

Supporting Information

**Computational Study on H₂S Release and Amide Formation from
Thionoesters and Cysteine**

Yuan-Ye Jiang^{*a}, Ling Zhu^a, Xia Fan^a, Qi Zhang^b, Ya-Jie Fu^a, He Li^a, Bing Hu^a and

Siwei Bi^{*b}

^aSchool of Chemistry and Chemical Engineering, Qufu Normal University, Qufu 273165, People's Republic of China

^bInstitute of Industry & Equipment Technology, Hefei University of Technology, Hefei 230009, People's Republic of China

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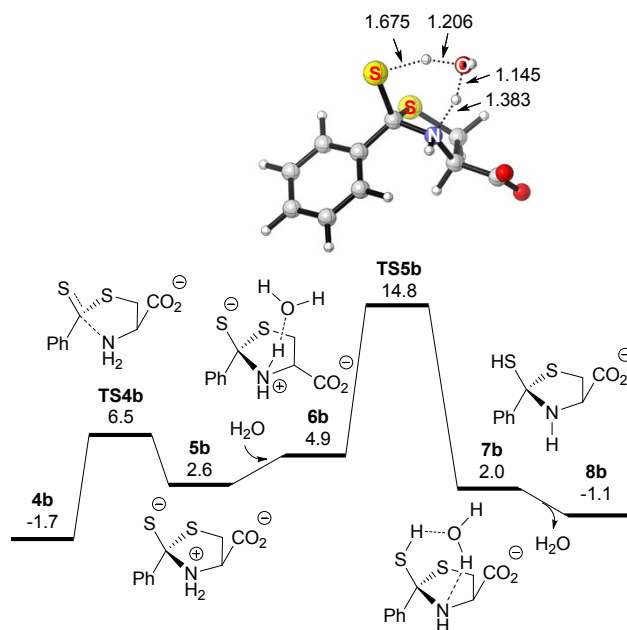


Fig. S1 Calculated Gibbs free energy profile for the formation of cyclic thiol intermediate from **4b** (in kcal/mol). Bond lengths of **TS5b** are given in angstrom.

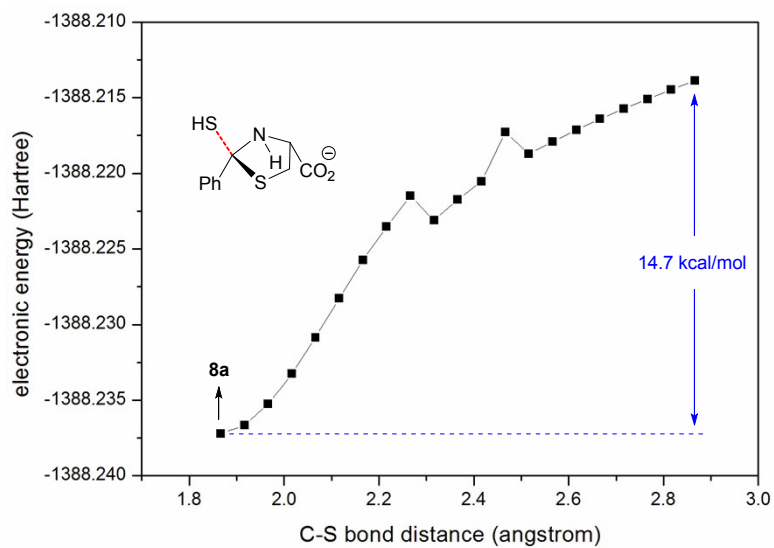
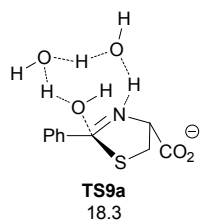


Fig. S2 Relax energy surface scan of the C-S bond (red colored) of **8a**.



Scheme S1 Three-water-assisted nucleophilic addition transition state from dihydrothiazole **12**.

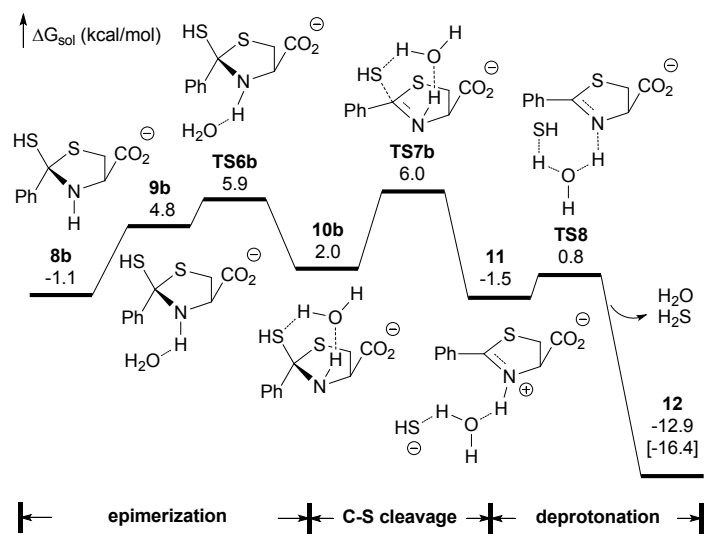


Fig. S3 Calculated Gibbs free energy profile for the H₂S release from **8b** (in kcal/mol).

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

	ΔG_{cor}	ΔE_{sol}	ΔG_{sol}
H ₂ O	0.00332	-76.47629141	-76.46994357
1	0.151931	-975.1131666	-974.9582078
2a	0.061669	-721.6810565	-721.6163597
2b	0.065814	-721.6763109	-721.6074691
TS1a	0.256141	-1773.243637	-1772.984468
3a	0.261605	-1773.276517	-1773.011884
TS2a	0.260888	-1773.247457	-1772.983541
TS1b	0.241171	-1696.792402	-1696.548204
3b	0.241932	-1696.796405	-1696.551445
TS2b	0.242856	-1696.791405	-1696.545521
PhOH	0.075748	-307.6216982	-307.5429224
4b	0.141843	-1389.179277	-1389.034406
TS3	0.142707	-1389.168103	-1389.022368
4a	0.140716	-1389.185561	-1389.041817
TS4a	0.144698	-1389.166297	-1389.018571
TS4b	0.144424	-1389.168782	-1389.02133
5a	0.146776	-1389.175316	-1389.025512
5b	0.146765	-1389.177283	-1389.02749
6a	0.168576	-1465.662645	-1465.491041
6b	0.167232	-1465.664109	-1465.493849
TS5a	0.161153	-1465.642495	-1465.478314
TS5b	0.161027	-1465.64198	-1465.477925
7a	0.163392	-1465.670018	-1465.503598
7b	0.163593	-1465.664943	-1465.498322
8a	0.141985	-1389.185583	-1389.04057
8b	0.14299	-1389.179481	-1389.033463
9a	0.162163	-1465.669449	-1465.504258
TS6a	0.162066	-1465.660863	-1465.49577
10a	0.163556	-1465.668551	-1465.501967
TS7a	0.16298	-1465.66146	-1465.495452
11	0.161826	-1465.668839	-1465.503985
TS8	0.154556	-1465.657894	-1465.50031
12	0.122777	-989.7522022	-989.6263973
TS9	0.164872	-1142.681458	-1142.513558
TS9a	0.186898	-1219.171721	-1218.981795
13	0.168912	-1142.705548	-1142.533608
14	0.169882	-1142.705154	-1142.532244

TS10	0.169533	-1142.700033	-1142.527472
15a	0.142693	-1066.248356	-1066.102635
OH ⁻	-0.007961	-75.97343399	-75.97836715
TS11	0.130753	-1065.701495	-1065.567714
16	0.132916	-1065.742313	-1065.606369
17	0.13339	-1065.759228	-1065.62281
TS12	0.237015	-1696.784247	-1696.544204
18	0.240194	-1696.791488	-1696.548266
TS13	0.239285	-1696.780015	-1696.537702
19	0.237794	-1696.782084	-1696.541263
TS14	0.237627	-1696.781347	-1696.540692
20a	0.141553	-1389.203163	-1389.058583
TS15	0.254423	-1773.257655	-1773.000204
21	0.258016	-1773.279139	-1773.018095
TS16	0.258164	-1773.270726	-1773.009534
TS17	0.139358	-1389.162155	-1389.019769
20b	0.139754	-1389.196062	-1389.053281
TS18a	0.183967	-1542.099131	-1541.912137
22a	0.18719	-1542.141523	-1541.951305
TS19a	0.182732	-1542.132474	-1541.946714
TS20a	0.149876	-1465.157485	-1465.004582
23a	0.153233	-1465.16972	-1465.013459
TS21a	0.171829	-1541.644424	-1541.469567
HS ⁻	-0.011991	-398.9506975	-398.9596606
TS18b	0.183957	-1542.103391	-1541.916406
22b	0.184554	-1542.135317	-1541.947735
TS19b	0.183265	-1542.126292	-1541.939999
15b	0.143504	-1066.243112	-1066.09658
TS20b	0.151573	-1465.152644	-1464.998043
23b	0.151332	-1465.171396	-1465.017036
TS21b	0.171816	-1541.644589	-1541.469746
TS22a	0.163938	-1465.647283	-1465.480317
TS22b	0.160881	-1465.64591	-1465.482001
24b	0.142523	-1389.182002	-1389.036451
25a	0.130875	-1388.711901	-1388.577998
TS23a	0.131516	-1388.694427	-1388.559883
26a	0.131993	-1388.69639	-1388.561369
TS24	0.130307	-1388.670169	-1388.536834
25b	0.131428	-1388.708214	-1388.573758
TS23b	0.132789	-1388.700892	-1388.565075

26b	0.132478	-1388.702899	-1388.567393
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Cartesian coordinates of all calculated intermediates and transition states (in angstrom) and imaginary frequency of transition states.

H₂O

O	0.00000000	0.00000000	0.12157700
H	0.00000000	0.75457500	-0.48630700
H	0.00000000	-0.75457500	-0.48630700

1

C	-0.43116300	0.46234600	-0.00604300
S	0.12106700	2.01380700	-0.08871900
C	-1.85210500	0.05035500	0.00451800
C	-2.20364700	-1.31462100	-0.00724500
C	-2.87481700	1.01796600	0.02315600
C	-3.54493500	-1.69610000	-0.00319300
H	-1.42294900	-2.07418300	-0.02398100
C	-4.21274600	0.63197100	0.02944900
H	-2.60116500	2.07372500	0.03367300
C	-4.55226400	-0.72608800	0.01509300
H	-3.80529300	-2.75670000	-0.01566200
H	-4.99611600	1.39276400	0.04591000
H	-5.60218400	-1.02786000	0.01859000
O	0.38323600	-0.61111600	0.05692400
C	1.77198600	-0.46196800	0.03410200
C	2.43264900	-0.48934400	-1.19197500
C	2.45879600	-0.35699400	1.24123300
C	3.82764000	-0.40669700	-1.20488400
H	1.85580100	-0.57178400	-2.11464000
C	3.85375800	-0.27512900	1.21485800
H	1.90212500	-0.33992600	2.17961000
C	4.53871300	-0.29780300	-0.00482400
H	4.36025600	-0.42759100	-2.15828200
H	4.40649300	-0.19402400	2.15347100
H	5.62889200	-0.23376900	-0.02004800

2a

C	0.78402800	-0.65660000	0.31690100
H	0.66514200	-1.68159200	-0.05764000
H	0.65442500	-0.67592800	1.41005900

C	-0.25593200	0.25817300	-0.32240500
H	-0.13267100	0.17314400	-1.42254500
C	-1.69403000	-0.26798300	-0.04959800
O	-1.85796900	-1.51529400	-0.06263100
O	-2.59466300	0.59594200	0.11812000
N	-0.11679000	1.63536200	0.14456400
H	0.49292300	2.15193100	-0.48882000
H	-1.04740900	2.04972500	0.06371200
S	2.52119600	-0.19698100	-0.06921100
H	2.46265200	1.04015000	0.47735400

2b

C	0.74890000	-0.81721000	0.28760900
H	0.62336500	-1.85489600	-0.05990300
H	0.43117000	-0.79992600	1.34729300
C	-0.24959000	0.05052400	-0.52087400
H	-0.17414600	-0.20089200	-1.58623200
C	-1.68697800	-0.15338600	-0.00793400
O	-2.25160700	-1.21739800	-0.35431200
O	-2.13821300	0.73583000	0.76429200
N	0.15394500	1.46675500	-0.34953600
H	-0.38762900	1.83165900	0.45078100
S	2.46849000	-0.20658900	0.11166500
H	1.22056600	1.38841100	-0.15500300
H	-0.04221300	2.04676400	-1.16946600

TS1a

imaginary frequency = -915.09 cm⁻¹

C	0.63866100	0.95408400	0.38090500
S	0.56644600	0.25757600	1.98874000
C	-0.16744100	2.20310700	0.11501400
C	0.16644600	3.05158800	-0.95539700
C	-1.28553600	2.51826100	0.90223100
C	-0.59581500	4.19005900	-1.22180100
H	1.02365600	2.81361100	-1.58442000
C	-2.05170100	3.65369600	0.62889500
H	-1.54076200	1.86661400	1.73775700
C	-1.70992800	4.49595600	-0.43260100
H	-0.31967100	4.84188800	-2.05423300
H	-2.91813200	3.88154500	1.25434300
H	-2.30746100	5.38583100	-0.64433900

O	1.89085100	1.11216800	-0.22750500	H	-3.94170500	2.81956400	1.09403900
C	2.83982900	0.10359200	-0.19410800	H	-3.44416700	4.84390500	-0.28415400
C	3.65179600	-0.07357900	0.93002300	O	1.50249900	1.47505800	-0.09566800
C	3.01007900	-0.68639500	-1.33386000	C	2.66363700	0.71595100	-0.03279600
C	4.62652200	-1.07450200	0.91493300	C	3.33621700	0.59174000	1.18633000
H	3.51044000	0.56771900	1.79839800	C	3.18290800	0.14472800	-1.19812400
C	3.98765400	-1.68570300	-1.33834900	C	4.51993700	-0.14830000	1.24334300
H	2.37942800	-0.51199000	-2.20692200	H	2.92423800	1.06996200	2.07447600
C	4.79220900	-1.88650700	-0.21278900	C	4.36752600	-0.59335800	-1.13052700
H	5.26239000	-1.21879200	1.79159300	H	2.66250000	0.28471400	-2.14607600
H	4.12032600	-2.30640500	-2.22742000	C	5.03243000	-0.75021400	0.08969900
H	5.55454000	-2.66886700	-0.21661700	H	5.04378500	-0.25257900	2.19632500
C	-1.90738400	-0.62895400	-0.18926400	H	4.77214000	-1.04572500	-2.03876800
H	-1.68662500	-0.54600400	0.88462400	H	5.95591700	-1.33142100	0.13906300
H	-2.56459100	0.19785700	-0.49369300	C	-1.70976600	-0.96302900	-1.05079800
C	-2.56675200	-1.96954700	-0.48432200	H	-2.29629600	-0.17652200	-0.56481300
H	-1.86539300	-2.76514300	-0.14869100	H	-2.11674800	-1.10538700	-2.06343900
C	-3.81751200	-2.17920700	0.41613300	C	-1.81112300	-2.27400300	-0.27763300
O	-4.72620000	-2.91329700	-0.05147000	H	-1.18554900	-2.17438300	0.62961400
O	-3.80641800	-1.65049600	1.55747300	C	-3.24368700	-2.45444600	0.29717700
N	-2.93019300	-2.10174800	-1.89196100	O	-3.79218800	-1.43089000	0.78776600
H	-2.11180600	-2.38997800	-2.42961500	O	-3.72720200	-3.61476100	0.28679200
H	-3.59863000	-2.87242200	-1.93956000	N	-1.42668200	-3.41529100	-1.10595900
S	-0.30387100	-0.41620700	-1.04291500	H	-0.41366000	-3.53309800	-1.07378100
H	0.94352800	-1.63941600	1.31166700	H	-1.82991200	-4.24042900	-0.65904700
O	0.91036000	-2.37890800	0.60613300	S	-0.01838100	-0.31352100	-1.32724400
H	0.40197400	-1.66657000	-0.25797200	H	0.91564800	-1.01224200	1.42674100
H	0.21143100	-2.99058100	0.90471800	O	1.73570800	-2.60352300	0.30718700
				H	1.31049600	-2.03417300	-0.36516800
				H	1.00814000	-3.16758500	0.61160700

3a

C	0.23675200	0.87673600	0.11934300
S	0.12011400	0.03586500	1.76441000
C	-0.79539300	1.98990100	0.05235000
C	-0.52698100	3.12550600	-0.73016200
C	-2.03572700	1.89288900	0.70259400
C	-1.47255000	4.14459300	-0.84600400
H	0.42649100	3.20824800	-1.25049000
C	-2.98215200	2.91548400	0.58100500
H	-2.27977100	1.01215900	1.29702600
C	-2.70503600	4.04486300	-0.19086900
H	-1.24499100	5.02320000	-1.45428500

TS2a

imaginary frequency = -456.12 cm⁻¹

C	1.18583200	-0.16068700	-0.45115100
S	0.92724400	0.18430600	-2.17123900
C	2.59298600	-0.47434200	0.02263200
C	2.88140300	-0.49176200	1.39993700
C	3.61736500	-0.77837200	-0.88418700
C	4.16186700	-0.81037000	1.85334600
H	2.09909300	-0.24093300	2.11675100
C	4.90138900	-1.09358600	-0.42910700

H	3.39110500	-0.76729300	-1.95102100	C	-4.70248500	0.73600000	-1.00024800
C	5.17854600	-1.11226000	0.94000300	H	-2.84595300	1.83090000	-0.93703800
H	4.36885800	-0.81675900	2.92618800	C	-4.75004800	-1.34231700	0.22569100
H	5.68727500	-1.32720400	-1.15142900	H	-2.92340500	-1.85794500	1.26817600
H	6.18183000	-1.35831800	1.29592400	C	-5.39621400	-0.40533400	-0.59103800
O	0.98992200	1.34087800	0.40861400	H	-5.19420500	1.47759600	-1.63509300
C	-0.29263200	1.75920900	0.60567700	H	-5.28037600	-2.24003800	0.55369500
C	-0.95195300	2.54023800	-0.35824600	H	-6.43116500	-0.56515700	-0.90290900
C	-0.95915100	1.39354700	1.78488500	O	-0.91241900	1.50748000	0.29633400
C	-2.27592400	2.93033500	-0.14676000	C	0.39887300	1.92317100	0.25680500
H	-0.42175800	2.82493600	-1.26675400	C	1.18010200	2.06042200	1.41006900
C	-2.28321000	1.78995000	1.98706200	C	0.90996100	2.28494100	-0.99459100
H	-0.42987500	0.79761100	2.52848900	C	2.49497900	2.52248700	1.29269900
C	-2.94901700	2.54814400	1.01890900	H	0.75862100	1.79622900	2.37683500
H	-2.78812900	3.53177600	-0.90182200	C	2.21810300	2.76549900	-1.09818900
H	-2.80007300	1.49694400	2.90418700	H	0.27474100	2.17600400	-1.87375900
H	-3.98884100	2.84399400	1.17411100	C	3.02116400	2.86941000	0.04381700
C	-1.51200900	-1.12338800	-0.57548500	H	3.11032300	2.61925200	2.19042800
H	-1.62469900	-0.06185200	-0.81079300	H	2.61363000	3.04916000	-2.07645400
H	-1.48214600	-1.68528500	-1.52192900	H	4.04792900	3.23295300	-0.03787200
C	-2.66695500	-1.60421400	0.29594800	C	0.90692700	-1.89367900	-0.39743100
H	-2.67014700	-0.99838900	1.21673500	H	0.55275800	-2.07585900	0.63565700
C	-4.00022200	-1.28629000	-0.44054300	H	1.07870300	-2.86937000	-0.88180600
O	-4.23246500	-0.06964100	-0.68049900	C	2.23417500	-1.12266800	-0.27727400
O	-4.74062100	-2.25519100	-0.74637200	H	2.12422900	-0.33030700	0.47129500
N	-2.48360300	-3.00641600	0.66351100	C	3.37797900	-2.08290700	0.10977100
H	-3.27631600	-3.26967300	1.25306500	O	4.17505900	-2.39933300	-0.81447000
H	-2.64080800	-3.55142300	-0.18926800	O	3.37012700	-2.50096100	1.28913800
S	0.08052700	-1.36781100	0.30165100	N	2.56514800	-0.48797900	-1.57911900
H	1.94220000	1.68722600	-1.91396800	H	1.66590300	-0.31342200	-2.08002700
O	2.33767600	2.51048600	-1.30481000	H	3.05860000	0.40313100	-1.46027300
H	3.28156400	2.31199500	-1.15600500	S	-0.38959600	-1.00500600	-1.28901100
H	1.82576100	2.19446300	-0.43660900	H	3.18709700	-1.15200200	-2.07360600

TS1b

imaginary frequency = -78.71 cm⁻¹

C	-1.29435600	0.20779000	0.64249100
S	-0.68747200	-0.53356300	2.04965800
C	-2.72118800	0.00608000	0.21745200
C	-3.37683300	0.94001100	-0.60403400
C	-3.43155700	-1.13651500	0.62704600

3b

C	-1.17876000	-0.00511800	0.46312800
S	-0.64851100	-0.88109500	1.91087100
C	-2.67477500	-0.08066400	0.14356900
C	-3.30632600	0.92441300	-0.60774100
C	-3.43406800	-1.19249600	0.53901900
C	-4.66014900	0.82104500	-0.94671100

H	-2.73595900	1.79489400	-0.93028900	H	0.38886500	-1.21659500	-1.80413600
C	-4.78313500	-1.29904300	0.19785400	C	3.48281600	-1.88885800	0.43771700
H	-2.93748000	-1.96446100	1.12888200	H	2.24535500	-1.21518200	2.07381900
C	-5.40595400	-0.29064800	-0.54724100	C	3.55916200	-2.13275000	-0.93806700
H	-5.13234600	1.61750600	-1.52784600	H	2.48225500	-2.08867500	-2.81241500
H	-5.35394100	-2.17459400	0.51833600	H	4.35033300	-2.07146100	1.07687800
H	-6.46320000	-0.37146800	-0.81168800	H	4.48679900	-2.50161600	-1.38228400
O	-0.89251000	1.42235500	0.46116900	O	-0.90265400	0.15838800	-0.46325300
C	0.38801100	1.90071500	0.40263900	C	-2.24274100	0.03451900	-0.51904300
C	1.26563400	1.81704600	1.49345600	C	-2.82563800	-1.06809200	-1.17075500
C	0.78959100	2.55821200	-0.76971100	C	-3.08101800	1.00312700	0.06444300
C	2.54974100	2.36187000	1.38955900	C	-4.21441800	-1.17574700	-1.27083500
H	0.92784100	1.31099000	2.39563900	H	-2.17075200	-1.82649400	-1.60180100
C	2.06681000	3.11785000	-0.85834400	C	-4.46958400	0.88930300	-0.03911000
H	0.08974400	2.61862200	-1.60446800	H	-2.63375400	1.84275800	0.59979400
C	2.95828200	3.00849300	0.21640200	C	-5.04342000	-0.19793700	-0.70832000
H	3.23532000	2.28651900	2.23717100	H	-4.65426400	-2.03131000	-1.79029100
H	2.37237100	3.62731200	-1.77527300	H	-5.10883200	1.65496400	0.40850500
H	3.96138100	3.43461800	0.14415800	H	-6.12963900	-0.28319600	-0.78996300
C	0.89993900	-1.83086500	-0.66541700	C	1.47866000	1.78472500	1.51308100
H	0.51354300	-2.38707600	0.20228800	H	1.46863800	2.54781400	2.30636000
H	1.07057400	-2.52130600	-1.50681000	H	2.44191400	1.26275900	1.57706200
C	2.21139300	-1.17200400	-0.23038800	C	1.41356700	2.45900200	0.13775300
H	2.04854500	-0.67820800	0.73425500	H	1.86264600	3.45928600	0.23901600
C	3.32526700	-2.24177200	-0.12151400	C	2.23652700	1.76700500	-0.98881300
O	4.21707200	-2.19688100	-1.01190300	O	3.36987600	1.34922800	-0.66758300
O	3.20770200	-3.07207700	0.80423300	O	1.70876000	1.76278000	-2.12942600
N	2.65889900	-0.15484900	-1.21976300	N	0.02601600	2.64787200	-0.34853000
H	1.85923700	0.20810900	-1.76371700	H	-0.52531400	3.27788800	0.24292800
H	3.11687400	0.64647000	-0.76654900	H	0.07410000	3.00294700	-1.31137400
S	-0.40639000	-0.70213800	-1.22017100	S	0.11509100	0.67986100	2.07410600
H	3.36650800	-0.64164300	-1.80629700	H	-0.44435200	1.68803400	-0.40019900

TS2b

imaginary frequency = -376.76 cm^{-1}

C	-0.09760000	-0.68480900	0.87124800
S	-1.10799300	-1.91111200	1.53886100
C	1.17293900	-1.14932000	0.20110700
C	1.25238400	-1.41701700	-1.17374800
C	2.30192600	-1.40583100	1.00039100
C	2.43684700	-1.90068200	-1.73664400

PhOH

C	-1.18070000	-1.18877200	-0.00008800
C	0.21474300	-1.22799700	0.00024700
C	0.94515600	-0.03028800	0.00031200
C	0.27123200	1.19969200	0.00008100
C	-1.12601900	1.22512800	0.00001900
C	-1.86084800	0.03493400	-0.00012000
H	-1.74205400	-2.12654800	-0.00012900

H	0.75552200	-2.17689100	0.00048900
H	0.84910200	2.12804000	0.00011000
H	-1.64292800	2.18805900	-0.00003500
H	-2.95263800	0.06001300	-0.00039500
O	2.30781500	-0.11564500	-0.00046900
H	2.68909200	0.77631400	0.00099800

4b

C	-1.50259500	-1.18024000	0.01336300
S	-2.78455000	-2.20225200	0.27309400
C	-1.67652800	0.29162300	0.00431100
C	-2.75838800	0.84723200	-0.70586900
C	-0.82840700	1.14168200	0.73890400
C	-2.98090600	2.22317100	-0.69046100
H	-3.41680600	0.18643600	-1.27198400
C	-1.07277900	2.51647600	0.76862100
H	0.02613500	0.72733900	1.28074300
C	-2.14234300	3.06221400	0.05274800
H	-3.81495200	2.64309900	-1.25736200
H	-0.41786500	3.16544400	1.35500300
H	-2.32330900	4.13951900	0.07194900
C	1.29282700	-0.68596400	-0.77094900
H	1.63809000	-1.01825400	-1.75736000
H	0.79468900	0.28300800	-0.89155100
C	2.48227900	-0.60424200	0.18682600
H	3.00671900	-1.58307000	0.14503800
C	3.53071600	0.41413500	-0.34787400
O	3.63670000	0.52644300	-1.59568300
O	4.22117500	1.01454600	0.51484200
N	2.08523600	-0.25511200	1.54620400
H	1.78765100	-1.09142100	2.04833200
H	2.92423200	0.09725200	2.00896300
S	0.05158000	-1.93824800	-0.23598100

TS3

imaginary frequency = -41.53 cm⁻¹

C	1.07879200	1.37927800	0.06713000
S	1.65166700	2.57247000	-0.90700200
C	1.68627800	0.03778700	0.16173900
C	1.45772900	-0.79493300	1.27743000
C	2.49846700	-0.45034400	-0.88593800

C	2.02304900	-2.06837400	1.34339900
H	0.83322600	-0.42961800	2.09203900
C	3.04717300	-1.72655000	-0.82397100
H	2.66897200	0.18276100	-1.75748400
C	2.81289700	-2.54165200	0.29204800
H	1.84114800	-2.69541100	2.21883500
H	3.65654700	-2.09500400	-1.65217500
H	3.24413500	-3.54428600	0.33798400
C	-1.76302900	1.07404600	0.19790800
H	-2.61161100	1.45212600	0.78398600
H	-1.76603700	1.57057100	-0.78446500
C	-1.90688800	-0.43489500	0.03156900
H	-1.70586000	-0.90086200	1.01691900
C	-3.40790800	-0.78029400	-0.24914200
O	-4.27260400	-0.15316100	0.41337600
O	-3.63259400	-1.69087300	-1.08770000
N	-1.05742000	-0.97285500	-1.02706300
H	-0.21301100	-1.37902900	-0.62909000
H	-1.59281800	-1.74236300	-1.43497500
S	-0.33107400	1.73871500	1.15196700

4a

C	-0.97648600	0.60728600	0.14862600
S	-0.63779600	2.16080700	0.60745000
C	-2.36429200	0.08658700	0.03259400
C	-2.67312700	-1.25552800	0.33071200
C	-3.40298500	0.94461800	-0.37851600
C	-3.98384700	-1.72254400	0.22102400
H	-1.88909600	-1.93010900	0.67862000
C	-4.70805600	0.47124800	-0.49827600
H	-3.16725800	1.98424200	-0.61040700
C	-5.00406300	-0.86352900	-0.19735200
H	-4.20822200	-2.76194800	0.47072900
H	-5.49974500	1.14649400	-0.83073500
H	-6.02869900	-1.23176200	-0.28675100
C	1.81403700	0.25710200	0.05132500
H	1.83727800	1.17654300	-0.54541200
H	1.84110700	0.53024100	1.11661000
C	2.97993600	-0.65765800	-0.30889000
H	2.88916100	-0.90935000	-1.38714500
C	4.32225200	0.12868900	-0.22197600

O	4.29771100	1.34330900	-0.54380700
O	5.33757200	-0.53169100	0.11717900
N	3.02634700	-1.84476200	0.54044500
H	2.46606900	-2.58984000	0.12548000
H	3.99647200	-2.16485400	0.51189300
S	0.23004700	-0.58623700	-0.27548700

TS4a

imaginary frequency = -208.10 cm⁻¹

C	-0.31085600	1.03209500	0.06152400
C	2.31517400	1.04980300	0.52860400
H	3.19693300	0.84369500	1.14719200
H	2.29562100	2.11036100	0.24130400
C	2.28004300	0.12409300	-0.69593200
H	3.02928900	0.48127900	-1.42318600
C	2.67056200	-1.33484400	-0.32214000
O	3.73286100	-1.47758000	0.32469700
O	1.89982600	-2.24765000	-0.72320200
N	0.94565300	0.14625900	-1.28116800
H	0.69262600	-0.81531000	-1.53738800
S	0.81002800	0.67783000	1.47790700
H	0.82921400	0.80118200	-2.05272700
C	-1.49556700	0.09979000	0.05085400
C	-1.33594200	-1.28515900	0.24827500
C	-2.79345700	0.60329300	-0.13218700
C	-2.44164300	-2.13574700	0.25838200
H	-0.33421600	-1.69749400	0.37253700
C	-3.90169000	-0.24694500	-0.11296600
H	-2.91270100	1.67690000	-0.28513500
C	-3.73094500	-1.62020100	0.08238500
H	-2.29525400	-3.20889500	0.40312600
H	-4.90355800	0.16783000	-0.24885300
H	-4.59670900	-2.28677800	0.09634500
S	-0.44855200	2.63393100	-0.50026900

TS4b

imaginary frequency = -223.95 cm⁻¹

C	0.19209500	0.76552100	0.45358700
S	0.14294900	2.46145900	0.64033400
C	1.52548200	0.14666800	0.09489100
C	2.11058700	-0.87134300	0.86125000

C	2.23268500	0.63456100	-1.02058400
C	3.36885200	-1.38610800	0.52728200
H	1.58012500	-1.25317100	1.73486900
C	3.47842800	0.11176100	-1.36276200
H	1.79606400	1.44232000	-1.61141500
C	4.05592000	-0.90244100	-0.58711400
H	3.80937700	-2.17198300	1.14580800
H	4.00614300	0.49983200	-2.23753900
H	5.03496800	-1.30884700	-0.85168000
C	-1.20385100	-1.56693900	0.47914500
H	-1.98760600	-2.19407400	0.92220600
H	-0.30388400	-2.17696000	0.31559800
C	-1.70129800	-0.92046400	-0.82137000
H	-1.69437800	-1.67712500	-1.62371300
C	-3.16392100	-0.40672300	-0.67656900
O	-4.00024000	-1.23486300	-0.24682400
O	-3.37913500	0.78404700	-1.01886200
N	-0.81977100	0.19220100	-1.15559300
H	-1.40389500	1.00861500	-1.37277000
S	-0.84825400	-0.18222600	1.60996200
H	-0.14850400	-0.00215800	-1.89800600

5a

C	-0.15188800	0.87567900	-0.11742700
C	2.30556500	0.99116000	0.72276900
H	3.15803900	0.69248300	1.34475300
H	2.33695600	2.06888000	0.51219400
C	2.26424300	0.17181000	-0.56113200
H	2.93342900	0.58972200	-1.32663400
C	2.64841500	-1.32054100	-0.33989600
O	3.72737400	-1.53872900	0.24301400
O	1.83186800	-2.16880400	-0.79653700
N	0.86017400	0.19451100	-1.08592300
H	0.67231900	-0.81940000	-1.25731100
S	0.73156800	0.59804600	1.54539100
H	0.78790000	0.73424500	-1.95528100
C	-1.43912800	0.05086500	-0.06455500
C	-1.39617800	-1.35107000	0.04483400
C	-2.68729000	0.68450000	-0.06470700
C	-2.57481700	-2.09479600	0.13405400
H	-0.43666800	-1.87176200	0.06751400

C	-3.86761200	-0.05773600	0.03961300
H	-2.70072400	1.77240900	-0.15205900
C	-3.81700700	-1.45085100	0.13497700
H	-2.52081300	-3.18357400	0.20973500
H	-4.83130700	0.45784200	0.04334400
H	-4.73868300	-2.03285600	0.21142300
S	-0.28540700	2.58299000	-0.62284200

5b

C	0.10482500	0.77170100	0.23717800
S	0.24626700	2.54719300	0.29429300
C	1.45474000	0.09513200	-0.01117900
C	2.15154100	-0.58792600	0.99460700
C	2.06562700	0.22067300	-1.27335100
C	3.41838500	-1.13013800	0.75091300
H	1.69329300	-0.69312600	1.97898600
C	3.32191100	-0.33165600	-1.52242500
H	1.57175600	0.78580900	-2.06769700
C	4.00881900	-1.01066100	-0.50861300
H	3.94177800	-1.65384500	1.55485300
H	3.77118000	-0.22266900	-2.51267000
H	4.99514600	-1.43923000	-0.70118100
C	-1.19056600	-1.45232900	0.75548000
H	-2.01027300	-2.00839400	1.22702500
H	-0.30657500	-2.10263600	0.68836200
C	-1.62588800	-0.92857400	-0.61621100
H	-1.42274800	-1.66329400	-1.40733200
C	-3.14012800	-0.56185800	-0.64924500
O	-3.93163600	-1.48437700	-0.36732500
O	-3.41411200	0.62721800	-0.95897600
N	-0.85947400	0.32686000	-0.89657400
H	-1.60448400	1.05271200	-0.98197200
S	-0.80278700	0.06075600	1.70283000
H	-0.35805200	0.28055000	-1.78883900

6a

C	-0.26385500	-0.44134100	0.43064200
C	1.95885400	-1.71650800	-0.52004700
H	2.16048500	-1.80304000	-1.59717700
H	2.63743100	-2.38862500	0.01952200
C	2.12987900	-0.27959700	-0.03944800

H	2.28110400	-0.26712600	1.05039200
C	3.26548600	0.51737800	-0.71038200
O	4.32665700	-0.11457500	-0.91611400
O	3.02622600	1.72682900	-0.95273600
N	0.81587400	0.38387500	-0.24221200
H	0.63661900	0.47806500	-1.25080200
S	0.20064800	-2.17352500	-0.20558500
O	0.58024500	2.64693800	1.32655200
H	0.26140400	1.86755200	1.86391100
H	1.51233200	2.72979700	1.58567200
H	0.83119700	1.35123700	0.17041600
C	-1.63048100	-0.06819900	-0.10350100
C	-2.70251900	-0.95863200	0.08471800
C	-1.87979800	1.15980200	-0.73395500
C	-3.98439500	-0.63493200	-0.35522700
H	-2.52774600	-1.90821900	0.59535200
C	-3.16950000	1.48483700	-1.17231800
H	-1.08208600	1.89110600	-0.87102600
C	-4.22558200	0.59168600	-0.98843700
H	-4.80279900	-1.34256200	-0.20169700
H	-3.34238000	2.44814300	-1.65828300
H	-5.23082100	0.84670900	-1.33169900
S	-0.16936000	-0.23839200	2.22477400

6b

C	0.22239400	0.89252600	0.17049400
S	0.35355300	2.60947000	-0.35363600
C	1.53612800	0.13214700	-0.01384200
C	2.24716000	-0.43649900	1.04894300
C	2.05760000	0.00445600	-1.31528100
C	3.45546800	-1.10748400	0.82417800
H	1.85016200	-0.34699700	2.06090400
C	3.25191100	-0.67805600	-1.54227400
H	1.53184700	0.46753100	-2.15346800
C	3.96122400	-1.23484600	-0.47014100
H	3.99752000	-1.53636300	1.67059200
H	3.63775000	-0.76842700	-2.56065200
H	4.90146400	-1.76259700	-0.64666900
C	-1.29259000	-0.87591400	1.57678800
H	-2.34069500	-0.80582700	1.89685700
H	-0.80581800	-1.67617200	2.14922000

C	-1.18435100	-1.15488300	0.06672400
H	-0.33819100	-1.83021100	-0.12114200
C	-2.44958600	-1.79575000	-0.54891000
O	-2.89749100	-2.78926300	0.06791900
O	-2.88940400	-1.27507800	-1.60242100
N	-0.85953800	0.13212300	-0.60411400
H	-1.71022300	0.74732900	-0.64595700
S	-0.50076800	0.76064100	1.88165100
O	-2.70979100	2.22483900	-0.59803600
H	-1.80066500	2.61818100	-0.45629300
H	-2.83349500	2.32300800	-1.55604900
H	-0.57611900	-0.03425800	-1.57655500

TS5a

imaginary frequency = -1182.74 cm⁻¹

C	-0.24863300	-0.42683800	0.37484900
C	1.94057600	-1.64782800	-0.63372000
H	2.08478400	-1.66074300	-1.72409600
H	2.65634400	-2.34383100	-0.17798300
C	2.10287300	-0.23090500	-0.07163700
H	2.32183800	-0.30238300	1.00555000
C	3.23459300	0.57990200	-0.73442500
O	4.29591600	-0.05166300	-0.96098400
O	3.00980000	1.79490400	-0.96426400
N	0.80236400	0.44452500	-0.18150600
H	0.61497900	0.64092000	-1.16948300
S	0.21578400	-2.15501200	-0.24795000
O	0.70375700	2.24748900	1.52731600
H	0.26869000	1.28888800	2.07292000
H	1.60257100	2.35842500	1.88327700
H	0.83181900	1.59645500	0.61164200
C	-1.62369600	-0.03955200	-0.12846100
C	-2.68385200	-0.95955000	-0.04912600
C	-1.88696500	1.24387000	-0.63066900
C	-3.96586900	-0.61129000	-0.47042200
H	-2.50284900	-1.95669000	0.35845000
C	-3.17585000	1.59399700	-1.05121900
H	-1.09322900	1.99020900	-0.68233900
C	-4.21912400	0.66996800	-0.97760400
H	-4.77411300	-1.34368700	-0.40323000
H	-3.35856100	2.59924000	-1.43882900

H	-5.22401900	0.94327500	-1.30777600
S	-0.21359100	-0.33737800	2.22673100

TS5b

imaginary frequency = -1263.06 cm⁻¹

C	0.26957600	0.75910800	-0.02805400
S	0.56105000	2.35202900	-0.89609900
C	1.54370400	-0.07416900	-0.08211300
C	2.67185000	0.34264700	0.64563800
C	1.65228700	-1.22196800	-0.87884300
C	3.87014000	-0.36579800	0.57885900
H	2.60432900	1.23590000	1.26965500
C	2.85438400	-1.93854400	-0.94247100
H	0.80354600	-1.57896700	-1.46489000
C	3.96813300	-1.51492900	-0.21672300
H	4.73416200	-0.02158600	1.15270400
H	2.91258300	-2.83329500	-1.56706300
H	4.90556100	-2.07385800	-0.26566800
C	-1.64986700	-0.18936100	1.67256100
H	-2.60416400	0.35734000	1.67885500
H	-1.62951200	-0.87789500	2.52633900
C	-1.45035800	-0.93016500	0.35229300
H	-0.71039700	-1.73593000	0.50109000
C	-2.73630900	-1.58420600	-0.19827300
O	-3.41344400	-2.23848200	0.63184400
O	-2.97390700	-1.42702000	-1.42204400
N	-0.92030700	0.07670200	-0.57850100
H	-1.82500400	1.09834300	-0.80113600
S	-0.26504700	1.02083400	1.77204700
O	-2.24889300	2.14949200	-0.96431300
H	-1.10273900	2.52428200	-0.97814600
H	-2.51513100	2.16331600	-1.89978100
H	-0.73842500	-0.32798500	-1.49875500

7a

C	-0.22512800	-0.51330000	0.35900700
C	2.00261500	-1.59878200	-0.65599200
H	2.10896900	-1.51952400	-1.74850700
H	2.75976200	-2.29503700	-0.27268300
C	2.11454100	-0.20826700	0.00829700
H	2.41419400	-0.33670700	1.05828600

C	3.17162200	0.64713400	-0.72330400
O	4.36733100	0.32071400	-0.52498000
O	2.74661600	1.55532900	-1.48201200
N	0.79934300	0.41223900	-0.03216200
H	0.63710300	0.75146800	-0.98499700
S	0.32136900	-2.22138800	-0.26634000
O	0.76831300	2.93257800	1.22533200
H	-0.69130100	0.51519500	2.49717700
H	0.25317200	2.73713200	2.02222400
H	0.84036200	2.04431100	0.79621700
C	-1.59710600	-0.09135900	-0.12239900
C	-2.57676300	-1.03259700	-0.46944700
C	-1.92063300	1.27551200	-0.16821500
C	-3.85027300	-0.61905500	-0.86546100
H	-2.34679900	-2.09887500	-0.43140000
C	-3.19483500	1.68635500	-0.56899800
H	-1.18116000	2.01795200	0.13354700
C	-4.16399800	0.74274800	-0.92057500
H	-4.60014000	-1.36655500	-1.13473000
H	-3.42915200	2.75306800	-0.60216700
H	-5.15972000	1.06578300	-1.23326400
S	-0.24755700	-0.73818700	2.21266800

7b

C	0.27862000	0.70769500	-0.07019700
S	0.57919300	2.26811200	-1.03076100
C	1.60096600	-0.05678600	-0.08437300
C	2.73158300	0.48617000	0.54882400
C	1.72369800	-1.28560800	-0.74532100
C	3.95374100	-0.18557900	0.52389900
H	2.65186600	1.44183000	1.07172200
C	2.94848400	-1.96297800	-0.76496000
H	0.86527500	-1.73234300	-1.24973800
C	4.06683700	-1.41717100	-0.13244500
H	4.82185900	0.25218800	1.02244000
H	3.02304000	-2.92333600	-1.28057500
H	5.02208100	-1.94697700	-0.14833600
C	-1.68487300	-0.05318100	1.62240500
H	-2.60650200	0.53557100	1.51377400
H	-1.74282900	-0.65294800	2.53869900
C	-1.43374700	-0.91389700	0.38685500

H	-0.71177300	-1.71049900	0.65723100
C	-2.69238700	-1.62692800	-0.15180000
O	-3.46147100	-2.11463300	0.71380400
O	-2.81781800	-1.69331000	-1.40053400
N	-0.87128600	0.00873300	-0.59925600
H	-2.21789100	1.21847200	-0.82277300
S	-0.23836400	1.08125900	1.70328400
O	-2.85673900	1.97628300	-0.86468200
H	-0.71308000	2.67543900	-0.94517300
H	-2.92733200	2.14162500	-1.81709200
H	-0.68826900	-0.44722700	-1.49177200

8a

C	-0.15601700	-0.48234000	0.26467000
C	2.07907800	-0.78173800	-1.17611400
H	2.17625700	-0.07787300	-2.01674200
H	2.85528500	-1.55396000	-1.26271100
C	2.17265900	-0.02346800	0.17172700
H	2.49147700	-0.72682700	0.95319700
C	3.21061600	1.11265700	0.04040000
O	4.40535100	0.80918300	0.27556100
O	2.77580200	2.22699600	-0.35301500
N	0.85363800	0.49420700	0.49285400
H	0.69981000	1.31973300	-0.09218700
S	0.41684400	-1.54482800	-1.22305700
C	-1.52978000	0.11271900	0.04738400
C	-2.54133700	-0.63212000	-0.58076800
C	-1.82960500	1.40311400	0.50819300
C	-3.81506900	-0.09397700	-0.75981400
H	-2.33127700	-1.64512900	-0.93007400
C	-3.10883600	1.94202300	0.32955800
H	-1.06574200	1.99171600	1.01700800
C	-4.10489000	1.19866200	-0.30593600
H	-4.58657100	-0.68628600	-1.25752500
H	-3.32278800	2.94997000	0.69309900
H	-5.10301500	1.61996800	-0.44686700
S	-0.21513300	-1.74085400	1.64150800
H	-0.72642300	-0.90245200	2.58142900

8b

C	0.17173700	-0.81821400	0.32977100
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S	0.82490300	-2.05469900	1.55028200
C	1.35062500	0.12031400	0.05548900
C	2.51649100	-0.36624700	-0.55923900
C	1.30494900	1.46615500	0.44213000
C	3.60903400	0.47190400	-0.78197800
H	2.56601000	-1.41218400	-0.86981800
C	2.39870400	2.30927700	0.21364900
H	0.41211700	1.87216800	0.92063100
C	3.55372400	1.81695800	-0.39690300
H	4.50735200	0.07478600	-1.26078200
H	2.34244000	3.35726500	0.51760000
H	4.40727900	2.47550800	-0.57383600
C	-1.96416400	-0.73215400	-1.31146500
H	-2.79139700	-1.38775300	-1.00444100
H	-2.14934600	-0.36833300	-2.33002700
C	-1.75691900	0.40535200	-0.31992300
H	-1.14430800	1.18330400	-0.82397700
C	-3.03205200	1.12961200	0.15338800
O	-4.02090500	1.11826900	-0.62151700
O	-2.94953800	1.71752200	1.26366900
N	-1.04120900	-0.20538000	0.79773200
S	-0.37650400	-1.66508500	-1.26198600
H	-0.30098900	-2.80601700	1.58954500
H	-0.88430200	0.46137000	1.55152600

9a

C	0.25234700	-0.73758200	-0.17616100
C	-1.94710300	-0.69051700	1.34394900
H	-2.05833500	0.23420200	1.92959200
H	-2.68732300	-1.42704900	1.68510200
C	-2.08783400	-0.38883400	-0.16497400
H	-2.32230800	-1.32311400	-0.69085000
C	-3.24162300	0.60413400	-0.41113900
O	-4.35025500	0.11562600	-0.71588000
O	-3.00034000	1.83753600	-0.24151100
N	-0.80143400	0.11139200	-0.63844600
H	-0.65876300	1.04109000	-0.23168000
S	-0.24959300	-1.34042600	1.56438300
C	1.60511400	-0.05728000	-0.13227700
C	2.66607400	-0.63788900	0.58239100
C	1.83740000	1.13729200	-0.82927200

C	3.92325400	-0.03494100	0.60940300
H	2.50956900	-1.57387100	1.12400900
C	3.09856400	1.74260400	-0.80047400
H	1.03648800	1.59801400	-1.40728800
C	4.14528800	1.16222400	-0.08181900
H	4.73393000	-0.50105300	1.17439600
H	3.25867000	2.67498100	-1.34732300
H	5.12925800	1.63629400	-0.06013900
S	0.32591500	-2.18992000	-1.36323000
H	0.97961200	-3.02971200	-0.52818900
O	-0.78244400	2.80477100	0.87706800
H	-0.33493400	3.22376000	0.12658500
H	-1.64153000	2.49353000	0.48128400

TS6a

imaginary frequency = -225.42 cm⁻¹

C	-0.22684000	-0.71463600	0.37338400
C	1.98700700	-1.36493600	-0.98977700
H	1.92747400	-0.93501200	-2.00096500
H	2.80906900	-2.09052300	-0.94974200
C	2.12401500	-0.25843700	0.06846100
H	2.52855900	-0.72255800	0.99361900
C	3.15315600	0.81041000	-0.35227300
O	4.24905100	0.36749200	-0.76292700
O	2.84978000	2.03308500	-0.24189800
N	0.78995900	0.23778400	0.27528600
H	0.57322100	1.23118600	0.25031600
S	0.41663400	-2.21044700	-0.56746500
C	-1.56599500	-0.15630000	-0.08240000
C	-2.27228300	-0.66910300	-1.17705500
C	-2.10237800	0.93979800	0.61756600
C	-3.49070900	-0.10197500	-1.56534900
H	-1.86063100	-1.51428000	-1.73016600
C	-3.31653200	1.50709300	0.22687000
H	-1.56735700	1.34898200	1.47631200
C	-4.01742700	0.98676200	-0.86630500
H	-4.02882000	-0.51651900	-2.42130300
H	-3.71706200	2.35961400	0.78067300
H	-4.96941400	1.42862300	-1.16996700
S	-0.59868900	-1.35903100	2.17037300
H	0.61687200	-1.92734600	2.34338200

O	0.57811600	3.22455800	0.46856700
H	0.56617100	3.06749400	1.42506200
H	1.45742400	2.84436200	0.20058300

10a

C	-0.30220400	-0.41143500	0.30042100
C	1.77829700	-1.78721500	-0.66260200
H	1.84923600	-1.79718300	-1.75846500
H	2.46971700	-2.53115300	-0.24649000
C	2.02920900	-0.38916100	-0.11401200
H	2.28133900	-0.46744500	0.96531900
C	3.20241700	0.37886600	-0.75439700
O	3.95407400	-0.22723900	-1.54653100
O	3.32798000	1.58684200	-0.38908800
N	0.76388800	0.31759500	-0.30418100
H	0.80947300	1.27045400	0.06485300
S	0.05183800	-2.18565200	-0.15224000
C	-1.68148700	0.02651400	-0.15226200
C	-2.82070900	-0.68212000	0.26519600
C	-1.84275600	1.14262300	-0.98316500
C	-4.09316600	-0.28514600	-0.14565400
H	-2.70851700	-1.54969200	0.91902100
C	-3.12039900	1.54530200	-1.38710900
H	-0.96625200	1.69487500	-1.32133200
C	-4.24845600	0.83491000	-0.97126100
H	-4.96873300	-0.85063000	0.18188700
H	-3.22983400	2.42094300	-2.03143900
H	-5.24536500	1.14968900	-1.28871400
S	-0.34448600	-0.23254100	2.21967800
H	0.75697300	-0.98285600	2.45450500
O	1.62059400	2.61294000	1.42652800
H	1.34443600	1.86514600	1.98205600
H	2.31703700	2.22661200	0.83085900

TS7a

imaginary frequency = -78.24 cm⁻¹

C	-0.24125900	-0.60213000	-0.07824600
C	2.00129300	-1.86531600	-0.01928100
H	2.22179000	-2.28170200	-1.01196000
H	2.65332200	-2.32602800	0.73142500
C	2.07167200	-0.34854200	-0.00632400

H	2.09819600	0.00734000	1.04407200
C	3.27025700	0.29793200	-0.72652200
O	4.20812300	-0.44356800	-1.08132300
O	3.20345900	1.55445900	-0.85491200
N	0.78935400	0.08932000	-0.55690800
H	0.67956600	1.10797900	-0.66288900
S	0.23832100	-2.22350400	0.40774900
C	-1.64139500	-0.24539900	-0.33486700
C	-2.65122700	-1.21988400	-0.25095600
C	-1.98866900	1.07539700	-0.68345900
C	-3.98090900	-0.88288000	-0.50531600
H	-2.40016200	-2.25029400	0.00811600
C	-3.31689700	1.40400500	-0.93970900
H	-1.22598100	1.85383800	-0.71786200
C	-4.31800400	0.42811400	-0.85236200
H	-4.75489100	-1.65010800	-0.43552000
H	-3.57539000	2.43186700	-1.20324400
H	-5.35896100	0.69189900	-1.05223000
S	-0.33130300	0.79524700	2.34046300
H	0.79489600	0.32309600	2.92739300
O	0.97079400	2.80706500	0.16257000
H	0.68284800	2.27884400	0.95226100
H	1.85882700	2.44870900	-0.08103100

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C	0.74637800	-0.63456500	-0.30988600
C	-1.22245800	-2.18084500	-0.83274800
H	-1.77131200	-2.99119200	-0.33988500
H	-1.36144700	-2.23769300	-1.92076100
C	-1.60338300	-0.82524600	-0.25029300
H	-2.38051900	-0.31271800	-0.85148800
C	-2.16232100	-0.87534600	1.20775800
O	-2.83266000	-1.88262200	1.50702500
O	-1.93447200	0.12886000	1.93643500
N	-0.39458900	-0.00574300	-0.31025200
H	-0.50857600	1.02094900	-0.08970900
S	0.58339400	-2.36242000	-0.48534100
C	2.04344200	0.01591200	-0.14025200
C	3.23072400	-0.68277100	-0.43069400
C	2.11472400	1.34474700	0.32677700
C	4.46724800	-0.06567500	-0.25467500

H	3.18895700	-1.70577900	-0.80989500
C	3.35494900	1.95350600	0.49859000
H	1.20380600	1.89741400	0.56191700
C	4.53141500	1.25172800	0.21057500
H	5.38318600	-0.61309700	-0.48516200
H	3.40471800	2.98102500	0.86426100
H	5.50156400	1.73433600	0.34851700
S	-3.56783400	1.97495900	-1.30121800
H	-4.13563600	1.44136400	-0.19218200
O	-1.17971600	2.39189600	0.59957300
H	-1.94611600	2.40237900	-0.06601700
H	-1.49498700	1.70884900	1.24191700

TS8

imaginary frequency = -946.86 cm^{-1}

C	-0.68315500	-0.71550800	0.08852400
C	1.31592800	-2.26941000	0.42661500
H	1.43683800	-2.94150200	-0.43328800
H	1.91779500	-2.64578200	1.26173100
C	1.64866900	-0.81873700	0.06329200
H	2.03227900	-0.25665400	0.94022200
C	2.77226000	-0.71242900	-1.00274800
O	2.87271600	0.36706700	-1.66094400
O	3.54135000	-1.68891700	-1.08762200
N	0.40270700	-0.14575800	-0.31273400
H	0.60487600	1.07486700	-0.65965700
S	-0.45548700	-2.25730000	0.91816400
C	-2.02699500	-0.14023000	-0.07151500
C	-3.16543300	-0.87144200	0.31318800
C	-2.19079700	1.15403300	-0.60403200
C	-4.43915800	-0.32034200	0.17677900
H	-3.06143500	-1.88146100	0.71504300
C	-3.46572400	1.69830500	-0.74076700
H	-1.32203100	1.73715600	-0.90877600
C	-4.59231200	0.96546300	-0.34972000
H	-5.31414600	-0.89894300	0.47975100
H	-3.58132600	2.70276600	-1.15332200
H	-5.58997600	1.39693600	-0.45803200
S	2.43044600	2.42273800	1.72814600
H	3.52012600	1.91436100	1.10395700
O	1.14125000	2.12011600	-0.93820800

H	1.54264800	2.36038300	0.00786100
H	1.91384700	1.60683100	-1.35081500

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C	-0.10595800	0.26555700	-0.18779600
C	-1.53940600	-0.06117200	-0.04310600
C	-2.48187000	0.92239300	0.30170100
C	-1.98009200	-1.38036400	-0.25825800
C	-3.83390600	0.59632300	0.42746800
H	-2.15679200	1.94853600	0.48526400
C	-3.32920100	-1.70444800	-0.12762000
H	-1.25136300	-2.14270400	-0.53515500
C	-4.26144300	-0.71708300	0.21475800
H	-4.55417500	1.37213700	0.69636600
H	-3.65852300	-2.73213900	-0.29757400
H	-5.31904700	-0.97223700	0.31436700
C	2.13893300	1.44818300	-0.12874900
H	2.46875600	1.56221100	0.91279500
H	2.77396200	2.06269100	-0.77986600
C	2.14347900	-0.03485800	-0.52654400
H	2.36596100	-0.14839500	-1.60187400
C	3.21659500	-0.88260500	0.22591800
O	3.54577600	-1.95509200	-0.33733200
O	3.64040700	-0.44858900	1.32576900
N	0.81785700	-0.61010700	-0.30505500
S	0.39462300	1.98990900	-0.27206600

TS9

imaginary frequency = -237.87 cm^{-1}

C	0.12927800	0.49847000	-0.02280100
C	1.54085900	0.16721800	-0.25887400
C	2.55438900	1.06458800	0.11819900
C	1.88714000	-1.04713500	-0.87342100
C	3.89127200	0.74778100	-0.10732800
H	2.29525700	2.00074500	0.61653500
C	3.22980700	-1.36245000	-1.09248900
H	1.10989500	-1.74006500	-1.19680300
C	4.23375200	-0.46871900	-0.71127600
H	4.67209200	1.44905900	0.19444300
H	3.48965100	-2.30844700	-1.57246000
H	5.28321000	-0.71601600	-0.88646300

C	-2.17449900	1.60523800	-0.27138700
H	-2.43554400	1.72127700	-1.33251300
H	-2.83997800	2.22604400	0.33841600
C	-2.17833000	0.14219100	0.15850400
H	-2.30067100	0.08025100	1.25766900
C	-3.30777100	-0.70792400	-0.46694300
O	-4.37390300	-0.09871000	-0.72287900
O	-3.06477100	-1.92928800	-0.61575100
N	-0.84968200	-0.37563300	-0.16065000
S	-0.42863000	2.16280100	-0.04314000
O	0.49730200	0.07196700	2.26617000
H	0.24003900	-1.28025500	1.92249000
H	-0.37454100	0.40564400	2.52352400
O	0.01636800	-2.26284900	1.53859700
H	0.86910800	-2.56083200	1.18871300
H	-0.63800500	-1.33728000	0.19905300

TS9a

imaginary frequency = -277.08 cm⁻¹

C	0.01185500	-0.66275300	-0.02207800
C	-1.39216500	-0.40611800	-0.38760700
C	-2.41800100	-1.23072400	0.10148300
C	-1.70810700	0.66164800	-1.24166800
C	-3.74381000	-0.97363800	-0.23887900
H	-2.17426300	-2.04236300	0.78756700
C	-3.03959600	0.91669600	-1.57785300
H	-0.91685300	1.29087600	-1.64892400
C	-4.05931300	0.10463000	-1.07539700
H	-4.53762800	-1.61039400	0.15755600
H	-3.27808100	1.75241300	-2.23926400
H	-5.10042200	0.30786900	-1.33629400
C	2.37668800	-1.66977300	-0.15814700
H	2.70268500	-1.81124600	-1.19800600
H	3.03677400	-2.23713700	0.50725600
C	2.30268000	-0.18930500	0.21841500
H	2.43075000	-0.07982400	1.31278900
C	3.39762000	0.67937100	-0.44737800
O	4.51614200	0.12698600	-0.57836600
O	3.08051700	1.85343200	-0.74926500
N	0.95073300	0.24964000	-0.11587800
S	0.64954500	-2.30265600	-0.00325100

O	-0.53679400	-0.49137200	2.23084900
H	-1.16138600	0.67783800	2.11366100
H	0.36637700	-0.27051300	2.50125900
O	0.11328500	2.79355500	0.47427300
H	-0.37546600	3.10761300	-0.30103800
H	0.70692300	1.26645300	-0.01108900
O	-1.69145500	1.65698800	1.97452000
H	-0.60902300	2.40222700	1.07031300
H	-2.35891300	1.44428100	1.30594500

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C	-0.15297600	-0.40324500	0.50748900
C	-1.54094900	-0.12573900	-0.04100200
C	-2.66802300	-0.64539200	0.61527800
C	-1.72096900	0.63432300	-1.20387500
C	-3.94982700	-0.41420100	0.11193300
H	-2.53859000	-1.23032300	1.52685800
C	-3.00527400	0.87186400	-1.70256000
H	-0.84751800	1.03792700	-1.71466200
C	-4.12373300	0.34813700	-1.04821000
H	-4.81773300	-0.82741000	0.63152100
H	-3.13033700	1.47150200	-2.60744500
H	-5.12702700	0.53260100	-1.43956000
C	2.08246100	-1.57318900	-0.42261500
H	2.15390300	-1.57161300	-1.51975200
H	2.84402500	-2.24707600	-0.01124600
C	2.18890100	-0.15978200	0.13985700
H	2.44408200	-0.23642300	1.22029500
C	3.30893200	0.69574800	-0.48739500
O	4.36092900	0.08580000	-0.80935400
O	3.09566300	1.93127700	-0.57758200
N	0.86788100	0.41976400	-0.06830800
S	0.40457500	-2.14783600	0.07859100
O	-0.26202200	-0.28131000	1.93230500
H	-0.40044000	1.61086600	2.05615100
H	0.54519400	-0.64724000	2.32921100
O	-0.42920700	2.54699600	1.77428300
H	-1.11115800	2.52869400	1.08460000
H	0.80307900	1.37227300	0.29412000

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C	-0.27456600	0.42405200	-0.28545800	H	-3.54648600	-2.38703100	1.43773700
C	-1.70704200	-0.07682400	-0.18570100	H	-5.43794200	-1.12130100	0.41419800
C	-2.77884400	0.74988800	-0.54974300	C	2.00798100	0.09151800	1.25927800
C	-1.97918500	-1.35552400	0.32291800	H	1.89950000	-0.84411100	1.83390200
C	-4.09761800	0.30455200	-0.41208600	H	3.01268700	0.49160100	1.46539100
H	-2.57634700	1.74589700	-0.94267000	C	1.96846900	-0.28378200	-0.25600600
C	-3.29489500	-1.80143100	0.45754000	H	2.34844900	0.55330300	-0.85317800
H	-1.14601600	-1.99660100	0.60948900	C	2.85268000	-1.52886900	-0.47480800
C	-4.36110300	-0.97191900	0.09131600	O	4.08162800	-1.31686200	-0.61185100
H	-4.92245500	0.96073500	-0.70083000	O	2.27377700	-2.64633300	-0.42629300
H	-3.48948200	-2.80188600	0.85185500	N	0.59675900	-0.57547100	-0.61322400
H	-5.39119300	-1.32051500	0.19792200	S	0.70705000	1.26742200	1.74312700
C	1.85342200	0.10850500	1.37575100	O	-0.23983300	1.50673800	-1.23151400
H	1.76669700	-0.78547000	2.00902400	H	0.64710100	1.99001500	-1.10198200
H	2.67580400	0.73497200	1.74336400	H	0.33380800	-1.50498700	-0.28458500
C	2.01575900	-0.26773700	-0.09058100	O	1.80136500	2.90925500	-0.56332500
H	2.39497200	0.62183900	-0.63603000	H	1.52692600	2.58921500	0.35623700
C	3.03117200	-1.39484200	-0.37099800	H	1.42261900	3.80129800	-0.62519700
O	3.93713600	-1.57877100	0.48129800				
O	2.88996800	-2.00404800	-1.46261800				
N	0.67082600	-0.63842200	-0.52793300				
S	0.27277800	1.05487300	1.43719800				
O	-0.23945700	1.46433500	-1.22715600				
H	0.56980300	2.01222000	-1.09581600				
H	0.67055800	-0.88522600	-1.51760900				
O	1.80266300	3.13715000	-0.49930800				
H	1.46287500	2.85543900	0.37484400				
H	1.35946400	3.98793400	-0.64863600				

TS10

imaginary frequency = -71.03 cm^{-1}

C	-0.36411800	0.35914000	-0.58947400	H	-3.54648600	-2.38703100	1.43773700
C	-1.75583000	-0.05960400	-0.30697300	H	-5.43794200	-1.12130100	0.41419800
C	-2.82501200	0.65633600	-0.87092400	C	2.00798100	0.09151800	1.25927800
C	-2.02887900	-1.15902000	0.52701000	H	1.89950000	-0.84411100	1.83390200
C	-4.14224900	0.27239200	-0.61477600	H	3.01268700	0.49160100	1.46539100
H	-2.61727400	1.51112400	-1.51433700	C	1.96846900	-0.28378200	-0.25600600
C	-3.34557900	-1.53778800	0.78110600	H	2.34844900	0.55330300	-0.85317800
H	-1.21450400	-1.69979800	1.01265900	C	2.85268000	-1.52886900	-0.47480800
C	-4.40658200	-0.82451600	0.21027400	O	4.08162800	-1.31686200	-0.61185100
H	-4.96578000	0.83298600	-1.06266700	O	2.27377700	-2.64633300	-0.42629300
				N	0.59675900	-0.57547100	-0.61322400
				S	0.70705000	1.26742200	1.74312700
				O	-0.23983300	1.50673800	-1.23151400
				H	0.64710100	1.99001500	-1.10198200
				H	0.33380800	-1.50498700	-0.28458500
				O	1.80136500	2.90925500	-0.56332500
				H	1.52692600	2.58921500	0.35623700
				H	1.42261900	3.80129800	-0.62519700

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C	0.29599100	-0.40755500	-0.30612000	C	0.29599100	-0.40755500	-0.30612000
C	1.76262600	-0.16553600	-0.10072800	C	1.76262600	-0.16553600	-0.10072800
C	2.67096600	-1.03318200	-0.72629800	C	2.67096600	-1.03318200	-0.72629800
C	2.25072200	0.91091300	0.65687000	C	2.25072200	0.91091300	0.65687000
C	4.04509900	-0.84696900	-0.57228900	C	4.04509900	-0.84696900	-0.57228900
H	2.28563000	-1.85782800	-1.32846100	H	2.28563000	-1.85782800	-1.32846100
C	3.62664900	1.10257000	0.80152400	C	3.62664900	1.10257000	0.80152400
H	1.55918600	1.62174300	1.11400500	H	1.55918600	1.62174300	1.11400500
C	4.52595300	0.22124600	0.19313900	C	4.52595300	0.22124600	0.19313900
H	4.74459500	-1.53539000	-1.05210900	H	4.74459500	-1.53539000	-1.05210900
H	3.99706400	1.94763600	1.38625700	H	3.99706400	1.94763600	1.38625700
H	5.60189000	0.37048500	0.31063200	H	5.60189000	0.37048500	0.31063200
C	-2.55390400	0.83686500	-0.50221500	C	-2.55390400	0.83686500	-0.50221500
H	-2.19706600	0.52369700	-1.49291400	H	-2.19706600	0.52369700	-1.49291400
H	-3.64578000	0.74768100	-0.49880500	H	-3.64578000	0.74768100	-0.49880500
C	-1.96959600	-0.07307300	0.58168700	C	-1.96959600	-0.07307300	0.58168700
H	-2.35417500	0.26503700	1.55749600	H	-2.35417500	0.26503700	1.55749600
C	-2.46271600	-1.55345600	0.44063000	C	-2.46271600	-1.55345600	0.44063000
O	-1.74532400	-2.44220200	0.95574600	O	-1.74532400	-2.44220200	0.95574600
O	-3.57025300	-1.71740600	-0.13090500	O	-3.57025300	-1.71740600	-0.13090500
N	-0.52393000	0.01705500	0.67283700	N	-0.52393000	0.01705500	0.67283700

S	-2.07386100	2.60347000	-0.36305900
O	-0.11939100	-0.98109700	-1.32448700
H	-2.68915600	2.84263600	0.82016200
H	-0.12390400	0.47409000	1.48278100

OH-

O	0.00000000	0.00000000	0.10808500
H	0.00000000	0.00000000	-0.86467800

TS11

imaginary frequency = -314.81 cm⁻¹

C	-0.12350100	-0.26882400	0.23717900
C	-1.55334200	0.12207400	0.07583100
C	-2.57122600	-0.84222500	-0.02237600
C	-1.90500900	1.47701200	-0.01405400
C	-3.90071100	-0.46255300	-0.20325500
H	-2.31286000	-1.89745800	0.07542100
C	-3.23903600	1.86072100	-0.18954000
H	-1.11689800	2.22765200	0.05175900
C	-4.24279600	0.89369000	-0.28522800
H	-4.67786400	-1.22780900	-0.27474900
H	-3.49239600	2.92206500	-0.25503800
H	-5.28507200	1.19120900	-0.42420800
C	2.08803500	-1.05220600	-0.85314900
H	2.22278900	-0.56703200	-1.83422700
H	2.85769100	-1.82463700	-0.73020000
C	2.12692000	-0.00490900	0.28583800
H	2.33750800	-0.55950400	1.22532300
C	3.31603000	0.95181800	0.06104900
O	4.45026300	0.39226300	0.05635200
O	3.10038500	2.17584200	-0.11791900
N	0.81977900	0.60500900	0.37988200
S	0.41674300	-1.78051900	-0.75489000
O	-0.42079800	-1.31629600	1.98828200
H	0.04976600	-2.07330900	1.61747600

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C	0.38476500	0.34049000	0.32780000
C	1.83735300	0.04766900	0.13142700
C	2.80652600	1.03551800	0.37108300
C	2.25888000	-1.22603200	-0.28996600

C	4.16444600	0.75880300	0.18826500
H	2.48656900	2.02510200	0.69909900
C	3.61354300	-1.50190800	-0.47258200
H	1.50473400	-1.99351600	-0.46562200
C	4.57273200	-0.50978200	-0.23328500
H	4.90675800	1.53857500	0.37578900
H	3.92573300	-2.49739500	-0.79806200
H	5.63434700	-0.72699500	-0.37444900
C	-2.63700000	0.66609500	-0.71604900
H	-2.47331100	0.33097600	-1.75749100
H	-3.71380900	0.54978100	-0.51331100
C	-1.89595300	-0.30991100	0.21935900
H	-2.00729500	0.10371300	1.24098100
C	-2.65208400	-1.66825600	0.22297100
O	-3.78506000	-1.64492500	0.78453400
O	-2.13862600	-2.67160300	-0.33392900
N	-0.49286400	-0.48003200	-0.11651800
S	-2.15623500	2.43677500	-0.51281700
O	0.13709100	1.48209300	0.99494300
H	-0.74041800	1.92094300	0.55524400

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C	0.42391900	0.29282500	0.75668300
C	1.82501400	0.01521100	0.27615000
C	2.84246400	0.89177600	0.68266600
C	2.15723300	-1.08723300	-0.52836800
C	4.16177400	0.68753000	0.27552900
H	2.58201200	1.73747100	1.32105700
C	3.47876400	-1.29682400	-0.92872800
H	1.39393100	-1.80830600	-0.82877100
C	4.48312600	-0.40737500	-0.53353900
H	4.94246200	1.38349000	0.59154100
H	3.72536900	-2.16241300	-1.54794900
H	5.51583100	-0.57152200	-0.85035400
C	-2.68736000	0.74785900	-0.74050100
H	-2.58654400	0.23262400	-1.71970300
H	-3.76384400	0.68327200	-0.49133400
C	-1.98030700	-0.16581500	0.29591400
H	-2.12125400	0.26739200	1.29468700
C	-2.62438900	-1.56954600	0.23628800
O	-3.74134900	-1.69802200	0.80282200

O	-2.02347000	-2.45520300	-0.43339000
N	-0.55837000	-0.27443100	0.04538800
S	-2.10732500	2.47639600	-0.82266400
O	0.23733200	1.00006200	1.76182700
H	-0.32369700	-0.88848300	-0.72689500

N	-0.41475700	-0.49068100	1.17462200
H	-0.79772400	-0.12591200	2.05262400
S	-2.17635700	-2.42796800	-1.96506700
H	-3.10513200	-2.90060300	-1.09924500
H	0.32699400	-1.15012700	1.42453500

TS12

imaginary frequency = -231.14 cm⁻¹

C	0.55347600	1.04495800	0.43750200
S	1.40547500	1.69163200	1.77244800
C	-0.64225300	1.75597500	-0.13574100
C	-0.93507400	1.70260900	-1.50714300
C	-1.51871400	2.44495400	0.71859700
C	-2.07496900	2.33612800	-2.01311900
H	-0.27107200	1.16325000	-2.18143100
C	-2.66036900	3.06604400	0.21464000
H	-1.28370200	2.48811000	1.78329400
C	-2.94282500	3.01613500	-1.15619400
H	-2.28586300	2.29058400	-3.08427900
H	-3.33380100	3.59438700	0.89374800
H	-3.83584800	3.50590100	-1.55162300
O	1.24321400	0.41858400	-0.59297500
C	2.53809300	-0.04193100	-0.41613400
C	3.60639700	0.82169200	-0.67021300
C	2.76030800	-1.37910600	-0.08187800
C	4.91375200	0.33985700	-0.57867000
H	3.40007900	1.85983500	-0.93302500
C	4.07369400	-1.85225100	0.00969200
H	1.91476500	-2.04502200	0.09457200
C	5.15150200	-0.99647500	-0.23545100
H	5.75182300	1.01240100	-0.77655000
H	4.25130300	-2.89861200	0.26889200
H	6.17549700	-1.37023100	-0.16513300
C	-0.96707200	-2.06467100	-0.63918100
H	-0.60039500	-3.00482200	-0.19984600
H	-0.12372900	-1.57906100	-1.14676500
C	-1.50974100	-1.13765600	0.44383100
H	-2.08400300	-0.33149400	-0.04365200
C	-2.49840500	-1.79497800	1.45558000
O	-3.17008900	-2.78262100	1.06600100
O	-2.56670000	-1.24348300	2.58281400

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C	-0.26720100	-0.73200600	0.57410200
S	-1.14917300	-1.49543600	1.91318600
C	0.73514200	-1.65472100	-0.11345600
C	0.63418700	-1.95987300	-1.47686000
C	1.77963300	-2.22869700	0.63207800
C	1.54922500	-2.83084400	-2.08145100
H	-0.16553400	-1.51486400	-2.06741900
C	2.69943900	-3.08292900	0.02588300
H	1.85918700	-2.01722700	1.69919300
C	2.58688300	-3.39218600	-1.33607200
H	1.44834800	-3.06353200	-3.14450100
H	3.50664700	-3.51710500	0.62089200
H	3.30430800	-4.06745400	-1.80840000
O	-1.05661500	-0.11472500	-0.46167200
C	-2.41135300	0.07604700	-0.30059600
C	-3.29254300	-0.85404600	-0.85925900
C	-2.90211400	1.22132800	0.33455100
C	-4.67066500	-0.63449700	-0.78684500
H	-2.88527900	-1.74416500	-1.34187800
C	-4.28166700	1.43361100	0.40711800
H	-2.20366700	1.93821700	0.76963800
C	-5.16969000	0.50823200	-0.15176900
H	-5.35811100	-1.36176900	-1.22585800
H	-4.66356400	2.32885300	0.90390700
H	-6.24725800	0.67876900	-0.09526100
C	0.75952400	2.59671700	-0.13061200
H	0.78623900	3.28752300	0.72615500
H	-0.29144300	2.42974000	-0.40006000
C	1.40456700	1.26280100	0.23471100
H	1.54488200	0.66634600	-0.67796500
C	2.79544100	1.37517700	0.92984900
O	3.64029500	2.13904600	0.41289800
O	2.95364200	0.65661200	1.95254000
N	0.53434700	0.46632400	1.15149300

H	1.20277200	0.12774500	1.87656700
S	1.51236800	3.38190100	-1.60420900
H	2.77409800	3.26098200	-1.12103500
H	-0.15460300	1.04807900	1.64358000

H	-0.95668500	-1.37156500	1.04929000
S	-4.63852800	0.67945300	-1.13556300
H	-4.91910800	0.74922800	0.18950000
H	-1.35537300	-2.01199800	-0.44964500

TS13

imaginary frequency = -257.95 cm⁻¹

C	0.10465500	-0.55820200	-0.59542200
S	-0.11769500	0.37263000	-1.99007000
C	1.28574700	-1.46442300	-0.45135700
C	2.48940000	-1.11553700	-1.09103100
C	1.26792100	-2.62172300	0.35092800
C	3.63689600	-1.89214700	-0.93330300
H	2.50283700	-0.22611000	-1.72051200
C	2.41520700	-3.40545100	0.49584500
H	0.36519900	-2.93745200	0.87573000
C	3.60600700	-3.04342800	-0.14027400
H	4.56110300	-1.59636500	-1.43551000
H	2.37485100	-4.30493300	1.11458100
H	4.50236700	-3.65633000	-0.02046000
O	0.40230700	0.48082400	0.93781700
C	1.27335400	1.46080700	0.72825200
C	2.63446500	1.30495500	1.08569800
C	0.87611100	2.67455300	0.11985500
C	3.55247600	2.33085800	0.86244700
H	2.94344300	0.36607500	1.55004700
C	1.80453800	3.69459100	-0.10534700
H	-0.17324200	2.80312200	-0.14758400
C	3.14506600	3.52960900	0.26027900
H	4.59707300	2.19547200	1.15603600
H	1.47728000	4.62903400	-0.56973600
H	3.86709500	4.33083000	0.08502300
C	-3.36600200	-0.61754200	-0.91176800
H	-3.84066800	-1.58529900	-0.68706000
H	-2.85934900	-0.69694500	-1.88348800
C	-2.33114100	-0.26422500	0.15205200
H	-1.98976700	0.76758800	0.00350400
C	-2.82556500	-0.42332600	1.61946700
O	-3.91808900	0.10096400	1.92440000
O	-2.05454900	-1.06551500	2.38405900
N	-1.12137800	-1.13629900	0.03604100

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C	0.16317400	-0.68630600	-0.72860200
S	-0.03066300	0.48775700	-1.86891600
C	1.38976700	-1.47196800	-0.51929300
C	2.59988400	-1.02115600	-1.08615600
C	1.41538400	-2.65144800	0.25697600
C	3.78920200	-1.71866100	-0.88363300
H	2.58783000	-0.11336100	-1.68856800
C	2.60682700	-3.34960900	0.44936100
H	0.51142900	-3.04478500	0.72364600
C	3.80008000	-2.88783700	-0.11665000
H	4.71472000	-1.34545100	-1.32812000
H	2.60197200	-4.26245100	1.04925700
H	4.73169100	-3.43615500	0.04058100
O	0.50381900	0.40723100	1.27369900
C	1.15228000	1.47399700	0.93519700
C	2.57882800	1.54749900	1.02215500
C	0.48652000	2.62084500	0.39985000
C	3.27250400	2.68923200	0.63247400
H	3.10831800	0.67833400	1.42061600
C	1.19604000	3.76131500	0.01620400
H	-0.60364800	2.59802200	0.33873500
C	2.59024300	3.80765400	0.12441800
H	4.36270800	2.71486500	0.72309400
H	0.65190600	4.62644800	-0.37473100
H	3.14115600	4.70167900	-0.17745500
C	-3.26827200	-0.72537200	-0.99410400
H	-3.73507600	-1.70643500	-0.81628600
H	-2.75685400	-0.76118500	-1.96604400
C	-2.25063500	-0.40688200	0.09621700
H	-1.92543600	0.63685500	0.00572600
C	-2.75107700	-0.64287500	1.55104200
O	-3.86413200	-0.17207800	1.86586200
O	-1.95956200	-1.28321000	2.29565800
N	-1.02432100	-1.24995400	-0.04370700
H	-0.82490800	-1.46118500	0.97026600

S	-4.55261700	0.56637000	-1.17420400
H	-4.86187800	0.56151800	0.14592800
H	-1.26669000	-2.14918700	-0.48524700

S	-4.58992800	0.19869200	-1.53613300
H	-5.05849000	0.55348800	-0.31466700
H	-1.31233700	-1.85225300	0.45387500

TS14

imaginary frequency = -37.07 cm⁻¹

C	0.05576300	-0.64094900	-0.53176800
S	-0.00244700	0.52618500	-1.68097200
C	1.13726500	-1.61895000	-0.34892000
C	2.27471500	-1.55554600	-1.18038600
C	1.10787200	-2.60129000	0.66621900
C	3.33732500	-2.44037700	-1.00928500
H	2.30912200	-0.79788600	-1.96318500
C	2.17007600	-3.48779200	0.82885800
H	0.27051100	-2.67347700	1.36082800
C	3.29107100	-3.41317600	-0.00595400
H	4.20759600	-2.36941600	-1.66563400
H	2.12570300	-4.23874400	1.62069600
H	4.12311800	-4.10827100	0.12688500
O	0.94165800	0.50339700	1.46130600
C	1.61676200	1.45125800	0.90795100
C	3.03009700	1.34413400	0.69279300
C	0.99046100	2.64305700	0.41840400
C	3.75129500	2.36111100	0.07577500
H	3.52803100	0.43560900	1.04296100
C	1.73089300	3.65929400	-0.18977900
H	-0.08506400	2.75147000	0.57827500
C	3.11275400	3.53164800	-0.36963100
H	4.83075800	2.24683600	-0.06409600
H	1.21960200	4.56391900	-0.53312100
H	3.68719300	4.32827500	-0.84831800
C	-3.25945000	-0.84626600	-0.84038900
H	-3.68639100	-1.75051100	-0.38045500
H	-2.65626800	-1.16084600	-1.70460500
C	-2.37530900	-0.10703500	0.15573600
H	-2.09391300	0.87278200	-0.25547100
C	-2.98270400	0.12583600	1.56909900
O	-4.19955600	0.40273600	1.64189600
O	-2.16206800	0.04802000	2.52063600
N	-1.09960100	-0.84818300	0.38000400
H	-0.80756400	-0.52470300	1.33666000

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C	0.68984900	-0.61953900	-0.19306100
S	0.30902600	-2.23524000	-0.47409500
C	2.10044100	-0.16717500	0.00453300
C	3.15741900	-0.84913300	-0.62230000
C	2.39849300	0.94279400	0.81688200
C	4.47524500	-0.42518400	-0.45437200
H	2.92482400	-1.71440900	-1.24468200
C	3.72024300	1.35704800	0.99533300
H	1.59929000	1.47478200	1.33632000
C	4.76218500	0.67797800	0.35767600
H	5.28396100	-0.95870100	-0.95925800
H	3.93549700	2.21158900	1.64092900
H	5.79547000	1.00532900	0.49476700
C	-2.29602400	-0.39149700	0.97917100
H	-2.27915400	0.35513200	1.78803200
H	-1.70283500	-1.25950900	1.29831200
C	-1.65888700	0.19938300	-0.29205800
H	-1.85427800	-0.49384300	-1.12600700
C	-2.24537300	1.59747500	-0.63277400
O	-3.46597500	1.64288900	-0.93171300
O	-1.45915200	2.57616200	-0.56564200
N	-0.22700000	0.34769500	-0.12919200
H	0.05042700	1.33147100	-0.08518700
S	-3.99723100	-1.02318400	0.72320400
H	-4.37345700	0.06374200	0.00002900

TS15

imaginary frequency = -1291.83 cm⁻¹

C	0.23576200	0.33953400	0.83888700
S	1.04432100	0.68685200	2.45812700
C	0.09347300	1.58305200	-0.03791500
C	0.30093200	1.51846300	-1.42306100
C	-0.35254000	2.78847700	0.52454900
C	0.08690100	2.64288700	-2.22699600
H	0.63447500	0.58727900	-1.88042900
C	-0.57060100	3.90910400	-0.27830800

H	-0.51746500	2.84278800	1.60165400
C	-0.34771200	3.84202800	-1.65813300
H	0.26126000	2.57648300	-3.30353100
H	-0.91480300	4.84103800	0.17651900
H	-0.51414200	4.72075300	-2.28567800
O	0.86748300	-0.72956500	0.12965800
C	2.19990400	-0.76265700	-0.17020200
C	3.07032000	0.33500000	-0.10678800
C	2.67750200	-2.00918800	-0.60246800
C	4.40945000	0.16829700	-0.47518200
H	2.71774700	1.30586900	0.23092800
C	4.01451900	-2.15896000	-0.97099800
H	1.98213800	-2.85022300	-0.64415700
C	4.89165200	-1.07011500	-0.90738500
H	5.08191200	1.02821100	-0.42182400
H	4.37248500	-3.13542400	-1.30650300
H	5.93952000	-1.18637200	-1.19245500
C	-2.00605500	-2.17703700	-0.11082200
H	-2.67230200	-2.57435300	0.67048100
H	-1.00507400	-2.59367300	0.06311000
C	-1.93037100	-0.64865200	-0.02928300
H	-1.48389600	-0.27534700	-0.96364800
C	-3.31916500	0.04508100	0.09161800
O	-4.22174700	-0.32518300	-0.69980800
O	-3.42275300	0.94591700	0.96450000
N	-1.10705400	-0.23801100	1.12572100
H	-1.66691900	0.49060200	1.59223300
S	-2.51744900	-2.80648600	-1.75480000
H	0.43113600	-0.75868400	2.97458200
H	-3.59223400	-1.98103000	-1.81301800
O	-0.31312400	-1.73265600	2.95781100
H	-0.83018000	-1.20333100	2.09064100
H	-0.90691800	-1.59435700	3.71544200

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C	0.21495900	0.26081200	0.83315000
S	0.99775100	0.58029400	2.49959800
C	0.16869200	1.55853500	0.02430600
C	0.41863500	1.55160800	-1.35534900
C	-0.26150200	2.74822800	0.63093300
C	0.26570500	2.71883100	-2.10916600

H	0.73294900	0.63175500	-1.84778400
C	-0.41097100	3.91421200	-0.12242300
H	-0.48420900	2.76334400	1.69910400
C	-0.14464300	3.90470600	-1.49532900
H	0.46799700	2.69689900	-3.18247700
H	-0.74067700	4.83375500	0.36659800
H	-0.26100700	4.81745300	-2.08420800
O	0.87507900	-0.78392000	0.14280300
C	2.21261200	-0.79896500	-0.15871700
C	3.08876600	0.28677600	-0.02652900
C	2.68351600	-2.02338400	-0.65532400
C	4.43073200	0.12969500	-0.39047200
H	2.74562800	1.24698500	0.34910000
C	4.02239600	-2.16293900	-1.01892800
H	1.98209700	-2.85486000	-0.74945100
C	4.90676700	-1.08597900	-0.88648700
H	5.10814500	0.98041900	-0.28356900
H	4.37625200	-3.12168000	-1.40551200
H	5.95629000	-1.19437300	-1.16824000
C	-2.04624400	-2.04571800	-0.35026700
H	-2.68190100	-2.54232100	0.39858000
H	-1.03977800	-2.47571300	-0.26628300
C	-1.96557500	-0.53890200	-0.07675800
H	-1.55692300	-0.05445800	-0.98027900
C	-3.35099600	0.13260000	0.16219000
O	-4.30213100	-0.20516400	-0.58695500
O	-3.40594800	0.99235300	1.07993500
N	-1.11656200	-0.27211800	1.09315900
H	-1.63583100	0.42297200	1.64192900
S	-2.61530300	-2.46585300	-2.04257400
H	0.64894300	-0.64902500	2.96095800
H	-3.70650900	-1.66621900	-1.94465700
O	-0.61781200	-2.40483500	2.83266700
H	-0.86420700	-1.72111600	2.15429600
H	-1.14109300	-2.12820400	3.60080900

TS16

imaginary frequency = -268.21 cm⁻¹

C	0.07656600	-0.75442900	0.64500700
S	-0.64361400	-1.80446000	1.91919000
C	1.35106700	-1.23154800	-0.00142900

C	1.64147300	-0.95112700	-1.34516900
C	2.30497900	-1.90895500	0.77398800
C	2.86105200	-1.34238700	-1.90025700
H	0.90248300	-0.43686200	-1.95510200
C	3.52440400	-2.29681400	0.21702900
H	2.09211300	-2.12383400	1.82140500
C	3.80722400	-2.01501500	-1.12270600
H	3.07042200	-1.11878700	-2.94880100
H	4.25716400	-2.82038900	0.83526100
H	4.76110900	-2.32040400	-1.55908800
O	-1.05767500	-1.07679700	-0.81422500
C	-2.29332800	-0.59638200	-0.63349200
C	-3.35117600	-1.44739500	-0.24372700
C	-2.56600200	0.77638300	-0.81948600
C	-4.63769700	-0.93974900	-0.05996500
H	-3.14382900	-2.50994400	-0.10434000
C	-3.85583300	1.27713800	-0.62312800
H	-1.76017900	1.43523300	-1.14611800
C	-4.89752800	0.42513600	-0.24089000
H	-5.44687400	-1.61481100	0.23147500
H	-4.04826800	2.34221300	-0.77781100
H	-5.90556800	0.81886300	-0.09131200
C	0.02768400	2.95494100	0.74320100
H	0.39411800	3.16331700	1.76008100
H	-1.06865100	2.87235700	0.78788100
C	0.62678400	1.63343400	0.24387000
H	0.41974100	1.54053800	-0.83165200
C	2.17324300	1.67340600	0.43567900
O	2.64325500	1.28560700	1.52798600
O	2.81520000	2.16873900	-0.53062500
N	-0.02394800	0.54989900	0.97767300
H	-0.87360900	0.80819200	1.47569000
S	0.36648700	4.36948900	-0.37056000
H	-0.69749600	-2.89750700	1.10487600
H	1.62978100	3.97260100	-0.67104100
O	-0.67312400	-3.74692000	-0.72060600
H	-0.85382100	-2.78861900	-0.89794100
H	0.29433200	-3.79676700	-0.76663600

TS17

imaginary frequency = -217.45 cm⁻¹

C	0.71326000	-0.88520400	0.36970200
S	0.44704400	-2.49211500	0.07448600
C	2.02633300	-0.24978100	0.13067700
C	3.21091900	-1.01114200	0.03385800
C	2.10602000	1.15020000	-0.02808000
C	4.43364600	-0.39292200	-0.20760100
H	3.15376700	-2.09299500	0.16236200
C	3.33130600	1.76330100	-0.29078200
H	1.19012000	1.73762600	0.02266900
C	4.49796200	0.99734300	-0.37456000
H	5.34443800	-0.99332600	-0.26379600
H	3.37589200	2.84582600	-0.43056600
H	5.45860900	1.48073000	-0.56783200
C	-2.59882200	-0.81673400	0.31707700
H	-2.92938600	-0.69309000	1.35890500
H	-2.22111300	-1.84047200	0.19362400
C	-1.49389300	0.18649000	0.00043500
H	-1.17615300	0.06964300	-1.04545900
C	-1.93555800	1.67011900	0.17765100
O	-2.89835800	1.90608800	0.95254500
O	-1.26065100	2.53079500	-0.44637600
N	-0.29213900	0.00527300	0.84339700
H	-0.56014000	-0.24106200	1.79780900
S	-4.05057000	-0.68466600	-0.79729800
H	-4.40962200	0.55361700	-0.38613100

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C	-0.91935500	1.33466000	-0.13474300
S	-1.72916800	2.78861600	-0.37626200
C	-1.69007600	0.06327400	-0.02144100
C	-2.65867000	-0.25493600	-0.98835900
C	-1.50918900	-0.79575000	1.07733200
C	-3.41924400	-1.41834400	-0.86910700
H	-2.80796900	0.42162600	-1.83140400
C	-2.28956600	-1.94772700	1.20385700
H	-0.75638300	-0.55498200	1.82960500
C	-3.24076000	-2.26615800	0.23030100
H	-4.15955200	-1.66238200	-1.63458000
H	-2.14966700	-2.60065600	2.06863500
H	-3.84414800	-3.17172300	0.32810600
C	2.16312100	0.14641300	-1.25888900

H	2.83694300	1.01481300	-1.27760500
H	1.50592000	0.20020100	-2.13904400
C	1.31816300	0.14812200	0.01449900
H	0.71396700	-0.76523200	0.03696400
C	2.14937500	0.19260000	1.33797000
O	3.39006500	0.36004200	1.24560700
O	1.49106400	0.06948100	2.40153000
N	0.41290700	1.29670300	-0.00355600
H	0.87061900	2.20690900	-0.04486300
S	3.13763400	-1.39006400	-1.47775900
H	3.89265700	-1.19143700	-0.37220600

TS18a

imaginary frequency = -271.19 cm⁻¹

C	0.62173900	1.14364800	-0.05486000
S	0.23753400	1.92524400	1.52291400
C	1.72822600	0.09198400	0.00868300
C	1.83537100	-0.74713800	1.12754900
C	2.56109000	-0.15104700	-1.09603000
C	2.75593400	-1.79730700	1.14607700
H	1.18956300	-0.56120900	1.98614600
C	3.49162200	-1.19319000	-1.07188600
H	2.48318200	0.47703000	-1.98435500
C	3.59211500	-2.02320500	0.04838800
H	2.82140600	-2.44202600	2.02605100
H	4.13839000	-1.35839900	-1.93716600
H	4.31654100	-2.84099100	0.06508300
C	-2.85520200	-0.06013300	-0.61179800
H	-2.92932700	-0.39629700	-1.65851800
H	-3.10905100	1.00850900	-0.58192100
C	-1.41674800	-0.24523900	-0.10300900
H	-1.39638900	0.00521000	0.96479300
C	-0.97681100	-1.72134600	-0.29362400
O	-0.37810100	-2.00432700	-1.36324800
O	-1.29213700	-2.53827700	0.61606400
N	-0.53616700	0.68805800	-0.80746100
H	-0.19108200	0.17209000	-1.62330200
S	-4.12401700	-0.91539200	0.41138300
H	-3.32143500	-1.96961100	0.70962600
O	1.15394600	2.22744400	-1.02680100
H	0.40466400	3.07310600	-0.95178400

H	1.98436600	2.57548200	-0.64737100
O	-0.50286700	3.93317400	-0.54894400
H	-0.02709800	4.76166300	-0.36269600
H	-0.54610500	3.46206900	0.35249500

22a

C	-0.70444000	-0.45600800	0.03359000
S	-0.47516600	-0.56885100	2.00572200
C	-2.17214100	-0.13645100	-0.18728900
C	-2.68886500	1.11781200	0.17750500
C	-3.03087800	-1.08712400	-0.75048600
C	-4.03551700	1.41608400	-0.02847500
H	-2.04208900	1.86236200	0.64761900
C	-4.38337800	-0.78872000	-0.95224600
H	-2.63733600	-2.06324900	-1.03187300
C	-4.89006900	0.46229900	-0.59512100
H	-4.42244500	2.39581700	0.26155900
H	-5.04150300	-1.54145500	-1.39315500
H	-5.94596900	0.69463200	-0.75258600
C	2.33504600	-0.08465900	-1.34255700
H	2.48747200	0.63706500	-2.15906200
H	1.76654800	-0.93218400	-1.74631600
C	1.54102500	0.54843500	-0.18874700
H	1.73051800	-0.05601600	0.71476400
C	2.03767300	1.97346700	0.17196700
O	3.28065100	2.12559600	0.30613900
O	1.16302200	2.86174900	0.33046400
N	0.11695500	0.58044800	-0.48447800
H	-0.21983200	1.51117700	-0.23185900
S	3.95065000	-0.77956900	-0.81296100
H	4.25705400	0.33329300	-0.09366300
O	-0.39547000	-1.70717000	-0.48221600
H	0.44260500	-2.05579100	-0.08000400
H	-1.38648400	-1.55906800	2.14194300
O	1.76829300	-2.67591100	0.82982800
H	1.44410900	-2.16374600	1.59549700
H	2.55822200	-2.17617500	0.53174200

TS19a

imaginary frequency = -188.18 cm⁻¹

C	-0.70132000	-0.42975600	-0.13543700
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S	-0.69766300	-0.66717500	2.23012200
C	-2.14081700	-0.06491700	-0.32997100
C	-3.03992700	-1.03053400	-0.80311700
C	-2.61095000	1.23214100	-0.06093500
C	-4.38412300	-0.70583200	-1.00825300
H	-2.68171800	-2.03857300	-1.01034200
C	-3.95125600	1.55330100	-0.26776300
H	-1.94044900	1.99406900	0.34192600
C	-4.84479700	0.58578400	-0.74397000
H	-5.07266800	-1.46869500	-1.37934800
H	-4.30310200	2.56440100	-0.05043000
H	-5.89530200	0.83952600	-0.90370000
C	2.34465600	-0.00240100	-1.46861000
H	2.36099700	0.83474400	-2.18339600
H	1.78172600	-0.82460400	-1.93164800
C	1.63052500	0.41435100	-0.17555800
H	1.82119100	-0.35935800	0.58440700
C	2.14685800	1.74893600	0.43572000
O	3.38916900	1.90149800	0.53501800
O	1.26913600	2.56967900	0.81318700
N	0.19881400	0.55640200	-0.40092700
H	-0.08247400	1.49379500	-0.10204500
S	4.04079900	-0.65082700	-1.20872400
H	4.38923600	0.39566800	-0.41724400
O	-0.39376200	-1.68161000	-0.52120100
H	0.40228300	-2.04740400	-0.03044700
H	0.03283400	0.46461900	2.36244000
O	1.43117100	-2.63921600	1.11097800
H	1.15294300	-3.55560300	1.26991500
H	0.89382300	-2.10859900	1.75754600

TS20a

imaginary frequency = -250.49 cm⁻¹

C	-0.63802800	-0.53636200	0.10058000
C	-2.06147600	-0.11825600	-0.12188400
C	-3.11453400	-0.84707600	0.46069500
C	-2.38475400	0.97773600	-0.93802600
C	-4.44100200	-0.48142900	0.25135300
H	-2.86139300	-1.70274200	1.08686300
C	-3.71995100	1.34317100	-1.15489100
H	-1.59358600	1.54714200	-1.42812100

C	-4.75356200	0.61949000	-0.56064900
H	-5.24220200	-1.05650100	0.72277300
H	-3.94611500	2.19694200	-1.79877200
H	-5.79539000	0.90346400	-0.72803700
C	2.46867000	-0.39744200	-1.10169600
H	2.55762000	0.31438900	-1.93770400
H	1.89280000	-1.26741300	-1.44508100
C	1.69477300	0.24256600	0.05980300
H	1.78412900	-0.41371000	0.94213900
C	2.24925500	1.63922100	0.45456500
O	3.47522900	1.71883400	0.73427900
O	1.43246900	2.59634500	0.47978800
N	0.29036700	0.38553500	-0.27945200
H	0.02048500	1.35794500	-0.11707700
S	4.12217900	-1.05307300	-0.65058000
H	4.45263700	0.06818200	0.04102900
S	-0.25348500	-2.21368400	0.14048800
O	-0.72217200	-0.06838700	2.26088600
H	-0.48122300	-1.00239600	2.28090000

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C	-0.64858100	-0.35040900	0.51704900
C	-2.06902900	-0.01778800	0.06697600
C	-3.13872500	-0.05675800	0.97753600
C	-2.35814600	0.28076100	-1.27636400
C	-4.45180200	0.17395300	0.55973500
H	-2.92722200	-0.27559400	2.02447100
C	-3.67086900	0.51115500	-1.69727100
H	-1.53863700	0.32701500	-1.99305500
C	-4.72852400	0.45766600	-0.78259600
H	-5.26578500	0.13637400	1.28908500
H	-3.86876000	0.73650400	-2.74897300
H	-5.75516700	0.63794300	-1.11103000
C	2.37770500	-0.55136500	-0.99120700
H	2.48563900	0.00252400	-1.93765300
H	1.72043200	-1.41669000	-1.15429000
C	1.69602200	0.32171000	0.06977400
H	1.82721000	-0.18488700	1.04515400
C	2.34868700	1.72390400	0.23038800
O	3.60385500	1.81431100	0.13095200
O	1.57878000	2.68988400	0.48002000

N	0.27956100	0.47439800	-0.24378300
H	0.05886100	1.45098600	-0.03321600
S	3.99621700	-1.25997400	-0.49321900
H	4.49143300	-0.05355100	-0.12291400
S	-0.38828600	-2.15551900	0.35146500
O	-0.52876000	-0.01868700	1.93285600
H	-0.28324100	-0.87458300	2.32225100

TS21a

imaginary frequency = -255.60 cm⁻¹

C	-0.67690300	-0.40997800	0.17470800
C	-2.14167500	-0.00863300	0.03732100
C	-3.07183300	-0.38823200	1.01484500
C	-2.59540400	0.71564300	-1.07671900
C	-4.42236300	-0.05228800	0.88597500
H	-2.72266400	-0.95262500	1.87929600
C	-3.94557100	1.05265700	-1.20687600
H	-1.88339500	1.01389800	-1.84596000
C	-4.86671600	0.67044600	-0.22586200
H	-5.13184300	-0.35625000	1.66011900
H	-4.27958700	1.61829100	-2.08063500
H	-5.92238200	0.93413900	-0.32703400
C	2.39949600	0.01896000	-1.10606500
H	2.63615600	0.76398900	-1.88133000
H	1.81644800	-0.78720200	-1.56984600
C	1.56130800	0.63980500	0.02205600
H	1.71580000	0.02313400	0.92483900
C	2.06606500	2.04919600	0.42538500
O	3.31407700	2.20947300	0.51699800
O	1.20020500	2.92871700	0.67252500
N	0.14831800	0.68810900	-0.32442400
H	-0.20225600	1.55466100	0.09124500
S	3.94672400	-0.77488700	-0.51958700
H	4.32896200	0.32314300	0.17826200
S	-0.46798500	-1.96682900	-0.92069000
O	-0.39110000	-0.75853400	1.49295500
H	0.40735100	-1.47556900	1.49629900
O	1.37898300	-2.48557500	1.33299700
H	0.51829100	-2.45669700	0.00751400
H	2.16533200	-2.03033000	0.99022100

HS-

S	0.00000000	0.00000000	0.08003400
H	0.00000000	0.00000000	-1.28054900

TS18b

imaginary frequency = -752.13 cm⁻¹

C	-0.86207600	0.89966500	-0.25866700
S	-1.73594000	2.23767200	-1.13042000
C	-1.72283700	-0.32982700	0.01907100
C	-2.57827300	-0.80608000	-0.98691100
C	-1.63887800	-1.04296600	1.22421600
C	-3.34468200	-1.95486900	-0.78828100
H	-2.64294900	-0.25153600	-1.92432400
C	-2.41424000	-2.19086100	1.42684700
H	-0.94832800	-0.71535300	2.00070100
C	-3.27057000	-2.65040700	0.42455200
H	-4.00685700	-2.30751700	-1.58295000
H	-2.33871100	-2.73045300	2.37409900
H	-3.87574500	-3.54615600	0.58359100
C	2.29684800	-0.79988200	-1.35179600
H	2.81886600	0.09417000	-1.72412300
H	1.78244100	-1.27084900	-2.20158600
C	1.28128300	-0.39558000	-0.28124900
H	0.72023800	-1.28461600	0.03330000
C	2.01669800	0.18741600	0.95589200
O	2.67194600	1.24677700	0.75534900
O	1.92037500	-0.43308000	2.04531300
N	0.35301900	0.55427200	-0.90493000
H	0.84321000	1.39661900	-1.20497400
S	3.54185100	-2.02828700	-0.80229600
H	4.18525400	-1.21725300	0.07062600
O	-0.48063100	1.45866300	1.16148600
H	0.03008400	2.57545800	0.93603300
H	-1.31662300	1.66149600	1.61895100
O	0.30022900	3.61588500	0.44666000
H	-0.09117400	4.30133000	1.01769300
H	-0.40040800	3.45897100	-0.31156900

22b

C	-0.78864700	1.04597100	-0.10037900
S	-1.74665800	2.35503800	-1.06205000

C	-1.70813500	-0.16474500	0.00785000
C	-2.16739700	-0.79336000	-1.15967900
C	-2.06985200	-0.68463800	1.25489700
C	-2.98484400	-1.92147400	-1.07748400
H	-1.87814700	-0.39822100	-2.13496600
C	-2.89111200	-1.81408200	1.33584800
H	-1.69297100	-0.21710700	2.16399700
C	-3.35068800	-2.43511600	0.17220500
H	-3.33649400	-2.40366700	-1.99265200
H	-3.16646000	-2.21205800	2.31539300
H	-3.99071400	-3.31829200	0.23616800
C	2.35672200	-0.63685800	-1.27189400
H	2.98293300	0.26702300	-1.29708500
H	1.98013700	-0.81854700	-2.28858200
C	1.19256800	-0.43637500	-0.30395400
H	0.54180100	-1.31993800	-0.33794900
C	1.70797600	-0.27941900	1.15338900
O	2.58212100	0.60937400	1.34826200
O	1.21820100	-1.04326800	2.02414400
N	0.42482000	0.72405300	-0.78958000
H	1.02585500	1.55162100	-0.78603600
S	3.41793700	-2.07950800	-0.87886100
H	3.97250300	-1.55215600	0.23836900
O	-0.47922200	1.60155900	1.17512000
H	0.88343700	2.90190900	0.82923200
H	-1.28666000	1.97868900	1.56207700
O	1.46192600	3.48428200	0.29830800
H	0.95018000	4.30474500	0.23169900
H	-0.74336400	3.26415500	-0.98950200

TS19b

imaginary frequency = -170.68 cm⁻¹

C	0.83986800	1.01084700	-0.21783800
S	0.99874000	1.76851400	1.94526900
C	1.71878600	-0.21203000	-0.22318500
C	2.74776600	-0.27958800	-1.17462300
C	1.52396000	-1.30018600	0.64139600
C	3.55946800	-1.41466700	-1.26445800
H	2.90899900	0.55968500	-1.85068400
C	2.32896800	-2.43496800	0.54529900
H	0.75757700	-1.25743500	1.41338500

C	3.35082500	-2.49798600	-0.40895400
H	4.35644600	-1.44884600	-2.01107500
H	2.16220300	-3.27194000	1.22719600
H	3.98411000	-3.38550700	-0.47855400
C	-1.88841100	-0.48032100	1.02349900
H	-2.61328800	0.32206500	1.23098600
H	-1.08378200	-0.39170800	1.76301800
C	-1.32871700	-0.31185500	-0.40705500
H	-0.77650900	-1.22084400	-0.68129600
C	-2.52344900	-0.13808900	-1.38953700
O	-3.14387900	-1.18521100	-1.71181200
O	-2.80680500	1.03457000	-1.73709800
N	-0.47194200	0.84654900	-0.55246800
H	-0.99807100	1.69175500	-0.77603700
S	-2.63720400	-2.12550600	1.33329500
H	-3.25089300	-2.17939700	0.12295800
O	1.43415900	2.07826400	-0.81678500
H	0.82967400	2.86256200	-0.70156900
H	-0.12251900	1.18276900	2.41906000
O	-0.31686300	3.88369300	0.02093800
H	0.11115200	4.75263700	0.08020200
H	-0.05333800	3.43273800	0.86345700

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C	0.85886700	-1.28264400	-1.01857000
C	1.72942800	-0.22196000	-0.41370700
C	2.68007000	-0.60238900	0.54392300
C	1.66349500	1.11550700	-0.83096100
C	3.53927000	0.34827300	1.09685400
H	2.72837500	-1.64546000	0.86248700
C	2.53670900	2.06233100	-0.28947200
H	0.93667600	1.41437500	-1.58905300
C	3.47049100	1.68239700	0.67967900
H	4.26695200	0.04853600	1.85455800
H	2.48700500	3.10034800	-0.62636700
H	4.14688000	2.42564600	1.10848000
C	-2.49022600	0.34421700	-0.95833500
H	-3.21500500	-0.46384300	-1.13828700
H	-2.20667600	0.76992000	-1.93164600
C	-1.24933400	-0.18940600	-0.24997700
H	-0.63068100	0.66539300	0.05069800

C	-1.53120400	-0.99638500	1.05888000
O	-2.70453200	-1.01405900	1.51111300
O	-0.52938700	-1.55904400	1.56674900
N	-0.46510800	-1.01688200	-1.16769900
H	-0.97679500	-1.81370500	-1.54644000
S	-3.30975100	1.71371000	-0.05650800
H	-3.55060600	0.96337900	1.04468300
O	1.35645100	-2.34257500	-1.41798300

TS20b

imaginary frequency = -245.82 cm⁻¹

C	0.80284400	1.06584400	-0.49771700
C	1.70473700	-0.03279700	-0.01934900
C	2.82372300	0.25992700	0.78342800
C	1.52542000	-1.35506200	-0.45675900
C	3.72723000	-0.73629700	1.14199700
H	2.95219900	1.28378100	1.12994000
C	2.43866100	-2.35654100	-0.09830300
H	0.66729400	-1.60971600	-1.07994400
C	3.54078700	-2.05546300	0.70142900
H	4.58535100	-0.48686600	1.77171600
H	2.28073800	-3.37842600	-0.45324100
H	4.25239000	-2.83614900	0.98147600
C	-2.32310100	0.76327300	0.70421300
H	-2.95716300	1.40228400	0.07293900
H	-1.66971800	1.39256300	1.32587700
C	-1.41420000	-0.10551600	-0.16421300
H	-0.84256200	-0.78142700	0.48353600
C	-2.18690400	-0.97857700	-1.19909400
O	-3.38566200	-0.68286600	-1.44034900
O	-1.54060000	-1.91399600	-1.74158900
N	-0.46579200	0.74260600	-0.88712400
H	-0.91047300	1.50228200	-1.39778000
S	-3.38170400	-0.19732700	1.84929600
H	-4.08633000	-0.81929300	0.87533800
O	0.46033100	1.85263300	1.53757300
H	0.53880600	2.66908400	1.02725400
S	1.52809600	2.42262200	-1.27092800

23b

C	0.76478700	1.20052400	-0.13083800
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C	1.70850600	0.02912300	0.12754400
C	2.63101000	0.07375600	1.18754600
C	1.72579000	-1.09605200	-0.71436300
C	3.54818900	-0.95992600	1.39052700
H	2.62612400	0.93785500	1.85228100
C	2.64178500	-2.13248300	-0.51179100
H	0.99673100	-1.15984300	-1.52092300
C	3.56217300	-2.07164600	0.53980500
H	4.25624900	-0.89905800	2.22175000
H	2.63111300	-2.99857300	-1.17945500
H	4.27676300	-2.88310500	0.69896800
C	-2.38548300	0.70172600	0.75550100
H	-2.95795400	1.39319800	0.12014100
H	-1.83878800	1.28834400	1.50268300
C	-1.39942500	-0.09613500	-0.10034600
H	-0.83306200	-0.78097900	0.54688400
C	-2.11520200	-0.95787300	-1.17409400
O	-3.15774300	-0.48079600	-1.70169700
O	-1.57344200	-2.05297900	-1.48474800
N	-0.43618100	0.75061800	-0.81267000
H	-0.88626900	1.55691700	-1.24154900
S	-3.56432700	-0.34073300	1.70671600
H	-4.21993400	-0.82059900	0.62445200
O	0.45571800	1.79816100	1.16696600
H	0.55985600	2.74518800	0.96984100
S	1.59891500	2.47230500	-1.14218400

TS21b

imaginary frequency = -246.78 cm⁻¹

C	0.72794500	0.93099000	-0.10796000
C	1.76314000	-0.15885800	0.15171200
C	2.69498300	-0.00177100	1.18952500
C	1.84311800	-1.30410700	-0.65355000
C	3.68447800	-0.96111100	1.41471800
H	2.64002600	0.88579900	1.82000300
C	2.83271800	-2.26666600	-0.42835900
H	1.10698400	-1.44966600	-1.44250400
C	3.75952400	-2.09965000	0.60457100
H	4.40082900	-0.81912400	2.22815500
H	2.87511400	-3.15594900	-1.06278200
H	4.53282100	-2.85161300	0.78034000

C	-2.37724300	0.34911300	0.73418700
H	-2.94856900	1.01982800	0.07576000
H	-1.85374400	0.95994900	1.47833800
C	-1.36275100	-0.44855900	-0.08722300
H	-0.77766200	-1.09232400	0.58498800
C	-2.03821400	-1.36455100	-1.14189800
O	-3.10409000	-0.94727400	-1.67221900
O	-1.44326300	-2.43633200	-1.43330400
N	-0.42518900	0.40686900	-0.82728700
H	-0.92593000	1.17653700	-1.26656000
S	-3.54962500	-0.69600900	1.68721900
H	-4.17199200	-1.21509500	0.60358200
O	0.41106600	1.56072700	1.10060700
H	-0.06682900	2.46279600	0.82523100
S	1.52478100	2.19953000	-1.27187500
O	-0.59143500	3.66173400	0.19356500
H	-1.33774600	3.26917600	-0.28427300
H	0.55612000	3.14545000	-0.75830000

TS22a

imaginary frequency = -51.15 cm^{-1}

C	-0.47168700	0.31910000	-0.51137300
S	-0.19366100	1.89758700	-1.22075700
C	-1.88089100	-0.02361700	-0.21704300
C	-2.94588900	0.50994100	-0.96372800
C	-2.15644400	-0.90137900	0.84824500
C	-4.26010300	0.15489300	-0.66090500
H	-2.74943700	1.18814500	-1.79597200
C	-3.47309800	-1.24519100	1.15153600
H	-1.33764900	-1.27714300	1.46452500
C	-4.52739400	-0.72114300	0.39635400
H	-5.07975000	0.56433400	-1.25500800
H	-3.67700700	-1.91622800	1.98860600
H	-5.55868700	-0.99017700	0.63555100
C	2.15636000	-0.29790800	1.23157900
H	3.24380500	-0.12134700	1.26322900
H	1.97011600	-1.24821700	1.76145800
C	1.83323900	-0.55628300	-0.27941000
H	2.23316300	0.26038700	-0.89057700
C	2.48542100	-1.89582400	-0.68838600
O	3.70885500	-1.85213000	-0.95473600

O	1.74455100	-2.91349200	-0.64928000
N	0.40828000	-0.65317600	-0.44290800
H	0.07078000	-1.58626800	-0.18627600
S	1.22192500	1.05010000	2.00973100
H	2.20363800	2.30574900	0.70459500
O	2.58856100	2.75139100	-0.12172500
H	3.33847000	2.18278800	-0.35675700
H	1.13954800	2.10551700	-0.89191100

TS22b

imaginary frequency = -836.20 cm^{-1}

C	-0.28744300	-0.58393300	-0.71888600
S	-0.39513300	-2.13508100	-1.50344700
C	-1.55085500	0.07615200	-0.31311700
C	-2.56459000	-0.65086900	0.33489500
C	-1.78920500	1.41673400	-0.66337600
C	-3.77802500	-0.04422900	0.64768700
H	-2.37685300	-1.69004100	0.60684300
C	-3.00947200	2.02158600	-0.35096000
H	-1.02728200	1.98264400	-1.20116100
C	-4.00479700	1.29665300	0.30839700
H	-4.55314600	-0.61656800	1.16246400
H	-3.18313400	3.06252100	-0.63324400
H	-4.95780200	1.77087200	0.55428400
C	1.81924500	0.21275200	1.43468500
H	2.78110400	-0.24911100	1.15308500
H	2.03069100	0.94446500	2.22989100
C	1.31718500	1.03204000	0.20535000
H	0.50857000	1.69692200	0.52444300
C	2.49743200	1.85893900	-0.34775200
O	2.73220500	2.94474000	0.23471600
O	3.15907000	1.33694200	-1.28360600
N	0.84489800	0.11161000	-0.80733800
H	1.62596900	-0.32096000	-1.30329400
S	0.63985600	-1.05304400	1.99280600
H	0.92600900	-2.61249600	-0.83807600
O	1.89917300	-2.88646600	0.02168200
H	1.50073600	-2.34397800	0.82461800
H	2.67485400	-2.37221300	-0.26208700

24b

C	0.05470400	0.62071400	-0.14448100
S	0.19734500	2.39908500	-0.60610500
C	1.46286300	0.03436500	-0.14932200
C	2.45570100	0.54949400	0.70228400
C	1.78637700	-1.03156700	-0.99655700
C	3.74148900	0.01108000	0.70177300
H	2.21175000	1.37222000	1.37717200
C	3.07478900	-1.58074900	-0.98908700
H	1.01888900	-1.42256200	-1.66420400
C	4.05629300	-1.06094200	-0.14401100
H	4.50197600	0.42456600	1.36869900
H	3.30824800	-2.41746400	-1.65213000
H	5.06254200	-1.48670300	-0.13929900
C	-1.18149300	-1.21015100	1.13382400
H	-1.98110600	-1.56636400	1.79460800
H	-0.32560500	-1.89867500	1.20006500
C	-1.68726100	-1.06189300	-0.30688600
H	-1.63926900	-2.05240300	-0.79211900
C	-3.18237400	-0.62339700	-0.33005300
O	-3.98648800	-1.35914300	0.29134900
O	-3.46303800	0.42021400	-0.97742600
N	-0.86109700	-0.07743400	-1.01874400
H	-1.54548900	0.58996300	-1.38481600
S	-0.65820600	0.47185800	1.60560500
H	-1.10081300	2.69409500	-0.34505200

25a

C	0.69238800	0.67586400	0.26604400
S	0.43784000	2.33176400	0.46900900
C	2.06163400	0.12709700	0.01841800
C	3.19345800	0.76505100	0.55461300
C	2.24686600	-1.02547400	-0.76755500
C	4.47219800	0.25802300	0.32503600
H	3.04853000	1.66657700	1.15166800
C	3.52895000	-1.52566400	-1.00678900
H	1.38961400	-1.52451500	-1.22387200
C	4.64582100	-0.88860200	-0.45880900
H	5.33975400	0.76146000	0.75827100
H	3.65382300	-2.41312200	-1.63157400
H	5.64839600	-1.28108100	-0.64453200
C	-2.22931600	0.22787300	-1.12465400

H	-1.96092700	-0.69236100	-1.68155800
H	-1.59970300	1.03280200	-1.54968600
C	-1.72185800	0.00974200	0.32024600
H	-1.92256500	0.91100900	0.91137100
C	-2.37570800	-1.22554900	0.97887900
O	-3.20170900	-1.04720500	1.90594800
O	-1.99150100	-2.34338000	0.52644600
N	-0.28120500	-0.23292900	0.30954100
H	-0.04976300	-1.21613000	0.17003200
S	-4.00781700	0.61326000	-1.25142200

TS23a

imaginary frequency = -154.50 cm⁻¹

C	-0.20503300	0.71176100	-0.22770900
S	-0.13221300	2.39059400	-0.74013400
C	-1.56060800	0.02565700	-0.18564900
C	-2.72939000	0.70283100	-0.56024600
C	-1.68444800	-1.31573600	0.22698600
C	-3.97784600	0.07135000	-0.52905400
H	-2.61984600	1.74235100	-0.87651100
C	-2.92477100	-1.95358500	0.25071900
H	-0.80367700	-1.85896500	0.57434800
C	-4.08319700	-1.26233300	-0.12800900
H	-4.87223100	0.62638800	-0.82534800
H	-2.99091000	-2.99413100	0.57931100
H	-5.05603200	-1.75971200	-0.10261300
C	2.01878100	-0.01192500	1.40254700
H	2.85211600	0.53835100	1.86779100
H	2.13810500	-1.07830800	1.66346800
C	2.11379800	0.12312500	-0.15205400
H	2.39163500	1.15526500	-0.40087000
C	3.18420300	-0.85229500	-0.66334300
O	4.37261600	-0.43551700	-0.66669000
O	2.80276500	-2.01484400	-0.97279000
N	0.81025500	-0.14287500	-0.71693400
H	0.60274200	-1.13032100	-0.57056900
S	0.40560800	0.60496700	1.96639900

26a

C	-0.18906000	0.70968200	-0.13956900
S	-0.14510200	2.39116400	-0.75247200

C	-1.55400700	0.01610500	-0.13567600
C	-2.71157400	0.67716000	-0.56418800
C	-1.68282400	-1.31572800	0.30322800
C	-3.95712100	0.03821500	-0.56139400
H	-2.58937000	1.71009200	-0.89888300
C	-2.91960500	-1.96231300	0.29894900
H	-0.80859200	-1.84625800	0.68663000
C	-4.06817800	-1.28684600	-0.13393300
H	-4.84483700	0.58052300	-0.89889100
H	-2.99083400	-2.99641400	0.64651000
H	-5.03839400	-1.79011400	-0.13101000
C	2.02873300	0.06315100	1.38125500
H	2.83167900	0.66221500	1.83699100
H	2.15175600	-0.98137200	1.71449100
C	2.11979000	0.11679700	-0.17325100
H	2.41047200	1.13275100	-0.47142700
C	3.18219000	-0.89303600	-0.63402600
O	4.37440300	-0.48756800	-0.64993600
O	2.79210500	-2.06465300	-0.89299900
N	0.80762200	-0.15590100	-0.72115900
H	0.60681700	-1.13815400	-0.52818500
S	0.38234100	0.68362900	1.85165900

TS24

imaginary frequency = -338.06 cm⁻¹

C	0.67866900	-0.91156000	0.32913600
S	0.44242400	-2.51637100	-0.01983200
C	1.98955900	-0.25605900	0.11001900
C	3.19434600	-0.98871200	0.08280300
C	2.04223400	1.13913500	-0.09408600
C	4.41170100	-0.34653200	-0.12875100
H	3.15683000	-2.06739400	0.24275400
C	3.26097200	1.77530300	-0.33105000
H	1.11019200	1.70390100	-0.09737800
C	4.44966000	1.03820800	-0.33969300
H	5.33843500	-0.92508700	-0.12764900
H	3.28387400	2.85331200	-0.50737600
H	5.40527800	1.54007800	-0.50952700
C	-2.71332400	-0.81459200	0.35181000
H	-2.96785800	-0.62271400	1.41519600
H	-2.32866700	-1.84849400	0.31007000

C	-1.56940400	0.12714900	-0.00191900
H	-1.28747500	-0.02482500	-1.05278700
C	-1.93231700	1.62163000	0.18085500
O	-2.44195900	1.95971500	1.28378000
O	-1.60016400	2.41759700	-0.74383500
N	-0.32651500	-0.04526400	0.81362900
H	-0.57793000	-0.27834300	1.77557000
S	-4.15384000	-0.56712200	-0.75633000

25b

C	-0.87932700	1.33216600	-0.04365200
S	-1.66040400	2.82945100	-0.09921300
C	-1.68501600	0.07611500	-0.02557600
C	-2.74982000	-0.08098300	-0.92990000
C	-1.44258900	-0.93537500	0.92164500
C	-3.54141000	-1.22916200	-0.90208900
H	-2.94864300	0.71276300	-1.65166900
C	-2.24983400	-2.07523800	0.95851800
H	-0.62130900	-0.83691900	1.63199800
C	-3.29625700	-2.22995600	0.04517900
H	-4.35702100	-1.34254200	-1.62025600
H	-2.05472100	-2.84797500	1.70597600
H	-3.92092500	-3.12603600	0.07209800
C	2.31383500	0.24200200	-1.26066900
H	2.91257100	1.15617800	-1.07570400
H	1.70243700	0.45542600	-2.16002000
C	1.35083300	0.08850700	-0.07903900
H	0.75060500	-0.81126600	-0.23644800
C	2.10028200	-0.02408600	1.27483200
O	2.86560700	0.93321500	1.56522300
O	1.84149300	-1.01442500	2.00954000
N	0.45057000	1.24837600	0.01681500
H	0.93532200	2.14281400	0.07913100
S	3.36457400	-1.24040900	-1.47681200

TS23b

imaginary frequency = -147.47 cm⁻¹

C	-0.20919900	-0.86215600	-0.44560700
S	-0.56649100	-2.32415100	-1.33739800
C	-1.39193000	0.04808400	-0.22127500
C	-2.56044800	-0.43434500	0.39881800

C	-1.39426800	1.37210400	-0.68716200	O	3.54749600	2.07828600	0.27463200
C	-3.67925900	0.37760500	0.56049400	O	3.66606400	0.29718100	-1.09038100
H	-2.57124300	-1.46874900	0.74669600	N	0.97420200	-0.13794600	-0.80386100
C	-2.52077700	2.19210600	-0.52820700	H	1.61017500	-0.80849100	-1.23412900
H	-0.50784600	1.76025300	-1.19033000	S	0.32081800	-1.31121200	1.59406000
C	-3.66746900	1.70411600	0.09835700				
H	-4.57202000	-0.02087000	1.05033900				
H	-2.49527600	3.21944300	-0.90213700				
H	-4.54561300	2.34205200	0.22534800				
C	1.86190500	-0.33845400	1.46447500				
H	2.70068200	-1.03364700	1.27919600				
H	2.13788500	0.29594900	2.32196900				
C	1.67441000	0.55290700	0.20641100				
H	1.08208200	1.43343400	0.49427900				
C	3.05491300	1.02439700	-0.28825400				
O	3.52201000	2.05974900	0.25458500				
O	3.63723500	0.30358700	-1.14288700				
N	0.98095100	-0.20417300	-0.81350600				
H	1.62909200	-0.86486700	-1.23976600				
S	0.31613900	-1.23576500	1.75409100				

26b

C	-0.18941600	-0.84631100	-0.34864600
S	-0.56649100	-2.28118000	-1.34399700
C	-1.39829200	0.05675000	-0.17355700
C	-2.56145900	-0.42549500	0.45757100
C	-1.41858000	1.36883600	-0.66940400
C	-3.69363400	0.37316500	0.59524300
H	-2.56321900	-1.45202300	0.82926500
C	-2.55835600	2.17545000	-0.53616000
H	-0.53261800	1.75576000	-1.17378400
C	-3.70072500	1.68681500	0.09813600
H	-4.58200300	-0.02664600	1.09209900
H	-2.54575200	3.19454300	-0.93299000
H	-4.58882400	2.31454700	0.20566800
C	1.86368400	-0.36207200	1.45684700
H	2.71910400	-1.03652600	1.28065400
H	2.06614800	0.21894800	2.36954800
C	1.69255200	0.57471700	0.23337700
H	1.11878900	1.45863800	0.55052200
C	3.08107300	1.03504700	-0.25254600