

Mechanism and Structure-Activity Relationship of Amide Bond Formation by Silane Derivatives: A Computational Study

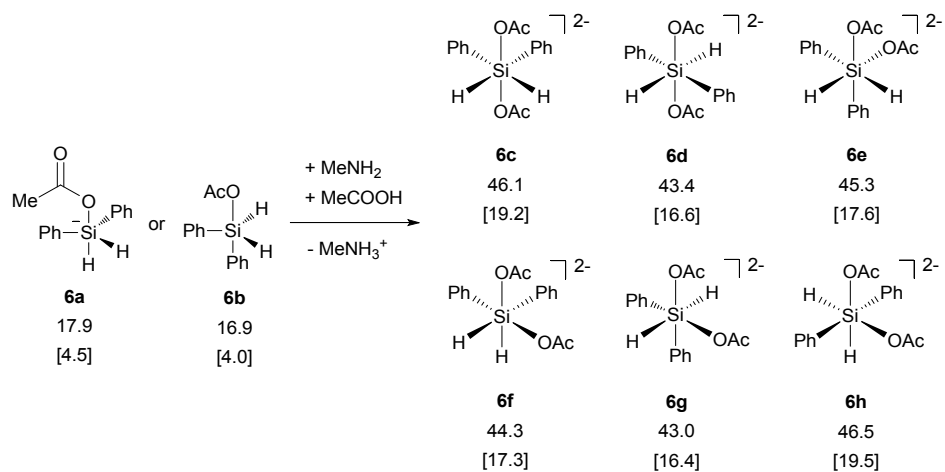
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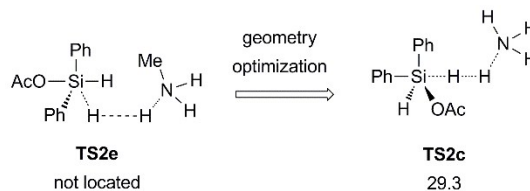
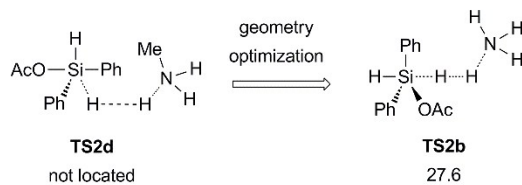
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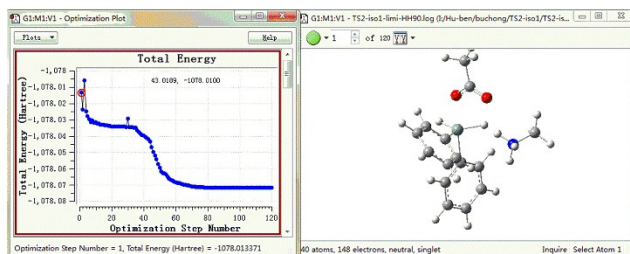
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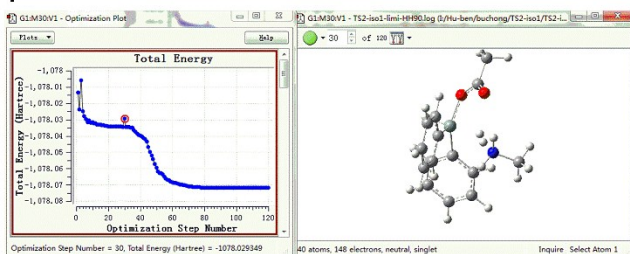
Scheme S1 Formation of hexavalent silicate species.



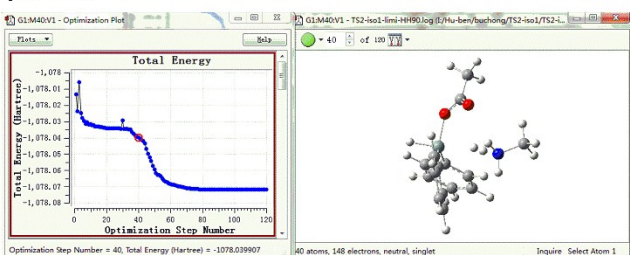
starting point



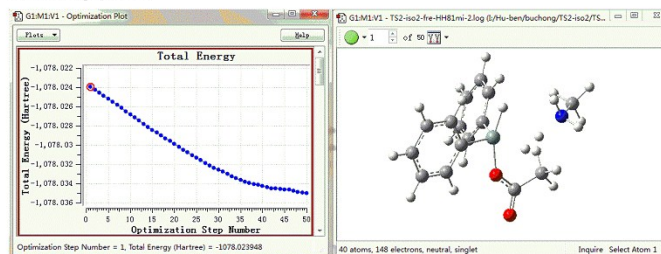
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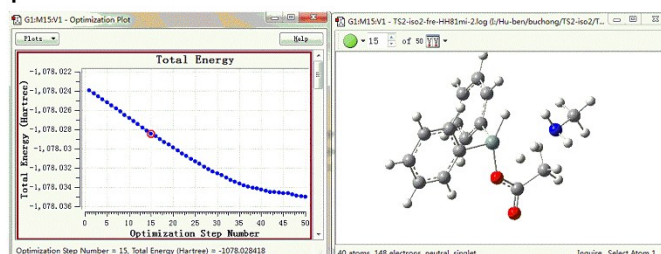
point 40



starting point



point 15



point 40

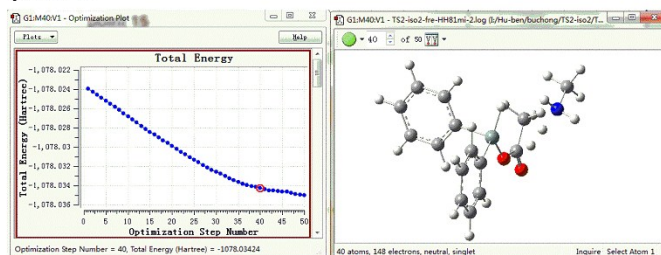


Fig. S1 Geometry optimization of the transition states for dihydrogen formation via equatorial Si-H bond cleavage.

All the hypothetic transition states of equatorial Si-H bond cleavage isomerized to the ones of axial Si-H bond cleavage during geometry optimization. See the provided file “trajectory of geometry optimization.pptx” for the detailed animations of geometry optimization.

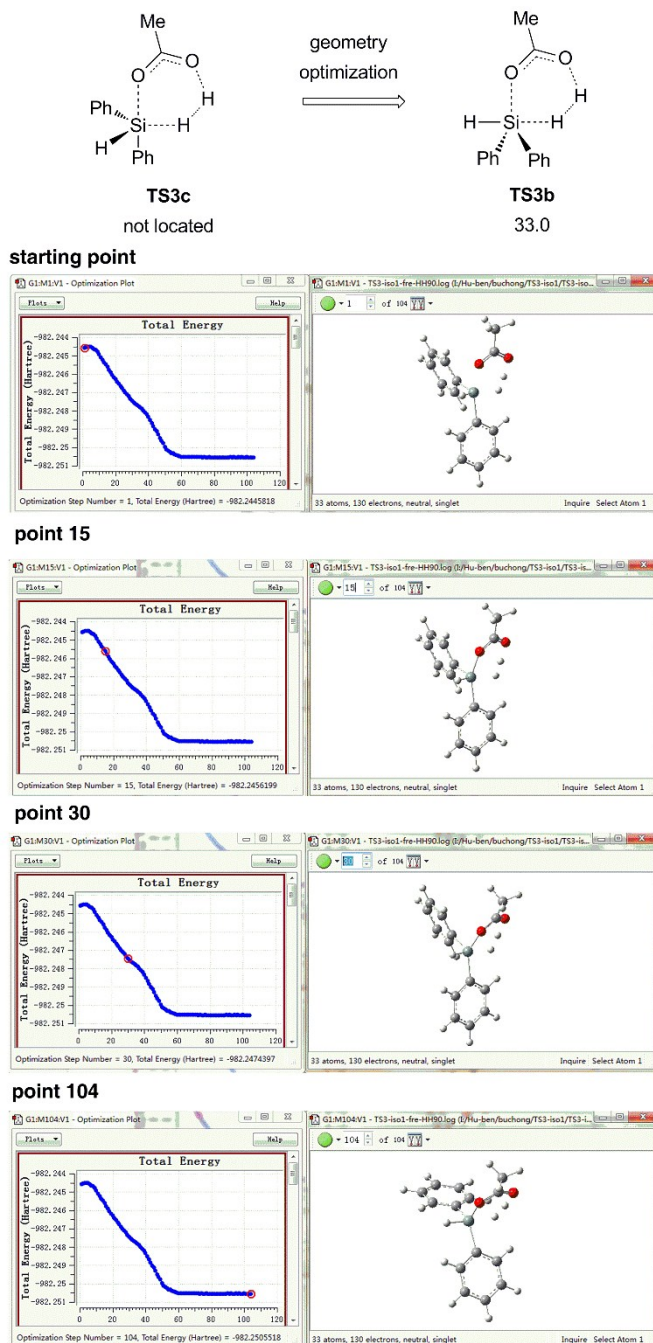
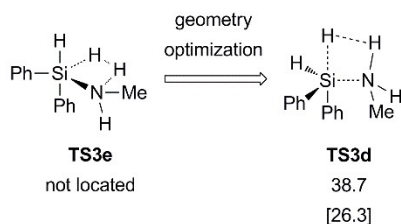
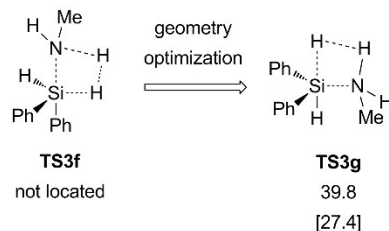
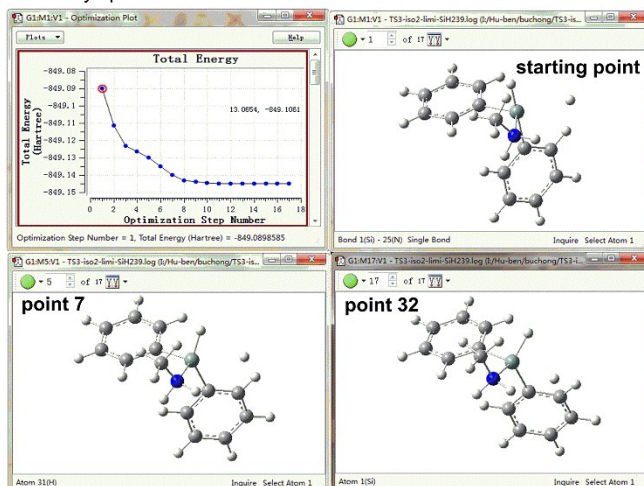


Fig. S2 Geometry optimization of the transition states for the addition of 2a on 1a via equatorial Si–H bond cleavage.

The hypothetical transition states **TS3c** of equatorial Si–H bond cleavage isomerized to **TS3b** during geometry optimization. See the provided file “trajectory of geometry optimization.pptx” for the detailed animations of geometry optimization.



Geometry optimization of **TS3e**



Geometry optimization of **TS3f**

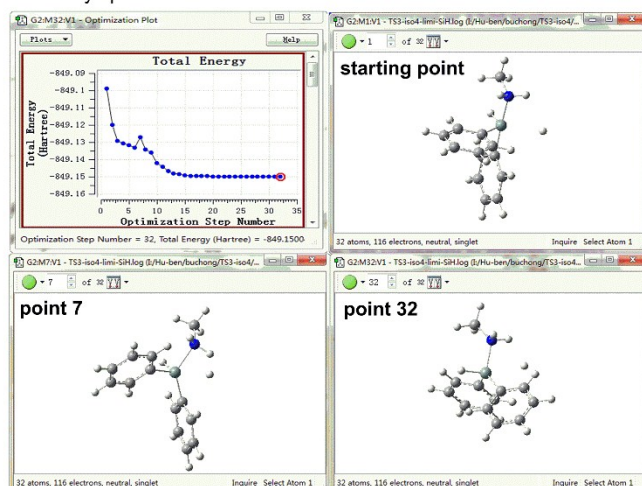
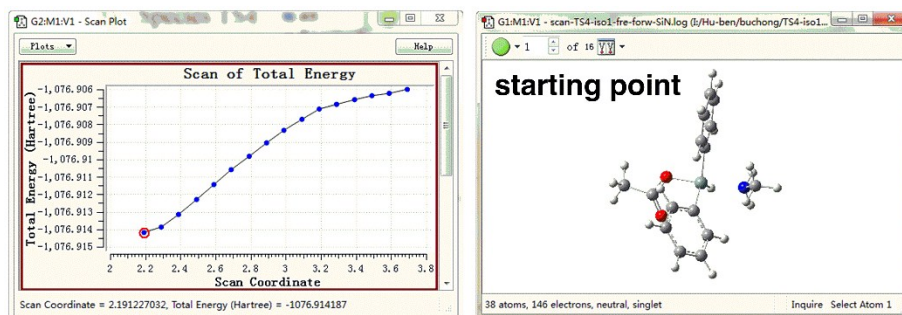
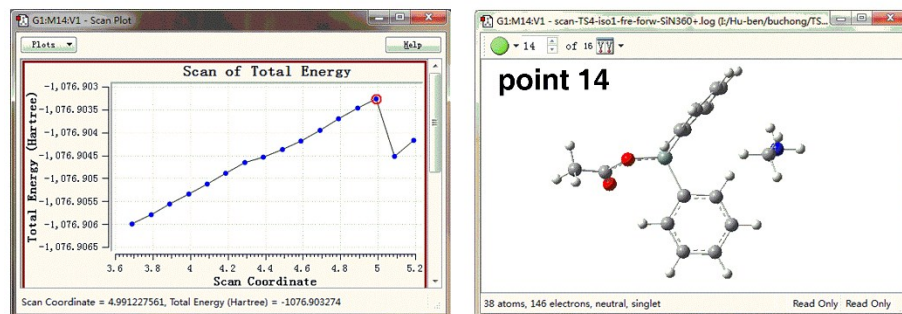


Fig. S3 Transition states of the addition of **3a** on **1a**.

The hypothetical transition states **TS3e** and **TS3f** of equatorial Si-H bond cleavage isomerized to **TS3d** and **TS3g** respectively during geometry optimization. See the provided file “trajectory of geometry optimization.pptx” for the detailed animations of geometry optimization.



Si-N distance varying from 2.19 to 3.69 Å



Si-N distance varying from 3.69 to 5.19 Å

Fig. S4 Relax potential energy surface scan of the Si-N bond from **8b**

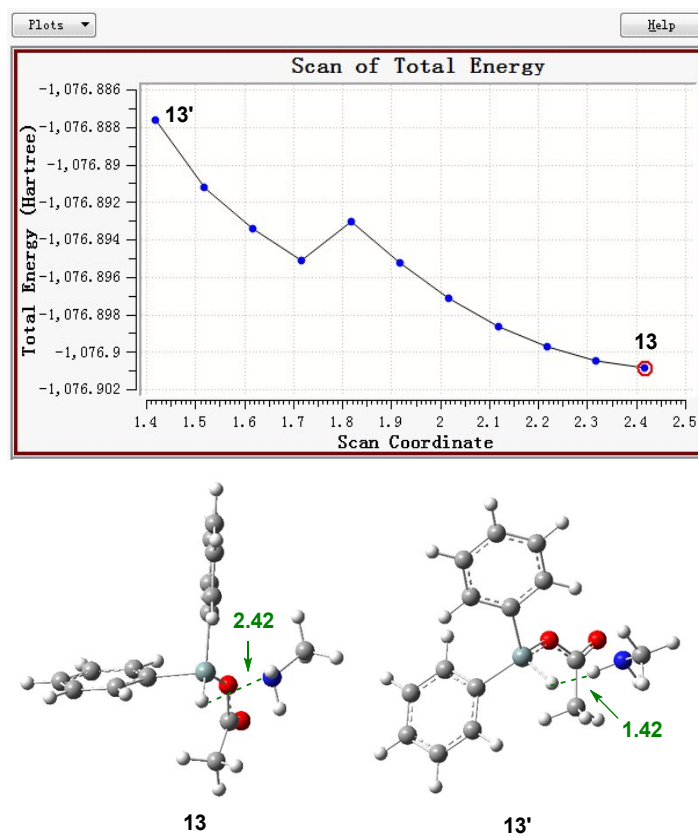
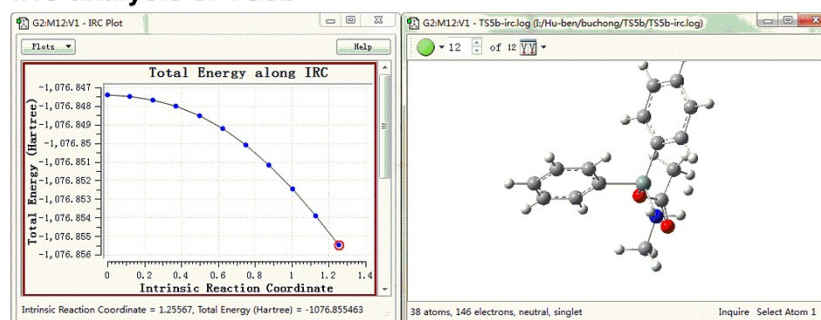


Fig. S5 Relaxed potential energy surface scan of the H–H bond from **8a**.

IRC analysis of TS5b



Geometry optimization continues from the point 12 of the IRC analysis of TS5b

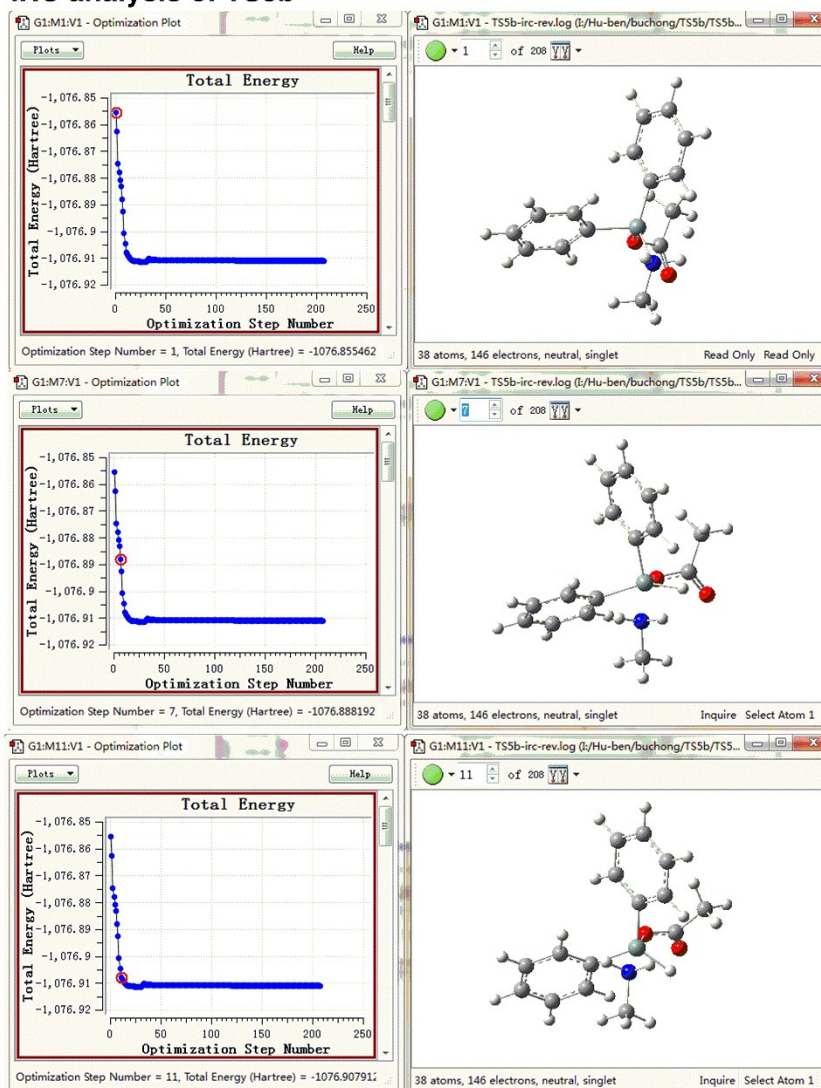
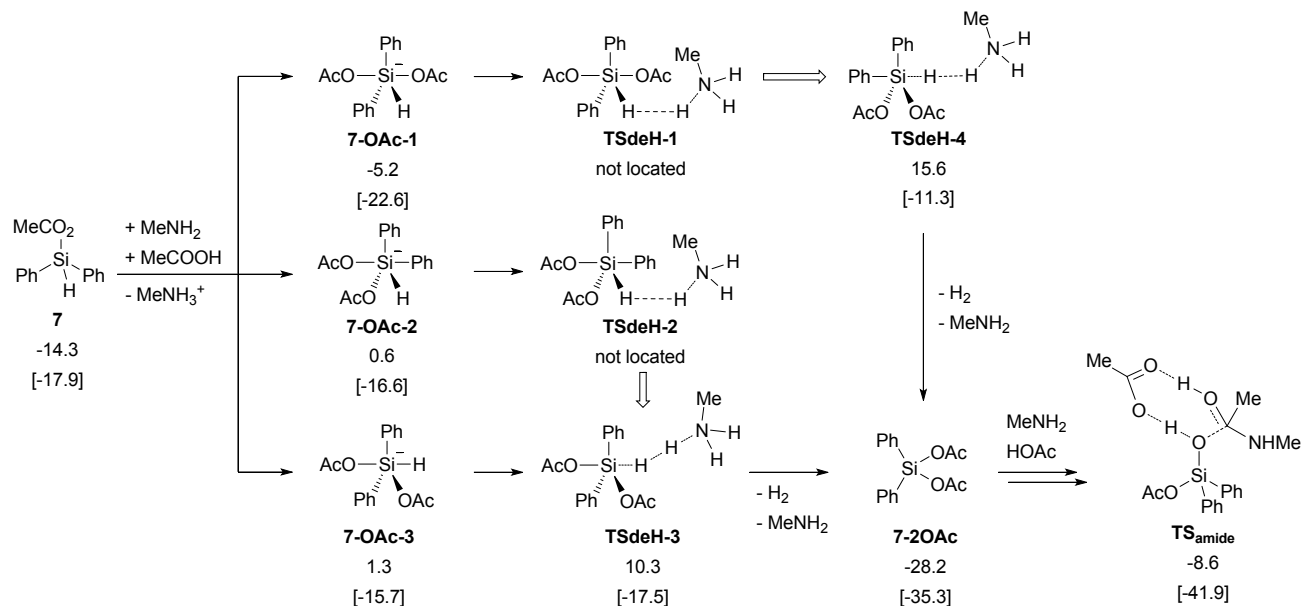
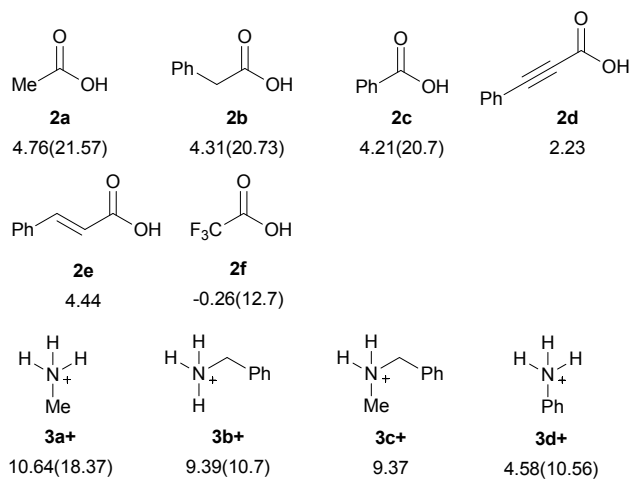


Fig. S6 IRC analysis for TS5b.

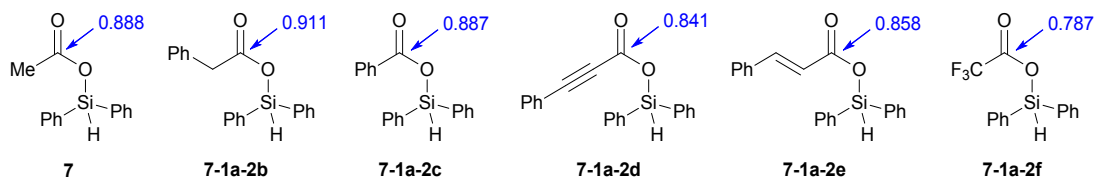


Scheme S2 Calculation results of the formation of bis(acyloxy)silane **7-2OAc** from **7**. Solution-phase Gibbs free energies and enthalpies in brackets are given in kcal/mol.

The dihydrogen formation transition states **TSdeH-1** and **TSdeH-2** isomerized to **TSdeH-4** and **TSdeH-3** respectively during geometry optimization. See the file “trajectory of geometry optimization” for the details.



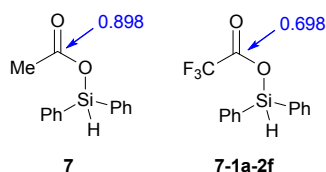
Scheme S3 pKa values of carboxylic acids and ammonium ions in H₂O and acetonitrile (in parenthesis). Data are obtained from reference 36. Because some values in acetonitrile are not available best to our knowledge, the values in H₂O are provided as reference.



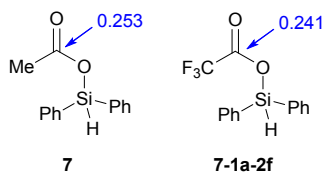
Scheme S4 Calculated NPA charge on the carbonyl carbon of acyloxysilane intermediates at the level of ω B97X-D/def2-SVP/SMD.

We are surprised that **7-1a-2f** has the less positive NPA charge on carbonyl carbon than **7**. To check the validity of the NPA charge, electrostatic potential-derived charge according to the Merz-Singh-Kollman scheme and Hirshfeld charge were calculated at the same level of theory as well. All the results show a similar trend.

electrostatic potential-derived charge according to the Merz-Singh-Kollman scheme



Hirshfeld charge



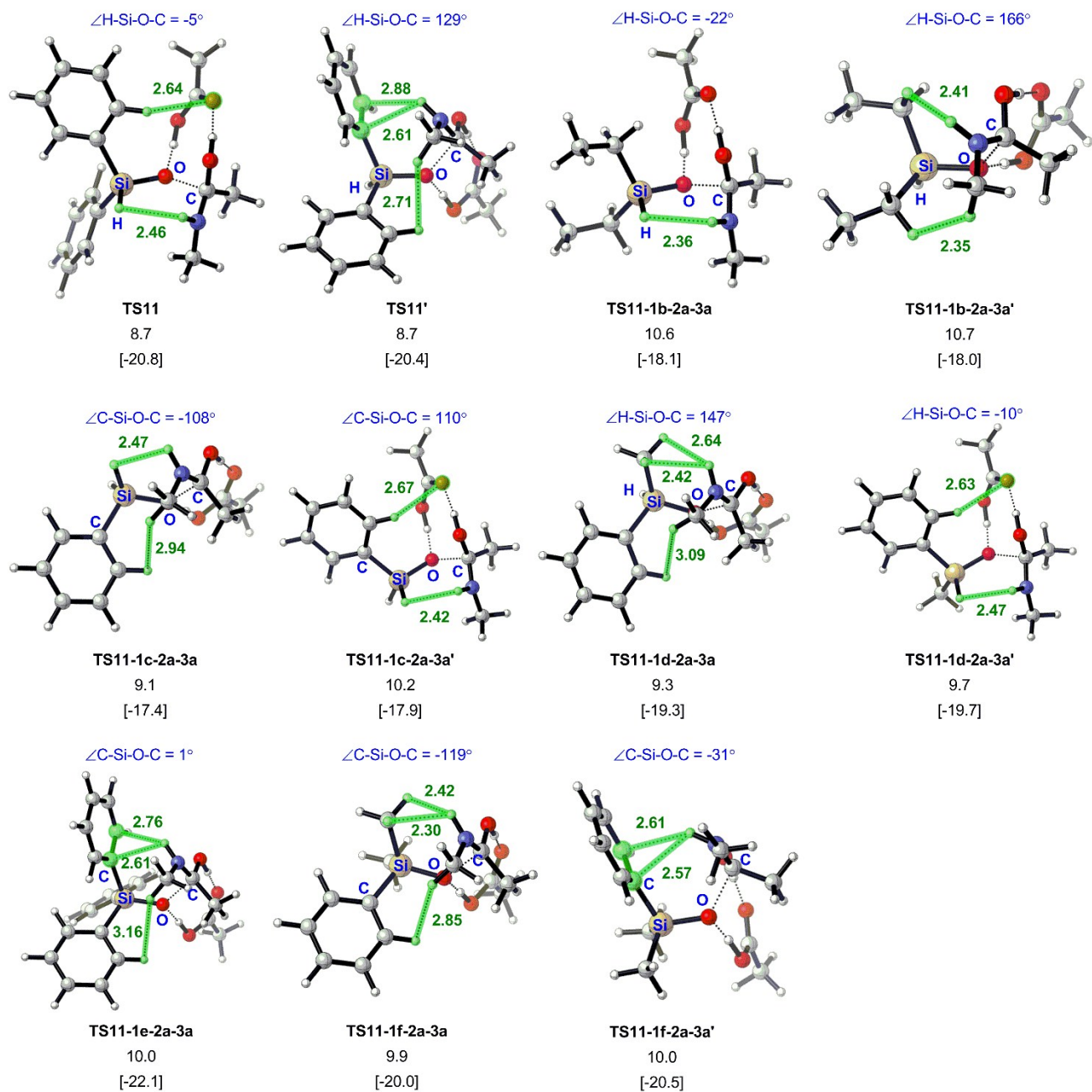


Fig. S7 Optimized structures of amide bond formation transition states. H–H and C–H bond lengths are given in angstrom. Dihedral angles are given in degree. The relative energies of transition states are calculated by setting the related the energies of silane reagent, acid and amines to be 0.0 kcal/mol.

Estimation of Gibbs free energy barriers and reaction constants

Supposing that the amide bond formation is first-order in silane reagents, acids and amines respectively, we can get the following equation

$$\frac{dx}{dt} = k[c_0 - x][a_0 - x][s_0 - x] \quad (1)$$

k is the rate constant, x is the concentration of amide, c_0 is the initial concentration of carboxylic acids, and a_0 is the initial concentration of amines, and s_0 is the initial concentration of silane reagents. Because the loading amounts of carboxylic acids, amines and silane reagents are equal, we can get the following equation

$$-\frac{dc}{dt} = k[c]^3 \quad (2)$$

c is the concentration of carboxylic acids. Then the k can be expressed as

$$k = \frac{3}{2c_0^2 t_{1/2}} \quad (3)$$

$t_{1/2}$ is the half life of the reaction. According to Eyring equation we can get the following equation by omitting the transmission coefficient,

$$k = \frac{k_B T}{h} e^{\frac{-\Delta G^\ddagger}{RT}} \quad (4)$$

k_B is Boltzmann's constant, h is Planck's constant, T is the temperature, R is the gas constant, $\Delta G^\ddagger$ is Gibbs free of activation. Finally, if the half life is roughly estimated to be the half of reaction time and the initial concentration of carboxylic acids is roughly estimated to be 2.7 M based on the volumes and amounts of substrates, $\Delta G^\ddagger$ is estimated to be 29.1 kcal/mol at 80 °C based on equations 3 and 4.

Similar to the estimation of Gibbs free energy barriers based Eyring equation, the reaction constants are predicted to be 2.1×10^{-2} to $2.6 \times 10^{-5} \text{ mol}^{-2} \cdot \text{L}^2 \cdot \text{S}^{-1}$ at 80 °C according to the calculated energy barriers of 23.5-28.2 kcal/mol by supposing that the amide bond formation is a third-order reaction and omitting the transmission coefficient.

Table S1. Calculated thermodynamic corrections to enthalpy (ΔH_{cor}), thermodynamic corrections to Gibbs free energy (ΔG_{cor}), solution-phase single point energies (E_{sol}), solution-phase enthalpies (ΔH_{sol}) and solution-phase Gibbs free energies (ΔG_{sol}) referring to 1 atm and 298.15 K (ΔG_{sol}) (in Hartree)

	ΔH_{cor}	ΔG_{cor}	ΔE_{sol}	ΔH_{sol}	ΔG_{sol}
1a	0.21298	0.161101	-754.02016228	-753.807182	-753.8590613
2a	0.067565	0.035433	-229.11901584	-229.051450	-229.0835828
3a	0.068683	0.041476	-95.87179702	-95.8031140	-95.83032102
4	0.054097	0.021916	-228.63550018	-228.581403	-228.6135842
5	0.084309	0.057916	-96.34627986	-96.2619708	-96.28836386
6a	0.269011	0.204995	-982.66114156	-982.392130	-982.4561466
6b	0.2051030	0.2693450	-982.6627748	-982.3934298	-982.4576718
6c	0.2492650	0.3241510	-1211.2859092	-1210.9617582	-1211.0366442
6d	0.2498690	0.3248490	-1211.2908132	-1210.9659642	-1211.0409442
6e	0.2511710	0.3249110	-1211.2891851	-1210.9642741	-1211.0380141
6f	0.2496490	0.3243280	-1211.2891750	-1210.9648470	-1211.0395260
6g	0.2498100	0.3252940	-1211.2914555	-1210.9661615	-1211.0416455
6h	0.2501080	0.3247840	-1211.2861387	-1210.9613547	-1211.0360307
7	0.262302	0.198892	-981.9872032	-981.724901	-981.7883112
7-OAc-1	0.2444500	0.3188290	-1210.6437594	-1210.3249304	-1210.3993094
TS-deH-4	0.3113360	0.3970170	-1306.9659176	-1306.5689006	-1306.6545816
7-OAc-2	0.2439300	0.3186800	-1210.6340566	-1210.3153766	-1210.3901266
7-OAc-3	0.2433220	0.3183760	-1210.6323543	-1210.3139783	-1210.3890323
TS-deH-3	0.3135780	0.3978530	-1306.9765939	-1306.5787409	-1306.6630159
7-2OAc	0.2358430	0.3110620	-1209.9527889	-1209.6417269	-1209.7169459
TS_{amide}	0.3581540	0.4507670	-1534.9577039	-1534.5069369	-1534.5995499
8a	0.333677	0.261156	-1077.85910702	-1077.52543	-1077.597951
8b	0.2633730	0.3343110	-1077.8706096	-1077.5362986	-1077.6072366
9	0.312183	0.241662	-1076.69730916	-1076.38512	-1076.455647
10	0.200718	0.147271	-828.07600516	-827.875287	-827.9287342
11	0.334066	0.263299	-1077.83936337	-1077.50529	-1077.576064
12	0.207724	0.153632	-828.8147881	-828.607064	-828.6611561
13	0.122954	0.088353	-248.98779904	-248.864845	-248.899446
14	0.220541	0.165411	-829.31476088	-829.094219	-829.1493499
15	0.403548	0.320736	-1307.00066232	-1306.59711	-1306.679926
16	0.3207020	0.4042460	-1306.9914330	-1306.5871870	-1306.6707310
TS1a	0.268592	0.205868	-982.65810546	-982.389513	-982.4522375
TS1b	0.20279	0.268206	-982.6579400	-982.3897340	-982.4551500
TSrot	0.2048450	0.2678120	-982.6483621	-982.3805501	-982.4435171
TS2a	0.348477	0.27321	-1079.00793724	-1078.65946	-1078.734727
TS2b	0.2746560	0.3486320	-1079.0036098	-1078.6549778	-1078.7289538

TS2c	0.2720640	0.3479190	-1078.9982600	-1078.6503410	-1078.7261960
TS3a	0.277414	0.213727	-983.09660049	-982.819186	-982.8828735
TS3b	0.2133640	0.2781000	-983.1034656	-982.8253656	-982.8901016
TS3d	0.2206120	0.2799290	-849.8482795	-849.5683505	-849.6276675
TS3g	0.2208670	0.2802560	-849.8468885	-849.5666325	-849.6260215
TS4a	0.332229	0.261156	-1077.85912321	-1077.52689	-1077.597967
TS4b	0.2598560	0.3320960	-1077.8638205	-1077.5317245	-1077.6039645
TS5b	0.329049	0.258319	-1077.81025733	-1077.48120	-1077.551938
TS6	0.311801	0.247007	-1076.64447671	-1076.33267	-1076.39747
TS7	0.332689	0.262442	-1077.83915346	-1077.50646	-1077.576711
TS9a	0.332962	0.26252	-1077.82743073	-1077.49446	-1077.564911
TS9b	0.3196990	0.4015700	-1306.9781282	-1306.5765582	-1306.6584292
TS9c	0.3260110	0.4030000	-1173.7156332	-1173.3126332	-1173.3896222
TS10	0.402159	0.317943	-1306.98799221	-1306.58583	-1306.670049
TS11	0.3191030	0.4007550	-1306.9847475	-1306.5839925	-1306.6656445
TS11'	0.401098	0.319037	-1306.98458285	-1306.58348	-1306.665546
H₂	0.013324	-0.001507	-1.17559908	-1.16227508	-1.17710608
pro	0.109907	0.072922	-248.55903623	-248.449129	-248.48611
pro'	0.109798	0.073336	-248.5562969	-248.446498	-248.48296
1b	0.157331	0.116333	-449.17758373	-449.020252	-449.0613
1c	0.123258	0.085955	-522.95238952	-522.829131	-522.8664
1d	0.154878	0.111884	-562.28591353	-562.131035	-562.1740
1e	0.301625	0.235862	-985.0897678	-984.788142	-984.8539
1f	0.185037	0.137044	-601.61932778	-601.434290	-601.4823
2b	0.154678	0.109951	-460.17549099	-460.020813	-460.06554
2c	0.124963	0.085031	-420.85882257	-420.733859	-420.7737916
2d	0.137129	0.090626	-496.99888984	-496.861760	-496.9082638
2e	0.160829	0.113985	-498.26055316	-498.099724	-498.1465682
2f	0.0084250	0.0468770	-526.8863145	-526.8394375	-526.8778895
3b	0.155261	0.115687	-326.93006094	-326.774799	-326.8143739
3c	0.184719	0.141798	-366.23655254	-366.051833	-366.0947545
3d	0.123906	0.088966	-287.61436675	-287.490460	-287.5254008
5-3b	0.170695	0.131075	-327.40254339	-327.231848	327.271468
5-3c	0.201038	0.158578	-366.71236917	-366.511331	366.553791
5-3d	0.140045	0.103806	-288.07771339	-287.937668	287.973907
TS2-1b-2a-3a	0.292548	0.228234	-774.16498699	-773.87243	-773.9368
TS2-1c-2a-3a	0.259863	0.196743	-847.93968449	-847.679821	-847.7429
TS2-1d-2a-3a	0.290277	0.222959	-887.27047692	-886.980199	-887.0475
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TS2-1f-2a-3a	0.320446	0.249403	-926.60066563	-926.280216	-926.3513

TS2-1a-2a-3b	0.43479	0.348426	-1310.06780562	-1309.63301	-1309.71938
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TS2-1a-2b-3b	0.522183	0.426792	-1541.12453812	-1540.60235	-1540.697746
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TS2-1a-2a-3d	0.404737	0.323447	-1270.7524896	-1270.34775	-1270.429043
TS11-1a-2a-3b	0.487532	0.394847	-1538.04337164	-1537.55584	-1537.648525
TS11-1a-2a-3c	0.517479	0.420544	-1577.34817151	-1576.83069	-1576.927628
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TS11-1a-2d-3b	0.625317	0.507401	-2073.79990624	-2073.17458	-2073.292505
TS11-1a-2e-3b	0.673346	0.55292	-2076.32300083	-2075.64965	-2075.770081
TS11-1a-2f-3b	0.3408940	0.4432500	-2133.5776644	-2133.1344144	-2133.2367704
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TS11-1b-2a-3a	0.2713540	0.3433190	-1002.1361983	-1001.7928793	-1001.8648443
TS11-1b-2a-3a'	0.343377	0.271505	-1002.13608727	-1001.79271	-1001.864582
TS11-1c-2a-3a	0.312582	0.24086	-1075.91315803	-1075.60057	-1075.672298
TS11-1c-2a-3a'	0.2432950	0.3124670	-1075.9138814	-1075.6014144	-1075.6705864
TS11-1d-2a-3a	0.342318	0.268347	-1115.24787567	-1114.905558	-1114.979529
TS11-1d-2a-3a'	0.2694160	0.3422450	-1115.2484006	-1114.9061556	-1114.9789846
TS11-1e-2a-3a	0.489599	0.398299	-1538.05664647	-1537.56704	-1537.658347
TS11-1f-2a-3a	0.371635	0.294565	-1154.58151384	-1154.20987	-1154.286949
TS11-1f-2a-3a'	0.2950710	0.3711550	-1154.5818809	-1154.2107259	-1154.2868099
7-1a-2b	0.349094	0.272843	-1213.03875442	-1212.68966	-1212.765911
7-1a-2c	0.319657	0.248538	-1173.72538923	-1173.40573	-1173.476851
7-1a-2d	0.331808	0.255143	-1249.8641065	-1249.53229	-1249.608964
7-1a-2e	0.355765	0.278677	-1251.12994725	-1250.77418	-1250.85127
7-1a-2f	0.1716000	0.2417740	-1279.7539954	-1279.5122214	-1279.5823954
7-1b-2a	0.205592	0.154555	-677.14189338	-676.936301	-676.98733838
7-1c-2a	0.173667	0.121838	-750.9111648	-750.737497	-750.78932680
7-1d-2a	0.204073	0.148819	-790.24891944	-790.044846	-790.10010044
7-1e-2a	0.35073	0.275813	-1213.05485037	-1212.70412	-1212.77903737
7-1f-2a	0.234249	0.174786	-829.58896249	-829.354713	-829.41417649
15-1a-2a-3b	0.490258	0.396502	-1538.05754402	-1537.56728	-1537.661042
15-1a-2a-3c	0.519706	0.422723	-1577.36539792	-1576.84569	-1576.942675
15-1a-2b-3b	0.664944	0.551653	-2000.17081698	-1999.50587	-1999.619164

15-1a-2c-3b	0.604294	0.495733	-1921.53314755	-1920.92885	-1921.037415
15-1a-2d-3b	0.629466	0.508135	-2073.81967143	-2073.19020	-2073.311536
15-1a-2e-3b	0.675474	0.558176	-2076.34125921	-2075.66578	-2075.783083
15-1a-2f-3b	0.3436810	0.4490260	-2133.6078747	-2133.1588487	-2133.2641937
15-1a-2b-3d	0.6335	0.524378	-1960.84937039	-1960.21587	-1960.324992
15-1a-2a-3d	0.458843	0.368277	-1498.73748792	-1498.27864	-1498.369211
15-1b-2a-3a	0.348284	0.276791	-1002.15637588	-1001.80809	-1001.879585
15-1c-2a-3a	0.314893	0.243622	-1075.92904489	-1075.61415	-1075.685423
15-1d-2a-3a	0.345163	0.271024	-1115.26561686	-1114.920454	-1114.994593
15-1e-2a-3a	0.491955	0.398552	-1538.07233048	-1537.58037	-1537.673778
15-1f-2a-3a	0.375684	0.298042	-1154.60089501	-1154.225211	-1154.302853
6a-1a-2a	0.269011	0.204995	-982.66114156	-982.392130	982.456147
6a-1a-2b	0.35646	0.283237	-1213.71897552	-1213.36251	1213.435739
6a-1a-2c	0.326431	0.254776	-1174.40401526	-1174.07758	1174.149239
6a-1a-2d	0.338855	0.260685	-1250.54953696	-1250.21068	1250.288852
6a-1a-2e	0.362616	0.284725	-1251.80464965	-1251.44203	1251.519925
6a-1b-2a	0.213303	0.158805	-677.81099587	-677.597692	-677.6521909
6a-1c-2a	0.180639	0.129476	-751.59659319	-751.415954	-751.4671172
6a-1d-2a	0.211017	0.155599	-790.92359576	-790.712578	-790.7679968
6a-1e-2a	0.357631	0.281571	-1213.72804859	-1213.37041	-1213.446478
6a-1f-2a	0.241317	0.182775	-830.25080768	-830.009490	-830.0680327

Cartesian coordinates of all calculated
intermediates and transition states (**in angstrom**)
and imaginary frequency of transition states.

1a

Si	-0.00003200	1.58066800	0.00003700
H	-0.10018300	2.45985900	1.20381000
H	0.09997400	2.46039100	-1.20335800
C	-1.54649400	0.51007100	-0.06324900
C	-2.67382600	0.81168900	0.71767400
C	-1.60369800	-0.61326900	-0.90645500
C	-3.82241700	0.02012400	0.65747400
H	-2.65937600	1.67511900	1.38974200
C	-2.74898500	-1.40641800	-0.96937600
H	-0.73959100	-0.88112300	-1.52286100
C	-3.86110500	-1.08946900	-0.18688100
H	-4.68906400	0.26959500	1.27463200
H	-2.77417200	-2.27624200	-1.63040000
H	-4.75862600	-1.71121100	-0.23348900
C	1.54655900	0.51025600	0.06307400
C	2.67370100	0.81139200	-0.71826600
C	1.60389100	-0.61266600	0.90686400
C	3.82225800	0.01977500	-0.65793700
H	2.65913600	1.67447000	-1.39078400
C	2.74913000	-1.40586000	0.96991000
H	0.73991100	-0.88014800	1.52361100
C	3.86109300	-1.08936800	0.18699000
H	4.68875800	0.26886400	-1.27545600
H	2.77444300	-2.27533500	1.63138900
H	4.75859700	-1.71112400	0.23372500

2a

C	-0.13353000	-0.12802500	0.00003600
O	-0.73659300	-1.16913600	-0.00001300
O	-0.81401900	1.02755300	-0.00000400
H	-0.20913200	1.78422100	-0.00003000
C	1.36605400	-0.00063400	-0.00001000
H	1.69729700	0.55834400	-0.88879600
H	1.69731300	0.55788800	0.88906200
H	1.82427800	-0.99582600	-0.00025700

3a

N	-0.74850900	-0.00000400	-0.13039300
H	-1.13756700	0.80876300	0.35403100
H	-1.13763000	-0.80874100	0.35402800
C	0.69867500	-0.00000200	0.01698900
H	1.12795100	-0.88471100	-0.47979800
H	1.12788500	0.88483600	-0.47960800
H	1.06687200	-0.00011400	1.06216600

4

C	-1.34660600	-0.05467700	0.00000000
H	-1.73035100	-1.08624200	-0.00000100
H	-1.74105300	0.47549100	-0.88334100
H	-1.74105100	0.47548800	0.88334400
C	0.20551100	0.00047100	-0.00000100
O	0.69718200	1.14955400	0.00000000
O	0.81019600	-1.09199100	0.00000000

5

N	0.00000000	0.00000000	0.69527300
H	0.00000000	0.95337300	1.07737800
H	-0.82564500	-0.47668700	1.07737800
H	0.82564500	-0.47668700	1.07737800
C	0.00000000	0.00000000	-0.78319400
H	-0.89850300	0.51875100	-1.13329300
H	0.89850300	0.51875100	-1.13329300
H	0.00000000	-1.03750200	-1.13329300

6a

Si	-0.12879400	0.04072200	-1.17414200
H	-0.25767400	-1.19286100	-2.14691700
C	-1.87212700	-0.26037000	-0.41596000
C	-2.51500000	-1.48521800	-0.67059000
C	-2.55866600	0.65797000	0.40049100
C	-3.77078000	-1.78708900	-0.13924000
H	-2.01912700	-2.22681700	-1.30422800
C	-3.81980500	0.37140200	0.92652900
H	-2.07705200	1.61003800	0.62774500
C	-4.43131000	-0.85467500	0.66082700
H	-4.23642400	-2.75273800	-0.35424200
H	-4.32753700	1.11026900	1.55284000
H	-5.41688600	-1.08247200	1.07547700

C	1.36748100	-0.74820000	-0.26879900
C	2.27280200	-1.56031400	-0.96921100
C	1.59244600	-0.57195600	1.10722500
C	3.37005400	-2.15079100	-0.33768100
H	2.11836200	-1.73947400	-2.03867000
C	2.66747300	-1.18247000	1.75546900
H	0.91430400	0.06435900	1.68190500
C	3.56696400	-1.96793200	1.03153900
H	4.06841000	-2.76343000	-0.91441100
H	2.80980300	-1.03841100	2.83006100
H	4.41694700	-2.43745200	1.53357400
O	0.02190600	1.62692300	-0.05546100
C	0.84344700	2.62438600	0.01036700
O	0.60322700	3.63322600	0.66122900
H	0.06470800	0.98842100	-2.33665600
C	2.16200200	2.49285300	-0.73610500
H	2.80405200	1.76418300	-0.21664700
H	2.01180500	2.11857000	-1.75964700
H	2.67847500	3.46093300	-0.76749500

6b

Si	-0.39652200	-0.71792800	-0.01385300
H	-0.55165500	-1.27659300	1.38523900
H	-0.44133600	-1.38672500	-1.37228500
O	-2.34484900	-0.77194800	-0.08715700
C	-2.95390400	-1.90910700	-0.05415700
C	-4.46877800	-1.79740800	-0.08650900
H	-4.81954500	-1.28112900	0.82082800
H	-4.78530200	-1.18975500	-0.94757500
H	-4.93451100	-2.78986400	-0.14179200
O	-2.39740500	-3.00109400	0.00641800
C	1.57404500	-0.88117600	0.06518300
C	2.27929400	-0.62074200	1.25327500
C	2.34231700	-1.23541000	-1.05432300
C	3.67185200	-0.69531700	1.32320500
H	1.72123700	-0.35070100	2.15909000
C	3.73821500	-1.31755700	-1.00490900
H	1.83427300	-1.45606800	-2.00152800
C	4.40880000	-1.04426800	0.18781800
H	4.18807700	-0.48407200	2.26438400
H	4.30481200	-1.59631800	-1.89829500

H	5.49934400	-1.10677200	0.23545200
C	-0.48559100	1.19833500	-0.06217900
C	-1.49441000	1.90704500	0.61351100
C	0.47011500	1.95724500	-0.75888500
C	-1.54169400	3.30245300	0.60606700
H	-2.26818000	1.35007500	1.14703300
C	0.41940400	3.35278200	-0.79236300
H	1.28050900	1.45006300	-1.29144200
C	-0.58531400	4.03189200	-0.10231400
H	-2.33349900	3.82389700	1.15108600
H	1.17235000	3.91233000	-1.35412700
H	-0.62333800	5.12436400	-0.11671900

6c

Si	-0.00002300	-0.00001900	-1.16232600
H	0.79986000	0.77756500	-2.29246900
H	-0.79984100	-0.77768600	-2.29248400
O	-1.21282000	1.47025700	-1.15099700
O	1.21276900	-1.47032800	-1.15089400
C	2.48478900	-1.58701600	-1.32627200
C	-2.48485000	1.58693200	-1.32635000
O	-3.26111400	0.71501500	-1.69213600
O	3.26106700	-0.71509100	-1.69200300
C	-2.98806900	2.99278100	-1.01492800
H	-2.81891300	3.21725700	0.05011900
H	-2.42232200	3.73790900	-1.59483700
H	-4.05920300	3.08710600	-1.23825900
C	2.98797600	-2.99291900	-1.01502400
H	2.81848300	-3.21771200	0.04989900
H	2.42245300	-3.73790800	-1.59533500
H	4.05917900	-3.08713200	-1.23807200
C	1.09030400	0.95436900	0.21575300
C	1.68257200	0.29878300	1.30920000
C	1.33927500	2.33311400	0.12124500
C	2.47608800	0.96545600	2.24724900
H	1.51835600	-0.77789600	1.43218100
C	2.12365100	3.02315700	1.05096600
H	0.89646200	2.88674800	-0.71461200
C	2.70008700	2.33893500	2.12363400
H	2.92275900	0.41324500	3.08029000
H	2.28729200	4.09999500	0.94049300

H	3.31684600	2.86949100	2.85464800
C	-1.09032100	-0.95435700	0.21576100
C	-1.33935900	-2.33308800	0.12133300
C	-1.68244900	-0.29870800	1.30925500
C	-2.12367200	-3.02307100	1.05115500
H	-0.89664600	-2.88677800	-0.71454400
C	-2.47589300	-0.96531600	2.24740400
H	-1.51816600	0.77796500	1.43218400
C	-2.69996800	-2.33879300	2.12385900
H	-2.28736000	-4.09990600	0.94072400
H	-2.92244900	-0.41306200	3.08047900
H	-3.31667000	-2.86929700	2.85495700

6d

Si	-0.00000500	0.00017500	0.00001700
H	-0.04870500	-0.21721700	1.55941600
H	0.04868500	0.21762300	-1.55939500
O	0.18525400	1.87348000	0.37987900
O	-0.18525900	-1.87315800	-0.37985900
C	-0.72592100	-2.85554400	0.25416800
C	0.72604800	2.85587600	-0.25401600
O	1.29325600	2.81486600	-1.33846600
O	-1.29292100	-2.81450200	1.33872300
C	0.60428000	4.17592400	0.50182400
H	-0.45400200	4.39306400	0.71383200
H	1.11788600	4.09718000	1.47277400
H	1.04154100	5.00199500	-0.07489300
C	-0.60430500	-4.17560900	-0.50167500
H	-1.11797600	-4.09684500	-1.47258800
H	0.45394900	-4.39281700	-0.71375700
H	-1.04156600	-5.00165200	0.07508500
C	-1.97569500	0.24748000	-0.03745200
C	-2.71165300	0.13011500	-1.22640600
C	-2.71600000	0.54696400	1.11709600
C	-4.10031600	0.29446900	-1.27213200
H	-2.17505400	-0.09737100	-2.15692000
C	-4.10147000	0.72767600	1.09612300
H	-2.18444300	0.63975100	2.07286000
C	-4.80444600	0.59887600	-0.10528100
H	-4.63669300	0.18748100	-2.22047700
H	-4.64006100	0.96741100	2.01861600

H	-5.88941700	0.73469300	-0.13058700
C	1.97567300	-0.24735400	0.03743400
C	2.71165700	-0.13086300	1.22644900
C	2.71590500	-0.54640800	-1.11728200
C	4.10027800	-0.29564000	1.27209500
H	2.17513000	0.09627000	2.15709300
C	4.10131900	-0.72751500	-1.09640400
H	2.18430900	-0.63850900	-2.07308900
C	4.80432600	-0.59960800	0.10508400
H	4.63666900	-0.18934000	2.22050800
H	4.63985500	-0.96688600	-2.01902400
H	5.88925100	-0.73579900	0.13032500

6e

Si	-0.21198400	-0.30207300	-0.77278900
H	-0.57314200	-1.72139200	-1.30862800
H	-0.03013500	0.28168300	-2.23977800
O	-0.46257100	-0.95486600	1.01734300
O	-2.07244900	0.14741400	-0.74011600
C	-3.08119900	-0.36045400	-1.35850500
C	-1.34350800	-1.72036400	1.55870700
O	-2.24589300	-2.33011000	0.99621500
O	-3.07126600	-0.89989800	-2.45903500
C	-1.17241300	-1.82296500	3.07163000
H	-0.14808700	-2.14272900	3.31746700
H	-1.31830500	-0.83062500	3.52709700
H	-1.89314200	-2.52999500	3.50411200
C	-4.37975700	-0.24065200	-0.57014600
H	-4.34002700	-0.98920300	0.23672000
H	-4.46693000	0.75019700	-0.10038000
H	-5.25509400	-0.43465400	-1.20554300
C	0.08130700	1.50390500	0.01037900
C	-0.20190600	2.66066100	-0.73589200
C	0.62411300	1.72256000	1.29051100
C	0.03517400	3.95090500	-0.25134600
H	-0.62373400	2.54738200	-1.74178900
C	0.87390600	3.00297300	1.79320300
H	0.85475000	0.85315300	1.91327700
C	0.57850900	4.12983200	1.02249800
H	-0.20299000	4.82193700	-0.87004700
H	1.30068400	3.12407600	2.79402300

H	0.77058200	5.13469100	1.40914900
C	1.71433600	-0.80189800	-0.64026600
C	2.73449100	-0.00025000	-1.18326300
C	2.13470800	-2.00131200	-0.03914600
C	4.08419000	-0.36368600	-1.13892700
H	2.46514400	0.94990300	-1.66196300
C	3.47822300	-2.38474900	0.01946000
H	1.37810000	-2.66049800	0.40248700
C	4.46413700	-1.56334200	-0.53265200
H	4.84419600	0.29079700	-1.57725000
H	3.76015200	-3.32776900	0.49861300
H	5.51732400	-1.85522700	-0.49125600

6f

Si	0.16240100	-0.44051300	-0.69209700
H	0.46129400	-1.94241800	-0.98334200
H	-0.10597000	-0.14652700	-2.22929300
O	2.02941200	-0.05625000	-0.84429500
O	0.50781500	-0.74583600	1.17566400
C	1.40716300	-1.42061100	1.80160700
C	2.95926200	-0.68396300	-1.47572100
O	2.82481400	-1.36495100	-2.48560600
O	2.24765900	-2.16968000	1.31650200
C	4.32971900	-0.51294900	-0.83305000
H	4.51497500	0.54220600	-0.58193800
H	4.32467600	-1.08194100	0.10977100
H	5.12935400	-0.88896700	-1.48612300
C	1.35594400	-1.20001400	3.31101600
H	1.62102800	-0.15521100	3.53948700
H	0.33514600	-1.36339100	3.68851000
H	2.05487200	-1.86866200	3.83121900
C	-1.76205800	-0.86281600	-0.37775700
C	-2.50267500	-1.54186600	-1.36086300
C	-2.45901700	-0.54489300	0.80202900
C	-3.84875100	-1.88061700	-1.19382200
H	-2.00440400	-1.82022000	-2.29898600
C	-3.80469300	-0.87471500	0.99227400
H	-1.92233000	-0.02525300	1.60308000
C	-4.51001900	-1.54575500	-0.00955700
H	-4.38605500	-2.40784800	-1.98850600
H	-4.30796000	-0.60915200	1.92750300

H	-5.56282100	-1.80633800	0.13129800
C	-0.05265200	1.48437500	-0.24739600
C	-0.96755800	2.26572300	-0.97275500
C	0.66669500	2.15847500	0.75534500
C	-1.16384200	3.62774100	-0.72443400
H	-1.55237900	1.78896900	-1.77008700
C	0.49102700	3.52014900	1.01827700
H	1.39143700	1.59156700	1.34657700
C	-0.43065300	4.26550700	0.27821600
H	-1.88986600	4.19495000	-1.31541400
H	1.07500000	4.00581200	1.80671400
H	-0.57455800	5.33069300	0.48031600

6g

Si	-0.33325000	0.01126400	-0.00234700
H	-0.45384300	-0.24981900	-1.52164000
H	-0.44874500	0.27763000	1.51552300
O	-1.77740000	1.30704800	-0.31393700
O	-1.82866300	-1.22703800	0.30569600
C	-2.48954700	-2.01597800	-0.45988600
C	-2.41932300	2.10907700	0.45445200
O	-2.04121100	2.58287800	1.52456000
O	-2.12346300	-2.50199700	-1.52855000
C	-3.80709700	2.46344700	-0.07573100
H	-3.77196700	2.66393000	-1.15665300
H	-4.47657200	1.60080400	0.07405100
H	-4.22641900	3.32971100	0.45399800
C	-3.88522700	-2.33541500	0.07237400
H	-3.85324900	-2.53701700	1.15321300
H	-4.53379000	-1.45667500	-0.07589100
H	-4.32683000	-3.19097100	-0.45669000
C	0.98433900	-1.44648500	0.26945000
C	1.93632500	-1.38995000	1.30230200
C	1.03617200	-2.58082900	-0.55933400
C	2.89472300	-2.38872300	1.49668700
H	1.93222700	-0.52699800	1.98148400
C	1.98416300	-3.59412300	-0.37931100
H	0.28109500	-2.67599500	-1.34810200
C	2.92342200	-3.50039000	0.65032600
H	3.62243000	-2.30332700	2.30991200
H	1.99051600	-4.46483100	-1.04302400

H	3.66878300	-4.28762900	0.79520700
C	1.04648600	1.41241100	-0.26894800
C	1.12002000	2.56240300	0.53634300
C	2.02342100	1.29582500	-1.27335100
C	2.10992600	3.53536700	0.35914800
H	0.35042800	2.70264700	1.30424600
C	3.02364000	2.25342500	-1.46393000
H	2.00401400	0.41798100	-1.93279800
C	3.07215800	3.38256500	-0.64181400
H	2.13225900	4.42021900	1.00350300
H	3.76905900	2.12187800	-2.25462300
H	3.85039000	4.13787100	-0.78366200

6h

Si	0.01569400	0.04302100	-0.84354200
H	0.05120000	-1.25770800	-1.74194800
H	-0.00917400	1.01343100	-2.10669500
O	0.05301700	1.61724700	0.24203400
O	0.13658200	-0.94020600	0.79741700
C	0.12445300	-2.16344000	1.17859500
C	-0.38512500	1.96351900	1.40410900
O	-1.24424900	1.40669700	2.07260200
O	-0.24467400	-3.14269500	0.53312600
C	0.30330800	3.22276100	1.92552500
H	1.36735900	3.00528800	2.11185300
H	0.26530300	4.02235300	1.17020300
H	-0.16097300	3.57126000	2.85795900
C	0.65505400	-2.33712600	2.59727700
H	1.73762300	-2.13071800	2.60283600
H	0.18235500	-1.60579600	3.26929200
H	0.48266600	-3.35658900	2.96761500
C	-1.95533300	-0.00775200	-0.79837700
C	-2.73163800	1.14722500	-0.99481100
C	-2.66315300	-1.21572000	-0.67360300
C	-4.12645100	1.11090600	-1.06777800
H	-2.22187200	2.11252400	-1.09648900
C	-4.05973100	-1.27252300	-0.73843700
H	-2.09158600	-2.13804300	-0.51434700
C	-4.80142400	-0.10610700	-0.93826600
H	-4.69298900	2.03438500	-1.22532700
H	-4.57471900	-2.23323200	-0.63468600

H	-5.89319600	-0.14388700	-0.99390000
C	2.00093100	0.08341900	-0.81368700
C	2.75460400	1.26872100	-0.87423400
C	2.73987200	-1.11290400	-0.79760500
C	4.15235900	1.26826100	-0.92587000
H	2.22367400	2.22648900	-0.87796500
C	4.13693900	-1.13646400	-0.84461200
H	2.19968100	-2.06645500	-0.75112700
C	4.85413000	0.06067200	-0.91040400
H	4.69916100	2.21530800	-0.97643000
H	4.67051200	-2.09216300	-0.83004800
H	5.94708900	0.05222400	-0.94955100

7

Si	0.08581400	0.50649200	-0.74351500
H	0.09790500	0.86816700	-2.18348800
C	-1.22952200	-0.75207200	-0.32136300
C	-1.94959100	-0.67737400	0.88158100
C	-1.48257000	-1.82764800	-1.18796000
C	-2.89724600	-1.64751400	1.20833000
H	-1.77425200	0.14962800	1.57616400
C	-2.42984600	-2.79911200	-0.86376000
H	-0.93749200	-1.91362200	-2.13356900
C	-3.13821000	-2.70929500	0.33549300
H	-3.45055000	-1.57397200	2.14766800
H	-2.61754700	-3.62814700	-1.55033000
H	-3.88147200	-3.46890700	0.58984200
C	1.78730900	-0.06976400	-0.22983700
C	2.92327800	0.30946400	-0.96385100
C	1.96360500	-0.88369600	0.90191900
C	4.19781700	-0.10515800	-0.57572300
H	2.81685200	0.93630200	-1.85455600
C	3.23629300	-1.29749100	1.29411200
H	1.09621300	-1.20419500	1.48726600
C	4.35452900	-0.90829700	0.55451200
H	5.07125800	0.19702100	-1.15857800
H	3.35672600	-1.92916200	2.17749300
H	5.35197100	-1.23504600	0.85887500
O	-0.19451000	1.91635200	0.20300800
C	-1.27911200	2.67522900	0.00395500
O	-2.06838600	2.44034500	-0.88057100

C	-1.39038100	3.80033100	0.98704200
H	-1.51213900	3.38299800	1.99812100
H	-0.46464700	4.39317600	0.98520800
H	-2.24916300	4.43567100	0.74289200

7-OAc-1

Si	0.05631800	0.15130300	-0.86063800
H	-0.02058300	0.34110000	-2.33987600
O	0.54371400	-1.61720600	-1.28610900
O	-0.40097800	1.96013100	-0.60192400
C	-1.44973700	2.53215900	-1.11447200
C	0.86714300	-2.56919100	-0.45809200
O	0.92506900	-2.45644300	0.75521300
O	-2.24854600	1.98913700	-1.86194500
C	1.15773100	-3.88533800	-1.15215500
H	0.22410800	-4.28299500	-1.58067600
H	1.85987000	-3.73472000	-1.98515400
H	1.56677300	-4.61687900	-0.44367700
C	-1.62016600	3.97160000	-0.67073300
H	-1.90904100	3.98443800	0.39244900
H	-0.67034600	4.51861300	-0.75767200
H	-2.40049300	4.47281000	-1.25756200
C	-1.45961000	-0.42052000	0.15719800
C	-1.88916100	0.28837000	1.29126400
C	-2.19982700	-1.55815000	-0.20410000
C	-2.99006800	-0.12740500	2.04291300
H	-1.35595500	1.19265500	1.59551700
C	-3.31869200	-1.96668500	0.52362900
H	-1.89403300	-2.14336500	-1.07558800
C	-3.71458000	-1.25578600	1.65752500
H	-3.28861600	0.43863200	2.92955200
H	-3.88155600	-2.84938600	0.20773400
H	-4.58379900	-1.57846900	2.23660700
C	1.72865600	0.51931700	-0.01359300
C	2.92426100	-0.01642200	-0.52058700
C	1.82701800	1.34339100	1.11975200
C	4.15976100	0.25683400	0.06934100
H	2.89131500	-0.67009400	-1.39671200
C	3.05429600	1.60190800	1.73346100
H	0.92530200	1.80286800	1.53130800
C	4.22867800	1.06294100	1.20628600

H	5.07297400	-0.16728300	-0.35720000
H	3.09490900	2.23547000	2.62381300
H	5.19243700	1.27127500	1.67835900

TS-deH-4

imaginary frequency = -970.01 cm⁻¹

Si	0.08736800	0.26445400	0.27984600
H	-1.22331400	1.12334300	1.34969400
O	0.79520800	0.34577900	1.85678800
O	-0.14161100	1.68499300	-0.68342400
C	0.22560700	2.93739700	-0.44665800
C	1.41384100	-0.66342400	2.46494800
O	1.21032700	-1.82202300	2.18169500
O	0.92811700	3.25314200	0.48592200
C	2.37494900	-0.20124800	3.52107200
H	3.21552900	0.31263800	3.02920000
H	1.88971000	0.52535800	4.18766200
H	2.75220800	-1.05482800	4.09590000
C	-0.32717300	3.89826900	-1.46088800
H	-0.02431500	3.58686600	-2.47123500
H	-1.42690100	3.87770800	-1.42619800
H	0.03099300	4.91410600	-1.25862700
C	1.63061600	-0.37138900	-0.64355400
C	1.67319800	-1.61264100	-1.29425800
C	2.79713100	0.41527500	-0.66543200
C	2.82767800	-2.05329200	-1.94681800
H	0.78969700	-2.25796200	-1.29228000
C	3.95443700	-0.01705900	-1.31303300
H	2.80306400	1.38983200	-0.16607500
C	3.97177500	-1.25597100	-1.95762700
H	2.83355100	-3.02542100	-2.44680200
H	4.84715600	0.61393200	-1.31555800
H	4.87652100	-1.59852700	-2.46637500
C	-1.29670500	-0.93272300	-0.13732900
C	-1.78633700	-1.87002700	0.78419000
C	-1.89359000	-0.87101300	-1.40618700
C	-2.84258200	-2.71745200	0.45004700
H	-1.33286800	-1.94521200	1.77577400
C	-2.95560100	-1.71287200	-1.74163100
H	-1.53264200	-0.15232300	-2.14792200
C	-3.43333400	-2.63734400	-0.81261500

H	-3.20989200	-3.44295800	1.18026800
H	-3.41167700	-1.64536900	-2.73253100
H	-4.26493200	-3.29696200	-1.07261100
N	-3.10752300	1.89320200	0.22686400
H	-2.93967700	1.82437800	-0.77833000
H	-3.23761400	2.88347500	0.44202500
C	-4.26448500	1.09971600	0.63237500
H	-4.09924300	0.05003100	0.35319400
H	-4.37705200	1.15329700	1.72403800
H	-5.19610800	1.44962100	0.16309400
H	-1.98557400	1.45986800	0.88034900

7-OAc-2

Si	-0.13811000	0.42365300	-0.40869600
H	-0.12583500	0.67073200	-1.89859000
O	0.12740600	1.36373400	1.09560700
O	-1.78650500	1.34293800	-0.37648000
C	-2.77056900	1.11595900	-1.19442800
C	0.64088600	2.56182000	1.00440300
O	0.92029400	3.08465900	-0.06090100
O	-2.81894200	0.20507400	-2.00685100
C	0.85504800	3.23034700	2.33757600
H	-0.10769600	3.32449100	2.86181400
H	1.51015000	2.60697000	2.96428300
H	1.30278600	4.22249000	2.20546200
C	-3.91519100	2.09831500	-1.03083000
H	-4.38103000	1.95356600	-0.04332000
H	-3.54042400	3.13197500	-1.06508000
H	-4.67233400	1.94835500	-1.81114800
C	-0.87467400	-1.23234000	0.18335600
C	-1.93105100	-1.26786000	1.10859900
C	-0.37212200	-2.46378400	-0.26669100
C	-2.45534000	-2.47479300	1.57402200
H	-2.35607900	-0.32712900	1.46936500
C	-0.90399300	-3.67748200	0.17526900
H	0.45847100	-2.48304500	-0.97944100
C	-1.94575400	-3.68648300	1.10344200
H	-3.27041000	-2.47105200	2.30313100
H	-0.49906700	-4.62039200	-0.20216200
H	-2.35829200	-4.63392700	1.46003700
C	1.75862400	-0.09866500	-0.43942900

C	2.43245700	-0.23562200	-1.66140600
C	2.49369500	-0.40423900	0.72183600
C	3.76479900	-0.65683800	-1.73600000
H	1.90002400	-0.00446900	-2.59207900
C	3.82307300	-0.82514500	0.66689000
H	2.01103500	-0.31146100	1.70023900
C	4.46594300	-0.95358600	-0.56776400
H	4.25745800	-0.75048500	-2.70815100
H	4.36401800	-1.05497000	1.58953000
H	5.50776500	-1.28166000	-0.61621400

7-OAc-3

Si	0.05211500	0.32121000	-0.65892500
H	0.03246700	0.06507800	-2.20120800
O	0.14871700	2.06754900	-0.99471300
O	-0.05830800	0.91372400	1.12059000
C	0.02747500	0.19087300	2.19985800
C	-0.89617000	2.85263200	-1.04877100
O	-2.04417200	2.45600400	-0.97144400
O	0.25592900	-1.00685400	2.23192200
C	-0.53477100	4.30749200	-1.21649200
H	0.00347000	4.65119700	-0.31988300
H	0.14230800	4.43382700	-2.07373100
H	-1.43622900	4.91567900	-1.35771800
C	-0.19640200	0.99764200	3.46377700
H	0.46449900	1.87683700	3.47819800
H	-1.23275900	1.36978300	3.48136500
H	-0.01864000	0.38255400	4.35494100
C	1.83011800	-0.34861700	-0.46477700
C	2.76087400	0.21659600	0.42257300
C	2.26982600	-1.41769100	-1.26057800
C	4.06933500	-0.26058000	0.51116800
H	2.45582700	1.05179700	1.05883900
C	3.56791300	-1.92370300	-1.15964600
H	1.58467900	-1.86719000	-1.98680900
C	4.47551500	-1.34102900	-0.27454400
H	4.77548100	0.20816100	1.20215400
H	3.87499400	-2.76817300	-1.78256600
H	5.49681300	-1.72373900	-0.20024600
C	-1.46815800	-0.83050400	-0.42374400
C	-1.56541800	-1.98202200	-1.21925100

C	-2.51451200	-0.58621400	0.48042300
C	-2.63348200	-2.87461000	-1.09641800
H	-0.78957300	-2.19038600	-1.96377000
C	-3.60290400	-1.45202800	0.58958500
H	-2.48040000	0.30972000	1.10406400
C	-3.66139000	-2.60831100	-0.19203900
H	-2.66903400	-3.77350000	-1.71797800
H	-4.41016300	-1.22734800	1.29236600
H	-4.50775700	-3.29416100	-0.10065800

TS-deH-3

imaginary frequency = -841.83 cm⁻¹

Si	0.27398800	0.26495800	-0.15441400
H	-0.16787200	-0.17518200	-1.93571700
O	0.13082600	1.87484900	-0.76793500
O	0.59127000	0.90687400	1.46437900
C	0.88295300	0.17031400	2.52367000
C	-0.76416000	2.80751200	-0.48873900
O	-1.85231000	2.56208700	-0.01043000
O	1.07220700	-1.02609500	2.47333800
C	-0.29556600	4.18678000	-0.84956600
H	0.57001300	4.44740100	-0.22201600
H	0.04031800	4.20429100	-1.89626000
H	-1.09841400	4.91680800	-0.69642000
C	0.96080700	0.97973600	3.78962300
H	1.72048600	1.76800100	3.68071600
H	-0.00443500	1.47712300	3.96741900
H	1.21086300	0.33664500	4.64152800
C	1.97521400	-0.38719400	-0.63174500
C	3.10818300	0.15734500	-0.00208200
C	2.18134000	-1.38677800	-1.59533600
C	4.39380200	-0.27624200	-0.32457900
H	2.98901200	0.93872000	0.75276400
C	3.46375700	-1.84011400	-1.90675500
H	1.32905400	-1.81881400	-2.12650700
C	4.57472400	-1.28191400	-1.27456800
H	5.25850000	0.17133000	0.17170800
H	3.59499100	-2.62603400	-2.65451000
H	5.58096900	-1.62743500	-1.52439800
C	-1.18524700	-0.85098100	0.27291300
C	-1.27088300	-2.15061100	-0.24789700

C	-2.18997400	-0.42303500	1.15280900
C	-2.31820600	-3.00100800	0.10504100
H	-0.51383900	-2.51452100	-0.94780700
C	-3.25562900	-1.26018300	1.48693100
H	-2.15056700	0.58650100	1.56722700
C	-3.31928900	-2.55394400	0.96853100
H	-2.35863800	-4.01339800	-0.30437500
H	-4.03740000	-0.90149800	2.16131000
H	-4.14896600	-3.21299800	1.23621700
N	-2.33992400	0.64323300	-2.36958600
H	-1.01190600	0.14817600	-2.12066800
H	-2.27843800	1.25502100	-3.18519000
C	-3.31344600	-0.42363300	-2.58152000
H	-3.46546000	-0.96909300	-1.64064700
H	-4.28689400	-0.04099700	-2.92600600
H	-2.93070900	-1.13158800	-3.33057500
H	-2.60326000	1.23147000	-1.57409800

7-2OAc

Si	0.14246000	0.28353900	-0.06117300
O	-0.18953000	1.05260700	-1.54815400
O	-0.09221400	1.44042300	1.13794000
C	-1.16744200	1.76069100	1.88970700
C	-1.33506700	1.69992700	-1.81214900
O	-2.19856100	1.83709000	-0.97924400
O	-1.95666700	0.94135800	2.27390600
C	-1.39983000	2.20814000	-3.21856600
H	-0.52965700	2.84897800	-3.42111500
H	-1.35184700	1.35820900	-3.91560600
H	-2.32800500	2.76834400	-3.37673000
C	-1.21635200	3.22644100	2.19484800
H	-0.25796600	3.55405700	2.62248000
H	-1.36558000	3.77864800	1.25493100
H	-2.03658500	3.44461200	2.88816800
C	1.96660000	-0.06163000	-0.05424400
C	2.88934200	0.88033100	0.43092900
C	2.45053100	-1.28438600	-0.54762600
C	4.25691600	0.60972200	0.41588800
H	2.53710200	1.83543100	0.82963000
C	3.81868600	-1.55568100	-0.56530600
H	1.75369500	-2.04098300	-0.92090900

C	4.72224500	-0.60816200	-0.08327500
H	4.96314900	1.35064800	0.79797200
H	4.18012500	-2.51142300	-0.95195400
H	5.79406900	-0.82096200	-0.09291400
C	-0.89323900	-1.25356100	0.05880000
C	-0.88546800	-2.01200000	1.24163600
C	-1.63434900	-1.72282600	-1.03621200
C	-1.60716500	-3.20006600	1.33002900
H	-0.31481100	-1.67058200	2.10997900
C	-2.35971600	-2.91206400	-0.94862600
H	-1.64951100	-1.16231700	-1.97523100
C	-2.34716300	-3.65012600	0.23418600
H	-1.59470600	-3.77800700	2.25709500
H	-2.93495400	-3.26296500	-1.80860000
H	-2.91434700	-4.58156100	0.30352400

TS_{amide}

imaginary frequency = -261.75 cm⁻¹

Si	-0.29778700	0.28464400	0.09945200
O	0.81987800	-0.19448100	-0.99108700
C	1.24579000	-1.96241900	-1.40532700
O	1.81257400	-2.35777500	-0.27787000
C	2.13546900	-1.62814000	-2.57160300
H	3.02155600	-1.07955800	-2.23305700
H	1.61366700	-1.02967900	-3.32592100
H	2.46662200	-2.57462500	-3.02575700
N	0.09612300	-2.61903900	-1.66265300
H	-0.39250500	-2.92481200	-0.82595600
C	-0.73814500	-2.32277600	-2.80522000
H	-1.61675700	-2.97870000	-2.77444200
H	-0.20659700	-2.51729800	-3.74738000
H	-1.08356300	-1.27424500	-2.80428000
H	2.55708000	-1.73724600	-0.03966700
C	3.81139300	0.50045000	0.09803100
O	3.71463700	-0.68709600	0.39209400
C	4.94522700	1.35198800	0.58419700
H	5.70864300	0.73461700	1.07066400
H	4.55260100	2.08641000	1.30423300
H	5.38256000	1.91287100	-0.25364700
O	2.95543700	1.13542500	-0.65283400
H	2.11370900	0.57179800	-0.83508800

C	-1.48798100	-1.07011700	0.59902500
C	-1.13659400	-2.01338000	1.57917900
C	-2.71962200	-1.21909000	-0.05689000
C	-1.98109300	-3.08085400	1.88133100
H	-0.18260100	-1.92437600	2.10649100
C	-3.56806500	-2.28660400	0.24205300
H	-3.02410700	-0.49701500	-0.82067600
C	-3.19754900	-3.22056900	1.20964700
H	-1.69045200	-3.80758000	2.64393500
H	-4.52142200	-2.38942900	-0.28202100
H	-3.85886600	-4.05830400	1.44445000
C	-1.17677300	1.80344400	-0.55312800
C	-2.23036100	2.42551600	0.13872200
C	-0.79636200	2.32891900	-1.79878400
C	-2.87669700	3.54009000	-0.39542700
H	-2.53756500	2.03828800	1.11351600
C	-1.43964100	3.44526500	-2.33525500
H	0.01547800	1.85225300	-2.35485400
C	-2.48140300	4.05190700	-1.63320300
H	-3.69315900	4.01325500	0.15588800
H	-1.12828200	3.84099500	-3.30524800
H	-2.98801600	4.92537400	-2.05157400
O	0.63620800	0.68617200	1.49475800
C	0.17705400	1.08611400	2.67666400
O	-0.99923100	1.25622600	2.90430600
C	1.27873900	1.30054900	3.67353300
H	1.86247600	0.37477800	3.78275500
H	1.96298900	2.07612400	3.29805100
H	0.86683500	1.60390300	4.64275600

8a

Si	0.03148700	0.47252300	-0.66392300
C	-1.38115400	-0.79719700	-0.32191900
C	-1.65821900	-1.76045000	-1.30626800
C	-2.11887700	-0.86816800	0.87222200
C	-2.61810600	-2.75565600	-1.11272000
H	-1.11132500	-1.73523700	-2.25646500
C	-3.08517900	-1.85634100	1.07559400
H	-1.94128500	-0.13590300	1.66577000
C	-3.33591300	-2.80538900	0.08340900
H	-2.81057600	-3.49162000	-1.89800200

H	-3.64585900	-1.88607200	2.01379200
H	-4.09149800	-3.57953400	0.23997000
C	1.53886000	-0.49872500	-0.09198800
C	2.51268100	-0.94276000	-1.00027500
C	1.69957800	-0.82656200	1.26334200
C	3.60958400	-1.69191100	-0.57107300
H	2.42121300	-0.70210000	-2.06446500
C	2.80123500	-1.56386100	1.69962500
H	0.95539700	-0.50137600	1.99687000
C	3.75760100	-2.00087500	0.78171900
H	4.35342300	-2.03361700	-1.29532000
H	2.91213800	-1.80171400	2.76064200
H	4.61811900	-2.58312500	1.12066200
O	-0.45167300	1.63521000	0.52211600
C	-1.45889600	2.50047700	0.58404600
O	-1.68121500	3.10881800	1.60271900
C	-2.26192100	2.66912200	-0.68096600
H	-1.61154300	3.01224100	-1.50076200
H	-2.70244500	1.70635300	-0.98364200
H	-3.06297800	3.40075100	-0.52430700
H	-0.18235900	0.59852800	-2.13888600
N	1.45953800	2.12219300	-1.19331100
H	2.04715400	1.75260600	-1.94419000
H	0.89275800	2.85091600	-1.63412600
C	2.30126800	2.71748400	-0.15571000
H	1.66378900	3.15712600	0.62243000
H	2.91809300	1.93525900	0.30901400
H	2.96805000	3.49849300	-0.55379000

8b

Si	0.09081900	0.28909200	-0.83056400
H	0.07793100	0.83257100	-2.21584500
C	-1.42829600	-0.50508500	-0.02906700
C	-1.63515400	-0.33942900	1.35075900
C	-2.39216400	-1.22935500	-0.74798400
C	-2.74220300	-0.89730200	1.99243900
H	-0.92199500	0.24265600	1.94121400
C	-3.51076600	-1.77515900	-0.11700300
H	-2.28487600	-1.37295100	-1.82716300
C	-3.68492200	-1.61710000	1.25846700
H	-2.87205500	-0.76244400	3.06928400

H	-4.25010600	-2.32716000	-0.70285300
H	-4.55629300	-2.05041000	1.75573300
C	1.77626600	-0.00403600	-0.03042400
C	2.92797900	0.54568300	-0.61764100
C	1.93639300	-0.75695300	1.14335400
C	4.19122600	0.35088300	-0.05680700
H	2.84490400	1.13990200	-1.53344300
C	3.19734700	-0.95307700	1.71127700
H	1.06576000	-1.20787300	1.62834500
C	4.32880200	-0.39930400	1.11202500
H	5.07219300	0.78859700	-0.53341500
H	3.29556000	-1.54236300	2.62656900
H	5.31631000	-0.55190300	1.55471800
O	-0.08906700	1.90735500	-0.02169600
C	-1.06179500	2.73880500	-0.31125100
O	-1.92591300	2.50956200	-1.13739200
C	-1.00641300	4.01686600	0.48944000
H	-1.11388900	3.78210200	1.55947400
H	-0.02677500	4.50001600	0.35869400
H	-1.80554100	4.70226200	0.18210200
N	0.45016900	-1.55902200	-1.95164300
H	-0.27113300	-1.62512600	-2.67391600
H	1.30933800	-1.34969200	-2.46662200
C	0.59243400	-2.85756700	-1.28836000
H	1.42057600	-2.81354700	-0.56881500
H	-0.32899100	-3.09514500	-0.74003800
H	0.79386900	-3.66618100	-2.00726500

9

Si	0.05392600	0.35775400	0.42657700
C	-1.33134300	-0.84435800	0.05255600
C	-1.71226800	-1.81803500	0.99107300
C	-1.99423100	-0.81897700	-1.18626100
C	-2.72409200	-2.73470800	0.70331000
H	-1.21500400	-1.86061700	1.96441300
C	-3.00580500	-1.73408600	-1.47724300
H	-1.72254600	-0.07248100	-1.93858400
C	-3.37197900	-2.69340200	-0.53183600
H	-3.00918100	-3.48309600	1.44674600
H	-3.51199900	-1.69772300	-2.44494100
H	-4.16554900	-3.40986100	-0.75814200

C	1.74877000	-0.21675800	-0.11301600
C	2.36247100	0.25224300	-1.28514600
C	2.42382600	-1.18315100	0.65260500
C	3.61089500	-0.22917300	-1.68145700
H	1.85834100	1.00778200	-1.89294100
C	3.67155200	-1.66644900	0.25951500
H	1.97227600	-1.56192400	1.57484800
C	4.26637700	-1.18931400	-0.90993400
H	4.07495600	0.14861000	-2.59590100
H	4.18305700	-2.41640600	0.86785300
H	5.24445600	-1.56593900	-1.21965200
O	-0.19102700	1.71324400	-0.59402700
C	-1.14876500	2.64364000	-0.69519700
O	-1.14624900	3.40822000	-1.62572400
C	-2.17795800	2.66502900	0.40346700
H	-2.73227500	1.71386600	0.42087500
H	-1.68770800	2.78063800	1.38121000
H	-2.88039200	3.49008500	0.23875600
N	0.04263800	0.67120600	2.10530500
H	-0.85088800	0.60656200	2.58517400
C	1.05710900	1.38610100	2.85686400
H	0.80028300	2.44720900	3.02325600
H	1.22349800	0.92157600	3.84234800
H	2.01609500	1.36138600	2.31767600

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Si	-0.00005600	1.20779000	0.00029600
O	-0.00035200	2.74810000	0.00073200
C	1.57481600	0.23501900	0.02948000
C	1.65353800	-1.07698800	0.53020000
C	2.75338500	0.86005300	-0.41867500
C	2.87453800	-1.74861900	0.56850900
H	0.76056300	-1.58128800	0.90813300
C	3.97081300	0.18379900	-0.38986900
H	2.71652400	1.88612000	-0.79435900
C	4.03073500	-1.12110200	0.10293800
H	2.92375100	-2.76546300	0.96441000
H	4.87714000	0.67667700	-0.74887700
H	4.98615800	-1.65070600	0.12890700
C	-1.57472200	0.23471000	-0.02930800
C	-1.65314700	-1.07765600	-0.52912300

C	-2.75358400	0.86014400	0.41754600
C	-2.87415700	-1.74924800	-0.56778900
H	-0.75993200	-1.58227700	-0.90604900
C	-3.97103700	0.18396500	0.38831300
H	-2.71685100	1.88647900	0.79250400
C	-4.03066300	-1.12129900	-0.10357000
H	-2.92314400	-2.76639700	-0.96293300
H	-4.87761100	0.67717400	0.74624200
H	-4.98610200	-1.65085800	-0.12988100

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Si	-0.10395900	-0.05436500	0.81810200
H	-0.04457600	-0.14971600	2.31053800
C	0.13147700	1.73464500	0.29150500
C	1.18513200	2.13809200	-0.54480000
C	-0.78416500	2.70678800	0.73172800
C	1.31681800	3.47582500	-0.92682600
H	1.91228700	1.39193300	-0.88535300
C	-0.65333600	4.04176000	0.35129900
H	-1.61950100	2.42171600	1.38069700
C	0.40003500	4.42782200	-0.48098900
H	2.14215200	3.77639500	-1.57769400
H	-1.37442800	4.78387800	0.70309200
H	0.50434800	5.47357700	-0.78144300
C	-1.79803400	-0.65507300	0.28002300
C	-2.59793700	-1.43705200	1.12840100
C	-2.29171700	-0.34652600	-0.99924300
C	-3.84758100	-1.90138200	0.71309600
H	-2.24537700	-1.68979900	2.13334800
C	-3.53767200	-0.81037100	-1.42016500
H	-1.69657600	0.26950900	-1.68092500
C	-4.31774000	-1.58898700	-0.56264800
H	-4.45694600	-2.50750400	1.38811200
H	-3.90426700	-0.56080800	-2.41901100
H	-5.29605200	-1.95021500	-0.88957700
O	1.01039500	-1.06937900	0.12304600
C	2.45776000	-1.08352100	0.15209700
C	2.95784300	-0.88098600	1.58444600
H	2.78919900	0.17107000	1.86401800
H	2.45266700	-1.52603800	2.31891300
H	4.04146600	-1.06371000	1.62155300

O	3.03602400	-0.48677200	-0.77764900
N	2.63449600	-2.77033900	-0.06742100
H	3.62277800	-2.97727300	0.09909800
H	2.09782900	-3.27673600	0.64080300
C	2.25324800	-3.18311900	-1.41688700
H	1.16537800	-3.10050100	-1.52140300
H	2.73657900	-2.49529400	-2.12225700
H	2.57085400	-4.21527300	-1.61338300

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Si	-0.01234800	1.27263000	-0.83826900
H	0.00076100	1.07788300	-2.35681300
C	-1.51784900	0.21977100	-0.28488300
C	-2.46264400	0.80996400	0.56905000
C	-1.73993700	-1.11228000	-0.67292300
C	-3.57947100	0.10478700	1.02515000
H	-2.30768600	1.84989000	0.87469600
C	-2.85196900	-1.82761800	-0.22385900
H	-1.03116300	-1.61058100	-1.34334200
C	-3.77597600	-1.21907100	0.62937200
H	-4.30005900	0.58862600	1.69069900
H	-3.00101200	-2.86399600	-0.53964100
H	-4.64765200	-1.77632700	0.98283500
C	1.52531400	0.27370500	-0.28229000
C	1.92361800	-0.94147000	-0.86415200
C	2.30487600	0.77006000	0.77469900
C	3.03999400	-1.64162000	-0.40116200
H	1.35585400	-1.35461300	-1.70539500
C	3.42413000	0.07963700	1.24610400
H	2.02292500	1.72618600	1.22793900
C	3.79269900	-1.13236600	0.65956500
H	3.32816200	-2.58616100	-0.87096400
H	4.01371200	0.48850200	2.07158700
H	4.66789100	-1.67683500	1.02396300
O	-0.05319600	2.75245100	-0.29597900

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N	0.69881300	-0.70621600	0.00012400
H	0.74205500	-1.33861800	0.81422800
H	0.74187700	-1.33879300	-0.81385200
C	1.88105200	0.18718900	-0.00011500

H	1.86626800	0.80732800	0.90178900
H	2.77375800	-0.44762000	-0.00012000
H	1.86607100	0.80707200	-0.90219400
C	-0.70817700	-0.11857800	0.00022000
O	-1.59024900	-0.91303900	-0.00016400
C	-0.79434600	1.36030200	0.00000800
H	-0.29047600	1.76764900	0.88911500
H	-0.28975600	1.76748800	-0.88876100
H	-1.85067100	1.64983500	-0.00044100

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Si	0.00612000	1.31144400	-0.44250700
C	-1.53307700	0.26302100	-0.24441700
C	-2.62949000	0.71030800	0.50918100
C	-1.61615600	-0.99817700	-0.85852700
C	-3.77414500	-0.07688000	0.64532300
H	-2.58601900	1.68618300	1.00012400
C	-2.75977600	-1.78577000	-0.72849400
H	-0.77425400	-1.37882300	-1.44608600
C	-3.84083900	-1.32511300	0.02558700
H	-4.61744900	0.28540900	1.23859600
H	-2.80718900	-2.76373600	-1.21374900
H	-4.73683300	-1.94190800	0.13129700
C	1.54554000	0.28988100	-0.11604500
C	2.67030200	0.38835400	-0.95054000
C	1.60791700	-0.58370300	0.98402600
C	3.82248300	-0.35810600	-0.69566800
H	2.65099900	1.05683600	-1.81710200
C	2.75699900	-1.32906000	1.24422800
H	0.74460200	-0.68906400	1.64882900
C	3.86605700	-1.21689900	0.40261100
H	4.68789400	-0.27023700	-1.35716900
H	2.78805800	-2.00366200	2.10344600
H	4.76643500	-1.80275100	0.60391400
O	-0.19039000	2.56250600	0.64784100
H	0.49500900	3.24029200	0.64686700
H	0.13128500	1.85406700	-1.83018400

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C	-1.28306600	-0.74552700	0.10899100
O	-1.68425000	0.00338100	-0.95460300
N	-2.01427800	-2.06937100	-0.00474000

H	-3.08172200	-1.82508700	0.00419500
C	-1.71288600	-3.10717200	0.99207000
H	-2.08875700	-2.79383600	1.97279300
H	-2.22082300	-4.03172200	0.69297800
H	-2.65356600	0.30876200	-0.82450800
H	-1.80771500	-2.42049500	-0.94615600
O	-4.54715500	-1.42605000	0.07209100
C	-4.89420700	-0.25769400	-0.24426700
O	-4.11757600	0.65158600	-0.63043700
C	-6.37101200	0.08338400	-0.17230100
H	-6.76557900	0.18207700	-1.19604000
H	-6.93837800	-0.69455300	0.35426800
H	-6.51002700	1.05414500	0.32506200
O	0.06220300	-1.04087200	-0.01638200
Si	1.16029800	-0.05248600	-0.84048800
H	0.89746700	-0.06202400	-2.30460100
C	2.81624900	-0.84141600	-0.46218800
C	3.98187400	-0.30560400	-1.03636300
C	2.94340100	-1.94458900	0.39563800
C	5.23422300	-0.85490200	-0.76405800
H	3.91784700	0.55762000	-1.70737800
C	4.19557200	-2.49730700	0.67082600
H	2.05198600	-2.37776000	0.85646400
C	5.34191900	-1.95308800	0.09164900
H	6.12965600	-0.42483800	-1.21940400
H	4.27623000	-3.35594900	1.34200000
H	6.32246400	-2.38492300	0.30704000
C	1.10628900	1.70788200	-0.20211600
C	1.80821500	2.06552300	0.96097500
C	0.33253600	2.68895700	-0.84282600
C	1.73354600	3.36084100	1.47373200
H	2.42368800	1.32331700	1.47895500
C	0.25840800	3.98632100	-0.33576200
H	-0.22939200	2.43592600	-1.74611700
C	0.95760300	4.32243500	0.82478300
H	2.28409000	3.62155500	2.38093600
H	-0.34803700	4.73843000	-0.84636300
H	0.89884000	5.33814800	1.22383500
C	-1.58524900	-0.10673000	1.45711400
H	-1.15520100	0.90386500	1.45553900
H	-2.66911600	-0.02891600	1.61871900

H	-1.13368900	-0.67788200	2.27859900
H	-0.63077000	-3.27769500	1.03847500

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Si	-0.68788200	0.05118000	-0.87975900
O	-0.22484500	1.29950300	0.17457700
C	0.19166600	2.64863900	-0.20519300
O	1.39683100	2.55313500	-0.87119200
C	0.31201900	3.41011500	1.10950700
H	1.09471900	2.95966000	1.73596200
H	-0.63054000	3.39289200	1.67234700
H	0.58888200	4.45160500	0.89789900
N	-0.71460700	3.27260600	-1.10954700
H	-0.57957800	2.89084900	-2.04268200
C	-2.11465600	3.33512600	-0.74802900
H	-2.66877300	3.82846200	-1.55868000
H	-2.25669700	3.93971400	0.16000400
H	-2.58683000	2.34856500	-0.56887800
H	2.02098600	2.08824100	-0.27460400
C	2.59012500	0.23143700	1.61184900
O	2.96861600	1.10119100	0.84574900
C	3.50349200	-0.77834200	2.23128200
H	4.54923400	-0.48246300	2.09296000
H	3.33025600	-1.74626500	1.73441800
H	3.27376800	-0.90614700	3.29790200
O	1.32711800	0.07961100	1.96098600
H	0.74422000	0.65052400	1.39172600
H	-1.03059500	0.63913400	-2.20324500
C	-2.19865500	-0.74425500	-0.11852200
C	-3.38290700	-0.89506300	-0.85672800
C	-2.18051500	-1.19321600	1.21411900
C	-4.51483200	-1.47941300	-0.28495600
H	-3.42888200	-0.55003200	-1.89415100
C	-3.30943300	-1.77510200	1.78844500
H	-1.27289800	-1.09207300	1.81666500
C	-4.47847400	-1.91912000	1.03803100
H	-5.42879700	-1.58894400	-0.87372700
H	-3.27844700	-2.11776800	2.82550300
H	-5.36395400	-2.37500600	1.48782300
C	0.73633400	-1.15957700	-1.03741100
C	0.64208600	-2.48746600	-0.59123900

C	1.95123700	-0.73187500	-1.60025700
C	1.72801300	-3.35823700	-0.69506500
H	-0.29021700	-2.85363600	-0.15199500
C	3.03860600	-1.59791100	-1.70446400
H	2.05530700	0.29977200	-1.94761400
C	2.92849400	-2.91309800	-1.24939100
H	1.63676700	-4.38761900	-0.34004700
H	3.97689200	-1.24461300	-2.13884300
H	3.78042600	-3.59300600	-1.32811300

H₂

H	0.00000000	0.00000000	0.37928800
H	0.00000000	0.00000000	-0.37928800

pro

C	-0.48017000	0.16367100	-0.01043500
C	-1.81154000	-0.55315100	0.00831400
H	-2.47486600	-0.09213500	-0.73679700
H	-1.72851000	-1.62992600	-0.19237400
H	-2.27614000	-0.41108000	0.99622100
O	-0.40232100	1.38545200	-0.00159800
N	0.61278200	-0.63395100	-0.02826100
H	0.48443400	-1.63715800	0.02491600
C	1.95516200	-0.10696500	0.01324300
H	2.01926900	0.80178200	-0.60141000
H	2.26982300	0.15516100	1.03815900
H	2.65437100	-0.85393200	-0.38484400

pro'

C	0.61791400	-0.15916800	-0.00001000
C	0.71003500	1.34999600	-0.00000900
H	1.76724100	1.64050100	0.00018400
H	0.21580600	1.77553100	-0.88700000
H	0.21544100	1.77557900	0.88675200
O	1.60994900	-0.87653000	0.00005100
N	-0.63477900	-0.67914700	-0.00011400
H	-0.68089400	-1.69274000	0.00005100
C	-1.87585300	0.06234700	0.00005500
H	-1.97932900	0.69957400	0.89315800
H	-1.97863900	0.70099300	-0.89210000
H	-2.70834800	-0.65221200	-0.00086000

TS1a

imaginary frequency = -62.88 cm⁻¹

Si	-0.31392200	-0.43726700	-1.37145900
H	-0.57268500	-1.65850900	-2.22946100
C	-1.97472100	-0.25813700	-0.47669400
C	-2.91217200	-1.29785000	-0.62114600
C	-2.33116600	0.83528100	0.33404900
C	-4.15393700	-1.25292400	0.01576600
H	-2.67328000	-2.16488600	-1.24431100
C	-3.57276800	0.88368700	0.96977500
H	-1.60025200	1.63943300	0.45387100
C	-4.48816100	-0.15852100	0.81327500
H	-4.86264700	-2.07497300	-0.11379700
H	-3.82842200	1.74406900	1.59433400
H	-5.45991200	-0.11834800	1.31232600
C	1.11939500	-1.02149700	-0.29020900
C	2.18074800	-1.73310500	-0.86886900
C	1.16486000	-0.77646600	1.09049200
C	3.26684400	-2.16350000	-0.10278000
H	2.17114400	-1.95451300	-1.94143300
C	2.23810100	-1.21622700	1.86460700
H	0.35776400	-0.21121700	1.56232900
C	3.29698200	-1.90518800	1.26757500
H	4.08950500	-2.70479100	-0.57727100
H	2.25428500	-1.01472900	2.93895100
H	4.14296200	-2.24249000	1.87201200
O	0.31932100	1.86607000	-0.16134200
C	1.37819800	2.55548700	-0.10677800
O	1.52444900	3.62065600	0.51095200
H	0.01170500	0.59589400	-2.39053500
C	2.60037800	1.98998600	-0.85083900
H	3.09761200	1.24232400	-0.20985500
H	2.31304500	1.47971600	-1.78261900
H	3.32843000	2.78479900	-1.07033900

TS1b

imaginary frequency = -26.51 cm⁻¹

Si	-0.15972600	-0.77853500	-0.46336800
H	0.34771600	-1.77707600	0.51341700
H	0.03999400	-1.17575400	-1.88369800

C	0.47813400	0.98114600	-0.13960500
C	1.76887500	1.38689600	-0.52545000
C	-0.34735100	1.92854800	0.48995000
C	2.21187700	2.68962500	-0.29361400
H	2.42450100	0.64271300	-0.98940700
C	0.09585200	3.23145800	0.72868600
H	-1.35924700	1.65373500	0.80181500
C	1.37705600	3.61621600	0.33439500
H	3.21840400	2.98410300	-0.60333200
H	-0.56494300	3.94892100	1.22218600
H	1.72464600	4.63653000	0.51656900
C	-2.03957400	-0.71776200	-0.20013500
C	-2.89226100	-0.16910300	-1.17391600
C	-2.62326900	-1.18745500	0.98743600
C	-4.27015700	-0.08860500	-0.97026300
H	-2.47501000	0.20724600	-2.11406700
C	-4.00180600	-1.11004400	1.20018400
H	-1.99150100	-1.62461800	1.76752000
C	-4.82802400	-0.55957500	0.22027600
H	-4.91289900	0.34169000	-1.74270700
H	-4.43210900	-1.48259800	2.13341800
H	-5.90717200	-0.49872300	0.38262800
C	4.57710900	-1.17499300	0.33993900
H	5.23421200	-1.77794700	0.98440300
H	4.34548400	-0.23682800	0.87348300
H	5.11120800	-0.89917800	-0.58252400
C	3.25661800	-1.90766900	0.02155300
O	2.61477700	-1.46194900	-0.96854800
O	2.92001900	-2.83790600	0.77405000

TSrot

imaginary frequency = -74.30 cm⁻¹

Si	0.27386400	-0.82171100	-0.63238600
H	0.46278400	-0.67926500	-2.12952600
H	0.19897100	-2.37415600	-0.57890700
O	1.85984100	-1.05945400	0.31873800
C	2.83057100	-1.87389800	0.00968400
C	3.75697800	-2.16474100	1.17231500
H	4.11896300	-1.22330000	1.61156500
H	3.20074400	-2.69690600	1.95971100
H	4.60863100	-2.77672100	0.84947000

O	3.00376800	-2.35637000	-1.09629100
C	-1.64800400	-0.74933800	-0.24535000
C	-2.44027200	0.38187700	-0.51936500
C	-2.30802700	-1.86249900	0.29743100
C	-3.81586800	0.39453700	-0.28398100
H	-1.97225200	1.28104100	-0.93283600
C	-3.68084400	-1.85710700	0.56373600
H	-1.73027400	-2.76765600	0.51693400
C	-4.44157100	-0.72649100	0.26755200
H	-4.40377100	1.28473600	-0.52502400
H	-4.15803600	-2.73940900	0.99965100
H	-5.51671800	-0.71643400	0.46557700
C	0.56611800	1.07186500	-0.19375400
C	1.00394100	1.98157600	-1.16725100
C	0.36077500	1.58555500	1.10058400
C	1.22832300	3.33255900	-0.87533400
H	1.17440800	1.63218500	-2.19248300
C	0.58329900	2.92770200	1.40903800
H	0.00872600	0.92007300	1.89747000
C	1.01980600	3.81136700	0.41716300
H	1.56695000	4.01296500	-1.66223500
H	0.41371200	3.29071100	2.42707400
H	1.19283500	4.86489200	0.65259200

TS2a

imaginary frequency = -967.19 cm⁻¹

Si	-0.12145000	0.20821700	0.66419800
H	0.51736900	-1.48743700	1.15906700
C	1.46314200	0.35445900	-0.35618200
C	1.92340100	-0.71453200	-1.14027800
C	2.21222700	1.54167100	-0.35752900
C	3.08925900	-0.60612400	-1.89925800
H	1.36599500	-1.65644100	-1.15541300
C	3.39188000	1.64934700	-1.09636900
H	1.86886500	2.40127500	0.22416000
C	3.83159600	0.57560100	-1.87142100
H	3.42365000	-1.44949400	-2.50871300
H	3.96628000	2.57895400	-1.07200100
H	4.75119100	0.66053400	-2.45590900
C	-1.54254300	-0.80119700	-0.07210700
C	-2.09015500	-1.92334900	0.56792400

C	-2.10393200	-0.40205100	-1.29682000
C	-3.16501200	-2.61892800	0.01341800
H	-1.66995300	-2.26470300	1.51898900
C	-3.16459100	-1.10710400	-1.86769200
H	-1.71159500	0.47733100	-1.81570800
C	-3.70112800	-2.21474400	-1.21027800
H	-3.58249800	-3.48362500	0.53548900
H	-3.57824800	-0.78604600	-2.82705300
H	-4.53710600	-2.76334000	-1.65141600
O	-0.70838800	1.83920500	0.24012000
C	-1.73054200	2.57181900	0.64162500
O	-1.91145700	3.68421600	0.19589600
H	-0.04713700	0.42115700	2.13886700
C	-2.65239400	1.95589600	1.66914400
H	-3.14827900	1.06816700	1.24709500
H	-2.08568300	1.62694100	2.55335000
H	-3.41283200	2.68504900	1.97302300
N	2.55411000	-1.30762200	2.28293300
H	1.33550400	-1.39779800	1.63817800
H	2.39729000	-1.35884900	3.29116700
H	2.97167800	-0.39502300	2.09177800
C	3.41625800	-2.39211600	1.82134100
H	2.91380100	-3.35399800	1.99444600
H	3.58948900	-2.28112000	0.74229900
H	4.38771700	-2.40248500	2.33777500

TS2b

imaginary frequency = -988.16 cm⁻¹

Si	0.28990700	0.21189600	-0.62668300
H	0.35732000	0.06982900	-2.13734800
C	2.11561700	0.08180400	-0.16924500
C	2.73904200	0.88827600	0.79429100
C	2.89919600	-0.87321400	-0.83775000
C	4.09860200	0.75218600	1.07834600
H	2.15267800	1.63715400	1.33500500
C	4.25442100	-1.02963100	-0.54328300
H	2.44683600	-1.50985100	-1.60556400
C	4.85769300	-0.21249700	0.41392100
H	4.56679800	1.39751100	1.82601500
H	4.84306500	-1.78704200	-1.06707200
H	5.92055200	-0.32670000	0.64154300

C	-0.78550800	-1.31493900	-0.28159700
C	-0.71843500	-2.03125600	0.92340000
C	-1.62407600	-1.80782300	-1.29255900
C	-1.45702300	-3.19901900	1.11307900
H	-0.08049800	-1.66656500	1.73488900
C	-2.38421400	-2.96345400	-1.10312800
H	-1.69146900	-1.27635900	-2.24624300
C	-2.29872200	-3.66382400	0.10039400
H	-1.38121200	-3.74568900	2.05648100
H	-3.04119000	-3.32139000	-1.89997200
H	-2.88686000	-4.57280600	0.25021900
O	-0.19063800	1.90327600	-0.67991700
C	-1.39216300	2.31830600	-1.01983100
O	-2.33655600	1.56127300	-1.15518900
H	0.06280700	0.56753400	1.22896800
C	-1.47666600	3.80420500	-1.22389500
H	-0.99032300	4.33257800	-0.39229600
H	-0.93305400	4.06843800	-2.14425500
H	-2.52274600	4.11794200	-1.31692200
N	-2.19616600	0.81532500	1.75511200
H	-0.86139800	0.66688700	1.46885300
H	-2.51234400	0.01104000	2.29907900
C	-2.45035800	2.07409900	2.44816500
H	-2.10806700	2.91099400	1.82308700
H	-3.51738300	2.21931900	2.67439600
H	-1.88342900	2.09537500	3.38904900
H	-2.67251400	0.78228300	0.84886500

TS2c

imaginary frequency = -1071.19 cm⁻¹

Si	-0.01815900	0.51688300	-0.15140400
C	1.64079900	-0.42362500	-0.36989200
C	2.27240900	-0.47287600	-1.62129600
C	2.26387500	-1.09871500	0.69609800
C	3.47222300	-1.16614500	-1.81098100
H	1.81959800	0.04228200	-2.47582000
C	3.46030700	-1.79231800	0.51920500
H	1.80406300	-1.08468400	1.68959900
C	4.06888000	-1.82746900	-0.73881400
H	3.94218300	-1.18733700	-2.79787000
H	3.92375100	-2.30857000	1.36423600

H	5.00703100	-2.37033200	-0.88021900
O	0.45756800	1.42930300	1.24377600
C	0.90537300	2.66955100	1.40027800
O	1.14361600	3.10054000	2.50314200
H	-1.51926200	1.70391000	0.06030800
C	1.09461500	3.46901900	0.13608100
H	1.46942000	4.47047200	0.37762300
H	1.81132000	2.96272300	-0.52984400
H	0.13834600	3.55461100	-0.40395800
N	-3.07588700	1.26635200	-1.58845800
H	-2.21852800	1.48962900	-0.64538300
H	-3.99700800	1.19587300	-1.15090300
C	-3.01939400	2.36442900	-2.55240200
H	-2.03014700	2.37474000	-3.02839500
H	-3.79118400	2.27054000	-3.32939500
H	-3.16101400	3.31573200	-2.02140000
H	-2.88501200	0.36356700	-2.02762100
C	-1.22703800	-0.85977100	0.31136300
C	-2.21210600	-0.70180000	1.29832000
C	-1.14247900	-2.10074800	-0.34130300
C	-3.07977600	-1.74383000	1.62633800
H	-2.30633400	0.25590900	1.81855100
C	-2.02255300	-3.14013300	-0.03454500
H	-0.37514200	-2.26598300	-1.10394000
C	-2.99075700	-2.96425100	0.95444700
H	-3.83244800	-1.60203400	2.40602200
H	-1.94644800	-4.09305000	-0.56423500
H	-3.67482600	-3.77928300	1.20387300
H	-0.10865700	1.08382200	-1.53509800

TS3a

imaginary frequency = -986.55 cm⁻¹

Si	-0.14500300	0.45193400	-1.06673000
H	-1.57658500	1.13152600	-1.73133400
C	-1.21827300	-0.96111400	-0.39345100
C	-0.64621300	-2.22072500	-0.14088600
C	-2.58534500	-0.79802500	-0.11654500
C	-1.41207800	-3.27787700	0.35144300
H	0.41776900	-2.38528700	-0.33218700
C	-3.35195300	-1.84450000	0.39772400
H	-3.06871200	0.16517800	-0.30187300

C	-2.76699000	-3.08994700	0.62735200
H	-0.94705500	-4.25110800	0.52715800
H	-4.41127000	-1.68733900	0.61529300
H	-3.36643700	-3.91372400	1.02286500
C	1.59124100	0.01727800	-0.35763700
C	2.61045200	-0.37626100	-1.23550200
C	1.88242500	0.00350700	1.01876000
C	3.86880300	-0.77241800	-0.77022600
H	2.42241000	-0.37632600	-2.31512600
C	3.13266800	-0.38807000	1.49477100
H	1.11432500	0.30302200	1.73865100
C	4.13185400	-0.77867700	0.59822800
H	4.64440400	-1.07404000	-1.47919700
H	3.33256200	-0.39073300	2.56967000
H	5.11327400	-1.08568000	0.96886200
O	-0.17707000	1.93436200	0.04095900
C	-1.03903300	2.86842400	0.16189100
O	-2.03960400	2.95067400	-0.60193900
C	-0.84594000	3.85754700	1.25130000
H	-1.04681200	3.34851800	2.20720000
H	0.19978400	4.19272400	1.26448900
H	-1.53044900	4.70471800	1.13454400
H	0.27358700	0.44470600	-2.51262700
H	-1.91706300	2.03161400	-1.27766500

TS3b

imaginary frequency = -966.20 cm⁻¹

Si	0.01522100	-0.26443100	-0.47900900
H	0.02624500	-0.06929700	-1.98543300
H	0.00599200	-0.70032900	1.18027400
C	-1.61483400	0.64514700	-0.12158800
C	-2.19342700	0.73019400	1.15488200
C	-2.26547100	1.30141200	-1.18023000
C	-3.37171800	1.44520400	1.37000600
H	-1.71550500	0.22574200	2.00002100
C	-3.44379800	2.02004300	-0.97351000
H	-1.84364800	1.25029200	-2.18872100
C	-3.99942400	2.09250200	0.30432400
H	-3.80347600	1.49663800	2.37269600
H	-3.93145600	2.52259000	-1.81259300
H	-4.92372200	2.65173600	0.47011600

C	1.71992300	0.49720200	-0.12242200
C	2.32198900	0.50074400	1.14592900
C	2.40390800	1.13107300	-1.17364100
C	3.55547400	1.11607200	1.36048900
H	1.81862600	0.01047100	1.98471000
C	3.63620100	1.75254100	-0.96686100
H	1.96507000	1.14013300	-2.17614600
C	4.21453700	1.74529100	0.30293500
H	4.00521500	1.10463000	2.35650600
H	4.14801600	2.24143600	-1.79959700
H	5.18083300	2.22847400	0.46842700
O	-0.08357700	-2.07156600	-0.81442600
C	-0.20679600	-3.04915900	0.00362200
O	-0.25556700	-2.87011700	1.24723200
C	-0.30557600	-4.41652100	-0.56786800
H	-1.23058300	-4.47834400	-1.16081600
H	0.53876200	-4.58410000	-1.25121700
H	-0.31709500	-5.17131100	0.22578800
H	-0.12913300	-1.70372600	1.34326200

TS3d

imaginary frequency = -498.60 cm⁻¹

Si	-0.01559100	1.04750900	-0.73440700
C	-1.62768400	0.16742000	-0.35533700
C	-1.76451900	-1.15892900	-0.79999000
C	-2.67406500	0.72796700	0.39346900
C	-2.91898600	-1.89328900	-0.52616000
H	-0.95920200	-1.63572600	-1.36771700
C	-3.81805900	-0.01211400	0.69102100
H	-2.60310200	1.76139000	0.74308900
C	-3.94580100	-1.32160800	0.22498900
H	-3.01168200	-2.91818800	-0.89344100
H	-4.61762900	0.43905700	1.28353900
H	-4.84694500	-1.89765200	0.44935100
C	1.35902500	-0.15879200	-0.23416500
C	2.46383500	-0.36853200	-1.07376400
C	1.32108500	-0.84945000	0.99042200
C	3.49683900	-1.23480200	-0.70722200
H	2.52368100	0.15240200	-2.03479700
C	2.35046200	-1.71182400	1.36462300
H	0.47015600	-0.71681300	1.66690400

C	3.44113100	-1.90628000	0.51358300
H	4.34665800	-1.38585100	-1.37752700
H	2.30221700	-2.23812800	2.32116800
H	4.24771200	-2.58434400	0.80347400
H	-1.40253800	2.94668400	-1.20833600
N	0.30669100	2.40581800	0.51664900
H	-0.46485600	3.05708900	0.26086100
H	0.14694300	2.06518800	1.47258600
C	1.61324900	3.08949900	0.42654500
H	1.71364300	3.53604100	-0.57124600
H	1.66496500	3.87998400	1.18487000
H	2.42243000	2.36737500	0.59099400
H	0.35991000	1.45004500	-2.10670600

TS3g

imaginary frequency = -486.74 cm⁻¹

Si	-0.05250300	0.79428000	-0.17640000
C	-1.72650100	-0.03832900	-0.09966300
C	-1.93334400	-1.29956400	0.48157000
C	-2.81744900	0.60515200	-0.70518500
C	-3.19153300	-1.89772000	0.45931300
H	-1.10317200	-1.82081600	0.96528200
C	-4.08467700	0.01867100	-0.70888800
H	-2.68468800	1.58057500	-1.18463500
C	-4.27160800	-1.23570400	-0.12968300
H	-3.33332800	-2.88269400	0.91064100
H	-4.92513000	0.53988600	-1.17352800
H	-5.26030700	-1.70108900	-0.13788300
C	1.55527900	-0.16776100	-0.08694900
C	2.48765900	0.07246000	-1.11294000
C	1.87004800	-1.14432000	0.87391000
C	3.69543400	-0.62470400	-1.17039600
H	2.27209200	0.81601100	-1.88555200
C	3.06632200	-1.85601900	0.80781700
H	1.17376100	-1.33831900	1.69263400
C	3.98435400	-1.59393900	-0.21133700
H	4.40800600	-0.41310700	-1.97114000
H	3.28735800	-2.61571400	1.56137700
H	4.92600700	-2.14664100	-0.25639000
H	-0.16562900	0.53163200	2.29344100
N	-0.03652200	2.43410500	0.73741300

H	-0.86186500	2.98904200	0.48181800
H	-0.16576200	2.06925200	1.71061800
C	1.18985300	3.24578300	0.61641000
H	1.38244800	3.47698700	-0.43921100
H	1.06953900	4.17912100	1.17958900
H	2.03515400	2.67958300	1.02826800
H	-0.00681000	1.39359800	-1.55149900

TS4a

imaginary frequency = -47.39 cm⁻¹

Si	-0.04685400	0.32908800	-0.59723600
C	-1.70198700	-0.54624400	-0.26874500
C	-2.06743500	-1.62534600	-1.09238800
C	-2.57923600	-0.18855500	0.76686500
C	-3.25831800	-2.32281300	-0.89102600
H	-1.40961300	-1.93401400	-1.91298400
C	-3.77491900	-0.88106400	0.97422900
H	-2.32798500	0.64571400	1.42830600
C	-4.11628400	-1.95021300	0.14614100
H	-3.52013400	-3.15900700	-1.54449100
H	-4.44241300	-0.58419000	1.78739800
H	-5.05085800	-2.49350100	0.30729300
C	1.28126300	-0.88549700	-0.08477800
C	2.10849000	-1.51002700	-1.03068400
C	1.45358900	-1.20969200	1.26966500
C	3.08163500	-2.42878400	-0.63593600
H	2.00178700	-1.27324500	-2.09385600
C	2.43288500	-2.12004200	1.66957700
H	0.82015900	-0.74324100	2.03040300
C	3.24810900	-2.73203200	0.71644900
H	3.71653400	-2.90671700	-1.38623200
H	2.55902000	-2.35416200	2.72962900
H	4.01403500	-3.44659300	1.02793400
O	-0.12867300	1.60883700	0.53235800
C	-0.54652700	2.87295000	0.46259800
O	-0.35893300	3.62458400	1.38645400
C	-1.25014500	3.26825800	-0.80954200
H	-0.54715000	3.22229400	-1.65566900
H	-2.07906800	2.57622900	-1.02408900
H	-1.63780500	4.28960500	-0.72045100
H	-0.09669800	0.65062800	-2.04460100

N	2.09290200	1.76436200	-1.15957300
H	2.58369200	1.27772400	-1.91004700
H	1.77836400	2.64749400	-1.56312700
C	2.99729800	2.01622100	-0.04749200
H	2.45729300	2.53607100	0.75750300
H	3.35538200	1.05879300	0.36093300
H	3.88143400	2.62226900	-0.31564600

TS4b

imaginary frequency = -15.95 cm⁻¹

Si	0.84210000	-0.59703400	-0.73578600
H	1.12859900	-0.85524500	-2.17084300
C	0.95234600	1.21674900	-0.27833700
C	2.14939000	1.84088200	0.11264000
C	-0.21741100	1.99386700	-0.33084400
C	2.17242500	3.19456200	0.44945800
H	3.08001200	1.26967100	0.15036100
C	-0.19404600	3.34890000	0.00032400
H	-1.17812600	1.55886800	-0.62701000
C	1.00053400	3.95134800	0.39473800
H	3.11178500	3.66151300	0.75560400
H	-1.11889400	3.92971800	-0.04812100
H	1.02047300	5.01149300	0.65946800
C	-0.83601800	-1.29350500	-0.29606800
C	-1.83002600	-1.43077200	-1.27754400
C	-1.14545300	-1.66217600	1.02452200
C	-3.09862300	-1.91417900	-0.95041400
H	-1.61867900	-1.15687800	-2.31578200
C	-2.40896500	-2.15114900	1.35293500
H	-0.39066800	-1.57015500	1.81074500
C	-3.38865500	-2.27389500	0.36574400
H	-3.86131800	-2.01234200	-1.72670300
H	-2.63282500	-2.43423100	2.38422900
H	-4.38039600	-2.65338900	0.62361100
O	1.93702900	-1.51300700	0.22280500
C	3.25126500	-1.55842900	-0.01196700
O	3.77053500	-0.89233100	-0.87778500
C	3.97311300	-2.50204100	0.90013700
H	3.81184700	-2.19544400	1.94412500
H	3.55708700	-3.51383300	0.78667800
H	5.04469200	-2.50737400	0.67191900

N	-3.57676600	1.59996300	-0.52826400
H	-4.39974700	2.13004800	-0.81212200
H	-3.65215100	0.69755800	-0.99650200
C	-3.58548900	1.40126900	0.91190300
H	-2.68029600	0.85404400	1.21932000
H	-3.56106200	2.37573200	1.42488300
H	-4.45921600	0.84310600	1.30147700

TS5b

imaginary frequency = -462.30 cm⁻¹

Si	0.01520200	0.46600000	0.38419400
C	-1.54557400	-0.52915300	0.18409300
C	-1.81530300	-1.04754800	-1.09293100
C	-2.41053200	-0.85527100	1.23919800
C	-2.93514300	-1.85022100	-1.31471900
H	-1.14751300	-0.82649300	-1.93174900
C	-3.51313900	-1.67991200	1.02501100
H	-2.23459400	-0.45246600	2.24038700
C	-3.78177000	-2.17159400	-0.25429400
H	-3.14124100	-2.23201800	-2.31739800
H	-4.17292400	-1.93222800	1.85850500
H	-4.65434700	-2.80709700	-0.42378900
C	1.44601900	-0.65628600	-0.09558300
C	2.55336600	-0.19515100	-0.82535300
C	1.43512600	-2.00132200	0.31295700
C	3.61242700	-1.04821400	-1.13923100
H	2.58758000	0.84588900	-1.15632800
C	2.49403200	-2.85583100	0.00696300
H	0.58389100	-2.39747700	0.87626300
C	3.58438200	-2.37944700	-0.72260000
H	4.46323100	-0.67204100	-1.71263200
H	2.46590300	-3.89830100	0.33327300
H	4.41282700	-3.04836900	-0.96859500
H	-1.55551600	2.06489700	1.39122500
O	0.33797000	1.79945300	-0.56518700
C	-0.27174500	2.97911400	-0.84105700
O	0.22092800	4.01043900	-0.47794100
C	-1.49437300	2.84635800	-1.69611200
H	-1.23247100	2.32682600	-2.63024200
H	-2.24195600	2.23394500	-1.16978900
H	-1.91251500	3.83459500	-1.92019700

N	0.44290300	0.82801500	2.16294100
H	-0.40956300	1.36253000	2.44092700
H	0.50091500	-0.03676500	2.71530900
C	1.65296300	1.65431100	2.37044500
H	1.52628100	2.60474800	1.83744800
H	1.78121900	1.84473400	3.44224700
H	2.53204400	1.12684900	1.98014100

TS6

imaginary frequency = -261.63 cm⁻¹

Si	-0.07322500	0.32721000	-0.37201600
C	-1.70143200	-0.57331700	-0.17593100
C	-1.80687000	-1.96343000	-0.34945500
C	-2.87716300	0.15038300	0.09379100
C	-3.03994000	-2.60969800	-0.24817600
H	-0.91616700	-2.55776500	-0.57134300
C	-4.10973300	-0.49128700	0.20054400
H	-2.83931900	1.23664700	0.22195000
C	-4.19190100	-1.87466300	0.03031100
H	-3.10064000	-3.69165300	-0.38786200
H	-5.01022500	0.08926900	0.41460900
H	-5.15763700	-2.37942900	0.11240500
C	1.39853500	-0.80878600	-0.20395500
C	2.50489900	-0.60556200	-1.04451600
C	1.47300000	-1.82226200	0.76730700
C	3.64883000	-1.39574300	-0.92574600
H	2.46854500	0.18557600	-1.79852400
C	2.61752000	-2.60860400	0.89361400
H	0.62901800	-2.00216400	1.44003600
C	3.70529000	-2.39739900	0.04383500
H	4.49997800	-1.22829000	-1.59033600
H	2.66169100	-3.39009800	1.65605300
H	4.60118200	-3.01597800	0.13968500
O	0.03764800	1.51187700	-1.45386100
C	0.41467200	2.74759700	-0.11516000
O	1.57840500	3.08546400	-0.14219800
C	-0.74021000	3.69668400	-0.31736600
H	-0.58435400	4.23832000	-1.25935500
H	-1.71314900	3.19113000	-0.34906100
H	-0.73694400	4.42406400	0.51021300
N	0.05440800	1.63172300	0.97052100

H	-0.86591400	1.84289000	1.36893400
C	1.03041900	1.52198900	2.06297100
H	1.00403200	2.42743900	2.68382000
H	0.78658200	0.64773800	2.68077900
H	2.03370500	1.40515800	1.63864500

TS7

imaginary frequency = -151.19 cm⁻¹

Si	-0.10133700	-0.03386900	0.81704500
H	-0.02346100	-0.14005700	2.30673300
C	0.07400300	1.76138800	0.29299700
C	1.09110200	2.18813000	-0.57622100
C	-0.84922700	2.71265100	0.76162900
C	1.18099800	3.52778500	-0.96279000
H	1.82479500	1.46200900	-0.94218500
C	-0.76064400	4.04970900	0.37646300
H	-1.65676000	2.40956600	1.43697500
C	0.25691100	4.45875300	-0.48869600
H	1.97848300	3.84612400	-1.63924700
H	-1.48704600	4.77569300	0.75024000
H	0.32784100	5.50622500	-0.79264700
C	-1.76851300	-0.70232200	0.28088100
C	-2.52449000	-1.53210900	1.12418000
C	-2.28506900	-0.39893800	-0.99047100
C	-3.75436300	-2.04788600	0.71100200
H	-2.15274400	-1.78189900	2.12290400
C	-3.51141300	-0.91426400	-1.40901200
H	-1.72392900	0.25318700	-1.66734000
C	-4.24786400	-1.73994800	-0.55703300
H	-4.33007600	-2.69075900	1.38150800
H	-3.89684000	-0.66847200	-2.40164800
H	-5.21090000	-2.14142400	-0.88230400
O	1.05429400	-0.99311500	0.10197000
C	2.48039000	-0.97276600	0.15582600
C	2.98187300	-0.80256900	1.58566400
H	2.81295200	0.24347800	1.88931800
H	2.47493300	-1.46314200	2.30382000
H	4.06488000	-0.98633800	1.61726900
O	3.07056300	-0.41666100	-0.77781500
N	2.68259500	-2.77249400	-0.05410200
H	3.66710100	-2.97327900	0.13306600

H	2.13136400	-3.27798100	0.64166400
C	2.32654600	-3.16587500	-1.41091600
H	1.23910000	-3.09117400	-1.53341600
H	2.80853600	-2.46125400	-2.10264500
H	2.65203600	-4.19111600	-1.63624100

TS9a

imaginary frequency = -241.61 cm⁻¹

Si	-0.18246600	-0.21629300	0.76509300
H	-0.22737000	-0.24996800	2.27753200
C	-0.17796400	1.61601100	0.27235600
C	0.86550000	2.16197200	-0.49182900
C	-1.22383800	2.47091600	0.66170700
C	0.86570100	3.51242300	-0.85318700
H	1.69498000	1.52101000	-0.80601300
C	-1.22999800	3.81956400	0.30492600
H	-2.05708500	2.07777700	1.25496200
C	-0.18198200	4.34337000	-0.45608600
H	1.68796600	3.91765500	-1.44915300
H	-2.05448900	4.46544500	0.61842500
H	-0.18391500	5.39933500	-0.73865900
C	-1.86826200	-0.90706800	0.23915100
C	-2.68498700	-1.62349400	1.12807900
C	-2.33385200	-0.72840300	-1.07568400
C	-3.91720200	-2.14475300	0.72458500
H	-2.35781000	-1.77875600	2.16158500
C	-3.56124100	-1.24736400	-1.48817300
H	-1.72844400	-0.16732000	-1.79566600
C	-4.35685400	-1.95764600	-0.58593700
H	-4.53670100	-2.69732400	1.43594500
H	-3.90227200	-1.09518500	-2.51563800
H	-5.32075300	-2.36222000	-0.90527900
O	1.05297800	-1.04088600	0.13840800
C	3.06260500	-0.72845800	0.14224600
C	3.18978700	-0.22355000	1.55021700
H	2.78105500	0.79341800	1.60292400
H	2.68389500	-0.86759000	2.27885100
H	4.26395900	-0.17624100	1.79488300
O	3.38237200	-0.12514800	-0.84863200
N	3.13164800	-2.25953000	0.08198400
H	3.87366500	-2.59818200	0.70601200

H	2.20874600	-2.51731900	0.46640100
C	3.28299000	-2.80840800	-1.27254500
H	2.42747900	-2.47985400	-1.87167300
H	4.21475500	-2.44027900	-1.71446500
H	3.30011600	-3.90199500	-1.20334100

TS9b

imaginary frequency = -189.83 cm⁻¹

Si	0.69706400	0.01502400	0.91258200
H	0.90530700	-0.21917300	2.37898000
C	1.95820800	-1.04770000	-0.01759700
C	1.98733700	-2.44002400	0.18394300
C	2.88592700	-0.49690100	-0.91663400
C	2.90170300	-3.24935500	-0.49020100
H	1.26782000	-2.89458900	0.87152600
C	3.80331400	-1.30260000	-1.59571100
H	2.89925200	0.58240800	-1.09544600
C	3.81252400	-2.68098100	-1.38354400
H	2.90484300	-4.32901600	-0.31883500
H	4.51442800	-0.85094600	-2.29223400
H	4.52992300	-3.31313900	-1.91314500
C	1.09208800	1.83163200	0.59580500
C	1.75876000	2.60060600	1.56279500
C	0.76445100	2.44931200	-0.62402600
C	2.08918000	3.93655100	1.32475100
H	2.02669100	2.15250800	2.52498000
C	1.09138600	3.78299800	-0.86857700
H	0.23958900	1.88228100	-1.39813000
C	1.75570700	4.52949400	0.10702100
H	2.60695000	4.51635000	2.09311100
H	0.82682100	4.24396700	-1.82366400
H	2.01203200	5.57487400	-0.08277200
O	-0.85161100	-0.32109000	0.46802100
C	-1.70804300	-1.83600400	1.34222700
C	-2.70089500	-1.04878800	2.15632200
H	-2.16220600	-0.50722700	2.94356600
H	-3.28360800	-0.34074700	1.55505200
H	-3.39042500	-1.76298800	2.63490900
O	-0.85962800	-2.55619400	1.82205100
N	-2.31674300	-2.27734400	0.01474700
H	-3.10695500	-2.89191000	0.24951900

H	-2.73081800	-1.44436900	-0.47980800
C	-1.39333000	-2.98468500	-0.88417800
H	-0.59387400	-2.29140100	-1.16500700
H	-0.97357600	-3.85414400	-0.36727000
H	-1.94977000	-3.30507700	-1.77281500
C	-4.18152200	2.03293200	-1.76606300
C	-3.31935400	0.98037800	-1.13116700
O	-3.50689500	-0.21901500	-1.32520800
O	-2.37859200	1.44971100	-0.36944800
H	-1.73759900	0.69412500	-0.00547800
H	-3.55991200	2.68198700	-2.40059400
H	-4.62370900	2.66668100	-0.98340900
H	-4.97374100	1.57213500	-2.36672900

TS9c

imaginary frequency = -263.75 cm⁻¹

Si	0.27559800	0.01292300	-1.09121500
H	0.20894000	0.12739100	-2.58224200
C	-0.37820000	1.62863400	-0.35933300
C	-1.41515100	2.33685000	-0.98795600
C	0.10664700	2.12237500	0.86307400
C	-1.94968300	3.49279400	-0.41861200
H	-1.83045400	1.95544400	-1.92386100
C	-0.42913100	3.27417500	1.44384400
H	0.91873400	1.60035000	1.37949500
C	-1.45932700	3.96219200	0.80190400
H	-2.75752300	4.02811900	-0.92456300
H	-0.03993600	3.63689300	2.39878000
H	-1.88065400	4.86474400	1.25219700
C	2.10798600	-0.11360200	-0.62101200
C	2.97756100	0.97539500	-0.80656500
C	2.64957600	-1.29544400	-0.09053800
C	4.32967500	0.89158700	-0.47276300
H	2.59316900	1.91650500	-1.21431800
C	4.00144400	-1.38721000	0.24940100
H	2.00305500	-2.16491000	0.05955300
C	4.84478000	-0.29258800	0.05884300
H	4.98452500	1.75337100	-0.62552200
H	4.39808500	-2.31797500	0.66336500
H	5.90287400	-0.36072500	0.32417300
O	-0.42932800	-1.34860800	-0.49129200

C	-2.07475200	-1.58056900	-0.96359000
C	-1.96595200	-2.98794900	-1.54927600
H	-1.32499000	-2.95751200	-2.44054000
H	-1.55505000	-3.71605700	-0.83440400
H	-2.96879200	-3.32554200	-1.86036000
O	-2.39149100	-0.63009900	-1.71740300
N	-2.71333600	-1.66509100	0.37174900
H	-3.52094300	-2.28072800	0.27299500
H	-1.54503000	-2.36371200	1.54226500
C	-3.14488400	-0.38648200	0.91173500
H	-2.26671100	0.22982100	1.15525300
H	-3.76933400	0.18942500	0.20800700
H	-3.70960700	-0.55631500	1.84037300
N	-0.53187700	-2.47943600	1.83993300
H	-0.11379600	-2.14249200	0.93090400
H	-0.31281100	-3.46375900	2.00623700
C	-0.16301000	-1.61126900	2.96129600
H	-0.41105100	-0.57493700	2.70045400
H	-0.71801200	-1.90262700	3.86130300
H	0.91451300	-1.68768800	3.15252900

TS10

imaginary frequency = -230.77 cm⁻¹

C	-1.40111400	-0.30223400	0.68306400
O	-1.82722800	0.57961600	-0.09142200
N	-1.88618600	-2.00403100	-0.35527100
H	-2.90733900	-1.92526200	-0.41455500
C	-1.42806400	-3.29482300	0.12303900
H	-1.90406300	-3.52253100	1.08751600
H	-1.65631900	-4.11971600	-0.57271900
H	-3.36470600	0.81362600	-0.18645800
H	-1.51849200	-1.79772800	-1.28438700
O	-4.71695300	-1.13865500	-0.39428200
C	-5.12432100	0.01016400	-0.36071600
O	-4.34772000	1.06172000	-0.24783900
C	-6.58319500	0.36361600	-0.44032800
H	-6.75911800	1.02146700	-1.30427800
H	-7.19126800	-0.54350700	-0.53176900
H	-6.87663900	0.92149500	0.46125800
O	-0.06484200	-0.49156400	0.76986400
Si	1.00850400	-0.00063800	-0.45842600

H	0.40126900	-0.31687100	-1.77995700
C	2.52048000	-1.07823200	-0.22589500
C	2.70283800	-2.22573100	-1.01497500
C	3.47586100	-0.79235500	0.76440200
C	3.80086900	-3.06503800	-0.81913200
H	1.97862300	-2.47266500	-1.79757900
C	4.57331800	-1.62897100	0.96433600
H	3.36592200	0.09861600	1.39028500
C	4.73635100	-2.76696100	0.17189000
H	3.92776200	-3.95313900	-1.44299000
H	5.30603300	-1.39257700	1.73978700
H	5.59736700	-3.42199700	0.32635900
C	1.44582500	1.80995500	-0.25944000
C	2.65023700	2.29520300	-0.79812600
C	0.60576300	2.71290500	0.41229700
C	3.00275800	3.63913300	-0.67411400
H	3.33194500	1.61590400	-1.31979700
C	0.95851200	4.05653200	0.54258900
H	-0.34349100	2.36485500	0.82661600
C	2.15671900	4.52150900	-0.00084400
H	3.94273300	3.99781500	-1.10054300
H	0.29328500	4.74453800	1.07015700
H	2.43254500	5.57408900	0.10065500
C	-2.11296300	-0.64550600	1.96480500
H	-1.98183100	0.20314000	2.65480300
H	-3.18508400	-0.78867600	1.78221600
H	-1.69142300	-1.54266800	2.43415700
H	-0.33876600	-3.26498000	0.27841100

TS11

imaginary frequency = -317.64 cm⁻¹

Si	0.71270100	-0.04783700	-0.74934400
O	-0.28957600	-1.05231100	0.08506000
C	-1.08544600	-2.62353300	-0.62168200
O	-2.18892700	-2.11225000	-1.13248100
C	-1.16593900	-3.33813400	0.69769800
H	-1.82102500	-2.79258700	1.38658100
H	-0.17980700	-3.45086100	1.16029600
H	-1.59932800	-4.33454400	0.51850500
N	-0.25091000	-3.10993600	-1.55583200
H	-0.33058800	-2.66232700	-2.46378800

C	1.01496100	-3.73556200	-1.24559200
H	1.51704000	-3.98907200	-2.18708100
H	0.87148800	-4.66558600	-0.67718300
H	1.67754900	-3.06846800	-0.66664900
H	-2.69780300	-1.62328300	-0.42248600
C	-2.97881300	-0.07764800	1.58142300
O	-3.47090600	-0.74299800	0.66831700
C	-3.83236900	0.76934500	2.47763400
H	-4.88063500	0.45364500	2.42339300
H	-3.75501300	1.81325300	2.13399300
H	-3.46766700	0.73051800	3.51260700
O	-1.70928900	-0.02319900	1.83689700
H	-1.11622900	-0.49787600	1.10093600
H	1.00656700	-0.62921500	-2.10085900
C	2.37208700	0.16938000	0.11232800
C	3.55744600	-0.32930600	-0.45023000
C	2.45171700	0.80923900	1.36206300
C	4.78202100	-0.19502100	0.20852600
H	3.52931100	-0.83255100	-1.42195600
C	3.67081300	0.94606200	2.02492200
H	1.54631000	1.21153300	1.82812900
C	4.83913200	0.44281000	1.44752500
H	5.69373700	-0.58983000	-0.24689000
H	3.71234000	1.44738200	2.99519900
H	5.79556800	0.54996800	1.96544600
C	-0.13015700	1.62926300	-0.94356300
C	0.58111500	2.83899600	-0.98059600
C	-1.53019400	1.68363300	-1.05072300
C	-0.08082900	4.06067400	-1.11995500
H	1.67219800	2.83430300	-0.89262300
C	-2.19771200	2.90064500	-1.18879700
H	-2.11126300	0.75765300	-1.02171200
C	-1.47216700	4.09309600	-1.22210000
H	0.49129000	4.99165000	-1.14383700
H	-3.28778100	2.91923800	-1.26738600
H	-1.99211900	5.04875100	-1.32663600

TS11'

imaginary frequency = -305.85 cm-1

Si	-0.33974000	-0.27220500	-0.88293900
O	0.94649100	-0.37954600	0.14289900

C	1.43675800	0.81438200	1.49481000
O	2.19377800	1.65206800	0.80993000
C	2.10949400	-0.21414700	2.36213000
H	2.96976500	-0.65095000	1.84276900
H	1.42226000	-1.01755800	2.64833200
H	2.47098300	0.29306800	3.27014000
N	0.32104700	1.40115400	1.97264900
H	-0.01967600	2.16381900	1.39482600
C	-0.67064100	0.70402300	2.75908300
H	-1.48223500	1.40396600	2.99239500
H	-0.24795700	0.34974600	3.71006900
H	-1.10133900	-0.15955600	2.22262500
H	2.92891700	1.15109900	0.35704900
C	4.01598100	-0.81607500	-0.85410500
O	4.08721800	0.33061500	-0.41639500
C	5.18535400	-1.48820900	-1.51094000
H	6.06087800	-0.82936800	-1.50784000
H	4.92106700	-1.75468100	-2.54505600
H	5.41633600	-2.42343100	-0.98034700
O	2.94734600	-1.55281800	-0.78825500
H	2.12845000	-1.04998600	-0.37466900
H	0.14748900	-0.45290900	-2.29089000
C	-1.18355000	1.41360000	-0.81344000
C	-0.56151500	2.52163100	-1.41419600
C	-2.38484700	1.62819000	-0.11902100
C	-1.10951800	3.80040400	-1.31100100
H	0.37507200	2.39034800	-1.96541300
C	-2.93892100	2.90506600	-0.01312500
H	-2.89540200	0.78769800	0.36021500
C	-2.29963500	3.99389700	-0.60706000
H	-0.60829200	4.64959600	-1.78221600
H	-3.87248300	3.05091000	0.53608200
H	-2.73032500	4.99492600	-0.52417300
C	-1.58724100	-1.62725700	-0.48508200
C	-2.80731000	-1.73901700	-1.17280800
C	-1.30284600	-2.56894500	0.51576300
C	-3.71421100	-2.75445600	-0.86837400
H	-3.06111800	-1.02010600	-1.95895600
C	-2.20680400	-3.58712300	0.82578400
H	-0.35601100	-2.49995500	1.05929800
C	-3.41455000	-3.68026500	0.13366000

H	-4.65916400	-2.82460000	-1.41302700
H	-1.96815200	-4.31047800	1.60965500
H	-4.12468600	-4.47555900	0.37384000

TS2-1a-2a-3b

imaginary frequency = -1054.20 cm⁻¹

Si	-1.46671900	-0.12849800	-0.56577100
H	-0.43081000	1.42255400	-0.39659900
C	-0.27845600	-0.86857600	0.69744000
C	-0.17497600	-0.33610600	1.99121800
C	0.54871100	-1.95023300	0.35940900
C	0.72445200	-0.86379600	2.91857100
H	-0.79945000	0.51469800	2.28194900
C	1.46421600	-2.47060800	1.27641600
H	0.48722300	-2.39608200	-0.63801500
C	1.55267500	-1.92850400	2.55946400
H	0.78569000	-0.43703400	3.92284000
H	2.10861800	-3.30551100	0.98947000
H	2.26631800	-2.33655000	3.27949100
C	-2.85699200	0.98586700	0.07321600
C	-2.98305400	2.33330600	-0.29865400
C	-3.82891600	0.44832800	0.93460600
C	-4.04183600	3.11559600	0.16341200
H	-2.23871700	2.78499100	-0.96133200
C	-4.87733800	1.23209600	1.41892300
H	-3.77039200	-0.60186300	1.23391300
C	-4.98929200	2.56700900	1.02918800
H	-4.12519600	4.15952800	-0.14934900
H	-5.61431900	0.79562900	2.09782900
H	-5.81405700	3.18045000	1.40053600
O	-2.41840300	-1.63168500	-0.75678900
C	-3.38546000	-1.98831400	-1.58053400
O	-3.93781600	-3.06145200	-1.46703100
H	-1.00359800	-0.02739900	-1.97983700
N	1.77040600	1.03290400	-1.03702800
H	0.48828400	1.27338700	-0.68885200
H	2.04023000	1.68505700	-1.77734800
H	1.83251900	0.09137600	-1.43149000
C	2.64669900	1.16578100	0.13560400
H	2.53833200	2.19196100	0.51444900
H	2.26762000	0.48266000	0.90804800

C	4.09283700	0.85877800	-0.16892500
C	4.93465100	1.84152600	-0.70452000
C	4.60094400	-0.42900700	0.03704000
C	6.25751600	1.54248800	-1.02907600
H	4.54871100	2.85235900	-0.86591900
C	5.92440800	-0.73054400	-0.28563800
H	3.95021900	-1.20005400	0.45921500
C	6.75511400	0.25475800	-0.82049900
H	6.90522600	2.31880700	-1.44371700
H	6.30903300	-1.73915300	-0.11592400
H	7.79225500	0.02034600	-1.07215100
C	-3.75432800	-1.00536600	-2.66874700
H	-4.06014400	-0.04134000	-2.23401900
H	-2.88600100	-0.81342700	-3.31758100
H	-4.57605900	-1.40852300	-3.27254800

TS2-1a-2a-3c

imaginary frequency = -953.10 cm⁻¹

Si	1.68538300	0.13238800	-0.59069200
H	0.20886800	-0.98036300	-0.29458600
C	0.76710800	1.39911700	0.46915200
C	0.05588400	1.01170600	1.61483500
C	0.75893100	2.75840500	0.11897100
C	-0.65190400	1.94097900	2.37722000
H	0.03927000	-0.04129300	1.91241700
C	0.03516300	3.69076300	0.86408800
H	1.32489900	3.09640000	-0.75267600
C	-0.67384800	3.28339400	1.99485000
H	-1.19638900	1.61524300	3.26711400
H	0.02862500	4.74146100	0.56309800
H	-1.23850800	4.01238300	2.58153000
C	2.60798600	-1.25105400	0.31183900
C	2.35759900	-2.61189000	0.07909600
C	3.61245100	-0.91424300	1.23443600
C	3.08717500	-3.60347600	0.73550700
H	1.57593300	-2.90753900	-0.62755500
C	4.33104100	-1.90163700	1.91051300
H	3.84454300	0.13687800	1.42905800
C	4.07287500	-3.24941000	1.65840100
H	2.88192400	-4.65725300	0.53066000
H	5.10054900	-1.61680300	2.63252200

H	4.63945700	-4.02426800	2.18087000
O	3.07080500	1.20827900	-0.92069100
C	4.12773300	1.12028700	-1.70645400
O	4.92265100	2.03188000	-1.78385800
H	1.27414000	-0.07361800	-2.00901400
N	-1.97177300	-0.40426900	-0.86944100
H	-0.66687900	-0.70495800	-0.54930900
H	-2.16082600	-1.02966500	-1.65671800
C	-2.78090300	-0.82055100	0.28522400
H	-2.44177100	-1.82825800	0.56930000
H	-2.54082300	-0.14074500	1.11536900
C	-4.26751400	-0.82166800	0.01896900
C	-4.85513000	-1.87308300	-0.69658500
C	-5.07319100	0.24159300	0.44136200
C	-6.21898200	-1.86093200	-0.98498200
H	-4.23523700	-2.71157400	-1.02775000
C	-6.43921000	0.25591900	0.15520300
H	-4.62356600	1.06647500	1.00114800
C	-7.01444800	-0.79495200	-0.55940100
H	-6.66535100	-2.68927600	-1.54051500
H	-7.05657100	1.09221200	0.49209900
H	-8.08390500	-0.78563900	-0.78325600
C	4.29328400	-0.16120700	-2.49106800
H	4.40935400	-1.01370000	-1.80431200
H	3.40353600	-0.35607600	-3.10889000
H	5.17738800	-0.09242100	-3.13606800
C	-2.15783900	0.98189400	-1.29499600
H	-3.18284800	1.16957600	-1.65284000
H	-1.94896800	1.65228200	-0.44997900
H	-1.45302100	1.20599400	-2.10665200

TS2-1a-2b-3b

imaginary frequency = -1020.05 cm⁻¹

Si	-0.25780700	-0.06932600	-0.07120600
H	0.83098800	1.40631100	-0.43337500
C	1.08799700	-0.57149600	1.14786300
C	1.40217900	0.23843700	2.24938800
C	1.82622000	-1.74968800	0.96031100
C	2.42053500	-0.11411000	3.13591200
H	0.85116600	1.16937900	2.41684600
C	2.85800800	-2.09884500	1.83386900

H	1.60196500	-2.40923800	0.11640400
C	3.15641400	-1.28133600	2.92496300
H	2.64663400	0.52878200	3.99025900
H	3.42924700	-3.01490400	1.66354100
H	3.96205800	-1.55461400	3.61083600
C	-1.50580100	1.25194700	0.45677700
C	-1.64274200	2.47578400	-0.21661000
C	-2.36488200	0.99757100	1.53942600
C	-2.60923600	3.40691300	0.16515600
H	-0.98405800	2.70880600	-1.05857000
C	-3.31801600	1.93474300	1.94054800
H	-2.29545000	0.05002600	2.08070400
C	-3.44686100	3.13939100	1.24928100
H	-2.70651500	4.34738500	-0.38284500
H	-3.96942300	1.71823100	2.79082600
H	-4.19997700	3.87002800	1.55462300
O	-1.27983200	-1.50996800	0.25347500
C	-2.44490600	-1.91321500	-0.19726700
O	-3.03999400	-2.83210700	0.32223700
H	-0.01606000	-0.34463600	-1.51623300
N	2.89040400	0.72386600	-1.28081400
H	1.67417000	1.12920400	-0.81123800
H	3.05670000	1.16365300	-2.18896800
H	2.86793200	-0.28632700	-1.43883500
C	3.94118500	1.07834300	-0.31667000
H	3.92056200	2.17027600	-0.19171000
H	3.66870200	0.62700500	0.64735800
C	-3.01043400	-1.21874000	-1.43911200
H	-2.88811200	-1.94367400	-2.26113500
H	-2.42577500	-0.33031500	-1.70837000
C	-4.46497600	-0.84729200	-1.28874300
C	-4.83216600	0.48373600	-1.05885900
C	-5.47093400	-1.82049300	-1.34725600
C	-6.17115300	0.83663500	-0.88466600
H	-4.05739400	1.25351400	-1.01124300
C	-6.80969900	-1.47059200	-1.17511700
H	-5.19753000	-2.86295400	-1.52403300
C	-7.16496400	-0.14033400	-0.94132000
H	-6.43622200	1.88149600	-0.70413000
H	-7.58252900	-2.24185200	-1.22581000
H	-8.21433600	0.13292700	-0.80603600

C	5.31451000	0.61633300	-0.73954400
C	6.10210300	1.39988400	-1.59201100
C	5.80094200	-0.62800900	-0.32165200
C	7.35097000	0.94850200	-2.01839500
H	5.73332100	2.37556200	-1.92167500
C	7.04988600	-1.08172500	-0.74643800
H	5.19238400	-1.24343900	0.34714200
C	7.82732400	-0.29419400	-1.59656600
H	7.95791100	1.57126900	-2.68010700
H	7.41881000	-2.05340100	-0.40917100
H	8.80690400	-0.64728400	-1.92779700

TS2-1a-2c-3b

imaginary frequency = -1047.49 cm⁻¹

Si	0.63845600	-0.00239300	-0.31505800
H	-0.37737600	-1.30213400	0.56712300
C	-0.75688200	1.20344900	0.09107900
C	-1.27296700	1.30580100	1.39190000
C	-1.30075100	2.03433300	-0.90126400
C	-2.29364800	2.20753400	1.69613500
H	-0.87617000	0.66511300	2.18560600
C	-2.33780400	2.92197700	-0.60885200
H	-0.90846600	1.99402500	-1.92124200
C	-2.83311600	3.01360100	0.69279100
H	-2.67475700	2.27501400	2.71809500
H	-2.75597600	3.55042100	-1.39915900
H	-3.64079900	3.71210500	0.92496800
C	1.88591300	-0.37662700	1.04793200
C	2.43634300	-1.65597300	1.21546000
C	2.35291100	0.66047700	1.87000300
C	3.43884100	-1.88926200	2.15603500
H	2.08780100	-2.48556300	0.59238000
C	3.34316900	0.42799000	2.82677000
H	1.95036400	1.67241000	1.75983700
C	3.89442200	-0.84570600	2.96492300
H	3.86758900	-2.88921200	2.25945300
H	3.69161400	1.24773800	3.46005800
H	4.67874300	-1.02682200	3.70404000
O	1.62158400	1.20532900	-1.22954400
C	2.90614500	1.47785800	-1.26840500
O	3.33017200	2.61418200	-1.26190800

H	0.44774000	-0.93739500	-1.45628500
N	-2.47606400	-1.48721300	-0.41829400
H	-1.23863000	-1.41916100	0.13080800
H	-2.58016100	-2.30488900	-1.02273300
H	-2.57844200	-0.65988500	-1.01128500
C	-3.47295900	-1.48188100	0.66076500
H	-3.41117500	-2.44786300	1.17981100
H	-3.17330300	-0.69989600	1.37401000
C	-4.87784800	-1.22333100	0.17294800
C	-5.80234800	-2.26370300	0.03476400
C	-5.26098400	0.07666300	-0.18381600
C	-7.08715700	-2.01102000	-0.44944600
H	-5.51433000	-3.28151500	0.31231900
C	-6.54160700	0.33066300	-0.67116800
H	-4.54450900	0.89667900	-0.07413800
C	-7.45878200	-0.71417600	-0.80445900
H	-7.80154600	-2.83189800	-0.54899100
H	-6.82765000	1.34949700	-0.94348600
H	-8.46460600	-0.51590900	-1.18259200
C	3.84662500	0.30294300	-1.33651200
C	5.07015800	0.37905100	-0.66265300
C	3.52180300	-0.85545300	-2.05002100
C	5.94344200	-0.70648300	-0.67065200
H	5.32094700	1.28965000	-0.11433500
C	4.40818100	-1.93124800	-2.07995800
H	2.57278500	-0.91599000	-2.58689900
C	5.61381700	-1.86305600	-1.38056100
H	6.88649700	-0.65073500	-0.12194000
H	4.15344300	-2.82978600	-2.64675300
H	6.30087900	-2.71260900	-1.39060800

TS2-1a-2d-3b

imaginary frequency = -987.40 cm⁻¹

Si	-0.25177600	-0.70969100	-0.21388500
H	0.48931400	0.35742000	1.12476100
C	1.37164200	-1.66208600	-0.16968500
C	1.79289200	-2.31049200	1.00069100
C	2.20732800	-1.71513500	-1.29529800
C	3.01034000	-2.99075200	1.04842800
H	1.16660500	-2.27807300	1.89788400
C	3.43434900	-2.37945400	-1.24826100

H	1.90434400	-1.22724800	-2.22656000
C	3.83757700	-3.01965400	-0.07540400
H	3.31853900	-3.49328600	1.96860400
H	4.07697000	-2.40049900	-2.13205100
H	4.79654900	-3.54228600	-0.03795300
C	-1.55271900	-1.10079400	1.09880800
C	-2.02940700	-0.13226400	1.99533200
C	-2.10932100	-2.38918300	1.16347700
C	-3.03949500	-0.42924700	2.91038100
H	-1.60785100	0.87717800	1.97916500
C	-3.10176600	-2.69937600	2.09428100
H	-1.77018700	-3.16645100	0.47282800
C	-3.57508900	-1.71691300	2.96443800
H	-3.40710900	0.34646400	3.58677700
H	-3.51412200	-3.71074000	2.13308200
H	-4.36086100	-1.95478700	3.68576600
O	-0.93888100	-1.71084400	-1.56462900
C	-2.05183300	-1.58120100	-2.23568600
O	-2.36085600	-2.29993900	-3.16124100
H	-0.29129100	0.58081200	-0.95573500
N	2.40169800	1.42484900	0.30661800
H	1.25445600	0.81437500	0.79098900
H	2.30984000	2.43761100	0.41434100
H	2.47333800	1.23911900	-0.69642200
C	3.58816800	0.92222500	1.01230200
H	3.46457800	1.15746000	2.07895900
H	3.59344000	-0.17185400	0.91058100
C	-2.94135700	-0.49956400	-1.80082400
C	-3.68618800	0.37632900	-1.41070500
C	-4.54621000	1.40944900	-0.91142200
C	-5.87608900	1.50741900	-1.35495500
C	-4.05970500	2.32743200	0.03565700
C	-6.70441400	2.50678500	-0.85185700
H	-6.25301000	0.79496400	-2.09156700
C	-4.89553300	3.32362400	0.53177600
H	-3.02565200	2.25178800	0.37734200
C	-6.21691200	3.41437300	0.09033700
H	-7.73783300	2.57823900	-1.19791600
H	-4.51317000	4.03404600	1.26795100
H	-6.87035900	4.19713500	0.48241100
C	4.87985600	1.49991900	0.48558400

C	5.35000100	2.73692800	0.94388300
C	5.60146300	0.82759200	-0.50767900
C	6.51748700	3.29099300	0.41944500
H	4.79572400	3.26925600	1.72247500
C	6.77002800	1.37925300	-1.03364800
H	5.24256600	-0.14092700	-0.86741200
C	7.22985000	2.61303900	-0.57161300
H	6.87547600	4.25550200	0.78783300
H	7.32522000	0.84173800	-1.80623300
H	8.14570400	3.04557300	-0.98157600

TS2-1a-2e-3b

imaginary frequency = -1046.49 cm⁻¹

Si	-0.03564900	-0.39260100	-0.11312600
H	0.89881300	0.69460700	1.09428700
C	1.50660200	-1.47362000	-0.10167300
C	1.93393900	-2.10740600	1.07477100
C	2.27716900	-1.64256000	-1.26193300
C	3.09309600	-2.88401800	1.09497900
H	1.35980300	-1.98669500	1.99891400
C	3.44812900	-2.40295200	-1.24334500
H	1.96882500	-1.17005200	-2.19957800
C	3.85784700	-3.02664600	-0.06396100
H	3.40587900	-3.37255000	2.02118000
H	4.04115100	-2.51195200	-2.15488300
H	4.77271900	-3.62404200	-0.04812000
C	-1.26328900	-0.55224600	1.31454200
C	-1.69616200	0.55971700	2.05291800
C	-1.83091100	-1.80239700	1.60935500
C	-2.67304000	0.43425200	3.04079800
H	-1.26893500	1.54680900	1.84985100
C	-2.79018500	-1.93856400	2.61407200
H	-1.52765000	-2.68775200	1.04281100
C	-3.21956500	-0.81826000	3.32608100
H	-3.00783500	1.31659500	3.59191900
H	-3.21183700	-2.92245500	2.83441100
H	-3.98056800	-0.92064200	4.10375100
O	-0.90508300	-1.40514000	-1.31660200
C	-2.13464100	-1.38643500	-1.78600700
O	-2.54738700	-2.26433800	-2.51780000

H	-0.01425000	0.85538900	-0.92901100	C	0.91569200	-0.94002700	1.66699400
N	2.85879000	1.51334900	0.14220400	C	1.43216300	1.52253500	2.86527600
H	1.70506000	1.06127300	0.69175700	H	-0.07902800	2.31617800	1.55518600
H	2.86720300	2.53518900	0.18339900	C	1.89548200	-0.83778200	2.65586700
H	2.87636000	1.25501600	-0.84727400	H	0.72212200	-1.91657900	1.21247200
C	4.01170500	0.94052700	0.85121400	C	2.15484600	0.39475200	3.25731700
H	3.93572300	1.24322500	1.90502500	H	1.62813500	2.48920800	3.33566600
H	3.91169500	-0.15296300	0.80991600	H	2.45716000	-1.72450100	2.95996600
C	-2.99546400	-0.24171500	-1.35826700	H	2.92041500	0.47577100	4.03282300
C	-4.32691500	-0.27959000	-1.51225100	C	-2.33024000	1.44016100	-0.35069400
H	-2.51431700	0.61736100	-0.88423100	C	-2.48334000	2.11937300	-1.56900100
C	5.33758400	1.36640800	0.26901700	C	-3.16196100	1.80536900	0.72092300
C	5.97564000	2.53000600	0.71507800	C	-3.43965900	3.12359600	-1.71801900
C	5.92637900	0.62363100	-0.76148300	H	-1.84573500	1.86230900	-2.42026000
C	7.17821800	2.94395000	0.14195800	C	-4.10530200	2.82465100	0.58290200
H	5.52619100	3.11495400	1.52273100	H	-3.07811500	1.28605600	1.67965700
C	7.12848100	1.03546500	-1.33651000	C	-4.24898500	3.48252100	-0.63878600
H	5.43558200	-0.28909800	-1.11147300	H	-3.55015300	3.63271400	-2.67865300
C	7.75667600	2.19756000	-0.88595800	H	-4.73514200	3.10117500	1.43206500
H	7.66853700	3.85187100	0.50163200	H	-4.99266200	4.27541500	-0.75060200
H	7.57849200	0.44449500	-2.13786400	O	-2.17786500	-1.04783200	0.83558400
H	8.69954000	2.51999800	-1.33430100	C	-3.20584000	-1.80534600	0.65148100
C	-5.28362300	0.74376500	-1.06293700	O	-3.96709400	-2.18137800	1.50612000
C	-6.60679700	0.69000100	-1.52872500	H	-0.78906100	-0.91016400	-1.22149900
C	-4.92787800	1.76872700	-0.16862600	N	2.13891500	0.17390400	-1.41093900
C	-7.54373200	1.64321100	-1.13259600	H	0.85470600	0.76215600	-1.25672700
H	-6.89902700	-0.10968700	-2.21454100	H	2.36781100	0.12169700	-2.40600000
C	-5.86482700	2.71724400	0.23043900	H	2.11333600	-0.78701400	-1.06260500
H	-3.91318400	1.81429300	0.23423800	C	3.13646700	0.96435600	-0.67888400
C	-7.17486300	2.66046900	-0.25254100	H	3.12467600	1.98167300	-1.09570800
H	-8.56767400	1.58840300	-1.50966500	H	2.80428700	1.03021000	0.36666700
H	-5.57388500	3.50412200	0.93031200	C	4.52726400	0.38018300	-0.74610600
H	-7.90837600	3.40586800	0.06368600	C	5.36183700	0.64636000	-1.83875600
H	-4.75413500	-1.15392200	-2.01579300	C	4.98480400	-0.47790600	0.26075000

TS2-1a-2f-3b

imaginary frequency = -903.40 cm⁻¹

Si	-1.07692700	0.05023400	-0.12774100
H	0.03081900	1.17209900	-1.11679600
C	0.19190400	0.18737100	1.25061500
C	0.46445600	1.41815400	1.86526600

H	5.01546900	1.31831700	-2.62950400
C	6.25047100	-1.05949200	0.17837500
H	4.34035200	-0.68845900	1.11906000
C	7.07402400	-0.78930900	-0.91519600
H	7.26903400	0.28496000	-2.78098000
H	6.59588000	-1.72492600	0.97334800

H	8.06603000	-1.24278200	-0.98034900
C	-3.41591900	-2.29920800	-0.80582500
F	-4.53748700	-2.99432900	-0.92435300
F	-3.47568000	-1.27626800	-1.66648300
F	-2.40095800	-3.08492700	-1.18219600

TS2-1a-2b-3d

imaginary frequency = -1048.40 cm⁻¹

Si	0.22277200	-0.01484900	-0.30726000
H	1.18804200	1.39249700	-0.73366900
C	1.68465600	-0.58252900	0.76086600
C	2.53839600	0.35136700	1.37032100
C	1.95372600	-1.94495900	0.97051700
C	3.61838100	-0.05302600	2.15456300
H	2.36422300	1.42148500	1.22330000
C	3.04616300	-2.35804500	1.73522000
H	1.29348300	-2.69647900	0.53240100
C	3.88029500	-1.41246800	2.33161400
H	4.26399700	0.69531100	2.62102000
H	3.24339900	-3.42467400	1.87035600
H	4.73421600	-1.73346800	2.93352400
C	-0.99008900	1.26035000	0.40922100
C	-1.19906000	2.51033400	-0.19354800
C	-1.72766300	0.96018900	1.56687400
C	-2.11934400	3.42187200	0.32621900
H	-0.63286800	2.78090200	-1.09020800
C	-2.63105600	1.87683300	2.10673200
H	-1.60024000	-0.00843500	2.05811800
C	-2.83460200	3.10801400	1.48297500
H	-2.27471000	4.38300500	-0.17042500
H	-3.18671500	1.62381700	3.01321200
H	-3.55028600	3.82242800	1.89740600
O	-0.76776100	-1.47869400	0.10443900
C	-1.96162500	-1.89807400	-0.22703500
O	-2.46391600	-2.86900300	0.30044700
H	0.23616900	-0.29836600	-1.77697000
N	2.85631000	1.13218800	-2.30036200
H	1.91040200	1.26733500	-1.42503700
C	-2.70055800	-1.15448200	-1.34425500
H	-2.16154500	-0.25097100	-1.65372200
H	-2.69712700	-1.84262400	-2.20598100

C	-4.12080900	-0.79997000	-0.97672300
C	-4.47017600	0.52921500	-0.71150900
C	-5.11025200	-1.78679700	-0.87260500
C	-5.77403400	0.86741000	-0.34563700
H	-3.70770700	1.30942500	-0.78592700
C	-6.41359900	-1.45176800	-0.50803600
H	-4.84919000	-2.82788100	-1.07292100
C	-6.75054800	-0.12283600	-0.24136600
H	-6.02460700	1.91117600	-0.13979400
H	-7.17343300	-2.23394400	-0.43326300
H	-7.77237900	0.13904000	0.04402900
H	2.94073100	2.04990900	-2.74451600
H	2.52033600	0.46869800	-3.00242000
C	4.07706500	0.70766400	-1.68616700
C	4.36100400	-0.65491400	-1.58192700
C	4.93331300	1.65509700	-1.12454300
C	5.51075800	-1.06747500	-0.91240100
H	3.67684100	-1.38742200	-2.01727100
C	6.08266800	1.23247500	-0.45776200
H	4.69764200	2.71881300	-1.20828200
C	6.37449000	-0.12706700	-0.34798100
H	5.73020300	-2.13425000	-0.82902500
H	6.75320400	1.97502500	-0.01930400
H	7.27335900	-0.45466900	0.17868800

TS2-1a-2a-3d

imaginary frequency = -1058.66 cm⁻¹

Si	0.98635100	0.19032200	-0.57480500
H	0.08302000	-1.30222700	-0.81352400
C	-0.41975600	0.74455600	0.57236600
C	-1.09202000	-0.18161900	1.38612200
C	-0.81999400	2.08836900	0.64568800
C	-2.12115900	0.21327100	2.24063100
H	-0.81231700	-1.23902700	1.34864200
C	-1.86665500	2.48773600	1.47892100
H	-0.29938200	2.83824000	0.04547900
C	-2.51750700	1.55103000	2.28185600
H	-2.62330700	-0.52716600	2.86837100
H	-2.17048400	3.53743700	1.50611200
H	-3.33362400	1.86219200	2.93889600
C	2.32741100	-0.94968000	0.14070000

C	2.57981200	-2.22752900	-0.38130600
C	3.11539100	-0.51586900	1.22043300
C	3.58758500	-3.03919900	0.14146700
H	1.97664100	-2.60085900	-1.21491800
C	4.10783800	-1.33220800	1.76521200
H	2.95514800	0.47974000	1.64354300
C	4.35075900	-2.59454400	1.22205500
H	3.77324400	-4.02538700	-0.29166600
H	4.69933100	-0.97834600	2.61352200
H	5.13357900	-3.23168400	1.64121400
O	1.89734100	1.73778800	-0.36206700
C	2.96481600	2.25061800	-0.93381400
O	3.39258500	3.33817000	-0.60446500
H	0.83317200	0.34898400	-2.05611300
N	-1.76154700	-1.20575000	-2.18631200
H	-0.72938500	-1.24903200	-1.43175200
H	-1.78012400	-2.11123100	-2.66308500
H	-1.59757700	-0.48087800	-2.88888500
C	3.62867500	1.42776800	-2.01670900
H	3.95953300	0.45864300	-1.61303700
H	2.91796100	1.21749300	-2.83044900
H	4.49364200	1.96853400	-2.41917900
C	-2.94869100	-0.96681100	-1.42200600
C	-3.53292000	-2.01962000	-0.71731300
C	-3.46406400	0.32591800	-1.32448400
C	-4.64519200	-1.77329900	0.08624900
H	-3.11593300	-3.02626400	-0.79851500
C	-4.57496600	0.56243600	-0.51750400
H	-2.98954700	1.14261400	-1.87379900
C	-5.16824100	-0.48413700	0.19013200
H	-5.10385400	-2.59769500	0.63685000
H	-4.97641400	1.57524200	-0.43954500
H	-6.03754600	-0.29436300	0.82337100

TS11-1a-2a-3b

imaginary frequency = -319.76 cm⁻¹

Si	1.79096000	0.84662300	-0.27365600
O	1.19047200	-0.67083500	-0.49872900
C	-0.06686800	-1.59244200	0.56020900
O	0.74209500	-2.26780800	1.34996100
C	-0.70962000	-2.30982400	-0.59366700

H	0.03057100	-2.91905200	-1.12402100
H	-1.17079600	-1.61274600	-1.30203400
H	-1.48727200	-2.97504300	-0.18872800
N	-0.79922600	-0.68203500	1.23555100
H	-0.36244800	-0.35086200	2.08958000
C	-1.77070800	0.19770200	0.62114900
H	-1.89926600	1.04781400	1.30702900
H	-1.37436800	0.62005400	-0.31672000
H	1.37371400	-2.82156100	0.80556600
C	2.92089200	-3.35059600	-1.13223700
O	2.43766300	-3.65908000	-0.04376900
C	3.90691600	-4.23508800	-1.83668700
H	4.01632700	-5.18794200	-1.30685100
H	4.88022700	-3.72336300	-1.88211800
H	3.57933100	-4.41027200	-2.87131500
O	2.63742700	-2.25423800	-1.76743800
H	2.00833900	-1.61172700	-1.22506000
H	3.26976200	0.81899200	-0.52750500
C	1.54683800	1.44416200	1.49935900
C	2.26362200	0.81398200	2.53163100
C	0.62609400	2.44321900	1.85164100
C	2.05698900	1.15695400	3.86762800
H	2.98966900	0.03023500	2.29303900
C	0.41653300	2.79327200	3.18714400
H	0.05079600	2.95372600	1.07380900
C	1.12948000	2.14744000	4.19743400
H	2.62105500	0.65119500	4.65536100
H	-0.30819400	3.57134900	3.43968400
H	0.96511000	2.41724300	5.24368900
C	0.98392600	2.04640700	-1.48261700
C	1.27042100	3.42170900	-1.47486000
C	0.06996000	1.56689400	-2.43392900
C	0.65752500	4.28944600	-2.37954900
H	1.98066200	3.82964700	-0.74800600
C	-0.54866400	2.43011500	-3.34023100
H	-0.16129300	0.49792800	-2.46088900
C	-0.25603200	3.79409500	-3.31247800
H	0.89141900	5.35681100	-2.35657600
H	-1.25981800	2.03687300	-4.07121700
H	-0.73887500	4.47309800	-4.01976600
C	-3.12359400	-0.43154200	0.35929500

C	-3.86403900	-0.04594300	-0.76261800
C	-3.66566400	-1.37703500	1.23615000
C	-5.12733300	-0.58839200	-1.00167800
H	-3.44253700	0.68285000	-1.46128100
C	-4.92599200	-1.92419100	0.99697700
H	-3.08694100	-1.69454600	2.10750300
C	-5.66201400	-1.53027500	-0.12219900
H	-5.69278400	-0.27873700	-1.88404800
H	-5.33618300	-2.66425600	1.68867500
H	-6.64833400	-1.96091100	-0.31085300

TS11-1a-2a-3c

imaginary frequency = -324.23 cm⁻¹

Si	1.78215800	-0.85856600	0.49865200
O	1.35175400	0.71091300	0.21713000
C	0.03516200	1.48121800	-0.75888600
O	0.74742200	2.16273200	-1.64310700
C	-0.58285600	2.28176500	0.36207300
H	0.17321900	2.92156800	0.83114100
H	-1.03497000	1.65066200	1.13400600
H	-1.36440800	2.92389500	-0.07136500
N	-0.72062300	0.51333600	-1.34650100
C	-1.70199200	-0.22702900	-0.57871600
H	-1.82001900	-1.21102900	-1.05571200
H	-1.31454400	-0.43907400	0.42969700
H	1.34965300	2.80289800	-1.17525000
C	3.02566200	3.52948400	0.59552600
O	2.39210400	3.79544000	-0.42260500
C	4.00175400	4.49254600	1.20213700
H	4.02908400	5.42465400	0.62707400
H	5.00164900	4.03455300	1.22256800
H	3.71373100	4.70052100	2.24308500
O	2.91438000	2.40643400	1.24383200
H	2.25946400	1.74100700	0.79547000
H	3.24312300	-0.84556200	0.83779300
C	1.59572300	-1.97798600	-1.00308000
C	2.55636700	-1.90719500	-2.02629500
C	0.50609100	-2.84411700	-1.18275200
C	2.42415500	-2.65711300	-3.19536700
H	3.42396600	-1.24838000	-1.91695500
C	0.36784000	-3.59828200	-2.34897000

H	-0.25571300	-2.93204900	-0.40303900
C	1.32516300	-3.50196700	-3.35948900
H	3.18078700	-2.58375300	-3.98053300
H	-0.49132800	-4.26273200	-2.47009900
H	1.21770900	-4.08995200	-4.27443000
C	0.81895400	-1.56284000	1.95946600
C	0.81774700	-2.93491300	2.26224900
C	0.09197300	-0.70272600	2.79798200
C	0.10567000	-3.43120600	3.35496600
H	1.37676600	-3.63536000	1.63353700
C	-0.62496900	-1.19280000	3.89082600
H	0.08580100	0.37060100	2.58978500
C	-0.62098600	-2.56018400	4.16896400
H	0.11473500	-4.50248700	3.57113900
H	-1.18749700	-0.50540900	4.52765800
H	-1.18266700	-2.94816700	5.02245500
C	-3.06738700	0.42218200	-0.46348400
C	-3.89793400	0.08834300	0.61238900
C	-3.53254700	1.32894000	-1.42045300
C	-5.17276500	0.64236600	0.72541300
H	-3.53646000	-0.60886200	1.37430400
C	-4.80687600	1.88691800	-1.30799100
H	-2.88665400	1.61011000	-2.25597500
C	-5.63204600	1.54413600	-0.23627900
H	-5.80845200	0.37455500	1.57307000
H	-5.15597400	2.59623300	-2.06252100
H	-6.62869000	1.98301400	-0.14695900
C	-0.44768100	0.13609100	-2.72432900
H	-0.62593300	0.97656300	-3.41190900
H	0.58910500	-0.20640200	-2.86036200
H	-1.12195500	-0.68297300	-3.00068000

TS11-1a-2b-3b

imaginary frequency = -345.77 cm⁻¹

Si	-0.30803000	-1.61133800	-0.10100800
O	-0.60271000	-0.03861200	-0.52501900
C	0.33082300	1.43717800	0.19741600
O	-0.31615700	1.58999500	1.33541300
C	0.00778400	2.36631300	-0.95831800
H	-1.08420900	2.42406100	-1.05037600
H	0.38882600	1.93260200	-1.88981000

N	1.60943400	1.06660200	0.37741400
C	2.57438100	0.87758000	-0.69559900
H	2.93744300	1.85802300	-1.04517700
H	2.09661300	0.37928000	-1.55269400
H	-1.30117200	1.67031100	1.16821100
C	-3.49847200	1.24073000	0.00421200
O	-2.86963900	1.75707700	0.92857800
C	-4.99525700	1.42936900	-0.12131600
H	-5.32678300	2.05845700	0.71430800
H	-5.17964800	1.97344000	-1.06040500
O	-2.96841000	0.51388600	-0.92409700
H	-1.93454600	0.29934000	-0.75724100
H	-1.63248400	-2.31286600	-0.05334700
C	0.44257000	-1.75815500	1.62360900
C	-0.38590900	-1.50359400	2.73031700
C	1.79626700	-2.04096700	1.86749000
C	0.11724300	-1.52433000	4.03061200
H	-1.44570300	-1.27508000	2.57730300
C	2.30671100	-2.06284700	3.16711000
H	2.47499400	-2.23541700	1.03277200
C	1.46757700	-1.80335900	4.25069300
H	-0.54480000	-1.32080200	4.87603100
H	3.36473700	-2.28163400	3.33155800
H	1.86528400	-1.81911200	5.26854100
C	0.78581300	-2.42506700	-1.39888200
C	1.46400700	-3.63440600	-1.17432700
C	0.91891500	-1.81721900	-2.65769000
C	2.26232200	-4.20676800	-2.16539700
H	1.37752800	-4.14090800	-0.20817300
C	1.71111700	-2.38738100	-3.65520400
H	0.39774200	-0.87595000	-2.85523500
C	2.38971500	-3.58141600	-3.40714900
H	2.78945800	-5.14350400	-1.96788100
H	1.80395800	-1.89623200	-4.62704700
H	3.01649800	-4.02766500	-4.18326100
C	3.73793400	0.04142000	-0.22049400
C	4.13535500	-1.09181500	-0.93626300
C	4.42043300	0.37237900	0.95714800
C	5.18436700	-1.89001300	-0.47815900
H	3.60567000	-1.36462500	-1.85233900
C	5.46420700	-0.42723500	1.41992200

H	4.12626800	1.25872500	1.52626300
C	5.84704400	-1.56392500	0.70490500
H	5.47653200	-2.77674700	-1.04587300
H	5.98179600	-0.16155800	2.34480000
H	6.66251500	-2.19289200	1.06981000
C	0.58146000	3.75070000	-0.74099500
C	1.59816100	4.23967100	-1.56926700
C	0.09843400	4.57162200	0.28696300
C	2.13194400	5.51373300	-1.36830100
H	1.97303000	3.61654200	-2.38580100
C	0.63143800	5.84325900	0.49090000
H	-0.70523600	4.21179600	0.93344700
C	1.65246900	6.31771500	-0.33496000
H	2.92484600	5.87898400	-2.02542300
H	0.24353500	6.46995200	1.29769500
H	2.06964400	7.31482900	-0.17514900
C	-5.72556800	0.10587500	-0.13379000
C	-6.14197200	-0.47974000	-1.33403200
C	-5.95600300	-0.57781500	1.06677400
C	-6.77939500	-1.72090700	-1.33558100
H	-5.96437200	0.04253400	-2.27776300
C	-6.59192200	-1.81899300	1.06772500
H	-5.63232900	-0.13077100	2.01110800
C	-7.00577800	-2.39451100	-0.13475200
H	-7.10139700	-2.16406400	-2.28118600
H	-6.76653400	-2.33901800	2.01286800
H	-7.50601900	-3.36594600	-0.13564900
H	1.78073500	0.56717800	1.24641700

TS11-1a-2c-3b

imaginary frequency = -359.30 cm⁻¹

Si	0.64937600	0.81665300	1.58628400
O	-0.40335300	0.02549700	0.58384700
C	-0.24803300	0.00523000	-1.31527400
O	-0.70760000	1.20556500	-1.59506500
N	1.06066400	-0.13334300	-1.58852300
C	1.82140400	-1.35609300	-1.37855200
H	1.52676100	-2.10598400	-2.13149200
H	1.60169700	-1.77932900	-0.38765400
H	-1.63617000	1.29789300	-1.22379600
C	-3.53608200	0.64035600	0.29441100

O	-3.09795500	1.34483700	-0.61847400
O	-2.80490500	-0.06901400	1.08758700
H	-1.75706100	-0.01319000	0.87025700
H	-0.15884600	1.45609000	2.67493400
C	1.57516900	2.20855400	0.70950200
C	0.90048400	3.41678600	0.46552400
C	2.88636100	2.07876700	0.22147700
C	1.50633600	4.45359500	-0.24380100
H	-0.12335200	3.55277300	0.82872200
C	3.49761000	3.11127100	-0.49258200
H	3.44354800	1.15251100	0.38591500
C	2.80725500	4.30062600	-0.72684600
H	0.96169200	5.38401900	-0.42286600
H	4.51656400	2.98434600	-0.86664500
H	3.28346900	5.11060500	-1.28501000
C	1.86511900	-0.41304300	2.33558000
C	3.08815500	-0.01912500	2.90364900
C	1.54744000	-1.78090600	2.34235000
C	3.97016700	-0.95832300	3.43971700
H	3.36799300	1.03846100	2.92535400
C	2.42269300	-2.72533300	2.88027500
H	0.59826200	-2.11452400	1.91403700
C	3.64030100	-2.31467700	3.42462300
H	4.91997000	-0.63099700	3.86989700
H	2.15546000	-3.78493900	2.87136500
H	4.33177400	-3.05147900	3.84094300
C	3.30133200	-1.07073300	-1.46202300
C	4.14887000	-1.45359600	-0.41768900
C	3.84170800	-0.38874800	-2.55925300
C	5.51146700	-1.15629400	-0.46336400
H	3.73469100	-1.97451400	0.44964400
C	5.20193300	-0.08644700	-2.60418800
H	3.19107000	-0.08194500	-3.38296500
C	6.04056400	-0.46734800	-1.55452800
H	6.15843500	-1.45658500	0.36443800
H	5.60999900	0.45086300	-3.46363200
H	7.10581000	-0.22677300	-1.58869600
H	1.58280100	0.73923400	-1.54267300
C	-5.00864900	0.55883200	0.54473600
C	-5.52141600	-0.22577300	1.58474700
C	-5.88182300	1.27412500	-0.28289800

C	-6.89722000	-0.29055400	1.79482400
H	-4.83672400	-0.78331900	2.22567400
C	-7.25668000	1.20730700	-0.07130900
H	-5.46921100	1.88057400	-1.09123200
C	-7.76490000	0.42509800	0.96777100
H	-7.29516300	-0.90304400	2.60701800
H	-7.93584000	1.76644700	-0.71878600
H	-8.84362500	0.37301200	1.13395400
C	-1.16917600	-1.16352100	-1.56614600
C	-1.16000300	-2.33552100	-0.80432500
C	-2.05383400	-1.05058700	-2.64442700
C	-2.02524300	-3.38032400	-1.11859900
H	-0.49347000	-2.41822400	0.05233800
C	-2.92022300	-2.09760600	-2.95577400
H	-2.06874900	-0.13789800	-3.24292200
C	-2.90823000	-3.26429200	-2.19330100
H	-2.01566300	-4.28883400	-0.51234900
H	-3.60883700	-1.99664200	-3.79758000
H	-3.58981100	-4.08365300	-2.43351100

TS11-1a-2d-3b

imaginary frequency = -381.09 cm⁻¹

Si	-1.72433800	-1.35195400	1.32358500
O	-0.52021700	-0.68513100	0.39253900
C	-0.69888800	-0.21679900	-1.39809900
O	-0.36130000	-1.35572200	-1.97332500
N	-1.96462700	0.16273000	-1.62622000
C	-2.49961700	1.46157200	-1.23796000
H	-2.17806600	2.22221900	-1.96919800
H	-2.09238400	1.75444800	-0.25883600
H	0.55081800	-1.62003200	-1.66315700
C	2.53029500	-1.44818400	-0.08183300
O	2.05066300	-1.89911800	-1.11993600
O	1.86927200	-0.91639000	0.88978300
H	0.81387400	-0.83529300	0.68246800
H	-1.06911800	-2.33933500	2.23950800
C	-2.96949300	-2.30009900	0.27339300
C	-2.54414100	-3.48680500	-0.34955600
C	-4.28371400	-1.86636200	0.03559600
C	-3.39566600	-4.20985900	-1.18412700
H	-1.52577200	-3.85436500	-0.18812200

C	-5.14165000	-2.58784400	-0.79682200
H	-4.64803300	-0.94248500	0.49164400
C	-4.69803000	-3.75967000	-1.40943100
H	-3.04346000	-5.12819900	-1.66046800
H	-6.15935900	-2.22896700	-0.96886700
H	-5.36777700	-4.32458400	-2.06265600
C	-2.54645100	0.00437800	2.33405200
C	-3.76283300	-0.18349300	3.01107900
C	-1.91829200	1.25602000	2.43710500
C	-4.34298000	0.84995700	3.74729400
H	-4.27560800	-1.14901600	2.96212200
C	-2.49049000	2.29146400	3.17750300
H	-0.96930000	1.42474900	1.91970100
C	-3.70841700	2.09106100	3.82850800
H	-5.29442800	0.68711500	4.25964100
H	-1.98747700	3.25949700	3.24194400
H	-4.16301700	2.90186700	4.40316600
C	-4.00646500	1.41764000	-1.16050200
C	-4.66744300	1.80668100	0.00836200
C	-4.76281300	0.96292400	-2.24812800
C	-6.05786500	1.72810500	0.09730900
H	-4.08705800	2.15788100	0.86497500
C	-6.15112300	0.87808000	-2.15901300
H	-4.26203000	0.66225700	-3.17280800
C	-6.80269200	1.25632900	-0.98329200
H	-6.55851100	2.02760300	1.02115300
H	-6.72808200	0.51341600	-3.01218000
H	-7.89066800	1.18525100	-0.91211500
H	-2.61831300	-0.59763100	-1.79708600
C	3.97105700	-1.46539500	0.12190500
C	5.17697800	-1.42446500	0.25275900
C	6.59987000	-1.36054300	0.41392500
C	7.44608100	-2.03661900	-0.48176000
C	7.15402500	-0.61309600	1.46782500
C	8.82659000	-1.96409400	-0.32045900
H	7.01397500	-2.61555700	-1.30048700
C	8.53592700	-0.54467200	1.61811600
H	6.49461100	-0.08832300	2.16227400
C	9.37234400	-1.21934400	0.72674600
H	9.48111100	-2.49136200	-1.01784300
H	8.96339900	0.03831900	2.43672500

H	10.45654800	-1.16363700	0.84853300
C	0.30663700	0.83703200	-1.32864900
C	1.21642300	1.63401300	-1.27636000
C	2.32884500	2.53366700	-1.16749900
C	3.32306700	2.28046600	-0.20653100
C	2.44234900	3.64972100	-2.01184000
C	4.41895500	3.13187200	-0.10101200
H	3.22647800	1.41542200	0.45266800
C	3.54083700	4.49736900	-1.89466100
H	1.66869800	3.84542200	-2.75703100
C	4.52973400	4.23957700	-0.94355800
H	5.19150900	2.92804000	0.64369000
H	3.62652800	5.36478100	-2.55279900
H	5.39099500	4.90612500	-0.85799600

TS11-1a-2e-3b

imaginary frequency = -323.04 cm⁻¹

Si	0.54623200	2.69230900	-0.51868900
O	0.42103300	1.08214000	-0.18801600
C	1.15598400	-0.22341700	-1.39690000
O	0.23050600	-0.20724900	-2.33047400
C	1.13673500	-1.32515700	-0.38856400
H	0.34679600	-1.29275800	0.36160500
N	2.34193800	0.26339000	-1.80545600
H	2.28634300	0.84336100	-2.63749400
C	3.44377500	0.53560300	-0.89387600
H	3.83639800	1.53166200	-1.15144800
H	3.05063000	0.61275200	0.12981300
H	0.65731200	-0.46070600	-1.93069100
C	2.42930800	-0.42132400	-0.12915000
O	2.05354000	-0.73384500	-1.26469200
C	3.78165700	-0.75790500	0.36475700
H	4.00995500	-0.45072100	1.38780300
O	1.69975600	0.21646700	0.73218200
H	0.78310100	0.57851900	0.32903100
H	1.16478900	2.88633100	-1.87224800
C	1.64847800	3.54464900	0.74532100
C	2.15709700	4.83625500	0.53065100
C	1.98613800	2.88845800	1.93951900
C	2.96982100	5.45607000	1.48069300
H	1.91895300	5.37289000	-0.39374600

C	2.80082700	3.50262500	2.89230600
H	1.60706200	1.87861700	2.12265600
C	3.29253200	4.78851700	2.66390700
H	3.35648700	6.46166100	1.29681700
H	3.05423900	2.97590800	3.81587300
H	3.93073900	5.27161100	3.40806900
C	1.17895700	3.45368500	-0.54003300
C	1.52120700	4.61134200	0.17424000
C	2.18672400	2.81337800	-1.28277100
C	2.82391200	5.11549700	0.14746600
H	0.76352300	5.13121500	0.76847100
C	3.48959900	3.30846000	-1.30971600
H	1.95585100	1.90155800	-1.84244200
C	3.81005000	4.46366600	-0.59285000
H	3.07061500	6.01821200	0.71205500
H	4.25864700	2.79052200	-1.88839800
H	4.83061500	4.85426300	-0.61037300
C	4.56870700	-0.47627500	-0.93750900
C	5.14268100	-0.94059400	0.24939400
C	5.04462600	-0.96859200	-2.15787300
C	6.17301900	-1.88189600	0.22055900
H	4.76705400	-0.57288400	1.20843400
C	6.07069600	-1.91187900	-2.18998200
H	4.59483000	-0.62248500	-3.09235300
C	6.63829600	-2.37216700	-0.99955400
H	6.60567200	-2.24187100	1.15715400
H	6.42911900	-2.29173400	-3.14989700
H	7.43958500	-3.11455100	-1.02432000
C	4.66410900	-1.39706500	-0.41966500
H	4.33536200	-1.65701000	-1.43187200
C	6.03526000	-1.79332200	-0.07279800
C	6.80817800	-2.45228300	-1.04254600
C	6.60703500	-1.54288200	1.18723800
C	8.11423000	-2.85211100	-0.76514900
H	6.37343400	-2.65222000	-2.02557300
C	7.91056200	-1.94256900	1.46345400
H	6.02950600	-1.03137200	1.96036700
C	8.66846900	-2.59815700	0.48902500
H	8.70065200	-3.36436800	-1.53136900
H	8.34137000	-1.74176300	2.44709200
H	9.69157700	-2.91096100	0.71062800

C	2.00523100	-2.34111300	-0.45951900
H	2.76592200	-2.32806900	-1.24524500
C	2.06932300	-3.50400000	0.44149900
C	1.08943600	-3.77929000	1.40983500
C	3.17163200	-4.36642100	0.33619500
C	1.21592600	-4.88261100	2.24896300
H	0.21538300	-3.13089800	1.50685700
C	3.29956000	-5.46920900	1.17930000
H	3.94020300	-4.16003100	-0.41419600
C	2.32148200	-5.73019700	2.13851300
H	0.44436800	-5.08541300	2.99545300
H	4.16667900	-6.12715500	1.08553200
H	2.41703100	-6.59486500	2.79951600

TS11-1a-2f-3b

imaginary frequency = -475.41 cm⁻¹

Si	0.50725400	1.93826700	-0.34161900
O	0.75746700	0.23985900	-0.39133500
C	0.04729200	-0.92633000	0.72117400
O	0.94631100	-1.06761100	1.66776900
C	-0.00730300	-2.09788200	-0.29446100
N	-1.13260600	-0.47234000	1.18022700
H	-1.05746500	0.00296300	2.07479800
C	-2.36697600	-0.28971100	0.43409900
H	-2.89400200	0.54316900	0.92189000
H	-2.15151500	0.04684800	-0.58856500
H	1.89665600	-1.18018300	1.32663000
C	3.73016900	-0.78427900	-0.18436800
O	3.37919700	-1.21947300	0.91460700
C	5.21656600	-0.93865000	-0.58006200
O	3.03363000	-0.22130500	-1.06605300
H	1.80298200	-0.02229500	-0.72179000
H	1.84979400	2.48067900	-0.68227500
C	0.03861100	2.44590000	1.39492600
C	1.00207300	2.31867700	2.41028000
C	-1.24855600	2.88431300	1.74374800
C	0.68516300	2.60951300	3.73636800
H	2.01303900	1.97559100	2.16914600
C	-1.56754900	3.17838400	3.06966500
H	-2.02058300	2.98703100	0.97649100
C	-0.60154400	3.03842300	4.06679300

H	1.44384300	2.50140500	4.51508700
H	-2.57493100	3.51477300	3.32588000
H	-0.85165300	3.26580500	5.10593700
C	-0.77502300	2.37446100	-1.62841000
C	-1.35065600	3.65579000	-1.66825000
C	-1.16070000	1.43752500	-2.60104300
C	-2.29392900	3.98526200	-2.64138000
H	-1.06589900	4.41210400	-0.93042000
C	-2.10627900	1.76397300	-3.57331500
H	-0.72423400	0.43559800	-2.59505900
C	-2.67549700	3.03776600	-3.59249100
H	-2.73444100	4.98496000	-2.65614200
H	-2.39907900	1.02094600	-4.31892700
H	-3.41753200	3.29427500	-4.35250700
C	-3.27415800	-1.50147600	0.39339000
C	-4.03352500	-1.75891000	-0.75185900
C	-3.38584500	-2.36099200	1.49066200
C	-4.90023500	-2.85127300	-0.79725700
H	-3.93975500	-1.09973400	-1.61969100
C	-4.24838900	-3.45552200	1.44597800
H	-2.78223700	-2.17848100	2.38337800
C	-5.00914900	-3.70349400	0.30194400
H	-5.48557000	-3.04273400	-1.69989800
H	-4.32468100	-4.12155300	2.30897100
H	-5.68269200	-4.56313200	0.26601700
F	-0.50817100	-3.16479100	0.32284200
F	-0.75569700	-1.84526700	-1.36091300
F	1.21476500	-2.41158700	-0.71306500
F	5.93568600	-1.49660700	0.38576100
F	5.75308000	0.25135200	-0.85955600
F	5.32771700	-1.70065200	-1.67113100

TS11-1a-2b-3d

imaginary frequency = -362.80 cm⁻¹

Si	-0.23911400	-1.71120300	0.82585100
O	-0.30294100	-0.19654600	0.15860600
C	0.90752600	1.27582100	0.47317500
O	0.42789500	1.72864100	1.60381600
C	0.55107000	2.00950700	-0.80794900
H	-0.53610900	2.13468900	-0.84751900
H	0.84444100	1.41802100	-1.67969500

N	2.14745600	0.76984000	0.61804100
H	-0.54363900	1.98432500	1.49801500
C	-2.84996400	1.73197800	0.60204800
O	-2.05009800	2.32445000	1.33359100
C	-4.26823400	2.24696900	0.46807200
H	-4.49350400	2.82473800	1.37411800
H	-4.24421700	2.96129300	-0.37205100
O	-2.55672700	0.70558500	-0.11799900
H	-1.54223500	0.32702300	0.01100400
H	-1.38985400	-1.88033300	1.77294500
C	1.33648800	-1.98855600	1.81936100
C	1.44415600	-1.45349100	3.11464400
C	2.45371500	-2.64664200	1.28196000
C	2.63540900	-1.54376800	3.83487400
H	0.58990100	-0.93995500	3.56695700
C	3.64612000	-2.74708700	2.00036000
H	2.40334100	-3.07728200	0.27775800
C	3.74062800	-2.18858400	3.27524000
H	2.70241000	-1.11219200	4.83669800
H	4.50657500	-3.25658600	1.55966700
H	4.67553200	-2.25910700	3.83683300
C	-0.36935300	-2.99022200	-0.55055100
C	-0.21049000	-4.36280300	-0.29616600
C	-0.63693600	-2.58833600	-1.86836900
C	-0.30944900	-5.30108400	-1.32382100
H	0.00011800	-4.71143700	0.72039900
C	-0.73614600	-3.52240300	-2.90129900
H	-0.76936300	-1.52499700	-2.08876100
C	-0.57042600	-4.88075800	-2.62976600
H	-0.17944800	-6.36432600	-1.10680400
H	-0.94256600	-3.18867000	-3.92140400
H	-0.64496900	-5.61458200	-3.43629700
C	1.23456500	3.35942400	-0.82660200
C	2.46728200	3.52756800	-1.46758600
C	0.65637400	4.45188400	-0.16927900
C	3.11022300	4.76549900	-1.45264300
H	2.92592400	2.68009200	-1.98433900
C	1.29776100	5.68988900	-0.15345500
H	-0.30840000	4.32982000	0.33066300
C	2.52762000	5.84906300	-0.79417100
H	4.07101700	4.88375200	-1.95936400

H	0.83337400	6.53537100	0.35981000
H	3.03032900	6.81914500	-0.78307100
C	-5.30480600	1.18090200	0.21911300
C	-5.63789700	0.78931000	-1.08276600
C	-5.93279600	0.54253000	1.29506400
C	-6.57747100	-0.21696000	-1.30534200
H	-5.15413800	1.27979000	-1.93166200
C	-6.87309300	-0.46481200	1.07595600
H	-5.68257200	0.83959500	2.31746800
C	-7.19782400	-0.84804100	-0.22583100
H	-6.82820400	-0.50899800	-2.32816600
H	-7.35551200	-0.95153300	1.92718400
H	-7.93553500	-1.63521300	-0.39930200
H	2.43315200	0.64001500	1.58599000
C	2.99166600	0.18748100	-0.34984500
C	4.37268500	0.26528600	-0.13729900
C	2.49753400	-0.51521600	-1.45325700
C	5.25069800	-0.34895500	-1.02584400
H	4.74967000	0.80597300	0.73399300
C	3.38542700	-1.11186700	-2.34758500
H	1.42281600	-0.62079100	-1.59637800
C	4.76198700	-1.03501000	-2.13963900
H	6.32671600	-0.28557100	-0.84828800
H	2.98844400	-1.65990700	-3.20533500
H	5.45257300	-1.51234000	-2.83820300

TS11-1a-2a-3d

imaginary frequency = -354.53 cm⁻¹

Si	-0.58148700	0.75215100	-0.99054000
O	-0.71982500	-0.76240100	-0.35504500
C	-0.01459400	-1.47367000	1.29905100
O	-0.03935900	-2.73629100	0.96873700
C	-1.07402600	-0.94225000	2.21935100
H	-2.06235000	-1.29391500	1.90413900
H	-1.06724200	0.15448600	2.24396200
H	-0.86818300	-1.32692100	3.23066000
N	1.21088500	-0.92633100	1.44089100
H	-0.98853400	-3.04530600	0.81316600
C	-3.02731900	-3.07401200	-0.52562600
O	-2.42708700	-3.50931700	0.46114900
C	-4.31501100	-3.68702100	-0.99002000

H	-4.51913400	-4.61593000	-0.44578000
H	-4.26929000	-3.87916200	-2.07121400
H	-5.13371500	-2.97191100	-0.81690200
O	-2.62331200	-2.06792100	-1.23117500
H	-1.77010000	-1.56086900	-0.83898800
H	-0.64735500	0.64517400	-2.48604800
C	1.05828300	1.59562800	-0.59946400
C	2.13406100	1.49323500	-1.49614900
C	1.26187200	2.30891000	0.59363200
C	3.37217300	2.07113400	-1.21056900
H	2.00902500	0.94878300	-2.43732900
C	2.49821900	2.88463400	0.88858700
H	0.44224400	2.41868700	1.31126100
C	3.55587900	2.76619800	-0.01496100
H	4.19637400	1.97648100	-1.92186000
H	2.63663000	3.43117400	1.82481100
H	4.52477000	3.21716400	0.21367800
C	-2.00076100	1.84259600	-0.38795300
C	-1.96872100	3.24204600	-0.51039300
C	-3.14408800	1.25734200	0.17985100
C	-3.03768200	4.02879100	-0.07963200
H	-1.09226100	3.73313400	-0.94565800
C	-4.21654400	2.03853000	0.61367600
H	-3.19792800	0.17000600	0.28190800
C	-4.16369700	3.42701100	0.48558400
H	-2.99161000	5.11601400	-0.18181500
H	-5.09612000	1.56207800	1.05413500
H	-5.00065400	4.04184500	0.82627400
H	1.24516800	-0.06951600	1.98410100
C	2.37661600	-1.22019400	0.71011300
C	3.58904100	-0.72054300	1.20099400
C	2.35685500	-1.92855000	-0.49789200
C	4.76907000	-0.92103700	0.48985500
H	3.59744400	-0.16135500	2.13998400
C	3.54667300	-2.13201100	-1.19467200
H	1.41231900	-2.29610900	-0.89431500
C	4.75579900	-1.63053600	-0.71160700
H	5.70618700	-0.51754600	0.88062000
H	3.52154900	-2.68264000	-2.13824900
H	5.68146400	-1.78957200	-1.26906600

TS2-1b-2a-3aimaginary frequency = -1076.45 cm⁻¹

Si	0.10413100	0.17702000	-0.29170800
H	-1.54517400	-0.20799100	-1.12670100
O	1.75600600	0.63135200	0.33809200
C	2.84092900	-0.02229700	0.00915200
O	2.84767200	-1.03746300	-0.66542800
C	4.10414400	0.61141300	0.54201600
H	4.20050000	1.63280400	0.14397500
H	4.04699800	0.69315500	1.63779400
H	4.98366900	0.02012700	0.25943300
H	0.49303200	0.26526700	-1.73303200
C	-0.77436200	1.66409400	0.48155300
H	-1.65798200	1.29363800	1.02894100
H	-0.10560800	2.09958000	1.24174000
C	-1.19565300	2.74042200	-0.52013800
H	-1.74517300	3.56215900	-0.03245200
H	-0.32292400	3.18645900	-1.02439200
H	-1.85064000	2.32869100	-1.30606900
C	-0.11982000	-1.50643900	0.54479300
H	0.67182000	-1.62199200	1.30453900
H	-1.07555500	-1.47199300	1.09550100
C	-0.10696500	-2.70380200	-0.40411900
H	-0.26268600	-3.65410000	0.13285000
H	-0.90192100	-2.62340800	-1.16429800
H	0.85701300	-2.76866800	-0.93120600
C	-3.96879600	-0.81625700	0.77144900
H	-3.71569600	-1.84556600	0.48340300
H	-5.02034600	-0.78255700	1.09022400
H	-3.33136800	-0.52176000	1.61548900
N	-3.71296900	0.07537700	-0.35911400
H	-3.87120900	1.05450500	-0.11105000
H	-2.49182300	-0.06263700	-0.78876800
H	-4.32826300	-0.13555100	-1.14776500

TS2-1c-2a-3aimaginary frequency = -981.02 cm⁻¹

S	0.01213800	-1.11564100	-0.86959900
H	-1.81217100	-0.89645500	-1.23273000
C	-0.02155900	0.72483600	-0.41836100
C	-1.07735200	1.30850200	0.30048600

C	1.06558800	1.54432600	-0.76707900
C	-1.05071400	2.65616100	0.65969200
H	-1.94147100	0.70482500	0.59075200
C	1.08824500	2.89842400	-0.42836600
H	1.91464100	1.12112500	-1.31080200
C	0.03095200	3.45693000	0.28969400
H	-1.88072700	3.08414100	1.22739100
H	1.93955500	3.51804600	-0.72141300
H	0.04993800	4.51497300	0.56271800
O	1.76312100	-1.39669700	-0.70757200
C	2.58376200	-1.37389600	0.32738200
O	3.78327900	-1.44490300	0.17198300
H	-0.47709400	-2.08869000	0.14821700
C	1.95271600	-1.27806300	1.69801800
H	1.32018200	-0.38026700	1.77512600
H	1.30801400	-2.15196100	1.87901300
H	2.73418500	-1.23925800	2.46617200
N	-3.38109700	-1.73498000	0.28322300
H	-2.42001900	-1.26252500	-0.59842100
H	-3.03535500	-1.65398600	1.24117400
H	-3.52475000	-2.73045900	0.10379600
C	-4.61354900	-0.97452600	0.09512000
H	-4.41944300	0.08775600	0.29850600
H	-4.94336500	-1.07021400	-0.94864400
H	-5.42374400	-1.31851800	0.75526000
H	-0.01036000	-1.51806300	-2.29910400

TS2-1d-2a-3aimaginary frequency = -1029.49 cm⁻¹

S	-0.67646600	0.52628100	0.09769800
H	-1.86107100	-0.87274000	-0.27737400
C	0.61533000	-0.86536900	0.09000500
C	0.57013600	-1.94109800	-0.81020700
C	1.68704800	-0.81725200	0.99781500
C	1.55595600	-2.92878200	-0.81130600
H	-0.25355600	-2.01332000	-1.52709400
C	2.66435400	-1.81382000	1.01813300
H	1.76691100	0.01585900	1.70209400
C	2.60386400	-2.87029100	0.10881000
H	1.50367500	-3.75027400	-1.53046200
H	3.48114500	-1.76054400	1.74261800

H	3.37279700	-3.64699400	0.11657100
O	0.45995000	1.88792800	0.40362200
C	1.42980900	2.43395300	-0.29840800
O	2.11638700	3.32105200	0.16508800
H	-1.19842500	1.03008100	-1.20808600
C	1.63866100	1.91294000	-1.70347200
H	1.88346700	0.83983300	-1.68166400
H	0.71777900	2.02661600	-2.29544700
H	2.45466400	2.46175000	-2.18879800
N	-4.01077000	-0.06846800	-0.62978200
H	-2.75184400	-0.51777500	-0.45000800
H	-4.18228500	0.03417900	-1.63186300
H	-4.10537200	0.86066800	-0.21496600
C	-4.93879900	-1.01936000	-0.02155000
H	-4.79089400	-2.00948700	-0.47399900
H	-4.72611300	-1.09421800	1.05359100
H	-5.98822600	-0.71933200	-0.15612600
C	-1.64575600	0.86002200	1.67489100
H	-2.07802600	1.87320700	1.64403900
H	-2.44860300	0.13748700	1.87489600
H	-0.94442500	0.83885200	2.52483500

TS2-1e-2a-3a

imaginary frequency = -935.87 cm⁻¹

S	0.16672000	-0.06200900	0.06561700
H	-0.41710900	-0.35400900	-1.70456900
C	1.75838000	-0.82673000	-0.61965200
C	2.31615700	-0.47825000	-1.85876700
C	2.43650700	-1.77983200	0.15940100
C	3.51361400	-1.04357100	-2.29863500
H	1.81053700	0.24885400	-2.50001300
C	3.62160200	-2.36759800	-0.28515400
H	2.03841400	-2.06671300	1.13699000
C	4.16749800	-1.99439200	-1.51382400
H	3.93461100	-0.74506900	-3.26200700
H	4.12482900	-3.11451200	0.33407100
H	5.10068900	-2.44522800	-1.86065200
O	0.70097900	0.14452200	1.76007700
C	1.63699300	0.84797100	2.36978700
O	1.65367400	0.94001700	3.57868600
C	2.70178300	1.49422400	1.51132200

H	3.42794900	0.72449300	1.20665200
H	2.28986600	1.94027000	0.59552800
H	3.22653300	2.26092500	2.09454400
N	-2.65447300	0.20941900	-2.06664000
H	-1.32565000	-0.11721100	-1.84664600
H	-2.67828600	0.85487700	-2.85803000
H	-3.00646700	0.72323900	-1.25691200
C	-3.45146500	-0.98597300	-2.32768500
H	-2.98010200	-1.56967000	-3.13085700
H	-3.48206400	-1.60587600	-1.42167100
H	-4.48283800	-0.74324100	-2.62522700
C	-0.31053100	1.75388100	-0.24453400
C	-0.75855500	2.54505700	0.82880900
C	-0.23033400	2.36458800	-1.50697800
C	-1.12226000	3.88025900	0.64720800
H	-0.82716500	2.11525000	1.83119400
C	-0.56954200	3.70506300	-1.69172800
H	0.09415400	1.78193600	-2.37310300
C	-1.02266500	4.46669500	-0.61409000
H	-1.47864200	4.46626000	1.49808900
H	-0.48584900	4.15503700	-2.68413500
H	-1.29836900	5.51443200	-0.75761300
C	-1.21081500	-1.27224800	0.51949500
C	-2.31654700	-0.85705300	1.27624900
C	-1.16925300	-2.60783700	0.09212800
C	-3.35056800	-1.74202600	1.58827600
H	-2.38378900	0.17676100	1.62778800
C	-2.19047900	-3.50221100	0.41518700
H	-0.32738000	-2.96080500	-0.51198800
C	-3.28777500	-3.06913400	1.16135600
H	-4.20751800	-1.39458000	2.17110800
H	-2.13346300	-4.54000800	0.07707100
H	-4.09336300	-3.76482200	1.40909200

TS2-1f-2a-3a

imaginary frequency = -1039.11 cm⁻¹

Si	-0.55032700	-0.64539700	-0.06408400
H	-1.89364800	0.58778300	0.36714200
C	0.52092600	0.92914400	-0.06519800
C	0.41829200	1.91283800	0.93075300
C	1.48358400	1.11949000	-1.07069900

C	1.24791900	3.03488200	0.93421100
H	-0.32786600	1.80379600	1.72427000
C	2.30167700	2.25096100	-1.08848300
H	1.60725900	0.36690200	-1.85486600
C	2.18983300	3.20981900	-0.08129000
H	1.15526700	3.77967100	1.72899200
H	3.03530600	2.38030500	-1.88851400
H	2.83511200	4.09199800	-0.08695000
O	0.79563100	-1.77769700	-0.52193600
C	1.96026000	-2.10614300	-0.01641800
O	2.73304500	-2.82050500	-0.62543000
C	2.29498300	-1.59328500	1.36957000
H	2.08876300	-0.51827400	1.46865700
H	1.67676100	-2.11821500	2.11406000
H	3.35171400	-1.78832000	1.58979500
N	-4.11641800	-0.05149800	0.36264900
H	-2.84851600	0.28849700	0.38972700
H	-4.45255100	-0.12503600	1.32502700
H	-4.20708800	-0.97867500	-0.05787400
C	-4.86118000	0.95551800	-0.39126500
H	-4.71465100	1.93785500	0.07788000
H	-4.47217400	0.99828900	-1.41755100
H	-5.93693000	0.73195400	-0.42500600
C	-1.50661600	-1.06230200	-1.63490900
H	-1.85327800	-2.10834400	-1.59205900
H	-2.37568600	-0.41706100	-1.82283500
H	-0.83024800	-0.98611200	-2.50092700
C	-1.05594800	-1.46149900	1.56148900
H	-2.14695500	-1.60488600	1.60158500
H	-0.58291900	-2.44730000	1.68911000
H	-0.77995200	-0.82971100	2.42134000

1b

Si	0.03315400	-0.78003500	0.14816500
H	0.48840500	-2.04029800	-0.52405800
C	-1.73268100	-0.38844000	-0.38032400
H	-1.74745900	-0.32887100	-1.48315900
H	-2.36611200	-1.25437100	-0.11919000
C	1.22494400	0.61996100	-0.26489100
H	1.11219300	0.84888800	-1.33968900
H	0.88392500	1.52282400	0.27171500

C	-2.30957500	0.89388900	0.22529300
H	-3.34872100	1.06128400	-0.10019100
H	-2.31327200	0.85840300	1.32709500
H	-1.72821300	1.78134400	-0.07218200
C	2.69104000	0.33211400	0.06624800
H	3.33950400	1.18449000	-0.19254400
H	2.83263500	0.12906200	1.14034300
H	3.06717700	-0.54476700	-0.48521600
H	0.07341400	-1.04264400	1.62481900

1c

Si	0.03124800	2.34627900	0.00000000
H	-0.65014800	2.87138000	1.21777800
H	-0.65014800	2.87138000	-1.21777800
H	1.43603200	2.85291500	0.00000000
C	-0.01231900	0.46604500	0.00000000
C	-0.01391000	-0.25494500	1.20586700
C	-0.01391000	-0.25494500	-1.20586700
C	-0.01391000	-1.65024400	1.20759900
H	-0.01853200	0.27524400	2.16330800
C	-0.01391000	-1.65024400	-1.20759900
H	-0.01853200	0.27524400	-2.16330800
C	-0.01334100	-2.34962400	0.00000000
H	-0.01657900	-2.19388800	2.15558900
H	-0.01657900	-2.19388800	-2.15558900
H	-0.01517700	-3.44254800	0.00000000

1d

Si	1.88216000	-0.62170500	0.15191200
H	2.16351900	-1.76398200	-0.77118000
H	2.22202300	-1.09340300	1.53157300
C	0.03907700	-0.22968100	0.05802800
C	-0.43010500	1.09191100	0.13386500
C	-0.90778100	-1.25968800	-0.07630400
C	-1.79599300	1.37622100	0.08050900
H	0.27685700	1.92080800	0.23411900
C	-2.27364100	-0.98084700	-0.12971800
H	-0.57812800	-2.30138800	-0.14505100
C	-2.72005900	0.33957600	-0.05093700
H	-2.13912800	2.41211700	0.14017900
H	-2.99320700	-1.79654900	-0.23597700

H	-3.78953100	0.56031800	-0.09430700
C	2.92809400	0.86763200	-0.28908300
H	2.77064000	1.69071300	0.42598000
H	3.99868300	0.60843100	-0.27283200
H	2.68047800	1.23606700	-1.29743400

1e

Si	-0.00066600	-0.00186400	-0.96528700
H	-0.00269900	-0.00158900	-2.46042000
C	0.56161800	1.69006700	-0.36006800
C	-0.07530900	2.33788200	0.70998500
C	1.67060300	2.31924600	-0.95180200
C	0.37942100	3.57319600	1.17571000
H	-0.94245900	1.87518900	1.19081900
C	2.12770400	3.55343500	-0.49073800
H	2.19053500	1.84083100	-1.78809000
C	1.48128100	4.18237000	0.57533400
H	-0.12989800	4.06193700	2.00992800
H	2.99027100	4.02792500	-0.96505700
H	1.83736700	5.15004000	0.93736000
C	-1.74681800	-0.35997200	-0.35889300
C	-2.84536700	0.28139400	-0.95698200
C	-1.99064700	-1.22665200	0.71797400
C	-4.14332900	0.06441600	-0.49548500
H	-2.68968600	0.96380800	-1.79891500
C	-3.28838900	-1.44612600	1.18422800
H	-1.15696500	-1.74258100	1.20385700
C	-4.36606900	-0.80091900	0.57759600
H	-4.98482200	0.57074300	-0.97480600
H	-3.45832700	-2.12457900	2.02391800
H	-5.38262300	-0.97280500	0.94014900
C	1.18414200	-1.33436400	-0.36004800
C	1.14877200	-2.61959700	-0.92853300
C	2.09088900	-1.09625900	0.68447100
C	1.99094300	-3.63207800	-0.46987500
H	0.45255900	-2.83914300	-1.74455300
C	2.93542000	-2.10724000	1.14767200
H	2.14397100	-0.10603900	1.14696600
C	2.88656300	-3.37603300	0.57053300
H	1.95026500	-4.62433800	-0.92596000
H	3.63493100	-1.90213100	1.96183400

H	3.54832800	-4.16776300	0.93051700
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1f

Si	-1.65486800	-0.19014200	-0.36633100
H	-1.92022400	-0.82066500	-1.70106500
C	0.22050400	-0.04750800	-0.17431200
C	1.04544400	-1.15667600	-0.43190400
C	0.83457100	1.14171400	0.25065400
C	2.42893600	-1.08317500	-0.26982100
H	0.60428600	-2.10051000	-0.76966000
C	2.21927100	1.22157500	0.41610000
H	0.22750500	2.02805500	0.45841300
C	3.01880100	0.10867600	0.15612800
H	3.05025200	-1.95792600	-0.47811700
H	2.67504400	2.15766000	0.74867100
H	4.10254100	0.16930000	0.28377600
C	-2.34584200	-1.31296700	0.97126300
H	-3.43184600	-1.45599500	0.84776600
H	-1.86757200	-2.30535000	0.94413100
H	-2.17028700	-0.87779700	1.96890100
C	-2.45584800	1.50360200	-0.30338300
H	-2.04811600	2.17777900	-1.07351200
H	-3.54215900	1.41923100	-0.46995600
H	-2.30628700	1.97676300	0.68093200

2b

C	-1.17639900	-0.14823700	1.05790400
H	-1.38697600	0.63517100	1.79694400
H	-1.34043800	-1.12827700	1.53043000
C	0.24610800	-0.04627000	0.55094700
C	0.77097500	1.19992000	0.18488600
C	1.04766700	-1.18386000	0.41073900
C	2.07042500	1.30627100	-0.30920100
H	0.15321600	2.09649100	0.28924000
C	2.34944800	-1.07928900	-0.08129200
H	0.64809500	-2.16204000	0.69137500
C	2.86429800	0.16572200	-0.44327700
H	2.46576300	2.28562000	-0.58976500
H	2.96435400	-1.97700400	-0.18183500
H	3.88352800	0.24791400	-0.82834000
C	-2.18284300	0.00717500	-0.05909200

O	-2.98021500	0.90672100	-0.15381600
O	-2.09212600	-0.97257000	-0.96102200
H	-2.74688500	-0.79967300	-1.65902700

2c

C	0.22149200	0.02819600	-0.00004500
C	-0.51097200	1.22131400	0.00020300
C	-0.44817000	-1.20191200	-0.00016100
C	-1.90263200	1.18571900	0.00014600
H	0.02353200	2.17324200	0.00034200
C	-1.84109100	-1.23355800	-0.00013700
H	0.12188700	-2.13209800	-0.00025900
C	-2.56805300	-0.04192000	-0.00003300
H	-2.47168800	2.11794400	0.00026700
H	-2.36231500	-2.19337100	-0.00022500
H	-3.66035300	-0.07006000	0.00000900
C	1.71078800	0.11545100	0.00000300
O	2.33186700	1.15175700	-0.00039600
O	2.30719900	-1.07734300	0.00038300
H	3.26823600	-0.93070100	0.00011800

2d

C	-3.17711400	-0.10476300	0.00000200
O	-3.79738800	-1.13859200	-0.00041800
O	-3.73799800	1.10106600	0.00067600
H	-4.70486600	0.98306500	0.00093700
C	-1.72802900	-0.03108500	-0.00030400
C	-0.51448100	-0.02275000	-0.00026200
C	0.91843700	-0.00816800	-0.00015900
C	1.63556400	-1.21723400	0.00009800
C	1.61114200	1.21514600	-0.00034000
C	3.02706400	-1.19727300	0.00037000
H	1.09513900	-2.16596800	0.00018300
C	3.00271900	1.22323200	-0.00018600
H	1.05170300	2.15279500	-0.00061000
C	3.71090700	0.01996100	0.00023000
H	3.58196800	-2.13784000	0.00060700
H	3.53856500	2.17479100	-0.00027600
H	4.80332800	0.03097400	0.00040600

2e

O	3.32938400	-1.22705600	-0.04453600
O	3.92931400	0.88895300	0.05500300
H	3.52531100	1.76927500	0.08249700
C	2.99442800	-0.06805600	-0.00454900
C	1.58775700	0.40617300	-0.01014200
H	1.40710700	1.48517100	-0.00305400
C	0.57967900	-0.48052600	-0.01448900
H	0.85178100	-1.54200000	-0.01762400
C	-0.85986200	-0.18973800	-0.00959200
C	-1.76083800	-1.26635300	0.01916900
C	-1.37460600	1.11858600	-0.02911200
C	-3.13707400	-1.04622900	0.02995300
H	-1.37202800	-2.28788100	0.03430500
C	-2.74821500	1.33753500	-0.01931800
H	-0.69722500	1.97496800	-0.05298300
C	-3.63381500	0.25658500	0.01077700
H	-3.82378400	-1.89541900	0.05336200
H	-3.13351800	2.35958400	-0.03524800
H	-4.71194300	0.43326100	0.01881600

2f

C	0.59583000	-0.00111700	-0.00121100
C	-0.94051300	0.15215600	-0.00397400
O	-1.48869500	1.21433700	-0.00181400
O	-1.51092500	-1.03541100	-0.00185400
H	-2.48029000	-0.92785700	0.00418000
F	1.17692200	1.18519800	-0.05560200
F	0.99646200	-0.62054900	1.10776300
F	0.99832200	-0.72129200	-1.04590900

3b

C	1.90145900	0.60768600	0.18825200
H	2.08605600	1.52767000	-0.40071100
H	2.11186000	0.88067300	1.23724200
N	2.76662900	-0.50427600	-0.16725400
H	2.70883300	-0.67740500	-1.17115700
H	3.73645700	-0.25227200	0.01552400
C	0.42826700	0.26834000	0.08012900
C	-0.52102900	1.29407100	-0.02716300
C	-0.02174000	-1.05595300	0.11356500
C	-1.88356800	1.00496100	-0.08854500

H	-0.18589900	2.33508600	-0.06432400
C	-1.38529200	-1.34918900	0.04706000
H	0.71410200	-1.85912500	0.18817500
C	-2.32200900	-0.32057300	-0.05188400
H	-2.60826100	1.81909200	-0.17086500
H	-1.71676200	-2.39057500	0.07259900
H	-3.38932000	-0.54927000	-0.10418900

3c

C	1.36142400	-0.61975800	0.28221100
H	1.58584100	-0.72595600	1.35991300
H	1.54261400	-1.62354700	-0.15827700
N	2.23748500	0.40100800	-0.25489600
H	2.04890000	0.51052900	-1.25040800
C	-0.10410900	-0.27650300	0.12661600
C	-1.05801700	-1.29106700	-0.02299800
C	-0.54208000	1.05313300	0.16031000
C	-2.41575200	-0.98723900	-0.12697000
H	-0.73164300	-2.33454100	-0.06160500
C	-1.89875100	1.36047400	0.05171200
H	0.19739100	1.84970700	0.26624500
C	-2.84161000	0.34141700	-0.09030500
H	-3.14483800	-1.79309200	-0.24378300
H	-2.22137900	2.40451900	0.07859900
H	-3.90422300	0.58158400	-0.17606800
C	3.64272300	0.11560000	-0.05653600
H	3.88007000	0.11753700	1.02020700
H	3.96712000	-0.86603400	-0.46187400
H	4.25477500	0.89589200	-0.53291700

3d

C	-1.13932800	1.22850600	0.00000200
C	0.25416800	1.18587400	-0.00001600
C	0.93261000	-0.04157500	0.00000800
C	0.18364400	-1.22281900	-0.00001600
C	-1.21201300	-1.18278500	-0.00002000
C	-1.87778500	0.04285500	0.00002700
H	-1.65261300	2.19349700	0.00001200
H	0.83408700	2.11306300	-0.00001400
H	0.71426400	-2.17807000	-0.00003100
H	-1.78136400	-2.11571500	-0.00001900

H	-2.96999200	0.07573700	0.00004300
N	2.36284900	-0.12794800	-0.00002300
H	2.73395100	0.37363700	-0.80801000
H	2.73395200	0.37315100	0.80826600

5-3b

N	-2.65272900	-0.00022900	0.65617700
H	-3.66449900	-0.00089300	0.47519600
H	-2.44207000	-0.82737700	1.22912600
H	-2.44313300	0.82709400	1.22927200
C	-1.87036800	0.00035300	-0.61404300
H	-2.17729400	-0.89192800	-1.17249800
H	-2.17719500	0.89324500	-1.17156000
C	-0.39105900	0.00016300	-0.33628800
C	0.30064900	-1.20783300	-0.19077700
C	0.30089600	1.20797200	-0.19057300
C	1.66550100	-1.20822800	0.09449300
H	-0.23386800	-2.15457400	-0.30752800
C	1.66575600	1.20804500	0.09471200
H	-0.23343100	2.15484200	-0.30712500
C	2.34935400	-0.00017000	0.23756800
H	2.19812800	-2.15594700	0.20169600
H	2.19856300	2.15564100	0.20211200
H	3.41953800	-0.00030200	0.45752100

5-3c

C	-1.32717400	0.00039100	0.73721200
H	-1.61526100	-0.89266000	1.30625800
H	-1.61518500	0.89428500	1.30495400
N	-2.15611400	-0.00049900	-0.50608200
H	-1.89937000	0.81541000	-1.07724400
C	0.13883400	0.00017500	0.39901600
C	0.82197900	1.20810900	0.21657500
C	0.82175400	-1.20792900	0.21687300
C	2.16958400	1.20816500	-0.14144300
H	0.29363100	2.15467400	0.35969000
C	2.16935600	-1.20831600	-0.14116100
H	0.29325300	-2.15437400	0.36022800
C	2.84417500	-0.00016000	-0.32169900
H	2.69581800	2.15562700	-0.27837500
H	2.69542200	-2.15590400	-0.27786300

H	3.90053600	-0.00029300	-0.60056500
C	-3.61656700	0.00014100	-0.27083500
H	-3.88070900	-0.89818600	0.29828700
H	-3.88028000	0.90016700	0.29579900
H	-4.12685700	-0.00105700	-1.24015100
H	-1.89984500	-0.81764900	-1.07567400

5-3d

N	2.30513700	0.00000100	0.00627400
H	2.67689500	-0.00019400	0.96763800
H	2.69617500	-0.82802800	-0.46317400
H	2.69618700	0.82821500	-0.46284100
C	0.84301500	0.00000900	-0.00954300
C	0.16972000	1.21635800	-0.00586800
C	0.16972500	-1.21635400	-0.00586000
C	-1.22420100	1.20941400	0.00150300
H	0.72759900	2.15538400	-0.01071900
C	-1.22418500	-1.20942300	0.00149700
H	0.72762700	-2.15536700	-0.01071500
C	-1.91988800	-0.00000300	0.00551100
H	-1.76680800	2.15677400	0.00162400
H	-1.76679600	-2.15678000	0.00161400
H	-3.01195200	-0.00001600	0.00921800

TS11-1b-2a-3a

imaginary frequency = -486.91 cm⁻¹

Si	1.42306200	-0.04223400	0.04404800
O	-0.01583500	0.54163600	-0.55926900
C	-1.03171200	1.80973800	0.43071300
O	-1.37268000	1.08232500	1.47670000
C	-2.05008200	2.04372400	-0.64955100
H	-2.62489700	1.12974600	-0.83601200
H	-1.58255900	2.36682500	-1.58558200
H	-2.74234200	2.82540600	-0.30008700
N	-0.19664100	2.81734500	0.73982400
H	0.38959500	2.63616400	1.54906400
C	0.32878900	3.73879800	-0.24267200
H	1.00657200	4.43706800	0.26318300
H	-0.47593300	4.32645500	-0.70677800
H	0.88972300	3.21780000	-1.03712900
H	-1.84392500	0.24800800	1.17077800

C	-2.26606600	-1.70022900	-0.37227300
O	-2.49570200	-1.10953100	0.68950000
C	-2.94414600	-3.00410100	-0.68774100
H	-3.77059000	-3.19108000	0.00769400
H	-2.20352300	-3.81404900	-0.59666600
H	-3.30671700	-3.00399400	-1.72496500
O	-1.44576400	-1.28302100	-1.27495100
H	-0.82440600	-0.41479700	-0.95695000
H	1.95356400	0.94280700	1.05119200
C	2.66189600	-0.18178700	-1.36735300
H	2.18449000	-0.78016000	-2.16435200
H	2.78552100	0.83113700	-1.79067800
C	4.02575000	-0.77685300	-1.00901000
H	3.93829800	-1.83017400	-0.69899200
H	4.71983700	-0.74858100	-1.86452400
H	4.50830400	-0.23074400	-0.18150900
C	1.13344300	-1.68260800	0.93184200
H	0.16742600	-1.57510800	1.45612600
H	0.97319000	-2.46693200	0.17031500
C	2.21606400	-2.11390000	1.92444800
H	1.94527700	-3.05030700	2.43883800
H	3.18626200	-2.28318400	1.43216800
H	2.37668000	-1.35041700	2.70317400

TS11-1b-2a-3a'

imaginary frequency = -434.46 cm⁻¹

Si	1.13298200	-0.85014200	-0.40360400
O	-0.10694200	0.23032100	-0.64772500
C	-0.38963400	1.71630100	0.50736700
O	-0.92379300	1.10938900	1.54784000
C	-1.29381300	2.45209200	-0.44097200
H	-2.21217100	1.87927200	-0.61225500
H	-0.80615600	2.64245200	-1.40290600
H	-1.56447900	3.41288500	0.02429800
N	0.81502500	2.25212000	0.76871000
H	1.33390800	1.80724600	1.51902400
C	1.54628000	3.08348600	-0.16032000
H	2.53231800	3.29949600	0.26807200
H	1.03369000	4.04211800	-0.33064000
H	1.69397500	2.58426800	-1.13136400
H	-1.72055000	0.56945600	1.25932200

C	-3.08542600	-0.87569200	-0.28897200
O	-2.94256900	-0.32827800	0.80870800
C	-4.32246300	-1.66970400	-0.60291300
H	-5.03429400	-1.62499000	0.22922500
H	-4.04248200	-2.71583000	-0.79786000
H	-4.78888500	-1.27981800	-1.51933400
O	-2.22135000	-0.82315400	-1.24613500
H	-1.28330100	-0.32151000	-0.97183500
H	0.84391600	-2.05382800	-1.26320800
C	1.18379600	-1.43015300	1.39090900
H	1.35958400	-0.55015600	2.03423400
H	0.16602800	-1.77765200	1.64231000
C	2.20981900	-2.52215100	1.70184800
H	3.24158600	-2.15895000	1.57204100
H	2.12251400	-2.88015000	2.74060300
H	2.08659900	-3.39939100	1.04508300
C	2.79223100	-0.14619000	-0.96380800
H	2.58730300	0.52109000	-1.81938000
H	3.18504500	0.50463000	-0.16215700
C	3.84184300	-1.18741600	-1.36501000
H	4.78127700	-0.71263700	-1.69172500
H	4.09310300	-1.86532600	-0.53436500
H	3.48598100	-1.81517700	-2.19798000

TS11-1c-2a-3a

imaginary frequency = -305.58 cm⁻¹

Si	-0.63417500	-0.10551700	-1.36623900
O	0.57911400	0.09849400	-0.27631300
C	1.34554700	1.75631100	0.13882800
O	2.37867600	1.74465500	-0.68307300
C	1.58071500	1.45576400	1.59336100
H	2.27699500	0.61656700	1.70210700
H	0.64842600	1.21364400	2.11494500
H	2.03310500	2.34706000	2.05546200
N	0.45157700	2.71634600	-0.16705600
H	0.42889700	2.97220600	-1.14935400
C	-0.74038200	2.98115300	0.60697100
H	-1.30640000	3.77777200	0.10919600
H	-0.49035600	3.32775200	1.62012700
H	-1.39332100	2.09513200	0.69164400
H	2.93508700	0.93309900	-0.51471000

C	3.38809800	-1.51710400	0.05182600
O	3.80667900	-0.40696700	-0.27056200
C	4.31174700	-2.67534100	0.28853500
H	5.35289400	-2.37970500	0.11792000
H	4.04096200	-3.50465900	-0.38123800
H	4.18883100	-3.03429600	1.32103200
O	2.13111900	-1.79536300	0.22965800
H	1.50109200	-0.98875300	0.02500200
H	-0.30843600	-1.21609100	-2.31840700
C	-2.25378200	-0.50653000	-0.48889600
C	-3.47918000	-0.54448700	-1.17362200
C	-2.25282000	-0.78044400	0.88750300
C	-4.66560500	-0.84993200	-0.50579300
H	-3.51545100	-0.33041200	-2.24718500
C	-3.43704100	-1.08659300	1.56089700
H	-1.30808100	-0.75069700	1.43842000
C	-4.64528900	-1.12218900	0.86392800
H	-5.61078300	-0.87403800	-1.05413500
H	-3.41727700	-1.29790500	2.63311200
H	-5.57398700	-1.36084100	1.38832900
H	-0.84152500	1.12677100	-2.19443500

TS11-1c-2a-3a'

imaginary frequency = -323.58 cm⁻¹

Si	0.16628300	-1.72400700	-0.64537500
O	1.10361500	-0.37397600	-0.71067900
C	2.49576100	-0.00759600	0.51628200
O	1.80261500	0.49657200	1.52062600
C	3.23185900	0.93586900	-0.39274600
H	2.60983100	1.80890800	-0.62091700
H	3.52163500	0.45215500	-1.33146300
H	4.13619600	1.27845100	0.13391700
N	3.08144100	-1.17806500	0.82403600
H	2.60050500	-1.71154900	1.54200100
C	3.90857300	-1.92444300	-0.09714600
H	4.22201200	-2.85360300	0.39400300
H	4.81464500	-1.36241500	-0.36527300
H	3.36905200	-2.18510300	-1.02416300
H	1.27422800	1.28750900	1.20929800
C	-0.25575100	2.56147400	-0.36584000
O	0.32198600	2.47372500	0.71808000

C	-1.21608700	3.67634100	-0.65388800
H	-1.08991600	4.49020300	0.06922100
H	-2.23888800	3.27571700	-0.56959300
H	-1.08662500	4.04484300	-1.68033800
O	-0.11496100	1.71069300	-1.33525800
H	0.43774500	0.85997900	-1.06633400
H	0.75496300	-2.70219600	0.32795200
C	-1.59016900	-1.29024800	-0.11892700
C	-2.71422500	-1.91225400	-0.68330700
C	-1.80037200	-0.30695300	0.86249700
C	-4.00620700	-1.56881300	-0.27912500
H	-2.58623500	-2.67519300	-1.45803400
C	-3.08826800	0.04323300	1.26772700
H	-0.94360700	0.20125000	1.31387200
C	-4.19459800	-0.58874400	0.69604500
H	-4.86939800	-2.06313700	-0.73201700
H	-3.22954400	0.81327500	2.03040300
H	-5.20508400	-0.31478200	1.00962600
H	0.08129400	-2.42506800	-1.96674000

TS11-1d-2a-3a

imaginary frequency = -332.40 cm⁻¹

Si	0.58590600	-0.08154900	1.34874700
O	-0.65297700	0.07945800	0.27215900
C	-1.26794800	1.63468600	-0.59398200
O	-2.35311100	1.86692700	0.11772900
C	-1.41537200	0.99791500	-1.94788900
H	-2.14530500	0.18163000	-1.90904500
H	-0.46242600	0.60433600	-2.31792000
H	-1.78609800	1.76475000	-2.64616500
N	-0.33833800	2.59737300	-0.45149900
H	-0.36915200	3.08172400	0.43987600
C	0.90981800	2.63511300	-1.17926000
H	1.47717200	3.51307700	-0.84752700
H	0.73877100	2.73480500	-2.26088200
H	1.52723500	1.73734900	-1.00384700
H	-2.95208700	1.06598600	0.10107000
C	-3.53160300	-1.40139000	0.09815200
O	-3.90059300	-0.22689700	0.10985400
C	-4.51536500	-2.53433200	0.05179600
H	-5.54177900	-2.15742400	0.12372000

H	-4.31130200	-3.23927200	0.87044700
H	-4.38817900	-3.08312000	-0.89351900
O	-2.28945500	-1.77226300	0.10615200
H	-1.60822400	-0.96353300	0.16834800
H	0.21054600	-1.17392200	2.31142800
C	2.14902200	-0.62040800	0.43102400
C	3.43431400	-0.46853300	0.97694400
C	2.04097100	-1.18399900	-0.85111000
C	4.57046000	-0.86762000	0.27050900
H	3.55964400	-0.02635800	1.97063100
C	3.17250700	-1.58451600	-1.56331200
H	1.05059200	-1.30255100	-1.30109300
C	4.44077700	-1.42653600	-1.00210000
H	5.56185200	-0.73874500	0.71254700
H	3.06587400	-2.01906300	-2.56068600
H	5.32931000	-1.73649400	-1.55800600
C	0.95681600	1.45655600	2.35685800
H	0.03098900	1.89032100	2.76870900
H	1.60655600	1.19741700	3.20939000
H	1.47439000	2.22974600	1.76760500

TS11-1d-2a-3a'

imaginary frequency = -342.16 cm⁻¹

Si	-0.06451800	-1.64058800	0.40572200
O	-1.04842700	-0.31893900	0.50693300
C	-2.45721300	0.09732900	-0.70186700
O	-1.79170800	0.78969600	-1.60552700
C	-3.28264100	0.84079000	0.31006900
H	-2.74476300	1.72952900	0.65897800
H	-3.53029400	0.21432400	1.17327300
H	-4.21234100	1.16642600	-0.18232900
N	-2.93469800	-1.06498500	-1.17741900
H	-2.39343400	-1.46143600	-1.93972100
C	-3.72525100	-1.98467600	-0.39098900
H	-3.95482000	-2.86117900	-1.00882400
H	-4.67731100	-1.52887500	-0.08378600
H	-3.19127600	-2.32601900	0.51261500
H	-1.32750600	1.56516200	-1.17153000
C	0.04627800	2.71418000	0.61523100
O	-0.48666000	2.73682200	-0.49708600
C	0.88039300	3.86277200	1.10234400

H	0.72962600	4.74570600	0.47082100
H	1.93952900	3.56352800	1.05961600
H	0.64292800	4.09196800	2.15011400
O	-0.04187200	1.72406500	1.44335300
H	-0.51365000	0.85637700	1.03106700
H	-0.61496400	-2.57156200	-0.63803400
C	1.66235400	-1.09082400	-0.13326100
C	2.82381100	-1.79318000	0.22742300
C	1.81144100	0.06722700	-0.91472200
C	4.08694300	-1.35924400	-0.18037900
H	2.74995600	-2.69566700	0.84225900
C	3.07061100	0.50878900	-1.32289600
H	0.92591000	0.63717300	-1.20848100
C	4.21242300	-0.20562800	-0.95574200
H	4.97769700	-1.92139700	0.11170100
H	3.16147000	1.41452600	-1.92809700
H	5.20057400	0.13752000	-1.27264000
C	0.04414900	-2.57135700	2.02733900
H	-0.96134700	-2.85868100	2.37568300
H	0.63796400	-3.49439900	1.92377800
H	0.51174900	-1.95011600	2.80867900

TS11-1e-2a-3a

imaginary frequency = -295.51 cm⁻¹

Si	-0.40236000	0.35197300	0.09268900
O	0.45027700	-0.61143900	-0.94153300
C	0.39758200	-2.48215500	-1.14177800
O	1.26071900	-2.83688500	-0.20757000
C	0.85087000	-2.48924800	-2.57579100
H	1.86519100	-2.08441200	-2.66126800
H	0.18173800	-1.90810900	-3.21905800
H	0.86488300	-3.53532700	-2.91942500
N	-0.85578000	-2.89750200	-0.88233900
H	-1.07117000	-2.96878100	0.10772200
C	-1.97091000	-2.64101100	-1.76525200
H	-2.87992100	-3.04424100	-1.30312000
H	-1.83424400	-3.14197500	-2.73426600
H	-2.12050500	-1.56173400	-1.94413800
H	2.13857800	-2.38905400	-0.37299800
C	3.68136200	-0.49437900	-1.11323200
O	3.53016300	-1.60108700	-0.59427100

C	5.03707000	0.13449100	-1.23468400
H	5.82264900	-0.62657800	-1.16157600
H	5.15518700	0.84825500	-0.40361100
H	5.12439800	0.69653900	-2.17361800
O	2.70771100	0.23110200	-1.57077600
H	1.75850100	-0.15213700	-1.32454000
C	-1.43834600	1.57034500	-0.90486700
C	-2.40425700	2.40404200	-0.31482400
C	-1.24221400	1.66861900	-2.29140500
C	-3.14180900	3.30765400	-1.08054800
H	-2.59338700	2.34577000	0.76190100
C	-1.97849100	2.56903300	-3.06371700
H	-0.49947400	1.02556500	-2.77216000
C	-2.92910500	3.39119000	-2.45810900
H	-3.88814000	3.94695300	-0.60226100
H	-1.81024400	2.62886900	-4.14205600
H	-3.50733700	4.09689700	-3.05988700
C	-1.54588000	-0.65186800	1.21748300
C	-1.02369400	-1.33043100	2.33272600
C	-2.91467500	-0.80256800	0.94189500
C	-1.83025000	-2.14552200	3.12727700
H	0.03594300	-1.23172600	2.58598100
C	-3.72906400	-1.61156500	1.73639900
H	-3.35808800	-0.28788800	0.08469900
C	-3.18643400	-2.28894900	2.82860000
H	-1.40013700	-2.66854600	3.98506500
H	-4.79122200	-1.71500700	1.50060700
H	-3.82084500	-2.92548900	3.45050400
C	0.83335400	1.27489200	1.18687400
C	1.98940600	0.60587700	1.62543300
C	0.65118100	2.60452700	1.59746100
C	2.92518900	1.23629000	2.44569600
H	2.16874100	-0.42685300	1.31326900
C	1.58377300	3.24243500	2.41838300
H	-0.22973100	3.16341100	1.26818900
C	2.72312500	2.55906900	2.84415100
H	3.81714800	0.69513300	2.77173200
H	1.42206400	4.27964400	2.72279300
H	3.45525900	3.05757400	3.48441900

TS11-1f-2a-3a

imaginary frequency = -387.63 cm⁻¹

Si	0.53055000	-0.27738700	0.98690600
O	-0.57005100	0.22149300	-0.15137900
C	-1.55852300	1.85198300	-0.14758500
O	-2.45469500	1.58205400	0.77904700
C	-1.96366600	1.76063200	-1.59230700
H	-2.60496200	0.88782700	-1.75662500
H	-1.09645200	1.69504400	-2.25766300
H	-2.53903100	2.66739500	-1.83618600
N	-0.71279100	2.83389400	0.20999000
H	-0.59431900	2.92979300	1.21347200
C	0.39172000	3.27302600	-0.61235700
H	0.92417100	4.07140400	-0.08127800
H	0.03903800	3.68189900	-1.56964200
H	1.10318000	2.45436100	-0.81734800
H	-2.93212100	0.72716000	0.55429300
C	-3.18088300	-1.58654700	-0.42560000
O	-3.63626700	-0.66133800	0.25227500
C	-3.98939400	-2.82419300	-0.69360700
H	-5.01290300	-2.70876800	-0.31907800
H	-3.50897000	-3.68051600	-0.19620100
H	-4.00104300	-3.03615900	-1.77232100
O	-2.00196500	-1.58747000	-0.95491800
H	-1.37728200	-0.75818600	-0.61809100
C	2.20655300	-0.48485700	0.13030000
C	3.37904600	-0.74982400	0.85855500
C	2.31121200	-0.38623100	-1.26626200
C	4.60818500	-0.91310500	0.21798600
H	3.33937500	-0.83172500	1.94992800
C	3.53760700	-0.54780100	-1.91484500
H	1.41168000	-0.17789400	-1.85312200
C	4.68921100	-0.81200900	-1.17255200
H	5.50760900	-1.11853700	0.80433600
H	3.59572500	-0.46687700	-3.00350700
H	5.65081500	-0.93888600	-1.67642700
C	0.74292800	0.93667200	2.40579700
H	-0.22799500	1.19037800	2.86190100
H	1.36653400	0.47801100	3.19146200
H	1.24098800	1.86813800	2.09287700
C	-0.01269700	-1.93281100	1.69170100
H	-0.97732300	-1.83123400	2.21711400

H	-0.13604600	-2.68564400	0.89715100
H	0.72719700	-2.31835000	2.41281400

TS11-1f-2a-3a'

imaginary frequency = -447.88 cm⁻¹

Si	-0.11724800	-1.24324400	0.54788900
O	0.72000300	0.17772100	0.81324800
C	0.43428300	1.78817800	-0.14628400
O	0.75007000	1.40183900	-1.36853600
C	1.43443700	2.59606100	0.63438800
H	2.44890600	2.21868700	0.46593300
H	1.22135400	2.57761300	1.70843200
H	1.38504300	3.63476600	0.27270500
N	-0.86456800	2.11424900	-0.01691000
H	-1.48101000	1.60653400	-0.64448200
C	-1.44684400	2.55271900	1.23089100
H	-2.51985000	2.71748100	1.07400400
H	-1.00516300	3.50287900	1.56419800
H	-1.32112300	1.80292800	2.03031400
H	1.67656200	1.01494000	-1.36764700
C	3.65070100	-0.20858400	-0.36578000
O	3.11475500	0.33997500	-1.33372400
C	5.02313800	-0.80971300	-0.48434100
H	5.52677300	-0.45015500	-1.38928900
H	4.91911100	-1.90476700	-0.54226900
H	5.62222400	-0.58080100	0.40747600
O	3.10261400	-0.33142900	0.79705200
H	2.03340400	-0.05139100	0.81452100
C	-1.87016600	-0.86000200	-0.05281600
C	-2.90596200	-0.59199200	0.85770700
C	-2.16957700	-0.78231500	-1.42396300
C	-4.18380500	-0.23942300	0.42070600
H	-2.71473100	-0.64801700	1.93359600
C	-3.44422000	-0.42731100	-1.86920000
H	-1.39131200	-0.98794400	-2.16475700
C	-4.45388700	-0.15150000	-0.94569600
H	-4.97202900	-0.03103200	1.14866500
H	-3.65156300	-0.36701900	-2.94067000
H	-5.45248900	0.12810100	-1.29083400
C	0.76158700	-2.28122100	-0.74791000
H	1.73332900	-2.63199100	-0.36289300

H	0.17106800	-3.16957900	-1.02701400
H	0.95725600	-1.69576000	-1.65995600
C	-0.21463400	-2.18801400	2.16469200
H	0.79808500	-2.44897200	2.51432400
H	-0.69661600	-1.59152400	2.95621100
H	-0.78362300	-3.12544700	2.04865400

7-1a-2b

Si	1.22831000	-0.25550600	-0.67821400
H	0.81482700	-0.45154900	-2.09466800
C	1.12692500	1.55907100	-0.25297900
C	0.55909200	2.48000300	-1.14797000
C	1.60368000	2.02943900	0.98305600
C	0.46845200	3.83310700	-0.81884600
H	0.17920600	2.14007900	-2.11618700
C	1.51003800	3.37973000	1.31588600
H	2.05691800	1.33533100	1.69758700
C	0.94252700	4.28225100	0.41386900
H	0.02621600	4.53855200	-1.52623700
H	1.88279800	3.73120700	2.28090600
H	0.87126100	5.34134100	0.67359500
C	2.90841600	-0.97201900	-0.29551900
C	3.05727200	-2.22562300	0.31865000
C	4.06463000	-0.25330300	-0.64401200
C	4.32549500	-2.74752200	0.57484300
H	2.17197200	-2.79846200	0.60666500
C	5.33305500	-0.77478800	-0.39128600
H	3.97992700	0.73103300	-1.11560700
C	5.46391800	-2.02322400	0.21920600
H	4.42550600	-3.72311600	1.05667500
H	6.22246900	-0.20329200	-0.66714600
H	6.45731000	-2.43163700	0.42063000
O	0.17083000	-1.16987500	0.30070800
C	-1.15918500	-1.23572900	0.44572600
O	-1.64277700	-2.02059300	1.21591800
C	-1.95585400	-0.26660200	-0.40932300
H	-1.61955900	0.75098100	-0.15033600
H	-1.66832500	-0.43144200	-1.46105300
C	-3.44542200	-0.39167300	-0.23816400
C	-4.19727400	-1.20696700	-1.09106300
C	-4.10000900	0.28832500	0.79552200

C	-5.57481900	-1.34199900	-0.91489600
H	-3.69687600	-1.74207500	-1.90295100
C	-5.47646600	0.15517800	0.97465200
H	-3.52239200	0.92903300	1.46773500
C	-6.21827100	-0.66137600	0.11926600
H	-6.14859600	-1.98123000	-1.59045200
H	-5.97339400	0.69342700	1.78552400
H	-7.29721800	-0.76502800	0.25760900

7-1a-2c

Si	0.92141000	0.03065300	-0.96308400
H	0.89123100	0.19955200	-2.43853800
C	1.54289700	1.58260400	-0.13475500
C	1.56778400	2.80568900	-0.82402200
C	1.97002600	1.55748100	1.20387700
C	2.00854800	3.97037100	-0.19553900
H	1.23683900	2.85382800	-1.86527200
C	2.40700200	2.72119600	1.83576300
H	1.96613400	0.61731800	1.76379800
C	2.42711100	3.92835900	1.13509300
H	2.02486500	4.91449600	-0.74523600
H	2.73494400	2.68639000	2.87740700
H	2.77208300	4.84042700	1.62845600
C	1.87434500	-1.48605800	-0.43065300
C	1.23142300	-2.71081500	-0.18691900
C	3.27228100	-1.42742800	-0.29956600
C	1.96259200	-3.84165800	0.17762100
H	0.14459600	-2.78469800	-0.27909900
C	4.00561600	-2.55747000	0.06196800
H	3.80246600	-0.48620900	-0.47606900
C	3.35038400	-3.76618400	0.30173000
H	1.44599700	-4.78587800	0.36622600
H	5.09195100	-2.49368100	0.16021400
H	3.92349700	-4.65175700	0.58724600
O	-0.68061200	-0.32837300	-0.43801200
C	-1.71709300	0.44466000	-0.75453400
O	-1.60373200	1.42718100	-1.45281800
C	-3.01182500	-0.01286800	-0.17122400
C	-3.08251700	-1.12263300	0.67962900
C	-4.17490600	0.70037000	-0.48669100
C	-4.31070600	-1.51554300	1.20740300

H	-2.17413000	-1.67363700	0.92774600
C	-5.40059600	0.30353900	0.04054300
H	-4.10548200	1.56545300	-1.14905200
C	-5.46862900	-0.80446000	0.88796600
H	-4.36477900	-2.38061700	1.87196900
H	-6.30691000	0.86004900	-0.20811500
H	-6.43072500	-1.11556400	1.30200100

7-1a-2d

Si	1.33584800	-0.40855500	-0.46547300
H	0.69549200	-0.72644300	-1.76929000
C	0.48501500	1.05258900	0.31952700
C	-0.58975600	1.68839600	-0.32124300
C	0.89734300	1.52880500	1.57572400
C	-1.24198400	2.76643000	0.27765700
H	-0.93086300	1.33590800	-1.29875300
C	0.24545200	2.60399800	2.17757100
H	1.73650100	1.05581300	2.09523900
C	-0.82543500	3.22238900	1.52868700
H	-2.07972500	3.24836100	-0.23197600
H	0.57342700	2.96218000	3.15628000
H	-1.33651000	4.06475600	2.00128900
C	3.18347100	-0.17689200	-0.57959600
C	4.08334600	-1.22886600	-0.34401600
C	3.69939200	1.08227700	-0.93004800
C	5.45907500	-1.02806700	-0.45721400
H	3.70791700	-2.21549100	-0.06024000
C	5.07450600	1.28352600	-1.04733700
H	3.02287100	1.92384500	-1.10994200
C	5.95554100	0.22753000	-0.81026200
H	6.14703800	-1.85520400	-0.26651500
H	5.45953800	2.26889700	-1.32029500
H	7.03339600	0.38476400	-0.89776400
O	1.18409500	-1.80357800	0.53199700
C	0.10383100	-2.43383300	0.98547700
O	0.18415000	-3.38010400	1.72390300
C	-1.16844900	-1.89512100	0.52816900
C	-2.22132900	-1.42012600	0.15476600
C	-3.45035300	-0.83316400	-0.28924400
C	-3.51122500	-0.19337300	-1.53930800
C	-4.59205800	-0.87990800	0.52872000

C	-4.70151800	0.39156100	-1.96077900
H	-2.62349500	-0.16301500	-2.17413400
C	-5.77590400	-0.28755200	0.09894000
H	-4.54173400	-1.37836300	1.49874300
C	-5.83227700	0.34759900	-1.14298600
H	-4.74668500	0.88616100	-2.93333200
H	-6.66114900	-0.32231400	0.73746900
H	-6.76395300	0.81018800	-1.47658800

7-1a-2e

Si	-1.75340400	-0.02362500	-1.03121600
H	-2.06134600	-0.24681000	-2.46759900
C	-2.65747600	-1.26422800	0.03118900
C	-3.20373700	-2.43128700	-0.52638600
C	-2.78559200	-1.05868200	1.41543200
C	-3.86035100	-3.36580700	0.27458000
H	-3.11565000	-2.61806000	-1.60044100
C	-3.43735600	-1.99337200	2.21930900
H	-2.37445300	-0.15521000	1.87613200
C	-3.97612400	-3.14748800	1.64810400
H	-4.28296900	-4.26805000	-0.17404400
H	-3.52781500	-1.81985200	3.29428800
H	-4.48959200	-3.87951500	2.27645200
C	-2.09542700	1.73295000	-0.49009900
C	-1.07783300	2.69861600	-0.42397000
C	-3.40620100	2.12028000	-0.16318500
C	-1.36095700	4.01020200	-0.04126700
H	-0.04882100	2.42408700	-0.67084700
C	-3.69231000	3.43146700	0.21639100
H	-4.22044200	1.38946200	-0.19761600
C	-2.66838200	4.37790200	0.27871600
H	-0.55691500	4.74856000	0.00793800
H	-4.71707000	3.71469900	0.46835400
H	-2.89046400	5.40498400	0.57871600
O	-0.05287600	-0.16058500	-0.81695600
C	0.62112500	-1.24474700	-1.21253600
O	0.07610600	-2.17286300	-1.77114700
C	2.06552000	-1.21948900	-0.91440100
H	2.61233800	-2.09213000	-1.27885700
C	2.65821500	-0.22227600	-0.23680200
H	2.03016100	0.60776200	0.10259000

C	4.08115200	-0.12045000	0.11580800
C	4.50571200	0.98209500	0.87472000
C	5.03499300	-1.07796700	-0.27187300
C	5.84286500	1.12601300	1.24060500
H	3.77335600	1.73365300	1.18100000
C	6.36974500	-0.93283700	0.09247000
H	4.73448200	-1.94454000	-0.86475300
C	6.77826600	0.16841100	0.85003200
H	6.15467600	1.98966500	1.83239400
H	7.09972700	-1.68432000	-0.21696300
H	7.82755100	0.27810900	1.13408500

7-1a-2f

Si	-0.49823900	0.00303000	-0.96731400
H	-0.41937800	-0.13232300	-2.44155200
C	-0.29104800	1.75561400	-0.36644000
C	0.43724800	2.04688600	0.79888500
C	-0.91342200	2.81092800	-1.05323900
C	0.54072800	3.35770200	1.26387300
H	0.93683900	1.24686300	1.35317200
C	-0.81166300	4.12165200	-0.58785600
H	-1.48503700	2.61543800	-1.96604200
C	-0.08472900	4.39529400	0.57162600
H	1.11240400	3.56954800	2.17048400
H	-1.29950800	4.93284700	-1.13331600
H	-0.00358100	5.42230700	0.93580400
C	-2.01530700	-0.83823600	-0.29538600
C	-2.62465400	-1.88811800	-1.00295700
C	-2.56813200	-0.44439600	0.93469100
C	-3.75122000	-2.53173000	-0.49118700
H	-2.22000600	-2.21038200	-1.96727400
C	-3.69348300	-1.08791900	1.44805200
H	-2.11814400	0.37667500	1.50077300
C	-4.28487300	-2.13187700	0.73484000
H	-4.21613700	-3.34611500	-1.05172600
H	-4.11253900	-0.77171300	2.40615600
H	-5.16884300	-2.63423300	1.13533300
O	0.82926400	-0.89845200	-0.28325300
C	2.08242800	-0.68527600	-0.60322700
O	2.49552100	0.03120700	-1.47081000
C	3.02203100	-1.48501900	0.32493900

F	2.73220400	-2.78341800	0.29087800
F	4.28609200	-1.32501500	-0.03255200
F	2.88254300	-1.06338900	1.58316300

7-1b-2a

Si	-0.68221400	0.15449600	0.58153000
H	-0.53709700	-0.27141200	2.00615000
C	-0.49012700	2.00833100	0.42107900
H	-1.37110800	2.45619900	0.91618800
H	0.37930700	2.32829700	1.01986300
C	-2.27193000	-0.48600000	-0.15523900
H	-3.09643600	0.04967000	0.34897700
H	-2.30701800	-0.16414100	-1.21076300
C	-0.36839600	2.51927600	-1.01699500
H	-0.26929000	3.61562100	-1.04432200
H	0.51425900	2.09634000	-1.52243800
H	-1.25123100	2.25458100	-1.62041100
C	-2.47286400	-1.99951200	-0.05078800
H	-3.42777900	-2.30968200	-0.50322100
H	-1.66880200	-2.54726700	-0.56662900
H	-2.48094700	-2.33571000	0.99855800
O	0.54750200	-0.64516400	-0.30925600
C	1.87674800	-0.73167000	-0.18923100
C	2.50275900	0.07096000	0.92090200
H	2.40691800	1.14470000	0.69628600
H	2.00086700	-0.11830200	1.88187800
H	3.56620100	-0.18020800	1.00694000
O	2.50699900	-1.41358000	-0.95660000

7-1c-2a

Si	-0.60790600	-1.02105300	0.04760200
H	-0.88520400	-1.80496400	1.28136400
H	-0.89732500	-1.86596300	-1.14209700
C	1.12890300	-0.33947200	0.01685100
C	1.37625400	1.04183500	0.01793800
C	2.22349300	-1.22039700	-0.00819800
C	2.68337800	1.53020400	-0.00520200
H	0.53902200	1.74438200	0.03612700
C	3.52961500	-0.73308100	-0.03109400
H	2.06349600	-2.30374300	-0.01085800
C	3.76027400	0.64394400	-0.02971200

H	2.86122300	2.60829500	-0.00448000
H	4.37075300	-1.43013100	-0.05073600
H	4.78369700	1.02646900	-0.04822200
O	-1.61939200	0.34216200	0.02376900
C	-2.95508300	0.50177700	-0.00920200
C	-3.76538700	-0.76374100	-0.06927800
H	-3.51993200	-1.32801800	-0.98278900
H	-3.53833700	-1.40564700	0.79656900
H	-4.83464700	-0.52339900	-0.06994700
O	-3.42070000	1.60922000	0.00573400

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Si	0.58080600	0.64878100	-0.54722700
H	0.93237400	0.38874200	-1.97126800
C	-1.19327700	0.15292300	-0.23571600
C	-2.01708000	0.89105900	0.62962600
C	-1.73182100	-0.98548500	-0.86001100
C	-3.33594100	0.50222900	0.86845100
H	-1.62982400	1.78470300	1.12774100
C	-3.04855000	-1.37805800	-0.62229000
H	-1.11741600	-1.57822900	-1.54512600
C	-3.85178700	-0.63335200	0.24341800
H	-3.96324100	1.08809200	1.54459900
H	-3.45143700	-2.26606900	-1.11538000
H	-4.88462300	-0.93839800	0.42926300
C	0.94695800	2.39509500	-0.03105000
H	0.77082100	2.53235300	1.04772100
H	1.99435100	2.66002900	-0.24387400
H	0.30046100	3.09970500	-0.57888600
O	1.51270200	-0.42630600	0.40489500
C	2.80658700	-0.77334600	0.41890700
C	3.66438900	-0.20055100	-0.67809900
H	3.28592800	-0.51791700	-1.66186000
H	3.64404900	0.89980700	-0.64975500
H	4.69776300	-0.54546700	-0.55859400
O	3.21887800	-1.51286500	1.27475200

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Si	-0.07526100	-0.05200400	0.27043200
C	1.17065000	-1.20474000	-0.52258700
C	1.43894100	-1.12547300	-1.89987500

C	1.81102000	-2.20755500	0.22373300
C	2.31961100	-2.01780700	-2.51124000
H	0.95974000	-0.35356900	-2.50980200
C	2.69561000	-3.09872200	-0.38413500
H	1.62151400	-2.30089500	1.29710200
C	2.95050600	-3.00480600	-1.75273000
H	2.51707700	-1.94033500	-3.58308000
H	3.18736000	-3.87024300	0.21316800
H	3.64339800	-3.70239000	-2.22957500
C	-1.83361600	-0.64251500	0.02484300
C	-2.63012900	-1.08462600	1.09180700
C	-2.37938500	-0.66052900	-1.27034200
C	-3.93474300	-1.53034000	0.87238200
H	-2.22571700	-1.07939500	2.10712900
C	-3.68121700	-1.10695200	-1.49255400
H	-1.78469300	-0.31933500	-2.12402300
C	-4.46130200	-1.54207900	-0.41915600
H	-4.54278100	-1.86932300	1.71472800
H	-4.09004200	-1.11415500	-2.50579900
H	-5.48273000	-1.89051300	-0.59110900
C	0.11567900	1.70637800	-0.34573100
C	-0.97377200	2.59109900	-0.27077700
C	1.33079400	2.18917500	-0.86017100
C	-0.85232300	3.91585600	-0.68991400
H	-1.93552400	2.24326700	0.11828800
C	1.45514700	3.51225700	-1.28302000
H	2.19745400	1.52578400	-0.93162400
C	0.36299200	4.37699600	-1.19740300
H	-1.70963800	4.58989000	-0.62338600
H	2.40762300	3.86998900	-1.68111700
H	0.45887300	5.41384700	-1.52898600
O	0.12085000	-0.14568000	1.96070900
C	1.08476900	0.15159900	2.84676600
C	2.27180800	0.90766100	2.31700900
H	2.71179100	0.39554000	1.44822100
H	1.95217900	1.90884700	1.98964600
H	3.02729100	1.00769700	3.10474200
O	0.95092900	-0.17130900	3.99779100

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Si	-0.51560800	0.72287500	0.26229600
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C	1.25935900	0.14563600	0.05589700
C	1.76427300	-0.89516300	0.85539100
C	2.12220100	0.73305900	-0.88330700
C	3.07998900	-1.33631900	0.71877800
H	1.12194900	-1.37519200	1.60038800
C	3.44172900	0.29762600	-1.02209400
H	1.76585600	1.54636700	-1.52229700
C	3.92173100	-0.73853100	-0.22144800
H	3.45195500	-2.14785500	1.34915200
H	4.09681700	0.76926600	-1.75878200
H	4.95405000	-1.08094400	-0.32842700
C	-0.91104400	0.99936900	2.06192800
H	-1.95189400	1.33088200	2.19266100
H	-0.76699000	0.07476200	2.64353300
H	-0.24425000	1.77038000	2.48186100
C	-0.88837700	2.18551200	-0.82627800
H	-0.72624900	1.94850400	-1.88974800
H	-1.93644000	2.49493300	-0.69903300
H	-0.24311200	3.03945100	-0.56311700
O	-1.41426800	-0.65239800	-0.29334400
C	-2.74442600	-0.70378500	-0.31338100
O	-3.44023900	0.22216400	0.03834300
C	-3.26630900	-2.01967800	-0.81280400
H	-2.88307000	-2.20722100	-1.82663200
H	-2.89653700	-2.83009100	-0.16736500
H	-4.36227800	-2.01797800	-0.82041600

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C	0.38932100	-0.76322000	0.07974200
O	0.23130900	-1.59743600	-0.98466000
N	1.77981800	-0.16883200	-0.05161800
H	2.46658900	-1.02238000	-0.08456100
C	2.20656300	0.80363300	0.98048200
H	2.37828200	0.24180600	1.90870500
H	0.80088100	-2.43557600	-0.86088700
H	1.80680300	0.27296900	-0.97736800
O	3.37685600	-2.22933200	-0.03296400
C	2.93886400	-3.37246100	-0.34199800
O	1.75782800	-3.62120200	-0.68149700
C	3.93401800	-4.51583200	-0.33105500
H	4.50631100	-4.49018500	-1.27244000

H	4.64945300	-4.40229300	0.49492100
H	3.42314100	-5.48499500	-0.26290900
O	-0.48370100	0.30182100	-0.03294100
Si	-1.96620000	0.22397100	-0.84597300
H	-1.76092300	0.01534700	-2.30434600
C	-2.72066400	1.90489000	-0.51020400
C	-4.04941500	2.15834100	-0.89177200
C	-1.99623800	2.93789400	0.10483500
C	-4.63564200	3.40351400	-0.66691000
H	-4.64411300	1.37231700	-1.36891200
C	-2.58013700	4.18518500	0.33261500
H	-0.96152600	2.76566200	0.41245700
C	-3.90020000	4.41929300	-0.05319500
H	-5.67049000	3.58202200	-0.96899500
H	-2.00197400	4.97742800	0.81454200
H	-4.35878600	5.39508600	0.12513200
C	-3.03852700	-1.14929600	-0.16135000
C	-3.77370000	-0.96290200	1.02128700
C	-3.08577100	-2.40606100	-0.78573500
C	-4.52865600	-2.00128900	1.56675000
H	-3.75916300	0.00680600	1.52855100
C	-3.84184500	-3.44626600	-0.24499100
H	-2.51740000	-2.58060300	-1.70359400
C	-4.56259500	-3.24457900	0.93315700
H	-5.09321200	-1.84012600	2.48839600
H	-3.86847000	-4.41839700	-0.74331200
H	-5.15410700	-4.05905700	1.35875100
C	0.24926100	-1.45776300	1.42605500
H	-0.71888900	-1.97634400	1.43765000
H	1.04866100	-2.19768800	1.56851200
H	0.26871900	-0.73495700	2.25168200
H	1.38455900	1.51113900	1.14636300
C	3.46034200	1.52870800	0.55908000
C	4.64196800	0.81980700	0.30002300
C	3.45665100	2.92042900	0.42457800
C	5.79700400	1.49690700	-0.08669900
H	4.65094100	-0.27062400	0.38859000
C	4.61613100	3.59831700	0.04443900
H	2.53765400	3.47929400	0.62085900
C	5.78797500	2.88781200	-0.21259200
H	6.71213600	0.93499000	-0.28852200

H	4.60082300	4.68628700	-0.05456600
H	6.69558100	3.41712900	-0.51251200

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C	0.30974300	-0.74037600	0.15043300
O	0.06134600	-1.64372100	-0.83377400
N	1.69710000	-0.12108100	-0.14416200
H	2.34820700	-0.98752200	-0.18273300
C	2.18637800	0.78313400	0.93412000
H	2.28655000	0.17894900	1.84362500
H	0.64035400	-2.48212100	-0.71080100
O	3.25486400	-2.23970100	-0.17489500
C	2.78700400	-3.39771200	-0.35072100
O	1.57835500	-3.66045300	-0.56144600
C	3.77554300	-4.54632700	-0.30443400
H	4.51575800	-4.42206100	-1.10970400
H	4.32622700	-4.52214400	0.64773600
H	3.27290800	-5.51518600	-0.41712400
O	-0.59149200	0.29933700	0.07183700
Si	-2.05654300	0.22223400	-0.77125400
H	-1.82550000	0.00158600	-2.22406800
C	-2.79914900	1.91429200	-0.46328200
C	-4.11505900	2.18183800	-0.87825100
C	-2.07671700	2.94243200	0.16224300
C	-4.69048500	3.43591900	-0.67616400
H	-4.70817700	1.39997700	-1.36416700
C	-2.64977400	4.19873600	0.36719900
H	-1.05261700	2.75836000	0.49709200
C	-3.95701200	4.44678500	-0.05196600
H	-5.71549300	3.62537700	-1.00405500
H	-2.07337800	4.98691900	0.85783900
H	-4.40717500	5.42957000	0.10854400
C	-3.16022500	-1.13012200	-0.09545600
C	-3.89527700	-0.93106200	1.08523700
C	-3.24411500	-2.37925800	-0.73108900
C	-4.68661300	-1.94944500	1.61699500
H	-3.85365800	0.03349100	1.60085600
C	-4.03750500	-3.39888700	-0.20493200
H	-2.67730200	-2.56347000	-1.64801300
C	-4.75832500	-3.18466500	0.97098100
H	-5.25082800	-1.77844200	2.53708800

H	-4.09341200	-4.36472600	-0.71299700
H	-5.37951500	-3.98290500	1.38493000
C	0.29728400	-1.36668200	1.53784800
H	-0.63861700	-1.93551000	1.62338400
H	1.14232800	-2.05581700	1.67149000
H	0.31274800	-0.60637400	2.32775900
H	1.41398400	1.54558100	1.10227300
C	3.51128100	1.42874200	0.61187700
C	4.66733100	0.65018600	0.46164000
C	3.60112500	2.81663500	0.47233700
C	5.88899900	1.25553900	0.17377300
H	4.59964200	-0.43839200	0.54499600
C	4.82659200	3.42334300	0.19184100
H	2.70214600	3.42867800	0.58447500
C	5.97248700	2.64364200	0.04129400
H	6.78390300	0.64011400	0.05381500
H	4.88352700	4.50944300	0.08761300
H	6.93217600	3.11651000	-0.18078500
C	1.71742100	0.51827100	-1.47542600
H	1.18214100	1.47522000	-1.43811300
H	2.75763100	0.68550000	-1.77521000
H	1.23716900	-0.15776000	-2.18940400

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C	-0.51583500	-0.59649900	-0.41644200
O	-0.35344000	-1.49721000	-1.43136000
N	0.72428300	0.28713500	-0.45143300
H	1.53082300	-0.31901700	-0.02961600
C	0.68730700	1.64492000	0.14745100
H	0.62501200	1.53370800	1.23623800
H	0.46061000	-2.06530600	-1.24547300
H	0.93925800	0.38329600	-1.45083500
O	2.60096600	-1.25034500	0.47509400
C	2.74285700	-2.28497200	-0.23509800
O	1.86152100	-2.78056000	-0.96990600
C	4.10947700	-2.97108700	-0.17435500
H	4.16534800	-3.49550200	0.79314800
H	4.15913400	-3.72533600	-0.97079200
O	-1.57879700	0.22697500	-0.68140700
Si	-2.99819100	-0.17913400	-1.50925000
H	-2.71513700	-0.33329400	-2.96132900

C	-4.10708800	1.28741500	-1.16657500
C	-5.38113800	1.35082100	-1.75578300
C	-3.71652800	2.32545300	-0.30614000
C	-6.23869900	2.41894500	-1.49466400
H	-5.71692100	0.55402900	-2.42782900
C	-4.57301800	3.39561800	-0.04226300
H	-2.73195700	2.29525600	0.16774000
C	-5.83427600	3.44345600	-0.63637500
H	-7.22619000	2.45251100	-1.96119300
H	-4.25373200	4.19497400	0.63093000
H	-6.50543600	4.28080000	-0.42983900
C	-3.73890000	-1.76097800	-0.83694500
C	-4.61797500	-1.73185200	0.25837300
C	-3.38661400	-3.00814700	-1.37845700
C	-5.12129000	-2.91286000	0.80436400
H	-4.91749700	-0.77388900	0.69457000
C	-3.88933400	-4.19068000	-0.83644600
H	-2.69967700	-3.05989300	-2.22765200
C	-4.75523600	-4.14349600	0.25754300
H	-5.80251200	-2.87297600	1.65774500
H	-3.60426400	-5.15337900	-1.26766800
H	-5.14859000	-5.06977700	0.68365100
C	-0.65246400	-1.31981400	0.93668800
H	-1.55977000	-1.93220000	0.83076900
H	0.19774500	-2.00875800	1.02641000
H	-0.22131500	2.14653300	-0.20416200
C	1.91918000	2.42545500	-0.24346600
C	3.20219600	1.94084800	0.04988200
C	1.79067900	3.65078500	-0.90493300
C	4.33149000	2.67034000	-0.31710800
H	3.32208000	0.97781900	0.55420400
C	2.92195200	4.38576600	-1.26341400
H	0.79418200	4.03294300	-1.14220900
C	4.19457400	3.89588500	-0.97229900
H	5.32515600	2.27674400	-0.08875300
H	2.80608500	5.34246300	-1.77824900
H	5.08117700	4.46754000	-1.25681200
C	5.23344000	-1.97270900	-0.29043200
C	5.67150700	-1.54517000	-1.55042900
C	5.81249200	-1.39841100	0.84771600
C	6.66179100	-0.56977400	-1.67174700

H	5.22618200	-1.98092500	-2.44964100
C	6.80402800	-0.42397000	0.73114900
H	5.47805300	-1.71805300	1.83816000
C	7.23214800	-0.00511200	-0.52998500
H	6.98972000	-0.24928300	-2.66384600
H	7.24529400	0.01177200	1.63117600
H	8.00803100	0.75874500	-0.62215400
C	-0.74681700	-0.44939900	2.16068200
C	0.35198100	-0.31795800	3.01890300
C	-1.91470400	0.26919900	2.44574300
C	0.29341400	0.52852900	4.12631400
H	1.26998300	-0.86799900	2.79431600
C	-1.97384900	1.12017800	3.54850900
H	-2.78493700	0.16406700	1.79391400
C	-0.86831500	1.25501900	4.39060900
H	1.16111600	0.62379100	4.78365800
H	-2.89034900	1.67908100	3.75334600
H	-0.91459900	1.92209600	5.25482700

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C	-0.29421300	0.12117500	-0.42975800
O	0.11068100	-0.57755500	-1.52264700
N	0.61875500	1.33273600	-0.33517700
H	1.63771600	0.95861400	-0.21583100
C	0.33352600	2.35253300	0.70494900
H	0.59210800	1.91456200	1.67701600
H	1.09104300	-0.84817500	-1.48478200
H	0.57538100	1.77439500	-1.26165500
O	3.03765300	0.39003900	-0.00457000
C	3.35112200	-0.62221200	-0.68079900
O	2.58163200	-1.23653800	-1.46065100
O	-1.55487900	0.62857500	-0.65259300
Si	-2.81802300	-0.27376200	-1.34375300
H	-2.68662700	-0.26193900	-2.82537600
C	-4.35332200	0.63257600	-0.77975900
C	-5.61628100	0.19770300	-1.21639900
C	-4.28982000	1.72726500	0.09616300
C	-6.78016000	0.83762900	-0.79225500
H	-5.69972700	-0.65596200	-1.89726400
C	-5.45331600	2.36957600	0.52325200
H	-3.31844600	2.08331200	0.44949500

C	-6.69897300	1.92547200	0.07942600
H	-7.75422100	0.48658500	-1.14138500
H	-5.38655900	3.21994700	1.20623500
H	-7.61027300	2.42752700	0.41365000
C	-2.78737700	-2.03966800	-0.72565300
C	-3.34339700	-2.37283400	0.52019900
C	-2.12914500	-3.04296600	-1.45387200
C	-3.22720700	-3.66410700	1.03359100
H	-3.86464400	-1.61135200	1.10827800
C	-2.01536300	-4.33738000	-0.94659100
H	-1.68290100	-2.80991000	-2.42454900
C	-2.55922100	-4.64681300	0.30077600
H	-3.65629400	-3.90459300	2.00926500
H	-1.49605000	-5.10648300	-1.52347100
H	-2.46440900	-5.65850100	0.70299400
H	-0.74171000	2.56861600	0.68352400
C	1.13954000	3.59887200	0.44375600
C	2.49848300	3.64746800	0.77828700
C	0.54495300	4.70878900	-0.16552800
C	3.24933600	4.79024900	0.50829500
H	2.97072500	2.77777300	1.24209000
C	1.29542900	5.85428400	-0.43264200
H	-0.51551700	4.67496800	-0.42980200
C	2.64853500	5.89625300	-0.09616000
H	4.30892100	4.81894000	0.77310100
H	0.82040300	6.71722300	-0.90516500
H	3.23695200	6.79293300	-0.30494400
C	4.76141800	-1.14613400	-0.53733400
C	5.16930400	-2.27375000	-1.25860700
C	5.66976000	-0.51142900	0.31711000
C	6.46893300	-2.76068400	-1.12834300
H	4.45193000	-2.76147400	-1.92130400
C	6.96976300	-0.99751100	0.44851800
H	5.34335100	0.36703800	0.87681000
C	7.37095900	-2.12276200	-0.27439700
H	6.78053100	-3.64160900	-1.69476200
H	7.67416700	-0.49739000	1.11763100
H	8.39007300	-2.50382800	-0.17188700
C	-0.25135300	-0.66804700	0.88631500
C	0.51096400	-1.83244800	0.99552600
C	-1.03108300	-0.25534000	1.97249900

C	0.50167800	-2.56942000	2.18014500
H	1.10900700	-2.17720400	0.15113500
C	-1.03447700	-0.98758600	3.15735900
H	-1.66180500	0.63086400	1.88462900
C	-0.26754200	-2.14843300	3.26402300
H	1.09582400	-3.48334900	2.25043300
H	-1.65072100	-0.65693700	3.99644700
H	-0.27660300	-2.72915300	4.18936300

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C	-1.32731000	0.66054600	-1.01040600
O	-1.02283400	0.37919500	-2.30333200
N	-1.04327600	2.13681900	-0.78843800
H	0.00239500	2.24717100	-1.00976500
C	-1.36598300	2.67455300	0.55747800
H	-0.78561900	2.08671900	1.28213000
H	-0.01472300	0.29366700	-2.41088700
H	-1.56658300	2.64833700	-1.51027000
O	1.58832700	2.10252800	-1.18764400
C	2.09670500	1.06480400	-1.67119500
O	1.53897200	0.22127200	-2.40786100
O	-2.66667100	0.49242000	-0.77953800
Si	-3.55421400	-0.88057000	-1.27576000
H	-3.82907400	-0.79885900	-2.73347400
C	-5.12376000	-0.76534200	-0.27224900
C	-6.25808600	-1.49417200	-0.66698400
C	-5.18974800	-0.01206100	0.91074100
C	-7.42446900	-1.47117600	0.09723300
H	-6.23792800	-2.09039200	-1.58511500
C	-6.35611600	0.01364300	1.67635500
H	-4.31976500	0.56303600	1.23891300
C	-7.47383300	-0.71629600	1.27048100
H	-8.29855300	-2.04281900	-0.22380600
H	-6.39219600	0.60527400	2.59427500
H	-8.38750500	-0.69652900	1.86960700
C	-2.57107800	-2.42040600	-0.87609000
C	-2.64766900	-2.99889300	0.40161100
C	-1.64964300	-2.94682800	-1.79570600
C	-1.81096400	-4.05591000	0.75909100
H	-3.35852700	-2.61025600	1.13736400
C	-0.81217000	-4.00452700	-1.44150100

H	-1.56503000	-2.51286100	-2.79593400
C	-0.88778600	-4.55490900	-0.16114700
H	-1.87426000	-4.48814200	1.76060000
H	-0.09276900	-4.39674600	-2.16432900
H	-0.22408800	-5.37593300	0.12115400
H	-2.43344500	2.50135900	0.73761100
C	-1.02433800	4.13942000	0.65368200
C	0.31301200	4.55780200	0.63835900
C	-2.03853700	5.09594800	0.76088000
C	0.62682600	5.91240900	0.72713900
H	1.11092600	3.81700900	0.53847600
C	-1.72341000	6.45227700	0.85621600
H	-3.08372900	4.77577000	0.77317700
C	-0.39075900	6.86231000	0.83904200
H	1.67251600	6.22855000	0.71261200
H	-2.52385900	7.19080100	0.94278400
H	-0.14309300	7.92397600	0.91237500
C	3.49911300	0.78939800	-1.30739900
C	4.62379300	0.50738400	-0.94490000
C	5.94362300	0.14762200	-0.50908800
C	6.45996400	-1.12593300	-0.80567500
C	6.72473000	1.05595700	0.22599000
C	7.73375300	-1.48140700	-0.37061100
H	5.85466600	-1.83203700	-1.37807400
C	7.99878000	0.69285000	0.65439900
H	6.32494600	2.04523800	0.45856500
C	8.50469800	-0.57417300	0.35848000
H	8.12786800	-2.47313600	-0.60347600
H	8.60081500	1.40377000	1.22469300
H	9.50433500	-0.85597000	0.69734100
C	-0.48460400	-0.11232900	-0.06154200
C	0.25086300	-0.83283100	0.57363000
C	1.16686800	-1.72171500	1.22697900
C	2.26084100	-2.21592900	0.49586900
C	0.97456400	-2.12472500	2.55718200
C	3.15187000	-3.10114200	1.09533200
H	2.39678800	-1.89873600	-0.54036900
C	1.87121200	-3.01245200	3.14674400
H	0.12017400	-1.74340700	3.12003400
C	2.95822300	-3.50062200	2.41931000
H	4.00136600	-3.48380500	0.52547000

H	1.72006700	-3.32617600	4.18197200
H	3.65841700	-4.19680400	2.88665500

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C	-0.95853500	0.57557500	-0.56780200
O	-0.38565700	0.29094900	-1.76298100
N	-0.63358000	2.02704900	-0.25921400
H	0.45706400	2.09697100	-0.24746500
C	-1.18943600	2.59736000	0.99228500
H	-0.63678600	2.14895600	1.82850200
H	0.63287400	0.34625200	-1.71437800
H	-0.97043500	2.56573100	-1.06588300
O	1.97296700	2.08031700	-0.10082400
C	2.63471600	1.23465100	-0.76139600
O	2.15221600	0.44239200	-1.60945000
O	-2.33680600	0.53601600	-0.68817900
Si	-3.19883100	-0.66850900	-1.51382400
H	-3.00079700	-0.52291000	-2.98109100
C	-4.97124300	-0.33295000	-1.01626100
C	-5.97814400	-1.24980100	-1.36328500
C	-5.33559000	0.81828900	-0.30039600
C	-7.30748200	-1.02311400	-1.00776700
H	-5.72605300	-2.16096900	-1.91578700
C	-6.66473800	1.04699000	0.05886300
H	-4.57049000	1.54580300	-0.01685500
C	-7.65189500	0.12690000	-0.29501700
H	-8.07744400	-1.74708500	-1.28520300
H	-6.93023000	1.94723600	0.61851400
H	-8.69279700	0.30489000	-0.01370200
C	-2.63120100	-2.36705900	-0.97532300
C	-3.02889700	-2.88873700	0.26680400
C	-1.70680700	-3.09427100	-1.74050000
C	-2.50700700	-4.09332700	0.73765000
H	-3.74859400	-2.34310900	0.88526000
C	-1.18148900	-4.29929900	-1.27228600
H	-1.37389000	-2.70881800	-2.70867500
C	-1.57828100	-4.79722800	-0.03056000
H	-2.81987600	-4.48108500	1.71010500
H	-0.45526000	-4.84943200	-1.87558100
H	-1.16040400	-5.73579800	0.34185300
H	-2.24224700	2.29843600	1.06583200

C	-1.05439900	4.09882900	1.00722900
C	0.21181800	4.69915300	1.03907600
C	-2.19407100	4.90849700	0.98225400
C	0.33094400	6.08753100	1.04547200
H	1.10805800	4.07217100	1.04557600
C	-2.07411700	6.29904100	0.99576900
H	-3.18419100	4.44558800	0.95456800
C	-0.81173100	6.89046700	1.02660700
H	1.32216700	6.54648500	1.06884700
H	-2.97192000	6.92142500	0.97972700
H	-0.71651400	7.97888300	1.03539900
C	4.10598500	1.18820100	-0.48985200
H	4.47510900	1.92054900	0.23348600
C	4.91171900	0.29520900	-1.08244900
H	4.44473500	-0.40028500	-1.78867400
C	6.36273800	0.13652400	-0.89164100
C	7.02773700	-0.87944400	-1.59683700
C	7.11603200	0.95617800	-0.03253500
C	8.40047300	-1.07465000	-1.45096500
H	6.45490000	-1.52478400	-2.26834000
C	8.48633100	0.76173500	0.11295000
H	6.62757200	1.75576400	0.52888500
C	9.13440400	-0.25411800	-0.59503000
H	8.89846900	-1.87139000	-2.00854200
H	9.05592500	1.40840400	0.78470200
H	10.21036800	-0.40387600	-0.47811200
C	-0.52584500	-0.30090500	0.59240700
H	-1.07210300	-0.13310700	1.52441900
C	0.35352200	-1.29704400	0.45968400
H	0.85772400	-1.41757700	-0.50283100
C	0.70446000	-2.30559700	1.47381100
C	1.69935600	-3.24538100	1.16336400
C	0.05506200	-2.40366200	2.71562600
C	2.03842800	-4.25452200	2.06311800
H	2.20757000	-3.18343200	0.19724900
C	0.39279800	-3.41158100	3.61444500
H	-0.73491400	-1.69713800	2.97978200
C	1.38404100	-4.34196200	3.29171400
H	2.81464900	-4.97753100	1.80154600
H	-0.12635500	-3.47689400	4.57360600
H	1.64312300	-5.13480400	3.99740700

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C	0.05713500	-0.26506500	0.19557500
O	0.22488400	-1.16528900	-0.79174800
N	1.12447000	0.80146300	0.05445900
H	2.09668900	0.32777100	0.01099000
C	1.13303100	1.93705900	1.02432600
H	1.53721500	1.56435300	1.97268400
H	1.12900600	-1.64679000	-0.76485600
H	0.97458700	1.17906400	-0.89135000
O	3.48110600	-0.39818900	-0.12643100
C	3.46052300	-1.59364900	-0.46803000
O	2.49032300	-2.30614200	-0.77907000
C	4.85295100	-2.26539000	-0.55901600
O	-1.14948100	0.35006300	0.11919200
Si	-2.43609300	-0.08349200	-0.92596400
H	-1.94730200	-0.05711300	-2.32825200
C	-3.68832300	1.26101200	-0.58806000
C	-5.00087400	1.11587700	-1.06911200
C	-3.35894100	2.43242600	0.11203800
C	-5.95444900	2.11155600	-0.85990600
H	-5.29091700	0.21099200	-1.61286300
C	-4.31215200	3.42914600	0.32493700
H	-2.34647200	2.56828000	0.50097500
C	-5.61010600	3.26999800	-0.16138100
H	-6.97048100	1.98200400	-1.24032400
H	-4.04053700	4.33344700	0.87478200
H	-6.35676600	4.05029400	0.00518100
C	-3.09242400	-1.77580400	-0.49644000
C	-3.96101200	-1.94953000	0.59398300
C	-2.69608600	-2.90801500	-1.22570000
C	-4.41700800	-3.21880800	0.94810500
H	-4.28849400	-1.08390400	1.17798800
C	-3.15352600	-4.17841200	-0.87618400
H	-2.01604400	-2.80127100	-2.07550200
C	-4.01337900	-4.33402500	0.21197200
H	-5.09086400	-3.33894500	1.79974400
H	-2.83768900	-5.05051300	-1.45373100
H	-4.37077400	-5.32923700	0.48791100
C	0.16857200	-0.93767900	1.60218500
H	0.09361700	2.25438200	1.17139800

C	1.97785100	3.05936600	0.48327100
C	3.35729000	3.08475400	0.71648500
C	1.39333400	4.06668900	-0.29234200
C	4.14145400	4.10690000	0.18354500
H	3.81844000	2.29536700	1.31548000
C	2.17752600	5.08926400	-0.82508500
H	0.31561900	4.04942400	-0.47719400
C	3.55245600	5.11039600	-0.58722600
H	5.21727600	4.12089000	0.37266200
H	1.71248300	5.87424200	-1.42586500
H	4.16705400	5.91257600	-1.00260000
F	5.63733100	-1.90974500	0.45975600
F	5.46557600	-1.88587800	-1.68934200
F	4.77908100	-3.59382400	-0.56850400
F	1.42238300	-1.31001800	1.86392100
F	-0.23039100	-0.12515400	2.57739400
F	-0.59946500	-2.01856000	1.63031100

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C	-0.01088200	0.17454700	-0.61630200
O	0.81852400	-0.75191400	-1.16412400
N	0.28845100	1.47605400	-1.38106700
H	1.37001700	1.60747600	-1.29354100
H	1.78245700	-0.61746400	-0.84780000
H	0.10794200	1.24638700	-2.36607200
O	2.86192200	1.80264300	-1.04084500
C	3.58337100	0.87017700	-0.59711800
O	3.20952400	-0.31193300	-0.42285200
C	5.01058100	1.25593300	-0.20288400
H	5.34474200	2.04951900	-0.88552700
H	4.92570400	1.71618500	0.79623400
O	-1.31238100	-0.14774300	-0.90601400
Si	-1.86964400	-1.71888900	-1.22812800
H	-1.31633100	-2.22240300	-2.51250200
C	-3.72207100	-1.48669500	-1.35012900
C	-4.50914900	-2.49346800	-1.93391400
C	-4.36741900	-0.35245300	-0.83177700
C	-5.89722500	-2.37251500	-1.99731900
H	-4.03684400	-3.39016700	-2.34868300
C	-5.75611500	-0.22818000	-0.89379600
H	-3.77929000	0.44419600	-0.36928300

C	-6.52236300	-1.23827500	-1.47605700
H	-6.49360500	-3.16485800	-2.45613800
H	-6.24104200	0.66142000	-0.48445900
H	-7.60985200	-1.14196200	-1.52485300
C	-1.43523100	-2.88661200	0.17385200
C	-2.35364500	-3.13414200	1.20781100
C	-0.17912000	-3.51409000	0.23553200
C	-2.02366800	-3.96678200	2.27796900
H	-3.34418100	-2.66988500	1.18311000
C	0.15304600	-4.34901500	1.30172900
H	0.55650500	-3.33628100	-0.55292000
C	-0.76860100	-4.57355300	2.32631900
H	-2.74962400	-4.14321400	3.07522900
H	1.13538400	-4.82641800	1.33474600
H	-0.50784800	-5.22551200	3.16372500
C	0.23755200	0.34833000	0.89626200
H	0.26929700	-0.68483500	1.27415400
H	1.24527100	0.76705300	1.02847500
C	5.99369500	0.11754500	-0.16926400
C	6.00553500	-0.78942600	0.89896900
C	6.90641100	-0.07122300	-1.21350400
C	6.90197500	-1.85635000	0.92135600
H	5.29852700	-0.65581600	1.72173800
C	7.80648500	-1.13883200	-1.19565100
H	6.91285700	0.62921000	-2.05370500
C	7.80724100	-2.03531600	-0.12746500
H	6.89694800	-2.55269100	1.76392700
H	8.51241700	-1.26768200	-2.02009600
H	8.51219600	-2.87017900	-0.10949700
C	-0.77200700	1.14307900	1.68834300
C	-0.43830900	2.38997000	2.22849300
C	-2.06109700	0.64461600	1.91695400
C	-1.37761400	3.14158900	2.93412700
H	0.57028800	2.78393500	2.08290400
C	-3.00540500	1.39307000	2.61789800
H	-2.33152200	-0.34409800	1.54451300
C	-2.67004800	2.65076600	3.12114200
H	-1.09727700	4.11828100	3.33611900
H	-4.00830000	0.98778100	2.77373500
H	-3.40983500	3.24102400	3.66724200
C	-0.38732200	2.71575100	-1.02583500

C	0.39132300	3.79096800	-0.60502700
C	-1.77483600	2.81739900	-1.10837300
C	-0.23308000	4.98274600	-0.23977800
H	1.47669500	3.68385100	-0.55394700
C	-2.38935300	4.00730200	-0.72583400
H	-2.36457000	1.96874800	-1.45350800
C	-1.62211400	5.08900800	-0.28841100
H	0.37271200	5.82793100	0.09372400
H	-3.47731200	4.08947200	-0.77431600
H	-2.11064500	6.01943000	0.00930800

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C	1.04480000	-0.30825300	-0.25963200
O	1.15613000	-1.35714800	-1.11692100
N	2.07036300	0.73087500	-0.73967900
H	3.06570700	0.21988400	-0.69585000
H	2.02975000	-1.85396300	-0.94339400
H	1.86029900	0.87078500	-1.73421400
O	4.34576400	-0.45579800	-0.57762400
C	4.39751100	-1.71995700	-0.58490300
O	3.40872200	-2.48007400	-0.69726300
C	5.77420500	-2.34118300	-0.47063800
H	6.30864300	-2.19472400	-1.42283300
H	6.35682400	-1.83581600	0.31254400
H	5.71043400	-3.41656200	-0.26167100
O	-0.18681100	0.28862800	-0.40636900
Si	-1.58631500	-0.49601200	-0.94160700
H	-1.47107100	-0.86907300	-2.37704700
C	-2.90988500	0.80318300	-0.69011200
C	-4.21819100	0.55804300	-1.14045600
C	-2.64475900	2.01847800	-0.03958300
C	-5.22994400	1.49864200	-0.95043900
H	-4.45792500	-0.38188900	-1.64889700
C	-3.65546100	2.96216700	0.15230100
H	-1.63444500	2.23105600	0.31990400
C	-4.94851800	2.70326200	-0.30270800
H	-6.24173900	1.29186700	-1.30764100
H	-3.43193500	3.90334800	0.66082300
H	-5.74021100	3.44163400	-0.15317200
C	-1.93827900	-2.02620300	0.07842500
C	-2.61715800	-1.92732700	1.30425000

C	-1.49814300	-3.29204400	-0.34122400
C	-2.84492100	-3.05725800	2.09027200
H	-2.97611900	-0.95443100	1.65422500
C	-1.72683700	-4.42453600	0.44015700
H	-0.96145500	-3.39631600	-1.28825100
C	-2.39926200	-4.30716400	1.65784600
H	-3.37351900	-2.96283100	3.04195800
H	-1.37882100	-5.40265700	0.09919600
H	-2.57874400	-5.19395500	2.27083000
C	1.31729600	-0.66326900	1.19249600
H	0.61614700	-1.46006900	1.47597200
H	2.34271900	-1.03428100	1.32309200
H	1.15195500	0.20000900	1.84961700
C	2.10333100	2.00479300	-0.05430600
C	1.22465800	3.01995000	-0.42942100
C	3.01113000	2.18668100	0.98747500
C	1.25153000	4.23176400	0.25803500
H	0.52562100	2.85821300	-1.25172100
C	3.02923600	3.40185300	1.67069100
H	3.70070600	1.38210000	1.25021900
C	2.14939700	4.42262600	1.30977800
H	0.56618800	5.03126400	-0.03154400
H	3.73922400	3.55048000	2.48700200
H	2.16679200	5.37361100	1.84669700

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C	0.41464700	0.41077400	0.26717100
O	0.59461400	-0.63231800	-0.59013600
N	1.27308000	1.54690000	-0.26902100
H	2.29808200	1.16991600	-0.29559600
C	1.21451400	2.83655200	0.43388300
H	1.68805100	2.74015200	1.41768600
H	1.76396600	3.57971900	-0.15617800
H	1.53566000	-1.01694400	-0.48388900
H	0.98414300	1.66932400	-1.24548900
O	3.71738300	0.60251700	-0.26183500
C	3.89054700	-0.64389700	-0.30546700
O	2.97556700	-1.50304800	-0.36015600
C	5.32063600	-1.15225300	-0.32616400
H	5.59988900	-1.37103000	-1.36962000
H	6.01769200	-0.40162700	0.06881600

H	5.40617100	-2.08883100	0.24213100
O	-0.88750300	0.85570100	0.20452100
Si	-2.21481500	-0.06071000	-0.33417300
H	-2.08493700	-0.35120300	-1.79553300
C	0.82367700	0.09923100	1.70015700
H	0.27065300	-0.79358700	2.02127200
H	1.90043800	-0.10912800	1.76454700
H	0.57157600	0.92748500	2.37506900
H	0.17026900	3.15116300	0.54696500
C	-3.66495700	1.09960900	-0.07190100
H	-3.86065200	1.16485700	1.01301300
C	-2.32658200	-1.65737300	0.64310100
H	-2.31554600	-1.39351200	1.71563400
H	-3.33160400	2.10670800	-0.37894700
C	-4.94516200	0.72476800	-0.82484100
H	-5.33588800	-0.25641500	-0.51405000
H	-5.74385300	1.46304000	-0.64997200
H	-4.77576900	0.67935100	-1.91284000
H	-1.39315900	-2.21381700	0.45476000
C	-3.54129000	-2.53514400	0.32801200
H	-3.49221000	-3.49340400	0.86884100
H	-4.48399800	-2.04613800	0.61876500
H	-3.60980500	-2.77085200	-0.74667900

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C	0.99817200	0.13944500	0.21414200
O	1.42375300	-1.12273300	-0.06432600
N	1.60636400	1.03809000	-0.84560500
H	2.69152900	0.91552700	-0.76021100
C	1.23873600	2.46163900	-0.82737100
H	1.67977100	2.94423300	0.05232400
H	1.63768600	2.93418300	-1.73269400
H	2.42516800	-1.21711100	0.14607800
H	1.34042500	0.62125900	-1.74428400
O	4.18502200	0.72569900	-0.56666500
C	4.62108500	-0.33345000	-0.04389400
O	3.91053400	-1.27901300	0.38151200
C	6.12567000	-0.49981700	0.05201100
H	6.46137400	-1.13208600	-0.78593000
H	6.63951500	0.46778600	-0.01667600
H	6.40034000	-1.01300300	0.98395900

O	-0.37270800	0.20634600	0.03802900
Si	-1.34895000	-1.17190500	-0.00908100
H	-1.14944500	-1.98020100	-1.24074400
C	-3.09114000	-0.48569100	-0.00633500
C	-4.12027400	-1.15631100	-0.68671400
C	-3.41034800	0.68922000	0.69495900
C	-5.42944300	-0.67281300	-0.66399100
H	-3.90235800	-2.06913000	-1.25042600
C	-4.71670100	1.17722400	0.71664300
H	-2.62707200	1.23632400	1.22716200
C	-5.72841700	0.49517200	0.03812900
H	-6.21766600	-1.20686400	-1.20022900
H	-4.94704300	2.09401300	1.26501200
H	-6.75222700	0.87698200	0.05449700
C	1.39324500	0.62983100	1.59798800
H	1.02580300	-0.10247600	2.32965000
H	2.48557300	0.70424800	1.68855300
H	0.94017800	1.60446300	1.82110700
H	0.14714200	2.56335700	-0.80699100
H	-1.09426600	-2.01054400	1.19441200

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C	1.05499000	-0.34351800	-0.37160600
O	1.50476700	0.88349000	-0.75259400
N	1.56665800	-0.55529100	1.05083800
H	2.66101900	-0.50755000	0.99733900
C	1.13596800	-1.77207600	1.75395200
H	1.59430800	-2.64969900	1.28360200
H	1.47122600	-1.70871700	2.79601400
H	2.52152500	0.86874200	-0.86523600
H	1.27489100	0.27257500	1.58155000
O	4.16733400	-0.46995300	0.86413900
C	4.68089500	0.18544400	-0.08194900
O	4.04047000	0.81606800	-0.95839600
C	6.19618400	0.23022200	-0.14001400
H	6.55729200	0.94963700	0.61258300
H	6.61996200	-0.75132700	0.11437500
H	6.54919100	0.55266900	-1.12810700
O	-0.32109700	-0.34350700	-0.31469200
Si	-1.30761100	1.03608200	-0.33501500
C	-3.03085100	0.30090800	-0.20186300

C	-4.11388400	1.09775300	0.20645200
C	-3.28134700	-1.04431800	-0.51910800
C	-5.40327400	0.57107100	0.29238700
H	-3.95699800	2.14929800	0.46652200
C	-4.56898500	-1.57535000	-0.43347400
H	-2.45557200	-1.68864900	-0.83253400
C	-5.63247600	-0.76770600	-0.02816800
H	-6.23186100	1.20731800	0.61312300
H	-4.74325000	-2.62493600	-0.68333400
H	-6.64127400	-1.18246800	0.03973200
C	1.54065400	-1.47805500	-1.25841300
H	1.25532400	-1.23711000	-2.29093700
H	2.63330600	-1.57665400	-1.20358800
H	1.07364200	-2.43146600	-0.97914400
H	0.04298900	-1.85573900	1.72037600
H	-1.15643500	1.74086000	-1.63934100
C	-0.94908000	2.17975700	1.09156500
H	-1.02516300	1.64223300	2.05077000
H	0.06164600	2.60610900	1.00324400
H	-1.67036300	3.01319000	1.11112600

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C	1.51190700	-0.21487600	0.94992200
O	1.84868000	0.22131900	-0.29454700
N	2.24765000	0.68490300	1.92464200
H	3.31248200	0.58551600	1.68613200
C	2.01841500	0.46988400	3.36047700
H	2.46618100	-0.48361500	3.66335600
H	2.50145600	1.28369600	3.91415800
H	2.81954000	-0.02318800	-0.50083700
H	1.98248700	1.64184800	1.66710800
O	4.77419500	0.37146200	1.34765000
C	5.10030600	-0.04238500	0.20334500
O	4.29989700	-0.31734500	-0.72462500
C	6.58214300	-0.18816700	-0.08781400
H	6.93436300	0.73381900	-0.57841700
H	7.15704500	-0.32530100	0.83745900
H	6.76362500	-1.02319200	-0.77824400
O	0.16763900	0.00537100	1.17948000
Si	-1.04566400	0.04045100	0.00038600
C	-2.60728800	-0.07776800	1.03479000

C	-3.82972200	0.40078500	0.53541200
C	-2.59971600	-0.68488700	2.30119500
C	-5.00678000	0.27545800	1.27382100
H	-3.86993300	0.88484200	-0.44557500
C	-3.77435900	-0.81107100	3.04399000
H	-1.66094000	-1.06334800	2.71448100
C	-4.98001600	-0.33135600	2.53044400
H	-5.94791700	0.65529700	0.86872100
H	-3.74879700	-1.28529900	4.02825100
H	-5.90072400	-0.42935400	3.11099500
C	1.88226300	-1.66797300	1.20838400
H	1.41685800	-2.27714800	0.42173000
H	2.97119600	-1.80715500	1.16702400
H	1.50712500	-2.00864000	2.18222200
H	0.94219400	0.46668100	3.57050800
C	-0.93028800	-1.43430900	-1.15637500
C	-0.09823500	-1.41464400	-2.28915600
C	-1.66093000	-2.60397100	-0.89061900
C	0.00358900	-2.52636400	-3.12400200
H	0.48656900	-0.52009200	-2.51617900
C	-1.55916200	-3.72076800	-1.72194200
H	-2.32322600	-2.64971700	-0.02093600
C	-0.72576800	-3.68280000	-2.83964000
H	0.65626400	-2.49252000	-3.99988900
H	-2.13424400	-4.62229600	-1.49691300
H	-0.64543200	-4.55520700	-3.49305100
C	-1.00385300	1.66195000	-0.93830700
C	-0.42143200	2.80260200	-0.36209100
C	-1.59345800	1.78568800	-2.20637400
C	-0.42665900	4.02653400	-1.02984400
H	0.04956800	2.73547000	0.62312900
C	-1.60348100	3.00985700	-2.87784900
H	-2.04986800	0.91443200	-2.68605100
C	-1.01901900	4.13164400	-2.28999700
H	0.03441700	4.90265100	-0.56714100
H	-2.06596100	3.08637300	-3.86496700
H	-1.02260400	5.08997600	-2.81526500

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C	1.11901500	0.22931700	0.16932300
O	1.58681400	-1.00368700	-0.17378100

N	1.73666600	1.20040200	-0.82627400
H	2.81927300	1.10349500	-0.71639900
C	1.33140100	2.61086100	-0.74631200
H	1.72251300	3.05466800	0.17637900
H	1.75435300	3.14313300	-1.60661600
H	2.57950900	-1.07692500	0.05739100
H	1.50537400	0.82427800	-1.75200400
O	4.32116100	0.95618900	-0.47776800
C	4.77052400	-0.11128400	0.01571600
O	4.07903600	-1.10781700	0.34358800
C	6.27123700	-0.21739700	0.21870400
H	6.68433900	-0.91556600	-0.52663900
H	6.76277500	0.75712600	0.10332900
H	6.49026100	-0.63534100	1.21185500
O	-0.24096000	0.29721400	-0.02668600
Si	-1.31744800	-1.01571800	-0.11335400
C	-2.98602200	-0.15000900	-0.00312400
C	-4.16459600	-0.84736000	-0.31968900
C	-3.10411800	1.18365000	0.42015500
C	-5.41525700	-0.23692500	-0.21725400
H	-4.11354200	-1.88867500	-0.65449500
C	-4.35231900	1.80043400	0.52230000
H	-2.20318300	1.75018600	0.67093400
C	-5.51063200	1.09049200	0.20392700
H	-6.31882800	-0.79815000	-0.46844200
H	-4.42132100	2.84039400	0.85163400
H	-6.48866100	1.57182400	0.28324800
C	1.48912900	0.64688200	1.58564000
H	1.12366100	-0.13108700	2.26950500
H	2.57815100	0.73588400	1.69822500
H	1.01474800	1.59936100	1.85605500
H	0.23763800	2.68467400	-0.76617900
C	-1.16463800	-1.90866500	-1.74489100
H	-1.28689700	-1.20886600	-2.58733700
H	-0.17738400	-2.38702500	-1.83077100
H	-1.93648000	-2.69034500	-1.83748500
C	-1.09174100	-2.16297300	1.34280600
H	-1.16467000	-1.61272100	2.29444400
H	-1.88007000	-2.93403500	1.33730900
H	-0.11425300	-2.66637100	1.30030700

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Si	-0.12879400	0.04072200	-1.17414200
H	-0.25767400	-1.19286100	-2.14691700
C	-1.87212700	-0.26037000	-0.41596000
C	-2.51500000	-1.48521800	-0.67059000
C	-2.55866600	0.65797000	0.40049100
C	-3.77078000	-1.78708900	-0.13924000
H	-2.01912700	-2.22681700	-1.30422800
C	-3.81980500	0.37140200	0.92652900
H	-2.07705200	1.61003800	0.62774500
C	-4.43131000	-0.85467500	0.66082700
H	-4.23642400	-2.75273800	-0.35424200
H	-4.32753700	1.11026900	1.55284000
H	-5.41688600	-1.08247200	1.07547700
C	1.36748100	-0.74820000	-0.26879900
C	2.27280200	-1.56031400	-0.96921100
C	1.59244600	-0.57195600	1.10722500
C	3.37005400	-2.15079100	-0.33768100
H	2.11836200	-1.73947400	-2.03867000
C	2.66747300	-1.18247000	1.75546900
H	0.91430400	0.06435900	1.68190500
C	3.56696400	-1.96793200	1.03153900
H	4.06841000	-2.76343000	-0.91441100
H	2.80980300	-1.03841100	2.83006100
H	4.41694700	-2.43745200	1.53357400
O	0.02190600	1.62692300	-0.05546100
C	0.84344700	2.62438600	0.01036700
O	0.60322700	3.63322600	0.66122900
H	0.06470800	0.98842100	-2.33665600
C	2.16200200	2.49285300	-0.73610500
H	2.80405200	1.76418300	-0.21664700
H	2.01180500	2.11857000	-1.75964700
H	2.67847500	3.46093300	-0.76749500

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Si	1.52533300	0.22181900	-1.20894700
H	2.17550900	1.39142200	-2.02940100
C	3.17794200	-0.21927800	-0.33147000
C	4.25057800	0.68487000	-0.43599200
C	3.40181300	-1.38268500	0.42847200
C	5.47971800	0.45099700	0.18433000

H	4.12221900	1.60133300	-1.01971800
C	4.63078700	-1.63201500	1.04222400
H	2.58398300	-2.09521500	0.54240500
C	5.67592900	-0.71465500	0.92453200
H	6.28769800	1.18095500	0.08531400
H	4.77224600	-2.54916200	1.62079700
H	6.63714100	-0.90665200	1.40866500
C	0.32860100	1.41684800	-0.30271700
C	-0.14996500	2.56191200	-0.95916900
C	-0.07685000	1.22147200	1.02867200
C	-1.01468100	3.46099800	-0.33037300
H	0.16049500	2.76012200	-1.99056600
C	-0.91500500	2.13014900	1.67707200
H	0.26788100	0.33613200	1.56895800
C	-1.39549300	3.24955700	0.99545100
H	-1.38554600	4.33390100	-0.87429200
H	-1.20422700	1.95795700	2.71729000
H	-2.06337000	3.95527700	1.49616800
O	0.69048100	-1.29477900	-0.25576700
C	-0.47732800	-1.83251400	-0.23724400
O	-0.77838400	-2.75755900	0.50643300
H	1.10448500	-0.50325600	-2.46450400
C	-1.52950200	-1.30900700	-1.23381100
H	-1.16233900	-0.42556100	-1.76953600
H	-1.65704000	-2.11175100	-1.97933700
C	-2.85576100	-1.00009200	-0.58696100
C	-3.26405100	0.32719600	-0.40656200
C	-3.69779800	-2.02388400	-0.13039300
C	-4.47519700	0.62794100	0.21922000
H	-2.61843400	1.13789500	-0.75550100
C	-4.90917400	-1.72739300	0.49302200
H	-3.38776900	-3.06288400	-0.25788900
C	-5.30282100	-0.39910600	0.67246000
H	-4.77035000	1.67197100	0.35262100
H	-5.55254700	-2.53960500	0.84153200
H	-6.25191100	-0.16750200	1.16236200

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Si	1.42755200	0.11274700	-1.20769300
H	2.88100200	0.30094000	-1.79173200
C	1.87860000	-1.55400000	-0.37196700

C	2.86760900	-2.37078700	-0.94467000
C	1.29323400	-2.00392300	0.82477000
C	3.24391800	-3.58687800	-0.36957500
H	3.36335600	-2.04775600	-1.86619000
C	1.68110800	-3.20414700	1.42377900
H	0.51179100	-1.40376600	1.29570300
C	2.65388600	-4.00545000	0.82344300
H	4.00696100	-4.20525900	-0.85014900
H	1.21583600	-3.52001300	2.36159600
H	2.95225300	-4.95059300	1.28467000
C	1.56365100	1.70587400	-0.14337200
C	2.45699000	2.72054500	-0.52388000
C	0.84043000	1.90644100	1.04587300
C	2.61263900	3.88761200	0.22810500
H	3.05318700	2.59636200	-1.43373200
C	1.00799500	3.05539800	1.82045500
H	0.12633800	1.14705400	1.37347900
C	1.89100600	4.05593100	1.40986000
H	3.30619400	4.66408200	-0.10613800
H	0.44006800	3.17486800	2.74725100
H	2.01670800	4.96156400	2.00912500
O	-0.40944900	-0.18158100	-0.56082800
C	-1.43131600	0.52207400	-0.90040800
O	-1.41273700	1.53459600	-1.59052200
H	0.81382900	0.08566800	-2.58580500
C	-2.75031900	-0.00068700	-0.36231500
C	-3.92558600	0.71561300	-0.61388400
C	-2.81715700	-1.18892200	0.37387900
C	-5.15058200	0.25509700	-0.13395600
H	-3.85951800	1.63917100	-1.19292500
C	-4.04203400	-1.65254800	0.85355800
H	-1.89737400	-1.74595200	0.56214900
C	-5.21046900	-0.93116800	0.60070200
H	-6.06364200	0.82142100	-0.33385300
H	-4.08658800	-2.58228300	1.42621600
H	-6.17026700	-1.29451800	0.97644200

6a-1a-2d

Si	1.40284900	-0.11033500	-1.00611900
H	1.49995600	0.77377200	-2.27855300
C	3.28417000	-0.14803200	-0.68776500

C	4.02477700	0.99873700	-1.02377500
C	3.99299600	-1.23978600	-0.15886400
C	5.40598800	1.06363000	-0.83105000
H	3.51159700	1.86739600	-1.44967500
C	5.37775700	-1.19342300	0.01354400
H	3.44331500	-2.13464100	0.13661000
C	6.08905700	-0.03882800	-0.31628000
H	5.95154300	1.97488000	-1.09040600
H	5.90424900	-2.06266000	0.41712800
H	7.17195400	0.00164400	-0.17247700
C	0.39042500	1.17345500	-0.01857800
C	-0.42678600	2.08244700	-0.70998400
C	0.44640400	1.29085400	1.38045900
C	-1.17305900	3.05420800	-0.03929900
H	-0.48451400	2.03427000	-1.80212800
C	-0.27922900	2.27131800	2.05814400
H	1.06557100	0.59355400	1.94917100
C	-1.09830000	3.15341900	1.35001700
H	-1.81264500	3.73733600	-0.60444200
H	-0.20987500	2.34486300	3.14680300
H	-1.67409800	3.91654900	1.87994500
O	1.26301200	-1.43508200	0.63498500
C	0.29761200	-2.16842400	1.02183700
O	0.38025900	-3.16760600	1.72714100
H	0.72298500	-1.25652000	-1.69588900
C	-1.05893500	-1.74886300	0.58314300
C	-2.17358200	-1.38705700	0.26194400
C	-3.47281800	-0.90602500	-0.11594700
C	-4.39772200	-1.75103200	-0.75206600
C	-3.82629100	0.42878100	0.14873300
C	-5.64988200	-1.26449900	-1.11964300
H	-4.12726800	-2.78888800	-0.95771000
C	-5.08230100	0.90468900	-0.21810100
H	-3.10747200	1.08709200	0.64134800
C	-5.99551700	0.06162000	-0.85383200
H	-6.36230700	-1.92723300	-1.61622200
H	-5.34825800	1.94316400	-0.00774900
H	-6.97936900	0.43848200	-1.14292300

6a-1a-2e

Si	1.68075900	0.16694700	-1.08531100
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H	2.09338700	1.31256800	-2.07520600
C	3.50327400	-0.21076600	-0.60050100
C	4.50742700	0.67008000	-1.04219400
C	3.91980400	-1.30259500	0.18477800
C	5.85314800	0.48178500	-0.71947500
H	4.23046100	1.53084100	-1.65796500
C	5.26324000	-1.50376300	0.50686200
H	3.16337300	-1.99850300	0.54903400
C	6.23716900	-0.61115600	0.05703800
H	6.60391900	1.19068300	-1.07891500
H	5.55147600	-2.36461200	1.11658500
H	7.28916800	-0.76658600	0.31067100
C	0.67357800	1.36857300	0.01739800
C	-0.04144300	2.42192500	-0.57401800
C	0.60243400	1.24517800	1.41494100
C	-0.82010700	3.29752800	0.18659600
H	0.00496800	2.56241800	-1.65937800
C	-0.14707300	2.13357400	2.18786800
H	1.13746500	0.43010600	1.90948700
C	-0.87121100	3.15734500	1.57402800
H	-1.38258800	4.09610800	-0.30465400
H	-0.17536800	2.02046300	3.27505700
H	-1.47126200	3.84506400	2.17557100
O	1.13460000	-1.33904200	0.07938800
C	0.01391900	-1.88084400	0.41290300
O	-0.06619800	-2.87006700	1.13475700
H	0.97928500	-0.60830900	-2.17548200
C	-1.23686800	-1.22613500	-0.11189300
H	-1.12116400	-0.43206000	-0.85331900
C	-2.45225400	-1.57467900	0.33217400
H	-2.50616900	-2.39650900	1.05512800
C	-3.73328500	-0.96357800	-0.06163900
C	-4.93102400	-1.63102800	0.24069300
C	-3.80729100	0.27425000	-0.72454200
C	-6.16401500	-1.09347300	-0.12650300
H	-4.88970600	-2.58817000	0.76767200
C	-5.03852600	0.81278000	-1.08774800
H	-2.89282100	0.83127400	-0.94311700
C	-6.22168800	0.12984000	-0.79417400
H	-7.08423700	-1.63184000	0.11285800
H	-5.07669700	1.77784300	-1.59878700

H	-7.18656900	0.55579000	-1.07959500
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6a-1b-2a-3a

Si	0.86247900	-0.00441600	0.66587100
H	2.15175700	-0.22795300	1.56543300
O	-0.90012500	0.40641400	-0.36436400
C	-2.12236100	0.05030100	-0.21560600
O	-3.06826100	0.57875600	-0.79903100
H	0.00759800	0.31982000	1.86487000
C	-2.39145200	-1.12143000	0.72813800
H	-1.98365100	-2.04953000	0.29702700
H	-1.89504000	-0.97266300	1.69937200
H	-3.47093400	-1.24994300	0.88418300
C	0.90607800	-1.75725200	-0.08452000
H	0.60562100	-2.47007100	0.70520400
H	0.14383500	-1.83242400	-0.87563200
C	1.58419300	1.40828800	-0.38628100
H	2.68081900	1.29190900	-0.43164000
H	1.20472700	1.29576500	-1.41491800
C	1.23253900	2.80256600	0.13626100
H	1.66239600	3.60419100	-0.48828900
H	0.14025000	2.94480200	0.15321200
H	1.60203600	2.96055300	1.16400600
C	2.27466900	-2.15709000	-0.63972600
H	2.27543400	-3.18819300	-1.03167200
H	2.58523400	-1.49736600	-1.46733900
H	3.06031300	-2.10073200	0.13154600

6a-1c-2a-3a

Si	-0.67546800	1.78355400	-0.35742600
H	0.24011600	3.06276500	-0.19673100
C	0.82111500	0.59163800	-0.21189300
C	1.92717800	0.95406000	0.57451400
C	0.87976300	-0.64986600	-0.86922200
C	3.03283300	0.11325000	0.71981600
H	1.92765000	1.92077400	1.08870500
C	1.99291200	-1.48476500	-0.75451400
H	0.03355100	-0.97044700	-1.48132100
C	3.07129000	-1.10934900	0.04835700
H	3.87080600	0.41704600	1.35303000
H	2.01570800	-2.43817300	-1.28936900

H	3.93883500	-1.76672400	0.14912400
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O	-1.88762800	0.26921800	-0.63618700
C	-2.32226900	-0.67151400	0.13806600
O	-3.05301100	-1.57163800	-0.25771800
H	-1.48970800	2.13497800	0.86119500
C	-1.90203800	-0.62617500	1.60104300
H	-0.80613400	-0.58460200	1.69556700
H	-2.30139900	0.27928200	2.08380700
H	-2.28132000	-1.51144300	2.12736200
H	-1.17115200	2.20247300	-1.71315800

6a-1d-2a-3a

Si	-0.80366000	1.45761500	0.48652000
H	-0.03622800	2.65972200	1.18065600
C	0.83284200	0.53488600	0.10778900
C	1.91313500	0.60625600	1.00122900
C	1.01929400	-0.21343600	-1.06737300
C	3.11726800	-0.05710100	0.75294000
H	1.81449600	1.19586000	1.91899600
C	2.22841600	-0.85542200	-1.34073400
H	0.19423900	-0.30476100	-1.77856700
C	3.28066100	-0.78653300	-0.42526500
H	3.93383800	0.00288100	1.47773400
H	2.34864800	-1.42023600	-2.26936700
H	4.22424000	-1.29909900	-0.63026400
O	-1.82378100	-0.07529400	-0.30393700
C	-2.02167300	-1.29619300	0.05928100
O	-2.77669900	-2.05874800	-0.53624400
H	-1.58441200	1.16202600	1.74342900
C	-1.24930500	-1.80532800	1.27137800
H	-0.19887400	-1.97777300	0.98779700
H	-1.24669800	-1.07383600	2.09275600
H	-1.67767800	-2.75412300	1.62052000
C	-1.55694100	2.55160400	-0.86498600
H	-2.18322000	1.99851200	-1.57844500
H	-2.16757700	3.34587000	-0.40233600
H	-0.74787200	3.05828000	-1.41829500

6a-1e-2a-3a

Si	0.17357900	-0.01581500	-0.51626800
H	0.24482300	0.00673000	-2.08929800

C	-0.46611600	1.79736100	-0.49511300
C	-1.34068400	2.25179500	-1.49418800
C	-0.06553500	2.72774800	0.47889300
C	-1.82383600	3.56250900	-1.50801100
H	-1.65471400	1.56525500	-2.28762900
C	-0.51353600	4.04973400	0.45580300
H	0.60704300	2.40848900	1.27963500
C	-1.40507600	4.46936700	-0.53367300
H	-2.52052000	3.88054900	-2.28848500
H	-0.17252900	4.75501700	1.21878300
H	-1.76843400	5.50029100	-0.54709000
O	0.06824300	-0.05234900	1.41534300
C	-0.84538600	0.00272300	2.33017800
O	-0.60900500	-0.24737100	3.50494400
C	-2.24302300	0.44047700	1.91970200
H	-2.28480600	1.54128100	1.94030100
H	-2.50949200	0.12039000	0.90369200
H	-2.97858600	0.05648100	2.63906600
C	2.07211600	-0.30752400	-0.35235600
C	2.74099200	-0.57431700	0.85768600
C	2.86506100	-0.26005200	-1.51324200
C	4.12040900	-0.78548800	0.90395500
H	2.15423100	-0.60860000	1.77679700
C	4.24661100	-0.46213400	-1.47773700
H	2.38836100	-0.05930600	-2.47734200
C	4.88111600	-0.72935000	-0.26473700
H	4.60611900	-0.99350700	1.86153700
H	4.82844900	-0.41324700	-2.40224800
H	5.96157700	-0.89254000	-0.23004200
C	-1.00070000	-1.54147200	-0.57372700
C	-1.94447000	-1.65920500	-1.60660200
C	-0.94703300	-2.58541900	0.36636300
C	-2.81741300	-2.74677400	-1.68626000
H	-1.99998600	-0.88099000	-2.37496000
C	-1.79138400	-3.69383800	0.27784900
H	-0.22998100	-2.53160700	1.18968300
C	-2.73812400	-3.77381800	-0.74499400
H	-3.55465300	-2.79818600	-2.49218400
H	-1.71534000	-4.49713000	1.01593000
H	-3.40949000	-4.63414300	-0.80941300

6a-1f-2a-3a

Si	0.90860000	-1.33948200	-0.01415500
H	0.32612200	-2.78602900	0.31139600
C	-0.85589500	-0.59809300	-0.08373500
C	-1.79555500	-0.91284000	0.91012800
C	-1.27715000	0.25112900	-1.12023600
C	-3.08819200	-0.38402200	0.89341200
H	-1.51335700	-1.58937300	1.72462800
C	-2.57709000	0.75926000	-1.16659700
H	-0.56731700	0.53386800	-1.90267400
C	-3.48557400	0.45157900	-0.15175100
H	-3.79130800	-0.63202900	1.69340700
H	-2.88053000	1.40812800	-1.99298900
H	-4.49970500	0.85892700	-0.17703800
O	1.61536400	0.52478700	-0.47758200
C	1.55745500	1.70051700	0.03546200
O	2.13700100	2.67548100	-0.43956100
C	0.68962200	1.90441000	1.27645600
H	-0.33830200	2.13560000	0.95286900
H	0.63843800	1.01636800	1.91987900
H	1.06170700	2.76259100	1.85303100
C	1.70946000	-1.90457500	-1.63682300
H	2.33461400	-1.13492200	-2.10960400
H	2.32166400	-2.80495600	-1.45893500
H	0.91852600	-2.19639900	-2.34967500
C	1.93093900	-1.32568800	1.58967700
H	2.52612800	-2.25410600	1.63407400
H	2.61452300	-0.47003500	1.69422900
H	1.26135200	-1.34708600	2.46675600