	2.355675	1.314781
H	0.482517	2.971410	1.450889
C	-0.099927	0.876553	1.155670
H	0.810076	0.517496	1.643063
C	-0.967375	1.758831	-0.991294
N	-0.007887	0.694869	-0.332827
C	1.362337	1.058918	-0.856481
H	1.247940	1.079696	-1.942999
H	-1.057052	2.529855	2.189609
H	-0.946654	0.276310	1.491002
C	-0.359556	-0.692581	-0.779629
H	-0.303132	-0.659503	-1.871197
H	0.409435	-1.370624	-0.398120
C	-1.717815	-1.175424	-0.335097
C	-2.891036	-0.685631	-0.920042
C	-1.808688	-2.162042	0.650800
C	-4.130229	-1.171628	-0.510123
H	-2.813928	0.092616	-1.672560
C	-3.049114	-2.649496	1.060223
H	-0.899207	-2.553548	1.101852
C	-4.213250	-2.151481	0.479643

H	-5.035530	-0.783281	-0.966181
H	-3.104009	-3.415810	1.827076
H	-5.181926	-2.527400	0.794407
H	1.531378	2.086636	-0.528214
C	2.501212	0.167331	-0.428160
C	2.876131	-0.941955	-1.194400
C	3.240789	0.467677	0.720527
C	3.941126	-1.750627	-0.804764
H	2.332244	-1.168163	-2.108485
C	4.307458	-0.337534	1.114814
H	2.986414	1.350415	1.303442
C	4.655452	-1.452852	0.355158
H	4.218489	-2.607473	-1.410523
H	4.871406	-0.088611	2.008158
H	5.487997	-2.079925	0.657835

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C	-3.100300	-2.287508	0.469315
C	-1.743225	-1.757568	0.631814
H	-1.690005	-1.120706	1.521737
C	-1.305408	-0.922700	-0.578841
H	-1.433984	-1.505408	-1.508459
C	-4.221330	-2.709631	0.307055
N	0.067687	-0.450540	-0.426107
C	1.041132	-1.463384	-0.820057
H	0.706835	-2.427685	-0.421185
H	-1.046895	-2.587993	0.795707
H	-1.967242	-0.054589	-0.649267
C	0.301285	0.802690	-1.137855
H	1.378556	1.005276	-1.100772

H	0.027132	0.717093	-2.207033
C	-0.439025	1.964418	-0.514720
C	-0.422670	2.141612	0.872602
C	-1.127028	2.885357	-1.305297
C	-1.077242	3.223565	1.454545
H	0.102922	1.414363	1.485258
C	-1.781291	3.972976	-0.725479
H	-1.154728	2.748791	-2.383775
C	-1.758155	4.144207	0.656330
H	-1.057712	3.350402	2.532782
H	-2.314194	4.680279	-1.353545
H	-2.270315	4.986629	1.110568
H	1.082582	-1.576024	-1.920583
C	2.425745	-1.168932	-0.286602
C	2.595980	-0.828098	1.059253
C	3.548156	-1.247900	-1.111040
C	3.866349	-0.577710	1.569773
H	1.717441	-0.753317	1.694757
C	4.823832	-0.999829	-0.602026
H	3.423400	-1.501408	-2.161145
C	4.985390	-0.663972	0.739577
H	3.985992	-0.313835	2.616197
H	5.688128	-1.062613	-1.256020
H	5.975924	-0.466377	1.137166
C	-5.580050	-3.224072	0.125101
H	-5.608224	-4.307066	0.270922
H	-6.267408	-2.765914	0.841022
H	-5.944880	-3.007256	-0.882273

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C	-1.631365	3.047539	-0.159188
H	-1.143041	3.872357	0.379160
H	-2.643589	2.959537	0.254534
H	-1.690314	3.319186	-1.215517
C	-0.869368	1.783989	0.014324
C	-0.857213	1.041274	1.328363
H	-0.552983	1.688856	2.160309
C	0.142929	-0.087493	1.065887
H	1.051943	-0.014051	1.674346
C	-0.045615	1.172549	-0.985177
N	0.488783	0.113853	-0.357167
C	1.496332	-0.750396	-0.946119
H	1.236666	-1.797134	-0.744392
H	-1.861241	0.661852	1.566333
H	-0.285147	-1.088275	1.198942
C	-1.590228	-1.983071	-1.388506
H	-1.190926	-1.556837	-2.301144
H	-1.217861	-2.947538	-1.061521
C	-2.588816	-1.306947	-0.655993
C	-3.108203	-0.063325	-1.105163
C	-3.107605	-1.841655	0.555319
C	-4.104209	0.588846	-0.391483
H	-2.715143	0.367805	-2.021747
C	-4.088310	-1.173464	1.267657
H	-2.724007	-2.793334	0.915050
C	-4.595127	0.047539	0.799492
H	-4.498674	1.530647	-0.761193
H	-4.470357	-1.599470	2.190363
H	-5.370460	0.564263	1.355811
H	1.458338	-0.579159	-2.024764
C	2.881271	-0.454066	-0.403209

C	3.655181	-1.455622	0.181908
C	3.395168	0.844075	-0.489679
C	4.932028	-1.172090	0.669568
H	3.258217	-2.465385	0.256648
C	4.666815	1.129615	-0.001481
H	2.785049	1.623220	-0.941022
C	5.439106	0.121366	0.579027
H	5.525497	-1.960275	1.122529
H	5.059031	2.139316	-0.075013
H	6.430887	0.345472	0.959171

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C	3.490593	2.727006	-0.345739
H	3.668242	3.746569	0.015651
H	3.811607	2.701680	-1.395207
H	4.142579	2.055975	0.218616
C	2.047199	2.359481	-0.222820
C	0.971982	3.097846	-0.991867
H	1.027299	4.186541	-0.891526
C	-0.313651	2.518169	-0.389676
H	-0.649323	3.147069	0.455040
C	1.485603	1.297458	0.381899
N	0.097284	1.205968	0.121875
C	-0.783789	0.651651	1.134859
H	-0.312857	-0.242554	1.555003
H	1.052581	2.863245	-2.063881
H	-1.140693	2.422001	-1.097230
C	2.156706	0.180804	1.126199
C	1.898189	-1.179665	0.500642
C	1.867593	-1.329915	-0.889166

C	1.692327	-2.304499	1.302059
C	1.647786	-2.579815	-1.462822
H	1.999900	-0.453303	-1.518800
C	1.468034	-3.557540	0.731711
H	1.702122	-2.198168	2.384709
C	1.446093	-3.698671	-0.653887
H	1.625552	-2.679959	-2.543847
H	1.305363	-4.420145	1.370558
H	1.267859	-4.671499	-1.101177
H	-0.945188	1.368660	1.961767
C	-2.113727	0.257330	0.532838
C	-2.142127	-0.697717	-0.489360
C	-3.309844	0.824009	0.968507
C	-3.351471	-1.080631	-1.060109
H	-1.203026	-1.129183	-0.830341
C	-4.525617	0.441682	0.397310
H	-3.291308	1.571773	1.757975
C	-4.547867	-0.510833	-0.617374
H	-3.364873	-1.825280	-1.850249
H	-5.451191	0.891401	0.743512
H	-5.491278	-0.809546	-1.063847
H	3.233867	0.374169	1.148188
H	1.827707	0.161867	2.172733

CP1

C	0.186973	-1.429094	-0.793690
C	-0.228855	-0.442640	-1.865233
H	0.034453	-0.780789	-2.870003
H	0.206343	0.550067	-1.692071
C	-1.730567	-0.435949	-1.643835
H	-2.264153	0.510128	-1.761769

O	-1.820498	-0.787578	-0.206322
C	-0.672616	-1.648891	0.226002
C	-1.183714	3.224864	-1.125540
C	0.200708	3.321103	-1.267422
C	1.059094	2.783158	-0.301871
C	0.495131	2.157329	0.814714
C	-0.887676	2.066291	0.965592
C	-1.727994	2.595824	-0.008036
H	-1.847780	3.618853	-1.892089
H	0.624095	3.805797	-2.145323
H	1.152780	1.730133	1.568497
H	-1.343479	1.570682	1.819279
C	2.556130	2.824745	-0.478043
H	3.060527	3.054801	0.466312
H	2.932545	1.851942	-0.815831
H	2.848773	3.576114	-1.217449
S	-3.559360	2.465099	0.171876
O	-3.904936	1.735430	-1.127937
O	-3.658018	1.546716	1.381780
H	-2.226218	-1.252012	-2.178598
O	1.724130	-3.416457	0.015484
O	2.141355	-2.350939	-2.248053
C	2.907107	-1.088514	-0.096040
C	2.691350	-0.635776	1.203284
C	4.059425	-0.749035	-0.794120
C	3.648219	0.175578	1.802547
H	1.777852	-0.916727	1.723041
C	5.014020	0.058794	-0.175504
H	4.192397	-1.122442	-1.804707
C	4.819488	0.534555	1.122950
H	3.484640	0.542054	2.813569

H	5.918892	0.329864	-0.714153
S	1.732777	-2.228540	-0.839338
C	5.824588	1.454706	1.767966
H	6.816631	1.330142	1.326033
H	5.528899	2.501635	1.633718
H	5.900205	1.268324	2.842787
C	-3.191425	-1.174392	0.251809
O	-3.536068	-2.386811	-0.301174
C	-3.184508	-1.331215	1.757975
H	-3.805461	-0.367474	-0.148038
C	-3.144688	-3.458800	0.576180
C	-2.995022	-2.844175	1.979927
H	-4.145937	-0.959978	2.119023
H	-2.408442	-0.713569	2.206906
H	-3.932977	-4.213530	0.508405
H	-2.198262	-3.877774	0.223307
H	-3.742289	-3.242218	2.671933
H	-1.997451	-3.052652	2.368716

CP2

C	-0.794524	-1.938964	0.018497
C	-0.081758	-1.457060	1.266226
H	0.220392	-2.300471	1.895458
H	-0.696792	-0.782487	1.871580
C	1.087051	-0.707520	0.653067
H	0.865148	0.351801	0.531412
O	1.140346	-1.225035	-0.741682
C	-0.143092	-1.903192	-1.164307
C	2.408914	2.442076	1.218016
C	1.125829	2.977910	1.149522

C	0.399347	2.953227	-0.050549
C	1.012013	2.417288	-1.185739
C	2.306944	1.893539	-1.125358
C	2.993638	1.882323	0.081616
H	2.944957	2.413147	2.164235
H	0.663079	3.395322	2.042278
H	0.459283	2.384647	-2.122429
H	2.786712	1.444456	-1.992136
C	-1.027544	3.444238	-0.090120
H	-1.366465	3.590332	-1.120130
H	-1.701166	2.714445	0.375574
H	-1.138066	4.392062	0.447145
S	4.608862	0.995456	0.227261
O	4.201597	-0.085575	1.231315
O	4.744379	0.432632	-1.179168
C	2.394933	-1.856072	-1.188019
H	3.178020	-1.100866	-1.064244
C	2.657816	-3.103705	-0.406275
H	2.004369	-3.953663	-0.599496
C	3.636023	-3.160681	0.499293
H	2.203985	-2.049448	-2.244383
H	3.820307	-4.073249	1.060775
H	4.249780	-2.283893	0.708866
H	2.076682	-0.835675	1.099971
O	-2.910931	-3.116644	-1.073072
O	-2.762007	-2.887038	1.452766
C	-3.270682	-0.752946	0.021300
C	-3.290517	-0.082748	-1.201515
C	-3.800633	-0.175999	1.166712
C	-3.850208	1.186254	-1.265478
H	-2.855093	-0.557641	-2.076797

C	-4.359193	1.102046	1.086018
H	-3.773956	-0.731247	2.099457
C	-4.384403	1.799168	-0.122539
H	-3.864328	1.720922	-2.212419
H	-4.774377	1.563916	1.978439
S	-2.482657	-2.366562	0.106121
C	-4.927503	3.203338	-0.199520
H	-5.548340	3.437459	0.668983
H	-4.106272	3.929057	-0.230796
H	-5.528920	3.346921	-1.101817

CP3

C	-0.442770	-1.681493	-0.153443
C	0.168865	-1.110513	1.109505
H	0.840400	-1.836535	1.581979
H	-0.580495	-0.801185	1.845198
C	0.886692	0.095615	0.535731
H	0.232298	0.966782	0.504903
O	1.069787	-0.259558	-0.897560
C	0.052529	-1.298435	-1.350217
C	0.925490	3.490245	1.233955
C	-0.466190	3.512097	1.251065
C	-1.203905	3.255265	0.085575
C	-0.507514	3.016112	-1.101378
C	0.890424	3.008968	-1.126608
C	1.604612	3.221372	0.045153
H	1.491686	3.633388	2.151660
H	-0.994944	3.700789	2.183879
H	-1.064989	2.805025	-2.011670
H	1.446953	2.788286	-2.034417

C	-2.710928	3.186864	0.135952
H	-3.141622	3.222087	-0.869262
H	-3.040797	2.249460	0.600152
H	-3.127884	4.014543	0.719404
S	3.438588	3.006410	0.072298
O	3.535401	1.869202	1.092736
O	3.681103	2.510876	-1.345821
C	2.450703	-0.469941	-1.373476
H	2.944572	0.504145	-1.287978
H	2.303969	-0.742762	-2.419006
H	1.861046	0.373643	0.946783
O	-2.036878	-3.475303	-1.288251
O	-1.852034	-3.380444	1.244253
C	-3.186729	-1.497546	0.003998
C	-3.519033	-0.805210	-1.160208
C	-3.836744	-1.243630	1.203289
C	-4.519302	0.156185	-1.109518
H	-2.981317	-1.019620	-2.080012
C	-4.839607	-0.271617	1.237909
H	-3.556431	-1.808562	2.087166
C	-5.187584	0.441701	0.090147
H	-4.782082	0.707048	-2.009697
H	-5.352899	-0.062883	2.173339
S	-1.855230	-2.702693	-0.060268
C	-6.224028	1.535221	0.138168
H	-6.842214	1.457644	1.036134
H	-5.740298	2.519142	0.147224
H	-6.880132	1.498501	-0.736277
C	3.130483	-1.553195	-0.583578
C	2.837858	-2.900527	-0.825981
C	4.038494	-1.206073	0.422816

C	3.444771	-3.895909	-0.064289
H	2.117847	-3.159348	-1.598240
C	4.648103	-2.208440	1.178319
H	4.234886	-0.151363	0.619232
C	4.351934	-3.549437	0.938421
H	3.206162	-4.939030	-0.248861
H	5.349990	-1.936692	1.961233
H	4.823779	-4.326220	1.533966

IN1

C	2.537231	-0.746258	0.000025
H	2.516001	-1.380417	-0.890923
H	2.516001	-1.380329	0.891036
H	3.472389	-0.181039	-0.000003
C	1.306250	0.157476	-0.000022
C	-0.069400	-0.464407	-0.000037
H	-0.161670	-1.111844	0.882281
H	-0.161694	-1.111756	-0.882417
C	-1.215868	0.553154	0.000025
H	-1.086896	1.204319	0.884852
O	-2.434231	-0.072829	0.000019
C	1.635732	1.418348	-0.000017
Li	-3.899014	-0.723523	-0.000023
H	-1.086917	1.204393	-0.884753

IN2

C	2.282517	0.310520	0.049364
H	2.768546	-0.105037	-0.843376
H	2.731500	-0.188062	0.917859

H	2.523637	1.374989	0.103686
C	0.799467	0.113420	0.004016
C	0.190862	-1.274709	-0.126061
H	0.606789	-1.991801	0.590911
H	0.356041	-1.686856	-1.132164
C	-1.286297	-0.991821	0.149622
H	-1.982615	-1.539411	-0.490066
O	-1.445277	0.413620	-0.099877
C	-0.125362	1.082325	-0.009358
Li	-1.691734	2.190459	0.014951
H	-1.533598	-1.182562	1.201817

IN3

C	-4.004384	-0.533859	-0.148236
H	-4.126009	-1.260099	0.661378
H	-4.003753	-1.065231	-1.104393
H	-4.858901	0.146685	-0.130650
C	-2.679727	0.196225	0.024043
C	-1.388507	-0.586563	0.059623
H	-1.338733	-1.104197	1.030363
C	-0.141437	0.278796	-0.115872
H	-0.152002	0.680360	-1.148382
C	-2.803662	1.490423	0.143593
N	1.041625	-0.487440	0.144464
C	2.236941	0.127572	-0.391767
H	2.126772	0.304614	-1.482976
H	-1.414199	-1.361583	-0.717943
C	2.580253	1.480435	0.250645
H	2.723750	1.349253	1.330388
H	3.492429	1.911250	-0.178544

H	1.769525	2.199981	0.105252
C	3.416391	-0.832320	-0.209150
H	3.223094	-1.790803	-0.712044
H	4.348197	-0.433158	-0.619100
H	3.599916	-1.007245	0.864748
H	-0.256849	1.165383	0.544075
Li	1.426726	-2.015793	0.956438

IN4

C	-3.229407	0.466741	0.058072
H	-3.682733	0.269615	1.038557
H	-3.858168	-0.041873	-0.687259
H	-3.329740	1.548051	-0.125197
C	-1.800409	0.019621	-0.007283
C	-1.431427	-1.442960	0.173664
H	-1.896431	-1.921963	1.043312
C	0.092293	-1.345983	0.300556
H	0.361375	-1.236158	1.366826
C	-0.715599	0.746772	-0.382300
N	0.408493	-0.118583	-0.445666
C	1.729698	0.462877	-0.252937
H	1.766616	1.324046	-0.935174
H	-1.717367	-2.028327	-0.715553
C	1.981917	0.982723	1.170903
H	2.063492	0.159281	1.888118
H	2.916006	1.553047	1.215070
H	1.157462	1.627978	1.491413
C	2.822887	-0.518032	-0.673273
H	2.629409	-0.895578	-1.681241
H	3.803591	-0.032198	-0.657843

H	2.866902	-1.372097	0.011696
H	0.623207	-2.213795	-0.102628
Li	-1.087596	2.619834	-0.784950

S'-Bn

C	-3.695940	1.535724	-0.151384
H	-3.521115	2.172913	-1.026565
H	-4.700901	1.108221	-0.253676
H	-3.682631	2.164052	0.741963
C	-2.659067	0.455860	-0.049063
C	-2.517900	-0.567817	-1.161516
H	-3.341564	-1.292935	-1.136800
H	-2.512860	-0.104216	-2.153881
C	-1.181454	-1.221446	-0.860386
H	-0.352192	-0.684317	-1.330680
O	-1.073768	-1.045735	0.576042
C	-1.881462	0.318466	1.035079
C	0.218207	-1.245483	1.190740
H	0.044070	-0.971974	2.231734
H	0.434703	-2.315920	1.117701
C	1.315722	-0.426259	0.565650
C	2.350523	-1.054207	-0.130166
C	1.306628	0.969084	0.677059
C	3.372983	-0.302653	-0.708890
H	2.358993	-2.138440	-0.217865
C	2.323426	1.718944	0.092225
H	0.488589	1.448436	1.207452
C	3.357842	1.085811	-0.598969
H	4.175518	-0.800130	-1.244173
H	2.311373	2.800855	0.178687

H	4.150495	1.674792	-1.049839
H	-1.119386	-2.291600	-1.074669

S'-Me

C	-2.569788	-0.559179	0.130339
H	-3.163729	-0.160198	-0.700806
H	-2.982060	-0.143736	1.057475
H	-2.697687	-1.643622	0.150736
C	-1.119486	-0.204855	-0.026125
C	-0.694698	1.249397	-0.103777
H	-1.196273	1.868570	0.647704
H	-0.913797	1.678879	-1.089658
C	0.797098	1.177380	0.158097
H	1.407019	1.919263	-0.363272
O	1.142194	-0.132453	-0.353446
C	-0.174693	-1.148868	-0.150081
C	2.346101	-0.699472	0.165577
H	1.016053	1.183680	1.232674
H	2.454707	-1.670718	-0.311034
H	3.176805	-0.037429	-0.089558
H	2.254203	-0.821480	1.249122

S'-OtBu

C	-3.391316	-0.812788	0.095843
H	-4.033239	-0.520597	-0.744310
H	-3.874497	-0.459434	1.014706
H	-3.346181	-1.903662	0.126680
C	-2.014012	-0.234294	-0.051933
C	-1.824402	1.263819	-0.148125

H	-2.411760	1.808923	0.599060
H	-2.116613	1.638974	-1.137676
C	-0.337280	1.438360	0.096452
H	0.123586	2.254098	-0.463064
O	0.213711	0.183985	-0.377560
C	-0.932753	-1.019158	-0.161116
C	1.970897	-1.330577	-0.904460
H	1.905881	-1.011625	-1.948504
H	3.000730	-1.631673	-0.690288
H	1.298175	-2.175017	-0.754027
C	1.599748	-0.613241	1.481052
H	1.309103	0.202173	2.150152
H	0.917408	-1.452769	1.626354
H	2.615256	-0.918704	1.750414
C	2.483874	1.025473	-0.227725
H	2.275332	1.847018	0.463414
H	3.523548	0.722474	-0.077897
H	2.377296	1.383700	-1.256119
C	1.586049	-0.182724	0.019415
H	-0.118534	1.535032	1.165166

S'-THF

C	-3.043778	-1.564340	0.087106
H	-3.882720	-1.404979	-0.601306
H	-3.451531	-1.559945	1.105041
H	-2.622336	-2.552090	-0.112522
C	-1.997649	-0.501883	-0.084452
C	-2.358087	0.957703	0.110651
H	-2.955191	1.120640	1.014287
H	-2.933513	1.341418	-0.741790

C	-1.002668	1.628334	0.224900
H	-0.934484	2.627066	-0.213612
O	-0.147371	0.743161	-0.550720
C	-0.746250	-0.799386	-0.463368
C	1.281620	0.904294	-0.311147
O	1.607530	0.657606	1.002840
C	2.054724	-0.083032	-1.173805
H	1.471494	1.960034	-0.523597
C	1.931713	-0.738591	1.168108
C	2.358111	-1.253471	-0.217961
H	2.972153	0.406850	-1.510606
H	1.468440	-0.385221	-2.041543
H	2.724399	-0.780913	1.917643
H	1.043539	-1.263395	1.527563
H	3.418481	-1.514632	-0.239077
H	1.762554	-2.124562	-0.490207
H	-0.628977	1.625823	1.252575

S'-THP

C	4.099044	0.917879	-0.118722
H	4.859587	0.259400	-0.555775
H	4.422689	1.159649	0.900724
H	4.072592	1.841513	-0.701142
C	2.751079	0.257574	-0.118889
C	2.552322	-1.062347	0.600208
H	3.000245	-1.061872	1.600009
H	3.002845	-1.889325	0.036448
C	1.041430	-1.201527	0.681179
H	0.648280	-2.211172	0.567694
O	0.609687	-0.424543	-0.470581

C	1.716596	0.773919	-0.798893
C	-0.742970	0.033894	-0.528329
C	-1.077044	1.110808	0.490063
H	-0.836413	0.427776	-1.549520
C	-2.912035	-0.847711	-0.545772
C	-2.563418	1.460899	0.346194
H	-0.885818	0.734001	1.500985
H	-0.428920	1.971981	0.311729
C	-3.412873	0.191891	0.449705
H	-3.415752	-1.808530	-0.426219
H	-3.072831	-0.497024	-1.577776
H	-2.854608	2.190771	1.106615
H	-2.732024	1.935097	-0.630108
H	-4.468666	0.405967	0.252842
H	-3.340996	-0.223419	1.462102
O	-1.525214	-1.114479	-0.357411
H	0.641232	-0.734315	1.584864

S'-allyl

C	2.883556	0.979558	-0.202191
H	3.724631	0.465607	0.277664
H	2.758044	1.944473	0.304338
H	3.146907	1.169434	-1.244899
C	1.627144	0.160736	-0.117690
C	1.036422	-0.166654	1.239342
H	0.600369	0.730062	1.701398
H	1.788305	-0.561168	1.931904
C	-0.013392	-1.219469	0.925162
H	0.372630	-2.233852	1.037794
O	-0.275882	-1.073042	-0.502579

C	0.984966	-0.245603	-1.223222
C	-1.552351	-0.504372	-0.879160
H	-2.325588	-1.220408	-0.583696
H	-1.489092	-0.446450	-1.967431
C	-1.779700	0.843725	-0.267320
H	-1.042623	1.605521	-0.513638
C	-2.824032	1.115224	0.513355
H	-2.986752	2.107660	0.920609
H	-3.561351	0.353404	0.758506
H	-0.954104	-1.108822	1.468432

S'-dioxane

C	3.849140	0.912178	-0.330354
H	4.691272	0.316190	0.039173
H	3.818336	1.840638	0.251838
H	4.041238	1.167595	-1.374809
C	2.554333	0.157607	-0.192126
C	2.063845	-0.239034	1.181989
H	1.698554	0.644866	1.719684
H	2.861231	-0.693411	1.781215
C	0.948547	-1.239732	0.923591
H	1.318019	-2.265179	0.886493
O	0.497569	-0.966271	-0.432895
C	1.826678	-0.096074	-1.284015
C	-0.703626	-0.275206	-0.573064
H	-0.753549	0.033878	-1.627559
C	-3.007801	-0.539250	-0.394129
C	-1.886655	1.593234	0.153588
C	-3.089223	0.712535	0.471926
H	-3.741831	-1.293652	-0.108707

H	-3.162943	-0.285137	-1.454464
H	-1.784716	2.429406	0.846245
H	-1.958246	1.994722	-0.869152
H	-4.022201	1.251382	0.278057
H	-3.064777	0.428525	1.528642
O	-1.730206	-1.154862	-0.244163
O	-0.688259	0.831165	0.272150
H	0.095358	-1.167636	1.598178

S-Bn

C	-5.275210	1.031493	0.000056
H	-5.190930	1.658769	-0.891617
H	-5.191115	1.658273	0.892095
H	-6.260678	0.560194	-0.000178
C	-4.146185	0.006246	-0.000116
C	-2.715628	0.482043	0.000127
H	-2.551321	1.111762	0.882648
H	-2.551120	1.112040	-0.882158
C	-1.708036	-0.655104	0.000056
H	-1.845461	-1.288380	0.890674
O	-0.421221	-0.082571	0.000163
C	-4.580991	-1.222982	-0.000496
C	0.601116	-1.049949	0.000219
H	0.504595	-1.696470	-0.887349
H	0.504651	-1.696300	0.887915
C	1.956230	-0.386331	0.000095
C	2.094485	1.000753	0.000029
C	3.101246	-1.188488	0.000031
C	3.365686	1.577337	-0.000102
H	1.204817	1.620448	0.000075

C	4.368151	-0.613481	-0.000099
H	2.999079	-2.271817	0.000076
C	4.503858	0.775500	-0.000168
H	3.463997	2.658660	-0.000156
H	5.249359	-1.247537	-0.000154
H	5.490957	1.226906	-0.000276
H	-1.845383	-1.288204	-0.890700

S-Me

C	-3.010571	-0.534890	0.000054
H	-3.070266	-1.165112	0.891658
H	-3.070587	-1.164753	-0.891781
H	-3.863927	0.147086	0.000354
C	-1.678528	0.207881	0.000002
C	-0.393494	-0.580555	-0.000042
H	-0.376792	-1.231946	-0.881957
H	-0.376755	-1.231980	0.881847
C	0.848706	0.294377	-0.000055
H	0.859847	0.943325	-0.890607
O	1.967850	-0.558541	-0.000063
C	-1.824162	1.503551	-0.000018
C	3.184537	0.150432	0.000084
H	0.859855	0.943322	0.890497
H	3.989587	-0.585223	-0.000107
H	3.273643	0.784624	-0.893234
H	3.273664	0.784210	0.893691

S-OtBu

C	-4.178495	-0.579796	0.028875

H	-4.208699	-1.224376	0.911695
H	-4.264861	-1.196277	-0.870185
H	-5.033209	0.099433	0.066344
C	-2.849114	0.166536	-0.001845
C	-1.562326	-0.617890	-0.057987
H	-1.564142	-1.238347	-0.962247
H	-1.523914	-1.300169	0.799572
C	-0.321885	0.262556	-0.057870
H	-0.359431	0.954827	-0.911357
O	0.786844	-0.601539	-0.152020
C	-2.992943	1.462179	0.024227
C	3.037868	-1.173109	-0.326113
H	2.876544	-1.503019	-1.356098
H	4.079549	-0.859308	-0.213295
H	2.849529	-2.019016	0.340861
C	2.301079	0.424187	1.457796
H	1.661474	1.271120	1.722393
H	2.087847	-0.403625	2.140459
H	3.338821	0.738306	1.605029
C	2.302227	1.138306	-0.960676
H	1.683325	2.003172	-0.703174
H	3.347541	1.459526	-0.932069
H	2.063524	0.827152	-1.982567
C	2.090938	-0.025732	0.009576
H	-0.292740	0.859493	0.864907

S-THF

C	4.438377	-0.542504	-0.558178
H	4.301976	-0.807547	-1.610311
H	4.606496	-1.452376	0.024666

H	5.324244	0.091144	-0.473318
C	3.179603	0.153109	-0.049212
C	1.863640	-0.580351	-0.090209
H	1.957244	-1.506879	0.489125
H	1.652729	-0.869799	-1.126863
C	0.702641	0.238505	0.448264
H	0.887083	0.522727	1.496056
O	-0.454024	-0.572877	0.364664
C	3.421941	1.359994	0.380714
C	-1.614784	0.054973	0.854235
O	-1.943779	1.198100	0.107923
C	-2.777109	-0.903890	0.653795
H	-1.447681	0.387386	1.887225
C	-2.781390	0.829991	-0.997551
C	-3.104538	-0.663318	-0.825053
H	-3.607529	-0.598073	1.297048
H	-2.501002	-1.933702	0.884048
H	-3.677429	1.456894	-0.949554
H	-2.256228	1.040380	-1.933859
H	-4.142026	-0.892912	-1.075826
H	-2.452138	-1.274297	-1.453071
H	0.566403	1.156211	-0.136889

S-THP

C	5.035017	-0.333892	-0.295449
H	5.065491	-0.526081	-1.371499
H	5.190505	-1.272639	0.243482
H	5.849170	0.349265	-0.042723
C	3.668420	0.234900	0.072845
C	2.431201	-0.580483	-0.203642

H	2.508873	-1.533637	0.333300
H	2.393843	-0.815845	-1.273970
C	1.148123	0.126053	0.198551
H	1.156033	0.356858	1.275180
O	0.080196	-0.759527	-0.094370
C	3.751010	1.419575	0.611126
C	-1.164655	-0.291563	0.299768
C	-2.205318	-1.362688	0.027473
H	-1.146875	-0.030212	1.379276
C	-2.692001	1.461569	-0.059959
C	-3.601409	-0.828462	0.362741
H	-2.134326	-1.622312	-1.034996
H	-1.964001	-2.254765	0.613208
C	-3.841316	0.503367	-0.353216
H	-2.778064	2.388586	-0.630680
H	-2.677401	1.718121	1.013122
H	-4.365346	-1.562353	0.089427
H	-3.682263	-0.675247	1.447825
H	-4.788377	0.954130	-0.037450
H	-3.893953	0.339795	-1.436095
O	-1.447090	0.888679	-0.427190
H	1.027404	1.062868	-0.356362

S-allyl

C	-3.983645	-0.743383	0.119428
H	-3.938124	-1.364156	1.018450
H	-4.023034	-1.388250	-0.762791
H	-4.899410	-0.148944	0.155062
C	-2.733300	0.127017	0.048177
C	-1.378091	-0.531410	-0.006413

H	-1.338466	-1.189595	-0.882533
H	-1.255724	-1.166088	0.879226
C	-0.230267	0.461880	-0.073374
H	-0.325460	1.098370	-0.967718
O	0.966725	-0.278299	-0.122515
C	-3.005781	1.402033	0.043239
C	2.114759	0.545167	-0.181270
H	2.187407	1.170716	0.721936
H	2.035439	1.218052	-1.051799
C	3.325632	-0.325293	-0.314463
H	3.288253	-1.061982	-1.114989
C	4.400754	-0.221151	0.462419
H	5.271361	-0.851446	0.314673
H	4.444627	0.502425	1.272753
H	-0.241045	1.118130	0.811387

S-dioxane

C	4.872239	-0.065726	0.096432
H	5.120899	-0.247045	-0.952931
H	5.015203	-0.988211	0.665978
H	5.554806	0.692151	0.487830
C	3.412111	0.364175	0.197714
C	2.334785	-0.563796	-0.301996
H	2.422421	-1.522757	0.222573
H	2.505623	-0.761517	-1.367149
C	0.935286	-0.007193	-0.108487
H	0.719300	0.146990	0.953706
O	0.044092	-0.983580	-0.648837
C	3.279647	1.545589	0.733183
C	-1.284664	-0.726941	-0.460679

H	-1.849626	-1.535402	-0.955403
C	-2.945431	-0.492407	1.176733
C	-2.988606	0.818885	-0.909864
C	-3.381009	0.832054	0.562178
H	-3.055229	-0.505085	2.262246
H	-3.541019	-1.320838	0.758630
H	-3.129647	1.789121	-1.388621
H	-3.586618	0.071819	-1.457500
H	-4.461765	0.969800	0.671015
H	-2.870344	1.656338	1.069462
O	-1.568323	-0.723661	0.912500
H	0.812780	0.941401	-0.641754
O	-1.608636	0.505414	-1.043583

THF

C	1.126351	0.470563	0.160530
O	-0.000003	1.193507	-0.302879
C	-1.126366	0.470551	0.160494
C	-0.774503	-1.012801	-0.050565
C	0.774524	-1.012781	-0.050612
H	1.998536	0.807202	-0.402576
H	1.288843	0.683446	1.228927
H	-1.288921	0.683473	1.228873
H	-1.998527	0.807150	-0.402672
H	-1.195655	-1.644706	0.734822
H	-1.160956	-1.366596	-1.009009
H	1.195745	-1.644738	0.734696
H	1.160923	-1.366478	-1.009114

TS-R-Bn

C	-4.957442	1.196707	0.000091
H	-5.524226	0.898716	-0.886713
H	-4.503692	2.176679	-0.172731
H	-5.651499	1.280904	0.840013
C	-3.856031	0.174638	0.259915
C	-2.817197	-0.080365	-0.797199
H	-2.328385	0.868397	-1.047598
H	-3.328490	-0.418934	-1.705761
C	-1.721342	-1.071480	-0.380226
H	-1.921104	-1.493003	0.617252
O	-0.492590	-0.379584	-0.366262
C	-3.988610	-0.374521	1.436324
C	0.584600	-1.201260	0.015954
H	0.677361	-2.051054	-0.679801
H	0.394677	-1.617739	1.019192
C	1.869077	-0.410174	0.027331
C	1.868335	0.982901	-0.034879
C	3.086068	-1.089977	0.127122
C	3.072793	1.686005	0.004812
H	0.922803	1.507200	-0.117915
C	4.287244	-0.388313	0.171229
H	3.093137	-2.177122	0.169427
C	4.283423	1.005444	0.109365
H	3.062863	2.770507	-0.046224
H	5.225878	-0.928240	0.248743
H	5.218823	1.555171	0.140225
H	-1.662941	-1.912441	-1.087046

TS-R-Me

C	-2.943663	-0.364794	-0.337011
H	-3.302520	-0.991194	0.484802
H	-2.839782	-0.975142	-1.238537
H	-3.688826	0.411181	-0.529134
C	-1.583234	0.217310	0.031215
C	-0.440236	-0.709788	0.341289
H	-0.292689	-1.384546	-0.510044
H	-0.729051	-1.335737	1.193625
C	0.896023	-0.001096	0.603966
H	0.775589	1.093954	0.598594
O	1.797200	-0.385997	-0.408429
C	-1.611992	1.521983	0.031867
C	3.054082	0.232750	-0.269850
H	1.302772	-0.280817	1.587733
H	3.683635	-0.125267	-1.085128
H	2.965793	1.326414	-0.333669
H	3.521593	-0.029068	0.690332

TS-R-THF

C	-4.399196	0.756595	-0.185739
H	-4.674898	0.695880	-1.242532
H	-4.197040	1.799113	0.076062
H	-5.245785	0.408563	0.411397
C	-3.141558	-0.071959	0.053899
C	-1.879697	0.264381	-0.692194
H	-1.616474	1.307189	-0.479786
H	-2.092364	0.206171	-1.766084
C	-0.672912	-0.610096	-0.321839
H	-0.949410	-1.383036	0.411610
O	0.315000	0.235622	0.241648

C	-3.361595	-1.018724	0.924667
C	1.463398	-0.456691	0.666298
O	2.124479	-1.077772	-0.408317
C	2.447117	0.567811	1.207675
H	1.176584	-1.251967	1.366877
C	3.093903	-0.180093	-0.968440
C	3.081668	1.080368	-0.090404
H	3.186189	0.058819	1.833584
H	1.947878	1.340746	1.793255
H	4.063064	-0.689282	-0.946073
H	2.831769	0.028637	-2.009733
H	4.082286	1.492312	0.054836
H	2.448133	1.852793	-0.532654
H	-0.262539	-1.118294	-1.200942

TS-R-THP

C	-4.938595	0.435372	-0.189060
H	-5.348161	-0.286115	-0.901907
H	-4.840098	1.409335	-0.676792
H	-5.640915	0.534740	0.642354
C	-3.562244	-0.035783	0.267962
C	-2.471305	-0.232478	-0.748829
H	-2.319417	0.711361	-1.285333
H	-2.820468	-0.961709	-1.488948
C	-1.121480	-0.657038	-0.153129
H	-1.184020	-0.776367	0.939208
O	-0.183033	0.364809	-0.454960
C	-3.529838	-0.216708	1.559920
C	1.054925	0.187052	0.143982
C	1.932430	1.384512	-0.172506

H	0.930582	0.072910	1.241668
C	2.885567	-1.288985	0.234144
C	3.337072	1.164818	0.397132
H	1.967541	1.483235	-1.263532
H	1.467865	2.286381	0.237012
C	3.889936	-0.183316	-0.072822
H	3.202355	-2.251543	-0.173075
H	2.766213	-1.399338	1.325486
H	4.000133	1.983330	0.101773
H	3.290838	1.173979	1.494872
H	4.845842	-0.407283	0.412901
H	4.063244	-0.157628	-1.155205
O	1.625284	-1.009060	-0.354532
H	-0.778350	-1.605954	-0.575312

TS-R-allyl

C	-3.836738	-0.761066	-0.282109
H	-4.276209	-0.917751	0.707238
H	-3.562577	-1.727898	-0.713530
H	-4.589993	-0.297434	-0.923956
C	-2.584314	0.098040	-0.145650
C	-1.446297	-0.382459	0.712312
H	-1.128310	-1.369163	0.355917
H	-1.821708	-0.522045	1.732676
C	-0.213915	0.533109	0.697993
H	-0.398411	1.443037	0.105259
O	0.857052	-0.192022	0.136507
C	-2.691671	1.202493	-0.832500
C	2.044086	0.570930	0.052329
H	2.375604	0.881799	1.055667

H	1.848522	1.483166	-0.536159
C	3.099421	-0.254639	-0.615798
H	2.812530	-0.702160	-1.565641
C	4.321376	-0.434788	-0.121213
H	5.068393	-1.016433	-0.651035
H	4.615032	-0.002018	0.832040
H	0.049020	0.853370	1.717286

TS-R-dioxane

C	4.825713	-0.066369	0.107831
H	5.169245	-0.821576	-0.605095
H	4.896206	-0.467472	1.122892
H	5.485051	0.802135	0.033626
C	3.370491	0.281964	-0.191503
C	2.330132	-0.802713	-0.148165
H	2.357380	-1.275013	0.840624
H	2.616047	-1.576058	-0.870822
C	0.896168	-0.320607	-0.405387
H	0.860741	0.746112	-0.647670
O	0.161686	-0.551361	0.800087
C	3.252997	1.551661	-0.467851
C	-1.177942	-0.293821	0.723359
H	-1.603650	-0.468108	1.726252
C	-2.755973	1.381537	0.285413
C	-3.174487	-0.977723	-0.295696
C	-3.479812	0.462049	-0.690510
H	-2.798194	2.428898	-0.017232
H	-3.197366	1.293427	1.291828
H	-3.533017	-1.697808	-1.033032
H	-3.642302	-1.213920	0.674416

H	-4.558700	0.647114	-0.665726
H	-3.116452	0.648132	-1.705944
O	-1.377930	1.039460	0.345425
H	0.429331	-0.879854	-1.220616
O	-1.769761	-1.170834	-0.199067

TS-R-tBu

C	4.041214	-0.241319	0.500648
H	4.487017	-0.974720	-0.177507
H	3.910586	-0.695190	1.487120
H	4.729279	0.602267	0.596488
C	2.680013	0.180730	-0.039236
C	1.606276	-0.853976	-0.239909
H	1.419253	-1.355717	0.716452
H	1.988751	-1.616700	-0.928268
C	0.267640	-0.280314	-0.734452
H	0.344903	0.805977	-0.881740
O	-0.703007	-0.585693	0.242784
C	2.626909	1.464043	-0.272028
C	-2.830058	-0.637330	1.188774
H	-2.368253	-0.497175	2.170000
H	-3.839452	-0.216653	1.210332
H	-2.897200	-1.710260	0.988247
C	-2.588714	-0.202227	-1.268352
H	-2.042799	0.331408	-2.052469
H	-2.582069	-1.272142	-1.499967
H	-3.624376	0.149363	-1.289606
C	-1.873539	1.542732	0.408126
H	-1.302099	2.072469	-0.359428
H	-2.870631	1.992130	0.443498

H	-1.385006	1.698702	1.374164
C	-1.986187	0.043964	0.116494
H	-0.005176	-0.726040	-1.699973

TS-R1

C	4.330981	-0.118391	0.565383
H	4.838280	-0.885345	-0.026917
H	4.194464	-0.483277	1.587316
H	4.967342	0.769465	0.597337
C	2.965472	0.169341	-0.048464
C	1.956997	-0.940320	-0.173067
H	1.759875	-1.350025	0.824102
H	2.405230	-1.747501	-0.764711
C	0.606305	-0.497753	-0.765819
H	0.639239	0.572043	-1.022676
O	-0.415277	-0.751688	0.175212
C	2.852646	1.420243	-0.403631
Si	-1.888081	0.053466	0.108030
C	-2.924285	-0.714299	1.458601
H	-2.438856	-0.592782	2.431481
H	-3.912765	-0.246955	1.510495
H	-3.061564	-1.784868	1.280360
C	-2.658702	-0.201480	-1.585647
H	-2.040101	0.235544	-2.376909
H	-2.786349	-1.266531	-1.803855
H	-3.643673	0.274165	-1.639271
C	-1.611103	1.884285	0.410925
H	-0.988226	2.341256	-0.364832
H	-2.566695	2.419516	0.422353
H	-1.119042	2.048579	1.374489

H	0.398337	-1.048060	-1.692570

TS-R2

C	-2.371918	-0.522159	-0.188494
H	-2.620798	-1.099222	0.706779
H	-2.282305	-1.197679	-1.043930
H	-3.189583	0.175758	-0.385767
C	-1.038804	0.190382	0.027095
C	0.194586	-0.617558	0.322348
H	0.333458	-1.337023	-0.494612
H	0.001911	-1.205320	1.228955
C	1.488516	0.214857	0.462765
H	1.268168	1.283785	0.411896
O	2.408841	-0.029275	-0.583971
H	2.825642	-0.887132	-0.451233
C	-1.199313	1.480517	-0.080012
H	1.954377	0.024798	1.437465

TS-R3

C	-0.112242	0.263377	-0.324642
C	1.269920	0.867834	-0.327771
H	1.517511	1.149566	0.701112
H	1.225970	1.785668	-0.922159
C	2.355871	-0.090141	-0.843700
O	3.260543	-0.316605	0.219777
C	-0.558616	-0.905824	-0.701991
C	4.307779	-1.196307	-0.117221
O	5.096275	-0.688452	-1.162980
C	5.234739	-1.287884	1.083681

H	3.888940	-2.149638	-0.465886
C	6.174169	0.093705	-0.625669
C	6.074627	-0.018007	0.902809
H	5.852343	-2.186279	0.991293
H	4.681251	-1.323811	2.022767
H	7.107970	-0.328677	-1.010927
H	6.081994	1.123906	-0.981129
H	7.055920	-0.082265	1.376900
H	5.542573	0.840433	1.319229
H	1.929161	-1.050297	-1.171856
H	2.887464	0.345305	-1.696189
S	-1.400664	1.372409	0.304193
O	-1.102306	1.587263	1.714452
O	-1.452779	2.494366	-0.625733
C	-2.895867	0.434009	0.164694
C	-3.284936	-0.374865	1.229533
C	-3.630207	0.509571	-1.015841
C	-4.438963	-1.137491	1.092790
H	-2.694682	-0.392085	2.140141
C	-4.780879	-0.262244	-1.129238
H	-3.303138	1.166058	-1.815757
C	-5.196017	-1.096246	-0.084311
H	-4.761008	-1.772125	1.913438
H	-5.369272	-0.214386	-2.041002
C	-6.424669	-1.954699	-0.231928
H	-7.140181	-1.506630	-0.925085
H	-6.153270	-2.940878	-0.623115
H	-6.921036	-2.103731	0.729826

TS-R4

C	-2.775642	-0.610450	-0.243505
H	-3.112598	-1.037265	0.705537
H	-2.565251	-1.417895	-0.950500
H	-3.583599	0.002359	-0.650991
C	-1.502694	0.195347	-0.009607
C	-0.290251	-0.484494	0.563455
H	-0.070965	-1.362029	-0.058620
H	-0.555383	-0.878557	1.551355
C	0.947330	0.432692	0.672391
H	0.709967	1.449913	0.354530
H	3.205268	0.680821	-0.094031
C	-1.661763	1.444290	-0.353735
H	1.303377	0.471219	1.702539
S	2.272956	-0.235805	-0.395864

TS-R5

C	-2.737271	-0.058827	0.199978
H	-3.170484	0.724330	-0.428318
H	-2.883212	0.197875	1.253322
H	-3.264484	-0.994524	-0.000662
C	-1.239316	-0.163745	-0.084611
C	-0.366402	1.037310	0.180449
H	-0.298918	1.184837	1.266592
H	-0.874758	1.920396	-0.226682
C	1.024694	0.954317	-0.433012
H	0.944485	0.861630	-1.518308
H	1.055241	-1.065885	0.862561
C	-0.953332	-1.361244	-0.522280
H	1.574251	1.869405	-0.203303
S	2.034228	-0.446558	0.184478

TS-R6

C	-3.887028	0.487772	-0.184477
H	-4.298772	-0.138902	-0.980984
H	-3.773453	1.511786	-0.551663
H	-4.595836	0.496676	0.647501
C	-2.520135	-0.050968	0.223922
C	-1.421509	-0.143881	-0.799344
H	-1.779957	-0.779952	-1.618082
C	-0.074978	-0.655702	-0.245090
H	-0.168185	-0.907001	0.817979
C	-2.504403	-0.378588	1.486975
N	0.943472	0.381591	-0.348319
C	2.189136	0.107169	0.370227
H	1.912533	0.016015	1.429892
H	1.155547	0.563175	-1.329007
H	-1.269591	0.858764	-1.218378
C	2.897651	-1.182347	-0.060499
H	3.151566	-1.136589	-1.127008
H	3.826409	-1.321048	0.501624
H	2.274391	-2.065841	0.104364
C	3.109876	1.312626	0.212597
H	2.602607	2.224812	0.534865
H	4.023862	1.186346	0.799477
H	3.402869	1.433381	-0.837877
H	0.200051	-1.589245	-0.760334

TS-R7

C	-0.440482	5.068178	1.085625

H	0.410457	5.287309	1.736985
H	-1.279497	4.721620	1.696049
H	-0.737147	5.991876	0.582942
C	-0.050774	3.973830	0.100408
C	0.375666	2.624970	0.612340
H	1.218686	2.762555	1.300092
C	0.745167	1.619491	-0.497796
H	0.571350	2.061382	-1.498735
C	-0.145322	4.361696	-1.143503
N	0.000151	0.375291	-0.352279
C	-1.389785	0.546531	-0.767504
H	-1.754954	1.492208	-0.348630
H	-0.439271	2.210081	1.219852
H	1.810653	1.383505	-0.439550
C	0.630531	-0.724007	-1.079730
H	-0.061239	-1.574192	-1.051708
H	0.780380	-0.465558	-2.145467
C	1.948069	-1.137865	-0.465222
C	2.039593	-1.348216	0.914671
C	3.080941	-1.334263	-1.255333
C	3.240728	-1.753414	1.489565
H	1.158503	-1.181284	1.528138
C	4.286064	-1.743348	-0.682573
H	3.021311	-1.162608	-2.327423
C	4.368542	-1.953491	0.691469
H	3.299321	-1.914927	2.561739
H	5.159677	-1.890854	-1.310018
H	5.305470	-2.268363	1.140163
H	-1.466692	0.647385	-1.866860
C	-2.277747	-0.581196	-0.291778
C	-2.199653	-1.022102	1.033311

C	-3.196355	-1.184234	-1.151449
C	-3.029329	-2.042596	1.489303
H	-1.472165	-0.561292	1.696359
C	-4.031875	-2.205258	-0.696899
H	-3.256410	-0.854511	-2.185846
C	-3.949812	-2.636975	0.624530
H	-2.958502	-2.377154	2.519846
H	-4.740637	-2.666348	-1.377845
H	-4.595350	-3.434260	0.979262

TS1

C	3.250056	-1.211119	-0.140213
H	4.034345	-1.057281	0.610943
H	3.699988	-1.021261	-1.122046
H	2.939241	-2.257115	-0.098524
C	2.080255	-0.309006	0.107714
C	2.251494	1.205716	0.117284
H	2.862878	1.555446	-0.721138
H	2.727682	1.551582	1.043813
C	0.816924	1.703259	-0.000882
H	0.572789	2.598304	0.572169
O	0.061112	0.594428	0.567422
C	0.837035	-0.728886	0.375029
Si	-1.401524	-0.224611	-0.033312
C	-2.073908	-1.390724	1.255420
H	-1.781902	-1.037387	2.249263
H	-3.167598	-1.429351	1.212787
H	-1.661096	-2.392039	1.122974
C	-1.235660	-0.857105	-1.786154
H	-0.529567	-0.235628	-2.347772

H	-0.857435	-1.880625	-1.801623
H	-2.203618	-0.811359	-2.297552
C	-2.537226	1.285824	-0.107424
H	-2.181972	2.034997	-0.824543
H	-3.544304	0.989889	-0.421431
H	-2.623641	1.769184	0.871685
H	0.512833	1.824014	-1.046646

TS10

C	-3.731339	-1.250120	0.060454
H	-4.658639	-0.793819	-0.312127
H	-3.928718	-1.572975	1.091368
H	-3.524724	-2.137507	-0.543578
C	-2.581701	-0.294810	-0.018497
C	-2.628910	1.056011	0.682225
H	-2.927258	0.989425	1.734929
H	-3.327811	1.741613	0.181544
C	-1.181992	1.511365	0.529495
H	-1.041525	2.579529	0.339911
O	-0.677528	0.770195	-0.596403
C	-1.480359	-0.441890	-0.777102
C	0.983230	-0.554546	-0.965306
C	1.067386	-1.212158	0.368334
H	0.511354	-1.024137	-1.818528
C	2.399569	1.077158	-0.137451
C	2.556416	-1.289039	0.746888
H	0.509060	-0.629746	1.111296
H	0.570211	-2.180911	0.302705
C	3.177134	0.119931	0.774721
H	1.552673	1.541435	0.377259

H	3.025230	1.854685	-0.571876
H	2.664849	-1.780365	1.716060
H	3.080025	-1.911479	0.014508
H	4.225694	0.077296	0.470585
H	3.149439	0.533603	1.787525
O	1.833280	0.374647	-1.264731
H	-0.602476	1.223217	1.424926

TS11

C	2.580810	2.107445	-0.125447
H	3.252008	2.322045	-0.969665
H	3.135407	2.362751	0.788441
H	1.723209	2.784459	-0.201735
C	2.117738	0.683309	-0.130029
C	3.111591	-0.466649	-0.085218
H	3.858023	-0.368619	0.712582
H	3.660212	-0.566215	-1.034663
C	2.166652	-1.641000	0.158543
H	2.419386	-2.555773	-0.385729
O	0.876519	-1.185827	-0.283012
C	0.842991	0.264807	-0.275146
C	-1.388962	-1.123697	0.510056
H	-0.901964	-2.033773	0.829169
C	-1.847405	1.177975	0.967301
C	-2.782476	-0.005134	-1.008724
C	-2.158790	1.282813	-0.515009
H	-0.934751	1.724075	1.210007
H	-2.679631	1.449925	1.618598
H	-2.838384	-0.057148	-2.094168
H	-3.769813	-0.199337	-0.577570

H	-2.854538	2.108390	-0.692661
H	-1.211580	1.434533	-1.037338
O	-1.524255	-0.198069	1.371925
O	-1.954622	-1.143194	-0.636204
H	2.108385	-1.867809	1.235100

TS12

C	3.182772	-0.417287	-0.000009
H	3.788207	-0.355148	-0.900944
H	2.692761	-1.400919	-0.000016
H	3.788212	-0.355162	0.900924
C	1.491206	0.257938	-0.000000
C	0.278564	-0.576593	-0.000004
H	0.244337	-1.218551	0.887000
H	0.244334	-1.218538	-0.887018
C	-0.953802	0.324794	0.000004
H	-0.951232	0.971273	0.890476
O	-2.079344	-0.518068	-0.000000
C	2.393614	1.137969	0.000005
H	-0.951234	0.971286	-0.890458
C	-3.288801	0.205399	0.000007
H	-3.370463	0.839516	-0.893515
H	-4.101024	-0.522041	0.000002
H	-3.370461	0.839501	0.893538

TS13

C	-4.384895	-0.446554	0.015576
H	-4.975297	-0.399507	0.927342
H	-3.901201	-1.432856	-0.012238

H	-5.004611	-0.362450	-0.873816
C	-2.692641	0.219498	0.000811
C	-1.484771	-0.621406	-0.039936
H	-1.478138	-1.254111	-0.934297
H	-1.430411	-1.273843	0.838276
C	-0.246164	0.274354	-0.066656
H	-0.291384	0.936438	-0.941285
O	0.861718	-0.591734	-0.132167
C	-3.587643	1.106721	0.035297
H	-0.225506	0.898182	0.836775
C	2.165166	-0.005787	0.009708
C	2.370593	1.127809	-0.996839
H	1.750644	1.999151	-0.764901
H	3.415101	1.452209	-0.980547
H	2.130854	0.784525	-2.008115
C	2.374333	0.489168	1.442986
H	2.167124	-0.318356	2.151231
H	3.410402	0.813620	1.578685
H	1.730591	1.340393	1.682662
C	3.114395	-1.160597	-0.291568
H	2.953628	-1.522174	-1.310923
H	4.155146	-0.840460	-0.189003
H	2.929069	-1.986125	0.401211

TS14

C	-4.197538	-0.600540	0.123640
H	-3.626443	-1.539401	0.115943
H	-4.848485	-0.608349	-0.747189
H	-4.762383	-0.570448	1.052163
C	-2.570973	0.214154	0.029216

C	-1.293142	-0.515395	-0.014243
H	-1.243358	-1.167173	-0.893322
H	-1.165868	-1.136968	0.878689
C	-0.143393	0.487030	-0.081328
H	-0.240960	1.118146	-0.977314
O	1.048827	-0.259143	-0.124924
C	-3.544042	1.014735	0.058092
C	2.200196	0.561891	-0.182359
H	2.271245	1.188659	0.719861
H	2.124733	1.232298	-1.054835
C	3.408129	-0.313374	-0.309359
H	3.373586	-1.048128	-1.111725
C	4.477872	-0.214757	0.475552
H	5.347052	-0.848107	0.332770
H	4.518809	0.507244	1.287412
H	-0.161192	1.142913	0.801680

TS15

C	-5.536288	0.884287	-0.016321
H	-4.854115	1.745835	-0.031911
H	-6.141196	0.964103	0.883571
H	-6.141597	0.931737	-0.918227
C	-4.016435	-0.123751	0.001530
C	-2.657542	0.442029	-0.009688
H	-2.490017	1.076712	0.867369
H	-2.492706	1.047892	-0.907372
C	-1.641543	-0.697525	0.007435
H	-1.778784	-1.314586	0.907524
O	-0.362981	-0.109555	-0.001427
C	-5.081652	-0.797071	0.013829

C	0.669450	-1.067642	0.017188
H	0.579885	-1.730912	-0.858337
H	0.577551	-1.697411	0.917015
H	-1.778857	-1.341673	-0.873439
C	2.017520	-0.390016	0.005906
C	3.169978	-1.181148	-0.013002
C	2.142232	0.998249	0.017177
C	4.431155	-0.593787	-0.019165
H	3.078369	-2.265344	-0.023025
C	3.407738	1.587135	0.010282
H	1.247140	1.609887	0.030570
C	4.553419	0.796373	-0.007574
H	5.318347	-1.219205	-0.033830
H	3.495589	2.669289	0.018823
H	5.536051	1.257319	-0.012897

TS16

C	-4.662750	-0.280860	0.588597
H	-5.114494	0.310405	1.381374
H	-4.124305	-1.112332	1.064344
H	-5.410929	-0.712996	-0.071434
C	-3.038478	0.196121	-0.078190
C	-1.798378	-0.550172	0.191866
H	-1.877502	-1.581527	-0.169332
H	-1.589259	-0.581696	1.266954
C	-0.630883	0.134305	-0.514943
H	-0.808955	0.167078	-1.599622
O	0.520606	-0.635818	-0.230639
C	-3.976870	0.962301	-0.426982
C	1.687621	-0.138862	-0.844731

O	2.007049	1.149270	-0.388138
C	2.846776	-1.021162	-0.410617
H	1.529477	-0.063446	-1.928500
C	2.851004	1.059824	0.769675
C	3.163161	-0.431536	0.969143
H	3.682584	-0.878491	-1.101990
H	2.570938	-2.076219	-0.389151
H	3.751083	1.647545	0.562868
H	2.333649	1.500433	1.626709
H	4.196296	-0.599356	1.279469
H	2.499715	-0.867824	1.719424
H	-0.506769	1.161065	-0.153800

TS17

C	-5.065935	0.317118	0.124887
H	-4.766572	0.577272	-0.899924
H	-5.494103	1.209478	0.574878
H	-5.790397	-0.490842	0.057431
C	-3.306599	-0.067673	0.382144
C	-2.281236	0.067644	-0.665779
H	-2.215862	1.100910	-1.022709
H	-2.512427	-0.575769	-1.522194
C	-0.923449	-0.340352	-0.097515
H	-0.629868	0.342056	0.706574
O	-0.007237	-0.264908	-1.178090
C	-4.022747	-0.252906	1.402916
C	1.335170	-0.137542	-0.826742
C	1.870691	-1.278995	0.033090
H	1.875919	-0.105497	-1.786450
C	2.863749	1.405520	0.088228

C	3.348447	-1.031082	0.352891
H	1.297311	-1.320072	0.966923
H	1.725921	-2.225397	-0.498173
C	3.513922	0.354368	0.981057
H	2.870261	2.394039	0.552226
H	3.405056	1.472065	-0.870772
H	3.733034	-1.811487	1.016042
H	3.935885	-1.082798	-0.574272
H	4.571872	0.597939	1.125929
H	3.029515	0.376862	1.964639
O	1.500732	1.100867	-0.164146
H	-0.975582	-1.363041	0.296676

TS18

C	-4.487915	-0.942262	-0.082767
H	-4.013983	-1.056780	-1.067386
H	-5.432150	-0.424618	-0.233448
H	-4.632924	-1.939164	0.326304
C	-3.003695	0.005690	0.360126
C	-1.888399	0.255730	-0.568237
H	-2.237731	0.789119	-1.459471
H	-1.419127	-0.680680	-0.885428
C	-0.835939	1.116239	0.138386
H	-1.270277	2.067686	0.452601
O	0.211137	1.425797	-0.779906
C	-3.839518	-0.089846	1.299534
C	1.358530	0.698506	-0.632128
H	2.046229	1.001270	-1.439295
C	3.147003	0.277628	0.825516
C	2.220769	-1.487271	-0.622869

C	2.907863	-1.222434	0.710351
H	3.500752	0.569656	1.815329
H	3.891660	0.604062	0.080998
H	1.878982	-2.518956	-0.719548
H	2.907723	-1.270082	-1.456982
H	3.854594	-1.769112	0.769700
H	2.261131	-1.554433	1.528471
O	1.930579	0.982601	0.613941
H	-0.438788	0.603075	1.017285
O	1.062249	-0.670014	-0.746111

TS19

C	0.109487	-0.025543	-0.367927
C	1.358466	-0.127715	0.415926
H	1.231101	-0.865501	1.213028
H	1.583030	0.837302	0.882824
C	2.508259	-0.527097	-0.505888
O	3.657740	-0.623507	0.308700
C	-0.730455	-0.051235	-1.325593
C	4.810107	-1.023194	-0.398471
O	5.148263	-0.103727	-1.402644
C	5.975230	-1.005249	0.577091
H	4.621625	-1.984085	-0.895126
C	6.017431	0.905124	-0.864501
C	6.331106	0.486537	0.580637
H	6.792844	-1.605922	0.167643
H	5.693867	-1.395613	1.555906
H	6.913155	0.931080	-1.493085
H	5.519117	1.876977	-0.922410
H	7.372116	0.676798	0.848720

H	5.688033	1.019085	1.284921
H	2.296924	-1.496282	-0.982432
H	2.655093	0.221123	-1.292750
S	-1.410866	0.721821	0.707353
O	-1.094054	0.033007	1.955152
O	-1.289936	2.165248	0.597533
C	-3.047904	0.230911	0.232926
C	-3.586724	-0.920697	0.790206
C	-3.756889	1.033884	-0.657044
C	-4.886590	-1.277098	0.436935
H	-3.004776	-1.511787	1.488985
C	-5.050594	0.660213	-0.989453
H	-3.295358	1.923532	-1.072384
C	-5.631330	-0.498076	-0.451865
H	-5.328091	-2.172939	0.863502
H	-5.623599	1.273817	-1.679204
C	-7.037634	-0.880953	-0.831996
H	-7.334315	-1.821308	-0.363210
H	-7.746444	-0.106956	-0.522215
H	-7.128370	-0.995492	-1.916191

TS2

C	-4.759573	0.440426	-0.000004
H	-5.363862	0.367642	-0.900933
H	-4.286960	1.432503	-0.000006
H	-5.363864	0.367647	0.900925
C	-3.058031	-0.205125	-0.000002
C	-1.857547	0.646713	-0.000006
H	-1.830841	1.289207	0.886912
H	-1.830833	1.289187	-0.886939

C	-0.608082	-0.236260	0.000010
H	-0.617390	-0.881530	0.889379
O	0.514683	0.613943	0.000005
C	-3.943654	-1.102303	0.000003
Si	2.083441	0.011450	-0.000001
C	3.179075	1.523069	0.000080
H	2.989586	2.137459	0.885179
H	4.237101	1.242425	0.000049
H	2.989563	2.137571	-0.884935
C	2.351044	-1.036071	-1.534337
H	1.720019	-1.930866	-1.531340
H	2.129716	-0.467155	-2.442784
H	3.392296	-1.370680	-1.592414
C	2.350995	-1.036203	1.534254
H	1.719998	-1.931017	1.531144
H	3.392255	-1.370783	1.592359
H	2.129600	-0.467372	2.442738
H	-0.617382	-0.881552	-0.889344

TS20

C	-0.619859	0.963366	0.181722
C	-0.648689	2.332870	0.824242
H	-0.765332	3.144167	0.102211
H	0.253634	2.528506	1.417426
C	-1.888620	2.148509	1.706975
H	-1.785691	2.531480	2.724111
O	-2.117325	0.713153	1.786090
C	-1.387662	0.026464	0.792543
C	-4.011247	-0.311521	0.695452
O	-3.915546	0.018769	-0.514093

C	-3.738804	-1.736671	0.980608
H	-4.439162	0.421366	1.370836
C	-3.305775	-1.071979	-1.323220
C	-3.171746	-2.254425	-0.355938
H	-4.696289	-2.196438	1.266321
H	-3.043879	-1.815630	1.818123
H	-4.002057	-1.215740	-2.149492
H	-2.341372	-0.682697	-1.656653
H	-3.721218	-3.127578	-0.712148
H	-2.114114	-2.486642	-0.237475
H	-2.774901	2.599397	1.238811
O	-0.163611	-0.625331	-1.839012
O	0.643838	1.783780	-1.935593
C	1.972480	0.058474	-0.487730
C	2.068406	-1.165805	0.173235
C	3.073580	0.891659	-0.624557
C	3.292863	-1.552523	0.699913
H	1.186182	-1.792793	0.267650
C	4.298172	0.487513	-0.088761
H	2.964735	1.832651	-1.154431
C	4.424817	-0.732738	0.575738
H	3.380255	-2.505898	1.215498
H	5.167361	1.131179	-0.194859
C	5.746829	-1.176870	1.148534
H	6.512047	-0.407844	1.020953
H	5.657471	-1.394246	2.217298
H	6.098049	-2.089009	0.655733
S	0.391060	0.560304	-1.161349

TS21'

C	2.284842	-1.220262	0.358613
C	2.460616	-2.586367	-0.271546
H	2.629548	-3.380239	0.459510
H	3.288148	-2.604812	-0.993928
C	1.098605	-2.698693	-0.959344
H	1.126786	-3.107603	-1.971607
O	0.596545	-1.337864	-1.040953
C	1.266244	-0.468005	-0.138744
C	-1.466034	-1.069004	-0.706212
O	-1.591838	0.153329	-1.045908
C	-1.527093	-1.301416	0.759908
H	-1.615783	-1.804939	-1.484537
C	-1.548017	1.043894	0.122443
C	-1.424821	0.123997	1.341533
H	-0.717139	-1.957395	1.089963
H	-2.488839	-1.797512	0.967400
H	-0.668357	1.668185	-0.027011
H	-2.476946	1.616423	0.080443
H	-0.453138	0.268920	1.815536
H	-2.229483	0.314696	2.053410
C	-4.856897	0.401186	1.047626
C	-4.991553	1.742151	1.419283
C	-5.071255	2.749946	0.455394
C	-5.025440	2.383718	-0.898112
C	-4.894922	1.049908	-1.272805
C	-4.805007	0.055796	-0.297190
H	-4.799977	-0.399446	1.782338
H	-5.034514	2.010542	2.473413
H	-5.093838	3.157825	-1.660570
H	-4.868057	0.766396	-2.322492
C	-5.227568	4.198702	0.848962

H	-6.224530	4.570564	0.588119
H	-5.091818	4.331353	1.925615
H	-4.497020	4.831310	0.334668
S	-4.499021	-1.688111	-0.802249
O	-4.602910	-2.394557	0.540710
O	-5.624092	-1.959991	-1.768777
H	0.394587	-3.284076	-0.351431
S	3.452104	-0.566910	1.454385
O	4.175922	-1.690522	2.074833
O	2.854468	0.471562	2.298447
C	4.661045	0.271533	0.420579
C	5.919391	-0.282031	0.234842
C	4.305557	1.475150	-0.188455
C	6.842859	0.385051	-0.574309
H	6.163297	-1.215841	0.731833
C	5.233839	2.125678	-0.989793
H	3.307441	1.874996	-0.031313
C	6.515029	1.591063	-1.193359
H	7.832766	-0.039893	-0.722041
H	4.966184	3.064551	-1.469363
C	7.507973	2.316847	-2.066722
H	8.448953	1.765519	-2.137946
H	7.727945	3.311998	-1.666633
H	7.115359	2.450103	-3.079910

TS21

C	2.304091	0.840098	0.455873
C	2.139050	1.386239	1.858117
H	1.988385	2.467648	1.884676
H	2.995536	1.141443	2.501317

C	0.883985	0.609639	2.251163
H	0.864890	0.247324	3.281117
O	0.866459	-0.546852	1.369716
C	1.632730	-0.309945	0.187020
C	-1.038836	-1.003875	0.821483
O	-1.347158	0.052115	0.156431
C	-0.741558	-2.193018	-0.026466
H	-1.310271	-1.018119	1.866907
C	-1.171661	-0.151329	-1.283500
C	-0.783009	-1.624238	-1.458681
H	-1.524520	-2.927523	0.173449
H	0.236569	-2.596679	0.237753
H	-2.136433	0.107863	-1.724714
H	-0.387100	0.539491	-1.594679
H	-1.526622	-2.146965	-2.062410
H	0.203943	-1.688876	-1.916712
C	-4.712190	0.812041	0.247024
C	-5.518613	1.945991	0.192560
C	-6.866815	1.853129	-0.175658
C	-7.387719	0.593255	-0.480397
C	-6.584229	-0.547734	-0.433764
C	-5.248155	-0.435804	-0.068549
H	-3.672214	0.878614	0.558725
H	-5.102405	2.918927	0.448345
H	-8.437870	0.504244	-0.752805
H	-6.977012	-1.538278	-0.648376
C	-7.725218	3.092463	-0.252714
H	-7.474866	3.692028	-1.135145
H	-8.785936	2.833884	-0.315759
H	-7.582557	3.728682	0.626486
S	-4.172390	-1.917377	-0.077840

O	-3.384942	-1.706259	1.222962
O	-5.180516	-3.040813	-0.010152
H	-0.019221	1.197128	2.040638
O	3.047663	1.246765	-2.042231
O	3.752962	2.883459	-0.227624
C	4.966429	0.576094	-0.400540
C	5.036527	-0.736930	-0.866251
C	6.039292	1.163882	0.253524
C	6.204464	-1.460855	-0.668601
H	4.174160	-1.170000	-1.365679
C	7.208201	0.422347	0.443842
H	5.951580	2.191387	0.592763
C	7.306192	-0.892152	-0.011882
H	6.269190	-2.485607	-1.027488
H	8.055483	0.876662	0.951790
S	3.450208	1.506882	-0.657230
C	8.564487	-1.698646	0.192439
H	8.980606	-2.026103	-0.765790
H	9.328602	-1.114466	0.711420
H	8.362589	-2.596010	0.786228

TS22

C	-0.788266	-1.907108	-0.129579
C	-0.897171	-2.467194	-1.528475
H	-0.689805	-3.538058	-1.587935
H	-0.220894	-1.947949	-2.223075
C	-2.374078	-2.140235	-1.795516
H	-2.583687	-1.778951	-2.804892
O	-2.733953	-1.096941	-0.868335
C	-1.818976	-1.070971	0.141699

C	-2.051623	1.620171	1.372029
C	-3.012544	2.346535	-0.701949
C	-3.405217	1.993249	0.753201
H	-2.029652	1.834342	2.452646
H	-1.904760	-0.118047	0.858069
H	-3.542587	3.234034	-1.066846
H	-3.223073	1.516346	-1.383515
H	-3.889524	2.872451	1.220085
H	-4.123703	1.163458	0.786379
O	-1.191126	2.672456	0.774076
C	-1.484503	2.590454	-0.593948
H	-1.153515	3.515740	-1.083387
H	-0.941959	1.739718	-1.049085
H	-3.010740	-3.007078	-1.579119
O	0.339203	-1.834730	2.235315
O	1.409922	-3.188231	0.367599
C	1.625239	-0.575353	0.320783
C	2.837256	-0.751377	-0.333908
C	1.117136	0.694939	0.594276
C	3.566155	0.377623	-0.714075
H	3.192674	-1.757591	-0.533347
C	1.851381	1.805389	0.196861
H	0.147337	0.830937	1.079098
C	3.084039	1.662987	-0.455330
H	4.519036	0.255149	-1.224328
H	1.431739	2.789789	0.393373
S	0.659105	-2.001816	0.816771
C	3.865895	2.884987	-0.870420
H	4.765808	2.610908	-1.428139
H	3.258131	3.540936	-1.501762
H	4.172789	3.467916	0.004300

TS23

C	3.161165	1.940286	-0.183036
C	3.855280	2.447934	-1.428866
H	4.468421	1.688310	-1.927331
H	4.497799	3.307938	-1.208520
C	2.616997	2.814799	-2.264184
H	2.681572	3.790203	-2.751598
O	1.501059	2.846811	-1.349716
C	1.835289	2.225676	-0.185745
C	-1.371717	0.892201	-0.204113
O	-0.722063	-0.106477	-0.912535
C	-0.577369	1.220908	0.969272
C	0.167698	-0.794877	-0.007420
C	-0.037313	-0.151619	1.372310
H	-1.103286	1.786426	1.740654
H	0.768693	1.901273	0.462226
H	-0.080885	-1.860509	-0.042062
H	1.185790	-0.643338	-0.387819
H	-0.736371	-0.757983	1.968211
H	0.908826	-0.070352	1.923289
C	-5.629924	0.875087	-0.295936
C	-6.960673	1.087236	0.044525
C	-7.807160	0.012582	0.350686
C	-7.283550	-1.280157	0.308213
C	-5.949221	-1.505934	-0.037151
C	-5.129918	-0.426074	-0.333538
H	-4.968663	1.711347	-0.505909
H	-7.351630	2.101915	0.084377
H	-7.926496	-2.123575	0.550145

H	-5.521161	-2.504134	-0.063884
C	-9.246332	0.262495	0.729178
H	-9.764794	0.837019	-0.045320
H	-9.785526	-0.677799	0.870767
H	-9.313995	0.833104	1.661475
S	-3.421416	-0.739878	-0.852889
O	-2.772053	0.270040	0.228785
O	-3.192786	-2.169532	-0.471210
H	-1.688753	1.683435	-0.888427
S	4.041249	1.230667	1.119908
O	5.343237	1.912203	1.209810
O	3.195423	1.092671	2.307061
C	4.417197	-0.435886	0.566190
C	5.564771	-0.668043	-0.183616
C	3.542108	-1.474527	0.877132
C	5.826115	-1.957641	-0.646330
H	6.248057	0.153441	-0.377136
C	3.817115	-2.754954	0.410632
H	2.664595	-1.269425	1.483105
C	4.956685	-3.013280	-0.361602
H	6.722959	-2.146947	-1.231258
H	3.135571	-3.568348	0.648362
C	5.224852	-4.405172	-0.876993
H	5.165854	-5.141789	-0.069989
H	4.486021	-4.687974	-1.634058
H	6.216722	-4.474864	-1.330875
H	2.398255	2.048057	-3.015949

TS24

C	-3.876917	-0.041013	-0.278686

C	-4.693431	-0.478811	-1.477567
H	-5.690976	-0.843752	-1.221101
H	-4.185335	-1.260336	-2.062749
C	-4.731265	0.863716	-2.215771
H	-4.604951	0.792287	-3.299109
O	-3.633655	1.645034	-1.685010
C	-3.210900	1.139870	-0.479474
C	-0.771451	1.634196	-0.012635
O	-0.625930	2.626614	-0.846493
C	-1.052342	2.087429	1.393249
H	-0.836712	0.646766	-0.432904
C	-0.675767	3.886474	-0.123153
C	-1.444015	3.552371	1.153071
H	-0.119831	2.007941	1.958595
H	-1.842061	1.491152	1.850804
H	0.360930	4.184197	0.069953
H	-1.170897	4.598573	-0.784107
H	-1.158478	4.206377	1.979513
H	-2.520644	3.616108	0.978124
C	3.540606	-0.535497	-0.727087
C	4.637218	-1.384258	-0.622695
C	5.843869	-0.936148	-0.066727
C	5.920899	0.383482	0.380885
C	4.826862	1.246160	0.274061
C	3.640808	0.779832	-0.273190
H	2.598392	-0.888603	-1.142043
H	4.561382	-2.412197	-0.973427
H	6.849799	0.742754	0.818999
H	4.863900	2.275618	0.620774
C	7.023947	-1.870677	0.042303
H	7.885237	-1.366748	0.488800

H	6.782776	-2.739756	0.663369
H	7.324593	-2.244655	-0.942073
S	2.223338	1.910162	-0.457588
O	1.183404	1.072424	0.343048
O	2.657708	3.138252	0.310072
H	-5.660153	1.405032	-1.994477
O	-3.207161	-0.346573	2.251793
O	-4.570259	-2.142340	1.066224
C	-2.003870	-1.954272	0.593682
C	-0.783629	-1.448915	1.031682
C	-2.052470	-3.073418	-0.235674
C	0.401021	-2.050685	0.614310
H	-0.759574	-0.590329	1.695347
C	-0.861714	-3.673201	-0.637584
H	-3.017261	-3.469892	-0.538050
C	0.377726	-3.166021	-0.227614
H	1.347036	-1.623584	0.937803
H	-0.893045	-4.551683	-1.278750
C	1.664347	-3.794688	-0.702979
H	1.557773	-4.877022	-0.822692
H	1.965114	-3.383020	-1.674188
H	2.476854	-3.602057	0.002913
S	-3.527333	-1.101164	1.030662

TS25

C	-0.690714	0.083472	-0.530067
C	-1.975048	0.245356	0.183226
H	-2.126725	1.297934	0.444646
H	-1.957487	-0.332814	1.111225
C	-3.116947	-0.225536	-0.714280

H	-3.147900	0.373035	-1.637288
O	-4.303817	-0.067410	0.021357
C	0.181562	-0.208751	-1.411097
C	-5.451133	-0.463499	-0.706819
H	-5.396744	-1.533969	-0.958274
H	-5.495044	0.104481	-1.651222
C	-6.665848	-0.179742	0.120876
H	-6.739283	0.832295	0.514664
C	-7.620153	-1.074547	0.362955
H	-8.501018	-0.821624	0.943489
H	-7.550796	-2.091739	-0.014725
H	-2.970350	-1.280038	-0.994659
S	0.841966	0.944305	0.441245
O	0.417047	0.575426	1.788077
O	0.843874	2.330748	0.008813
C	2.450621	0.243746	0.182715
C	3.258609	0.772980	-0.820678
C	2.870545	-0.786445	1.013047
C	4.530332	0.244559	-0.985134
H	2.888544	1.575578	-1.449886
C	4.150911	-1.302934	0.824997
H	2.214144	-1.161618	1.790702
C	4.992597	-0.799232	-0.169714
H	5.179353	0.644505	-1.759350
H	4.500460	-2.106992	1.465860
C	6.377890	-1.355125	-0.371237
H	6.503552	-1.720735	-1.394646
H	7.133367	-0.581632	-0.202783
H	6.578299	-2.181468	0.313621

TS26

C	1.082449	0.384137	0.359953
C	1.323039	0.621439	1.834646
H	0.553182	0.151948	2.458389
H	1.381679	1.682828	2.086906
C	2.668064	-0.088294	1.965616
H	3.501295	0.591100	1.751562
O	2.626827	-1.077069	0.888107
C	1.823406	-0.575289	-0.218745
C	4.152187	-1.560156	0.349100
H	3.879954	-2.573462	0.062493
H	4.722052	-1.518379	1.275865
C	4.449425	-0.640533	-0.710052
H	4.939412	0.298921	-0.475225
C	3.555717	-0.723636	-1.742787
H	3.398022	0.095643	-2.438386
H	3.126876	-1.674750	-2.033225
H	2.831189	-0.631663	2.897129
O	0.218037	1.226261	-1.971955
O	-0.209752	2.611840	0.125336
C	-1.642543	0.457426	-0.286565
C	-2.519590	0.909183	0.691195
C	-1.934268	-0.660884	-1.065977
C	-3.715716	0.220148	0.893148
H	-2.270156	1.796763	1.264366
C	-3.129163	-1.334718	-0.850338
H	-1.230691	-0.980137	-1.829133
C	-4.035492	-0.904515	0.129654
H	-4.412979	0.568228	1.650336
H	-3.371210	-2.205765	-1.454017
S	-0.097157	1.313136	-0.548237

C	-5.336109	-1.638850	0.332151
H	-5.165945	-2.712992	0.449413
H	-5.862053	-1.277140	1.218411
H	-5.995448	-1.502326	-0.530978

TS27

C	1.768612	0.570132	-0.073979
C	2.089814	0.277833	-1.527422
H	2.431279	1.164434	-2.065971
H	1.210084	-0.127249	-2.049114
C	3.192528	-0.769174	-1.369876
H	3.053633	-1.675874	-1.963927
O	3.146766	-1.170343	0.045211
C	2.324088	-0.297752	0.790409
C	1.968234	-2.474038	0.942064
H	2.456130	-2.453505	1.907583
H	2.366000	-3.189224	0.225340
C	0.548487	-2.212492	0.853029
H	0.084790	-1.684274	1.679917
C	-0.156147	-2.549747	-0.239681
H	-1.218247	-2.333604	-0.312666
H	0.322408	-3.027913	-1.091788
H	4.195664	-0.371338	-1.540465
O	0.685418	2.100801	1.774948
O	0.654427	2.817935	-0.674580
C	-0.983353	0.943262	0.126558
C	-1.517475	0.819831	-1.152633
C	-1.637450	0.407746	1.232677
C	-2.715465	0.127828	-1.324168
H	-1.011368	1.285086	-1.993454

C	-2.836355	-0.275004	1.046256
H	-1.206744	0.547639	2.220206
C	-3.390641	-0.426641	-0.231585
H	-3.141408	0.031462	-2.319514
H	-3.358740	-0.687346	1.906071
S	0.589023	1.775856	0.354688
C	-4.709836	-1.133072	-0.415147
H	-5.541670	-0.444760	-0.232365
H	-4.815721	-1.519072	-1.431831
H	-4.813578	-1.967583	0.283319

TS28

C	-1.904065	-1.522340	0.350148
C	-1.507255	-1.442041	1.811153
H	-1.882112	-0.525794	2.288671
H	-1.851551	-2.297517	2.396732
C	0.010630	-1.419828	1.643867
H	0.442831	-2.423554	1.732345
O	0.211998	-0.976439	0.273908
C	-0.937631	-1.198797	-0.551212
C	1.879819	-1.397994	-0.537161
H	1.604741	-0.734899	-1.342494
H	2.413325	-1.003139	0.317893
C	1.657974	-2.848918	-0.648463
H	0.878192	-3.154256	-1.341487
C	2.334327	-3.726259	0.094512
H	2.132565	-4.790598	0.017054
H	3.138506	-3.389551	0.746891
C	3.971887	1.531991	-1.215948
C	3.664403	2.862811	-0.950314

C	3.840678	3.400888	0.331016
C	4.331005	2.569747	1.340521
C	4.642033	1.233008	1.083480
C	4.459574	0.717507	-0.194382
H	3.810125	1.104784	-2.202329
H	3.268732	3.494523	-1.743223
H	4.463380	2.971372	2.343038
H	4.999162	0.569217	1.866373
C	3.478981	4.839158	0.609641
H	3.812998	5.144391	1.604852
H	2.394804	4.986334	0.559601
H	3.935899	5.511646	-0.123297
S	4.911924	-1.022474	-0.548591
O	3.746951	-1.416842	-1.487084
O	4.769825	-1.654926	0.822632
H	0.541040	-0.724706	2.298068
O	-4.266403	-2.377628	1.009437
O	-3.695639	-2.237571	-1.463287
C	-4.224900	-0.040320	-0.152838
C	-3.830193	0.807825	-1.187909
C	-5.108722	0.387550	0.826789
C	-4.339335	2.098581	-1.233375
H	-3.124405	0.445665	-1.930969
C	-5.612988	1.689628	0.767032
H	-5.397882	-0.303291	1.612745
C	-5.237544	2.557467	-0.257872
H	-4.037154	2.767701	-2.036016
H	-6.309411	2.031589	1.529043
S	-3.562422	-1.713171	-0.102751
C	-5.773396	3.966132	-0.325253
H	-6.283627	4.147357	-1.276802

H	-4.963134	4.698035	-0.243076
H	-6.484601	4.157493	0.482417

TS29

C	1.471762	-1.946172	0.503544
C	1.377805	-3.176517	-0.370952
H	1.653689	-4.099040	0.145086
H	2.004936	-3.087599	-1.269272
C	-0.121552	-3.111090	-0.694572
H	-0.373114	-3.340379	-1.732430
O	-0.536179	-1.750899	-0.426752
C	0.393519	-1.135504	0.364456
C	-0.372446	1.527862	0.898100
C	0.196186	2.763348	0.379050
H	-0.128861	3.014657	-0.632962
C	1.128575	3.544946	0.963721
H	1.557729	4.394485	0.442049
H	1.486448	3.346772	1.971761
C	-3.700485	-0.658215	-0.020584
C	-4.616606	-1.553507	-0.565179
C	-5.915139	-1.153998	-0.904150
C	-6.277235	0.179028	-0.699438
C	-5.371265	1.091609	-0.158815
C	-4.092565	0.665662	0.181346
H	-2.680522	-0.964827	0.193549
H	-4.310747	-2.582427	-0.743773
H	-7.275888	0.510571	-0.974541
H	-5.633975	2.137287	-0.025987
C	-6.892122	-2.148673	-1.481076
H	-7.813975	-1.656615	-1.802333

H	-6.463209	-2.664824	-2.345742
H	-7.157650	-2.912135	-0.742014
S	-2.987304	1.878539	0.944339
O	-1.650177	1.212076	0.269857
O	-3.378127	3.176492	0.315610
H	0.179448	0.196494	0.642737
H	-0.473398	1.498096	1.991172
H	-0.695214	-3.766204	-0.027070
O	2.593622	-0.630015	2.474049
O	3.771599	-2.652304	1.467557
C	3.770292	-0.385465	0.155114
C	4.885965	-0.839101	-0.534028
C	3.265229	0.899134	-0.044214
C	5.513277	0.018141	-1.441832
H	5.254796	-1.842572	-0.345039
C	3.898850	1.736722	-0.951542
H	2.386645	1.240664	0.497712
C	5.030170	1.309026	-1.661937
H	6.391998	-0.323749	-1.983853
H	3.502638	2.738211	-1.104334
S	2.919667	-1.460194	1.312003
C	5.701950	2.236429	-2.644043
H	5.011004	2.527731	-3.441749
H	6.035799	3.154454	-2.149768
H	6.572731	1.762636	-3.105059

TS3

C	-2.248703	-0.003498	0.085236
H	-2.680179	0.456395	-0.810653
H	-2.520835	0.623962	0.940704

H	-2.699214	-0.988756	0.216331
C	-0.757606	-0.105875	-0.042441
C	0.117811	1.125362	-0.208943
H	-0.251270	1.962977	0.391325
H	0.154729	1.447420	-1.257230
C	1.468491	0.616676	0.274693
H	2.331616	1.135270	-0.147430
O	1.519736	-0.735502	-0.199619
H	1.082145	-1.616341	0.397682
C	-0.096303	-1.260024	-0.025724
H	1.522989	0.627240	1.369294

TS30

C	3.232464	-1.617622	0.148591
C	4.509528	-1.908127	-0.611851
H	5.337033	-2.227577	0.026432
H	4.845896	-1.040421	-1.199228
C	3.985707	-3.041608	-1.502449
H	4.337435	-3.008619	-2.536592
O	2.543160	-2.909384	-1.514007
C	2.129110	-2.140608	-0.456760
C	-0.000397	-1.342210	-0.519773
H	0.492230	-0.754864	-1.279592
H	0.177273	-1.086355	0.520058
C	-0.455370	-2.721076	-0.836933
H	-0.099863	-3.138393	-1.775374
C	-1.256020	-3.429377	-0.038849
H	-1.560147	-4.439351	-0.294930
H	-1.606465	-3.023021	0.907462
C	-4.289632	-0.968369	-0.115856

C	-5.669887	-1.106639	-0.223370
C	-6.525899	-0.021163	0.004257
C	-5.963830	1.213495	0.334890
C	-4.581022	1.365406	0.449821
C	-3.753457	0.272671	0.225282
H	-3.617480	-1.796813	-0.325924
H	-6.093653	-2.069874	-0.500666
H	-6.615122	2.069163	0.499277
H	-4.129355	2.325238	0.684333
C	-8.020905	-0.194073	-0.107694
H	-8.536682	0.766058	-0.022331
H	-8.295530	-0.642474	-1.067815
H	-8.401155	-0.851207	0.681866
S	-1.965431	0.466836	0.452541
O	-1.533861	-0.470499	-0.741551
O	-1.730863	1.925325	0.160637
H	4.221783	-4.021386	-1.068923
O	1.946962	-0.658520	2.226917
O	4.470121	-0.340339	2.031200
C	2.872805	1.131459	0.569932
C	3.953624	1.826990	0.037804
C	1.572552	1.606232	0.412501
C	3.717543	3.003069	-0.674449
H	4.961302	1.455864	0.200491
C	1.347562	2.775968	-0.303519
H	0.741769	1.077139	0.866235
C	2.418651	3.486444	-0.859827
H	4.557360	3.555798	-1.089850
H	0.319552	3.112509	-0.420027
S	3.141209	-0.437700	1.401692
C	2.162986	4.752227	-1.640131

H	1.533401	4.550439	-2.512613
H	1.639385	5.491432	-1.025623
H	3.097744	5.199354	-1.989667

TS31

C	-0.656038	-0.578357	0.441668
C	0.669106	0.050405	0.258871
H	0.852008	0.775260	1.059122
H	0.693123	0.586904	-0.693766
C	1.751046	-1.026181	0.288255
H	1.746845	-1.545523	1.258089
O	2.978408	-0.373918	0.079646
C	-1.577624	-1.443218	0.601662
C	4.071715	-1.262247	0.083273
H	3.942799	-2.017343	-0.709100
H	4.113231	-1.798573	1.045293
H	1.569191	-1.771049	-0.501509
S	-2.123461	0.772270	0.679259
O	-1.600324	1.753239	-0.266808
O	-2.173265	1.056244	2.102352
C	-3.735585	0.297824	0.113573
C	-4.617364	-0.289460	1.017684
C	-4.083464	0.560284	-1.204593
C	-5.889626	-0.617425	0.573402
H	-4.302258	-0.481279	2.037930
C	-5.366062	0.217755	-1.627500
H	-3.370537	1.030210	-1.873391
C	-6.280637	-0.371757	-0.751279
H	-6.595137	-1.073682	1.262360
H	-5.659510	0.416779	-2.653974

C	-7.669996	-0.734461	-1.205894
H	-7.882958	-1.787715	-1.001596
H	-8.417855	-0.138065	-0.674117
H	-7.796101	-0.561060	-2.276435
C	5.360164	-0.508040	-0.135601
C	6.558819	-1.223830	-0.206445
C	5.383902	0.879748	-0.264154
C	7.766980	-0.561987	-0.401684
H	6.545684	-2.307420	-0.107892
C	6.596142	1.543000	-0.460569
H	4.452908	1.432686	-0.209847
C	7.788421	0.827528	-0.529666
H	8.691200	-1.128983	-0.454950
H	6.605326	2.624124	-0.559631
H	8.729466	1.346386	-0.682254

TS32

C	0.197993	-1.342096	-0.091974
C	0.404766	-2.230281	-1.304171
H	0.746250	-3.229797	-1.025331
H	1.128969	-1.798582	-2.004936
C	-1.012455	-2.243618	-1.877479
H	-1.084643	-2.112266	-2.957171
O	-1.686117	-1.097179	-1.251270
C	-0.947908	-0.639941	-0.108180
C	-3.012826	-1.208058	0.124633
H	-2.595009	-1.507410	1.078777
H	-3.434556	-2.033889	-0.447949
C	-3.775265	0.033515	0.083932
C	-4.776703	0.199716	-0.879531

C	-3.558666	1.031846	1.046572
C	-5.571835	1.342890	-0.872182
H	-4.928945	-0.570333	-1.631151
C	-4.360342	2.163186	1.059843
H	-2.739414	0.911030	1.750137
C	-5.365659	2.320018	0.099227
H	-6.348108	1.470470	-1.619268
H	-4.198444	2.933254	1.806706
H	-5.983862	3.212374	0.106977
H	-1.567964	-3.138628	-1.574018
S	1.402103	-1.159680	1.152019
O	0.794421	-0.511454	2.313935
O	2.089620	-2.449674	1.283901
C	2.594887	-0.017591	0.466090
C	2.320104	1.348704	0.500607
C	3.763851	-0.505909	-0.102959
C	3.238531	2.232726	-0.050057
H	1.400440	1.698321	0.960508
C	4.675843	0.396720	-0.651453
H	3.955012	-1.574481	-0.094294
C	4.427886	1.770482	-0.632214
H	3.037703	3.300892	-0.025470
H	5.596579	0.025728	-1.093543
C	5.419608	2.749515	-1.206939
H	4.932971	3.436301	-1.905679
H	5.872073	3.353122	-0.413630
H	6.223030	2.234291	-1.738079

TS33

C	-1.004709	-2.189240	0.307733

C	-0.594991	-2.293807	1.765161
H	-1.214635	-1.658731	2.413609
H	-0.627565	-3.314152	2.153251
C	0.832202	-1.762939	1.643043
H	1.553643	-2.571170	1.471120
O	0.784709	-0.953315	0.438608
C	-0.243038	-1.362791	-0.459565
C	2.264146	-0.077798	-0.267062
H	1.658605	0.127706	-1.137294
H	2.263879	0.616347	0.561289
C	1.121763	2.911827	-1.268774
C	-0.239036	3.170385	-1.127049
C	-0.773311	3.555162	0.107904
C	0.095314	3.696873	1.193558
C	1.459065	3.432113	1.063073
C	1.966491	3.027208	-0.166689
H	1.525657	2.566594	-2.217282
H	-0.904006	3.041039	-1.978137
H	-0.306406	3.992899	2.160609
H	2.135228	3.487359	1.912055
C	-2.259966	3.746407	0.276980
H	-2.481127	4.473428	1.064143
H	-2.737177	2.797088	0.548227
H	-2.723789	4.093014	-0.651977
S	3.739341	2.568517	-0.315142
O	3.592206	1.270922	-1.150453
O	4.085190	2.251484	1.127209
H	1.170643	-1.125068	2.462485
O	-3.110550	-3.626938	0.789950
O	-2.529068	-3.145029	-1.638217
C	-3.585355	-1.245392	-0.190827

C	-3.410120	-0.276204	-1.179560
C	-4.507160	-1.068936	0.830508
C	-4.175495	0.880942	-1.131958
H	-2.667173	-0.437312	-1.955371
C	-5.269100	0.102467	0.865074
H	-4.623493	-1.848750	1.576967
C	-5.112709	1.089101	-0.108416
H	-4.043182	1.644740	-1.895685
H	-5.995405	0.247555	1.661313
S	-2.558955	-2.722782	-0.235667
C	-5.911746	2.367521	-0.063079
H	-6.386089	2.570385	-1.028330
H	-5.266575	3.222214	0.170955
H	-6.694401	2.318576	0.698420
C	3.240714	-1.187694	-0.260154
C	4.366743	-1.110911	0.564640
C	3.008322	-2.330602	-1.029470
C	5.255147	-2.181821	0.619412
H	4.541629	-0.191321	1.120690
C	3.899929	-3.399518	-0.969790
H	2.112109	-2.383480	-1.643254
C	5.023083	-3.326558	-0.145359
H	6.134281	-2.121378	1.254265
H	3.714281	-4.290543	-1.561991
H	5.717917	-4.160561	-0.099909

TS34

C	-1.304639	-2.215536	-0.972402
C	-1.133317	-3.562805	-0.307072
H	-1.592839	-4.381494	-0.866238

H	-1.544942	-3.570073	0.712131
C	0.401466	-3.634559	-0.318578
H	0.843382	-4.004221	0.609487
O	0.871453	-2.281322	-0.526524
C	-0.151859	-1.506295	-0.997860
C	0.691810	1.155058	-1.402287
C	3.910280	-0.837065	-0.092216
C	4.771762	-1.757216	0.497426
C	5.941404	-1.347517	1.149697
C	6.228113	0.017729	1.210504
C	5.374716	0.955073	0.627784
C	4.225470	0.520555	-0.021650
H	2.982502	-1.162825	-0.554491
H	4.522141	-2.815716	0.461518
H	7.124769	0.353612	1.726238
H	5.573605	2.020889	0.695015
C	6.855524	-2.366691	1.783967
H	7.733393	-1.889117	2.226995
H	6.337062	-2.920175	2.573759
H	7.202866	-3.097021	1.045996
S	3.194482	1.770751	-0.826399
O	1.806445	0.964484	-0.493324
O	3.386178	2.993900	0.009608
H	0.144153	-0.205102	-1.279820
H	1.046348	1.258074	-2.433963
H	0.761404	-4.239481	-1.159560
O	-2.661583	-0.434985	-2.328425
O	-3.726874	-2.680269	-1.762824
C	-3.511458	-0.875650	0.113552
C	-4.376893	-1.642139	0.884812
C	-3.118714	0.400647	0.515981

C	-4.858745	-1.118814	2.085546
H	-4.675981	-2.623614	0.529853
C	-3.610020	0.906247	1.713658
H	-2.447241	0.989651	-0.104444
C	-4.481083	0.155390	2.514295
H	-5.540914	-1.708422	2.693654
H	-3.306917	1.903746	2.022888
S	-2.842697	-1.557108	-1.405279
C	-4.995517	0.725237	3.813003
H	-4.170996	0.926420	4.504660
H	-5.519280	1.671671	3.644868
H	-5.688212	0.035129	4.302141
C	-0.242619	2.187245	-0.973933
C	-1.292141	2.573445	-1.839162
C	-0.249159	2.723704	0.330812
C	-2.294243	3.436176	-1.418753
H	-1.334457	2.141595	-2.835892
C	-1.257810	3.591864	0.743483
H	0.554485	2.455861	1.008921
C	-2.293816	3.955229	-0.118196
H	-3.096258	3.694530	-2.105639
H	-1.230492	3.991471	1.755354
H	-3.082167	4.625999	0.210854

TS35

C	-3.132547	1.643353	0.006545
C	-4.403856	2.096257	-0.681374
H	-5.118163	2.578371	-0.009418
H	-4.917551	1.266607	-1.189863
C	-3.778832	3.082121	-1.676661

H	-4.210578	3.051692	-2.680068
O	-2.379801	2.717677	-1.778015
C	-2.009454	1.952919	-0.705907
C	-0.050488	0.800397	-0.838679
H	-0.364693	0.723028	-1.869117
H	-0.577132	0.238389	-0.084335
C	3.998162	0.100903	0.030867
C	5.386475	0.168255	0.012101
C	6.168247	-0.994557	0.058437
C	5.523346	-2.230380	0.126026
C	4.129122	-2.313025	0.152020
C	3.378646	-1.147727	0.097621
H	3.396156	1.006010	-0.021666
H	5.874446	1.139189	-0.045198
H	6.117707	-3.140955	0.158694
H	3.607716	-3.265142	0.197690
C	7.674106	-0.898571	0.031909
H	8.021863	-0.423032	-0.891236
H	8.045946	-0.298928	0.869293
H	8.133773	-1.888497	0.094981
S	1.572802	-1.242699	0.191322
O	1.260136	-0.375764	-1.095816
O	1.272136	-2.701045	-0.032870
H	-3.823119	4.108659	-1.292435
O	-1.843355	0.645276	2.063323
O	-4.392045	0.744727	2.083701
C	-3.182035	-1.095910	0.664953
C	-4.378510	-1.588658	0.152224
C	-2.013190	-1.850707	0.591305
C	-4.388951	-2.839674	-0.462786
H	-5.287574	-1.002514	0.251646

C	-2.031753	-3.091537	-0.036513
H	-1.097817	-1.476862	1.038722
C	-3.219496	-3.598832	-0.575812
H	-5.320989	-3.232035	-0.863420
H	-1.096842	-3.642804	-0.111646
S	-3.127483	0.565476	1.350297
C	-3.225819	-4.941198	-1.264242
H	-2.565046	-4.932132	-2.136908
H	-2.867226	-5.727639	-0.592704
H	-4.230975	-5.210861	-1.599852
C	0.775727	1.953783	-0.398001
C	1.534017	2.674144	-1.323475
C	0.893573	2.250009	0.964594
C	2.400950	3.679069	-0.897339
H	1.453995	2.429119	-2.378968
C	1.766797	3.247680	1.389228
H	0.273208	1.705252	1.672321
C	2.526739	3.965036	0.462250
H	2.985628	4.232724	-1.626998
H	1.852321	3.469339	2.449216
H	3.207431	4.742718	0.797035

TS36

C	-2.763322	-0.200790	-0.405828
H	-2.944861	-1.034281	-1.079947
H	-2.560773	0.685734	-1.022806
H	-3.631478	0.023939	0.208639
C	-1.092583	0.069384	0.261005
C	-0.176598	1.133547	-0.185485
H	-0.539110	2.113852	0.147525

H	-0.113401	1.140487	-1.279165
C	1.218902	0.883874	0.402437
H	1.874125	1.711905	0.123570
H	1.128632	-1.483410	0.225048
C	-1.687078	-0.923132	0.761919
H	1.172250	0.846157	1.492866
S	2.038668	-0.611355	-0.238751

TS37

C	-2.655474	-0.148943	0.032630
H	-3.049543	0.244770	-0.909714
H	-2.978400	0.510497	0.843658
H	-3.077212	-1.141562	0.196282
C	-1.140473	-0.182090	-0.028859
C	-0.394084	1.113879	-0.288956
H	-0.973114	1.960422	0.100270
H	-0.290099	1.250524	-1.372564
C	0.975120	1.050727	0.374014
H	1.601934	1.890916	0.061014
H	0.815670	-1.411015	0.322930
C	-0.561185	-1.353764	0.127680
H	0.878042	1.076974	1.462490
S	1.858081	-0.453774	-0.125213

TS38

C	4.156194	-0.329157	0.326238
H	3.661557	-1.145233	0.871042
H	4.704798	0.262393	1.055096
H	4.817533	-0.782320	-0.408225

C	2.482711	0.172651	-0.159691
C	1.264836	-0.540012	0.261659
H	1.281899	-1.570284	-0.117635
C	0.028851	0.188441	-0.277589
H	0.010891	1.197491	0.143151
C	3.384725	0.920632	-0.626227
N	-1.170490	-0.523280	0.138629
C	-2.425362	0.084180	-0.316650
H	-2.366151	0.336533	-1.392201
H	-1.125523	-1.476139	-0.217314
C	-2.711737	1.365239	0.463212
H	-3.673860	1.786412	0.157078
H	-2.749006	1.142239	1.534281
H	-1.950169	2.131289	0.296171
C	-3.550263	-0.925908	-0.117493
H	-4.506259	-0.509785	-0.446108
H	-3.368531	-1.842403	-0.689334
H	-3.629548	-1.190287	0.941890
H	1.195821	-0.586536	1.353828
H	0.110252	0.293200	-1.372882

TS39

C	3.174025	-0.606259	-0.118690
H	3.433332	-1.008673	0.868351
H	3.864589	0.221901	-0.318290
H	3.339886	-1.385861	-0.864481
C	1.750345	-0.143757	-0.150314
C	1.254901	0.935907	0.807919
H	1.074116	0.533610	1.814960
C	-0.024281	1.417050	0.116120

H	-0.820662	1.743101	0.789788
C	0.792919	-0.602918	-0.968929
N	-0.465521	0.249515	-0.686491
C	-1.618547	-0.549406	-0.223467
H	-1.611378	-1.432119	-0.874951
H	-0.087011	-0.107950	-1.795811
C	-2.918448	0.221230	-0.425685
H	-3.025131	0.537277	-1.466699
H	-3.774574	-0.406250	-0.161973
H	-2.952414	1.112484	0.210393
C	-1.438319	-1.022348	1.218161
H	-2.238864	-1.717577	1.486341
H	-0.479437	-1.535432	1.333504
H	-1.479430	-0.182320	1.920541
H	1.980135	1.749913	0.908283
H	0.199925	2.234292	-0.575198

TS40

C	-3.710998	-3.929560	1.155698
H	-4.669140	-3.599495	1.540649
H	-2.900809	-3.688492	1.846434
H	-3.686435	-4.974520	0.868263
C	-2.854061	-2.695155	-0.104543
C	-1.619975	-1.979055	0.257765
H	-1.762632	-1.390115	1.170858
C	-1.227048	-1.016038	-0.873035
H	-1.213610	-1.548009	-1.839785
C	-3.893651	-3.185330	-0.640188
N	0.057430	-0.387670	-0.583030
C	1.180621	-1.219512	-1.003818

H	0.955929	-2.256343	-0.727895
H	-0.810084	-2.694355	0.445364
H	-1.994221	-0.239699	-0.940494
C	0.155690	0.955554	-1.150689
H	1.190517	1.291657	-1.014441
H	-0.040716	0.949187	-2.239575
C	-0.776074	1.931174	-0.469021
C	-0.813337	1.998803	0.927721
C	-1.595307	2.783650	-1.209301
C	-1.650444	2.907144	1.569047
H	-0.181263	1.325494	1.500527
C	-2.434347	3.697107	-0.569489
H	-1.580878	2.730052	-2.295267
C	-2.463871	3.760357	0.821085
H	-1.669780	2.952025	2.653778
H	-3.068787	4.351964	-1.158686
H	-3.118818	4.466847	1.321209
H	1.301304	-1.207278	-2.103669
C	2.478405	-0.808906	-0.344044
C	2.520108	-0.589611	1.036737
C	3.649286	-0.661730	-1.087738
C	3.712966	-0.236174	1.660696
H	1.602499	-0.690256	1.610614
C	4.847771	-0.309989	-0.465073
H	3.623250	-0.819750	-2.163282
C	4.881893	-0.096357	0.910451
H	3.733186	-0.068049	2.733185
H	5.750968	-0.196989	-1.056682
H	5.811745	0.181593	1.396548

TS4

C	-2.554120	-0.515783	-0.000121
H	-3.162303	-0.490569	0.900749
H	-2.005348	-1.467898	-0.000113
H	-3.162083	-0.490445	-0.901137
C	-0.905150	0.259831	0.000127
C	0.355924	-0.499257	0.000152
H	0.430153	-1.138149	-0.886764
H	0.430318	-1.137862	0.887262
C	1.532011	0.474941	-0.000117
H	1.480115	1.113403	-0.890834
O	2.702023	-0.320936	-0.000015
H	3.478084	0.248753	-0.000072
C	-1.859554	1.083015	0.000074
H	1.480216	1.113776	0.890340

TS41

C	-1.318396	2.962146	0.037392
H	-0.738496	3.657227	0.660012
H	-2.345371	2.977526	0.425605
H	-1.311222	3.330768	-0.990624
C	-0.743436	1.590384	0.108934
C	-0.807208	0.804388	1.398795
H	-0.402607	1.377920	2.242439
C	0.045507	-0.421545	1.072141
H	1.008113	-0.409742	1.596552
C	-0.034773	0.955247	-0.917003
N	0.304600	-0.270170	-0.382984
C	1.432763	-1.024138	-0.935502
H	1.311413	-2.083775	-0.685382

H	-1.846044	0.550308	1.652355
H	-0.451954	-1.376189	1.272730
C	-1.358982	-1.649870	-1.360650
H	-1.010061	-1.238932	-2.300220
H	-0.984167	-2.624702	-1.062100
C	-2.480446	-1.094481	-0.714219
C	-2.968089	0.179725	-1.102245
C	-3.074795	-1.728697	0.413300
C	-3.998177	0.787728	-0.384099
H	-2.547672	0.658941	-1.980383
C	-4.087356	-1.113193	1.118500
H	-2.719312	-2.712912	0.709490
C	-4.544686	0.161086	0.730831
H	-4.368330	1.759725	-0.695984
H	-4.532949	-1.609071	1.975274
H	-5.341482	0.641772	1.289659
H	1.381327	-0.905346	-2.020367
C	2.769206	-0.534979	-0.411485
C	3.586023	-1.377924	0.343313
C	3.197021	0.769826	-0.680389
C	4.818047	-0.931679	0.823711
H	3.257898	-2.392980	0.556323
C	4.424387	1.217003	-0.199132
H	2.550699	1.425034	-1.259055
C	5.238155	0.367910	0.553343
H	5.444543	-1.597935	1.408694
H	4.749584	2.230473	-0.413280
H	6.195294	0.719450	0.925943

TS42

C	-3.670940	2.253216	-0.072795
H	-4.033879	3.009184	0.635614
H	-4.331045	1.379495	0.037822
H	-3.791166	2.650143	-1.084199
C	-2.241226	1.895398	0.184706
C	-1.836376	1.254568	1.506392
H	-2.137320	1.838154	2.384397
C	-0.313105	1.147146	1.382797
H	0.195445	1.955412	1.930331
C	-1.223358	1.953182	-0.694966
N	-0.061085	1.345171	-0.072231
C	1.257226	1.880219	-0.422327
H	1.207921	2.182030	-1.471881
H	-2.294619	0.256648	1.601545
H	0.100491	0.188347	1.710196
C	-0.596083	0.137135	-1.579124
C	-1.209912	-0.970520	-0.829476
C	-2.593848	-1.173322	-0.884003
C	-0.418296	-1.832943	-0.059305
C	-3.178062	-2.223960	-0.182838
H	-3.203876	-0.486635	-1.465290
C	-1.001403	-2.889726	0.634493
H	0.656835	-1.664201	-0.009403
C	-2.382187	-3.083107	0.576515
H	-4.252355	-2.372901	-0.225499
H	-0.381900	-3.558672	1.223439
H	-2.837992	-3.902487	1.123624
H	1.425632	2.792981	0.168417
C	2.377263	0.885899	-0.194448
C	2.960205	0.213952	-1.273764
C	2.850289	0.610921	1.093591

C	3.962506	-0.734538	-1.072915
H	2.634917	0.443088	-2.285939
C	3.849137	-0.337642	1.300715
H	2.439009	1.149631	1.943020
C	4.402776	-1.019690	0.217488
H	4.401084	-1.244955	-1.924633
H	4.201539	-0.538495	2.307666
H	5.182238	-1.757728	0.377937
H	-1.172515	0.479273	-2.429870
H	0.451499	-0.011641	-1.826086

TS5

C	-2.326255	-0.867876	0.110023
H	-3.066346	-0.454672	-0.586636
H	-2.718300	-0.716212	1.123228
H	-2.251950	-1.942202	-0.072836
C	-0.991838	-0.215439	-0.068601
C	-0.814312	1.295227	0.073655
H	-1.307110	1.676849	0.973935
H	-1.225502	1.837950	-0.787158
C	0.697652	1.432603	0.172848
H	1.137510	2.287292	-0.341500
O	1.192048	0.221063	-0.481948
C	0.147311	-0.813216	-0.437471
C	1.991980	-1.150784	0.318381
H	1.042765	1.400520	1.213814
H	2.433493	-1.671091	-0.520964
H	2.679703	-0.456425	0.811208
H	1.512123	-1.813601	1.029483

TS6

C	-2.820793	-1.447310	0.083543
H	-3.679073	-1.299468	-0.585043
H	-3.214935	-1.471663	1.107806
H	-2.384444	-2.424716	-0.138441
C	-1.797400	-0.370400	-0.095858
C	-2.149498	1.102176	0.088861
H	-2.677425	1.295371	1.029370
H	-2.783460	1.468713	-0.729764
C	-0.771313	1.754424	0.078566
H	-0.696427	2.704176	-0.454919
O	0.078022	0.785756	-0.590640
C	-0.534053	-0.527693	-0.516137
C	2.357341	1.002528	0.401769
H	1.864900	1.553508	1.206644
H	3.362984	0.732699	0.750769
H	2.451952	1.642315	-0.476484
C	2.157731	-0.958400	-1.158057
H	1.712441	-1.941003	-1.295915
H	1.954717	-0.344827	-2.037922
H	3.251142	-1.038647	-1.049868
C	1.366345	-1.120906	1.290410
H	0.971584	-2.100198	1.028444
H	2.320632	-1.217978	1.832721
H	0.657318	-0.622709	1.956698
C	1.633501	-0.284104	0.073471
H	-0.387249	1.876489	1.101607

TS7'

C	2.560613	1.286649	0.039679
H	3.406184	1.022401	-0.607274
H	2.938968	1.314985	1.068957
H	2.221804	2.287769	-0.235598
C	1.442702	0.301357	-0.098987
C	1.646814	-1.165137	0.242191
H	2.166310	-1.313747	1.195799
H	2.215715	-1.690693	-0.535692
C	0.204871	-1.644939	0.304669
H	0.021057	-2.658934	-0.055815
O	-0.475238	-0.729997	-0.597654
C	0.217496	0.602059	-0.560532
C	-1.663801	1.658745	0.126854
H	-1.834477	1.925797	-0.908694
H	-1.330560	2.471002	0.767110
C	-2.174010	0.495991	0.644603
H	-2.081097	0.278758	1.704325
C	-2.061731	-0.588844	-0.301753
H	-2.331854	-1.595564	0.016440
H	-2.405135	-0.376505	-1.313072
H	-0.222722	-1.500576	1.304396

TS7

C	2.135426	1.745903	-0.042864
H	3.199317	1.600013	-0.268023
H	2.076249	2.181569	0.962419
H	1.734668	2.470391	-0.755934
C	1.380519	0.458048	-0.129116
C	1.751764	-0.751224	0.725167
H	1.899438	-0.477564	1.775691

H	2.672199	-1.233505	0.371665
C	0.528626	-1.644727	0.554132
H	0.725490	-2.714803	0.475827
O	-0.057666	-1.198911	-0.700968
C	0.369314	0.174067	-0.956299
C	-1.687054	-0.312676	-0.919490
H	-2.169486	-1.223944	-0.559201
H	-1.723959	-0.193005	-1.993990
C	-1.991918	0.854662	-0.094239
H	-1.734132	1.827498	-0.500065
C	-2.556687	0.722722	1.114284
H	-2.812628	1.586051	1.718830
H	-2.771464	-0.258291	1.530756
H	-0.214306	-1.453769	1.340317

TS8'

C	1.954130	2.221957	-0.226752
H	2.762893	2.604799	0.409398
H	1.067401	2.832798	-0.005919
H	2.238275	2.362863	-1.272007
C	1.684561	0.784657	0.051459
C	1.186123	0.332115	1.402196
H	1.801631	0.736512	2.214699
C	1.331026	-1.177835	1.274816
H	2.190897	-1.570958	1.823050
C	1.942205	-0.259226	-0.831787
H	0.152336	0.663349	1.581865
H	0.438258	-1.747940	1.541462
C	-0.261845	-2.005635	-1.116588
H	0.329650	-1.946330	-2.021507

H	-0.381307	-2.982054	-0.657117
C	-1.039085	-0.918014	-0.693445
C	-0.811192	0.368431	-1.253350
C	-1.939327	-1.036857	0.407320
C	-1.466349	1.485507	-0.722449
H	-0.177613	0.459455	-2.127750
C	-2.569391	0.071655	0.920393
H	-2.122367	-2.021684	0.830559
C	-2.315671	1.346294	0.364776
H	-1.299409	2.464236	-1.161001
H	-3.256922	-0.025878	1.754283
H	-2.813267	2.218387	0.777860
O	1.612305	-1.415730	-0.143427

TS8

C	3.559539	1.858555	-0.096447
H	4.130856	2.004783	-1.021972
H	4.284735	1.821856	0.726035
H	2.920551	2.732896	0.048319
C	2.731937	0.613649	-0.161379
C	3.365980	-0.750488	-0.422062
H	4.234425	-0.928810	0.221206
H	3.697495	-0.849529	-1.463880
C	2.224643	-1.702261	-0.090104
H	2.113773	-2.563086	-0.750786
O	1.029134	-0.878980	-0.226624
C	1.396662	0.536906	-0.101597
C	-0.085490	-0.320580	1.147186
H	0.266422	0.452011	1.818749
H	0.021358	-1.319209	1.577112

C	-1.388346	-0.077293	0.513027
C	-2.198685	-1.157560	0.151878
C	-1.854986	1.229721	0.320082
C	-3.469030	-0.939109	-0.377775
H	-1.827140	-2.170134	0.285671
C	-3.124354	1.447907	-0.196911
H	-1.194090	2.059697	0.552643
C	-3.933324	0.362821	-0.548260
H	-4.092922	-1.782102	-0.656683
H	-3.483384	2.461720	-0.341749
H	-4.921838	0.536225	-0.962107
H	2.269417	-2.038092	0.954599

TS9

C	2.268059	2.111251	-0.099446
H	3.055283	2.295779	-0.843327
H	2.683991	2.391580	0.877612
H	1.434379	2.784294	-0.321893
C	1.806986	0.687136	-0.127344
C	2.782867	-0.459590	0.091921
H	3.398313	-0.336026	0.990754
H	3.467549	-0.572570	-0.761260
C	1.825053	-1.641738	0.216726
H	2.149992	-2.556944	-0.284816
O	0.596644	-1.196200	-0.393326
C	0.568099	0.261114	-0.431665
C	-1.438309	-0.968159	0.440789
O	-1.665407	-0.041492	1.291337
C	-2.132131	-0.769159	-0.858441
H	-1.120401	-1.913307	0.860923

C	-2.123933	1.169296	0.608849
C	-2.540199	0.715546	-0.798073
H	-2.998685	-1.447292	-0.863616
H	-1.475948	-1.024571	-1.688319
H	-2.924680	1.567783	1.231643
H	-1.248246	1.819296	0.585158
H	-3.612252	0.843279	-0.962478
H	-1.976137	1.280194	-1.539049
H	1.617989	-1.864137	1.274682

p-TolSO2$^-$

C	0.312492	-1.203463	-0.093493
C	1.704605	-1.201300	-0.002080
C	2.420586	0.000008	0.036156
C	1.704598	1.201307	-0.002060
C	0.312480	1.203462	-0.093473
C	-0.386159	-0.000001	-0.142704
H	-0.258367	-2.129068	-0.088221
H	2.247248	-2.144517	0.052665
H	2.247233	2.144528	0.052699
H	-0.258386	2.129063	-0.088186
C	3.929626	-0.000001	0.096834
H	4.304984	0.885997	0.618458
H	4.304948	-0.885510	0.619319
H	4.368510	-0.000503	-0.908181
S	-2.224886	-0.000009	-0.338119
O	-2.584208	-1.280496	0.397292
O	-2.584214	1.280505	0.397242

S1

C	-0.690436	0.000001	0.015431
H	-1.112941	-0.000031	1.053469
H	-1.141230	-0.875487	-0.478523
H	-1.141241	0.875510	-0.478477
C	0.832936	0.000001	-0.146497
H	1.270207	-0.889064	0.344960
H	1.270204	0.889064	0.344964

S2

C	0.707422	0.000000	0.000066
H	1.279280	-0.924707	-0.000229
H	1.279281	0.924706	-0.000194
C	-0.707339	0.000000	-0.000090
H	-1.279530	-0.924572	0.000296
H	-1.279532	0.924571	0.000271

S3

H	0.000000	0.000000	0.000000

TS39'

C	3.230924	-0.741867	-0.132253
H	3.704299	-0.701170	0.856856
H	3.869099	-0.155155	-0.807520
H	3.213563	-1.775652	-0.480623
C	1.853638	-0.185875	-0.092991
C	1.560239	1.219186	0.364363
H	2.144685	1.533724	1.234050

C	0.057415	1.149390	0.614574
H	-0.169491	0.886754	1.656529
C	0.688901	-0.852208	-0.551752
N	-0.316206	0.018354	-0.271318
C	-1.721825	-0.410217	-0.385275
H	-1.763719	-0.960029	-1.329806
H	-0.326167	1.266431	-1.867239
C	-2.692075	0.765069	-0.423990
H	-2.435307	1.475491	-1.215134
H	-3.700146	0.388616	-0.616075
H	-2.716521	1.297145	0.533104
C	-2.054462	-1.369254	0.760051
H	-3.078609	-1.738786	0.653686
H	-1.364319	-2.215423	0.747281
H	-1.977451	-0.861649	1.728019
H	1.765097	1.930406	-0.454993
H	-0.488111	2.055479	0.344729