

Supporting Information

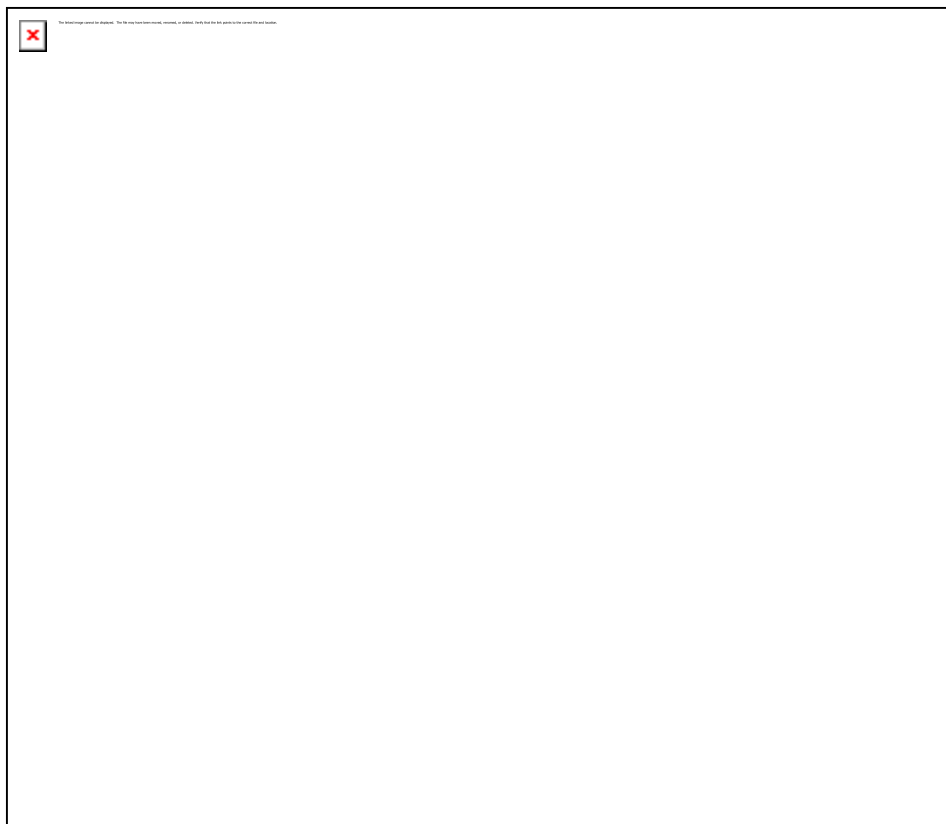
**Computational study of the mechanism of amide bond formation via CS₂-
releasing 1,3-acyl transfer**

Yuan-Ye Jiang*, Tian-Tian Liu, Xue Sun, Zhong-Yan Xu, Xia Fan, Ling Zhu, Siwei Bi*

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

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Scheme S1 Calculated Gibbs free energy profile for the CS₂ release after TS9a and TS13b (in kcal/mol) and the Wiberg bond orders and distances of the N–CS₂ bond of TS34 and TS35 (in angstrom).

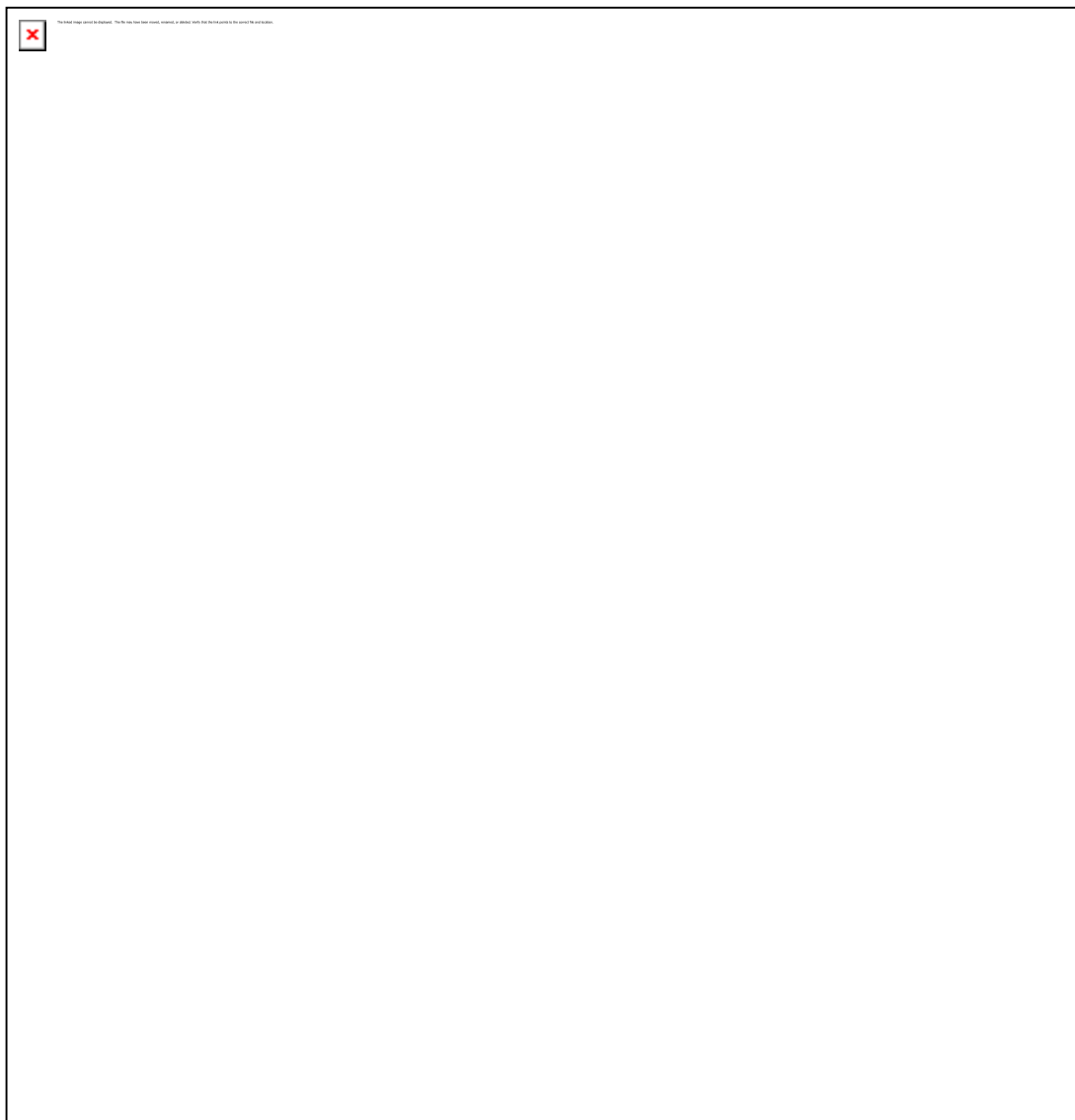


Fig. S1 Optimized structures of selected transition states.

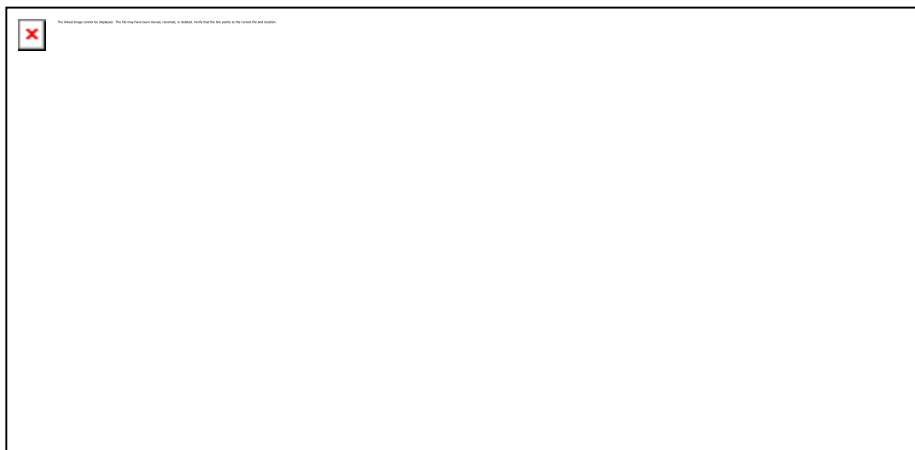


Fig. S2 Non-convlent interaction (NCI) plot of **6** and **TS9b**. Blue areas indicate typical hydrogen bonds while red areas indicate relative strong non-covalent repulsion.



Scheme S2 Calculated NBO charge of the carbonyl carbon atom and nitrogen atom in 6, 10 and 11.



Fig. S3 Non-convalent interaction (NCI) plot of **TS13b** and **TS22**. Blue areas indicate typical hydrogen bonds while red areas indicate relative strong non-covalent repulsion. The green-yellow areas circled by red lines indicate weak steric repulsion.

Comparison of different computational methods

Method A denotes our default method in which geometry optimization and energy calculation were performed by using B3LYP-D3(BJ) method,¹ Def2-SVP basis set,² SMD solvation model³ associated with the addition of 2.6 kcal/mol for entropy correction⁴ and 1.9 kcal/mol for standard state change from 1 atm. to 1 mol/L at 298.15 K.⁵ Method B is different to method A in two aspects. First, the solution-phase E(0) were calculated by using B3LYP-D3(BJ) method, Def2-TZVP basis set,² SMD solvation model based on the structures optimized with method A. Second, method B corrected entropy effect by using the Morokuma's strategy that only considers vibrational and rotational entropy terms.⁶ The relative Gibbs free energies of the key transition states and intermediates were calculated by the two methods for comparison (Table S1) and detailed results were listed in Table S2 and Table S3. As shown in Table S1, the two methods both predict that the amide bond formation from **1** and **2** proceeds via the nucleophilic addition of dithiocarbamic acid on thiocarboxylic acid, and the rate-determining dithiocarbamic-acid-assisted 1,3-acyl transfer.

References:

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Table S1. Relative solution-phase Gibbs free energies of the key transition states and intermediates in the amide bond formation from **1** and **2** calculated by different methods (in kcal/mol).

species	method A	method B
TS1	8.4	12.4
TS2	17.3	18.3
TS3	17.5	18.2
TS4	20.2	18.9
TS5	15.9	19.1
TS6	19.2	15.1
TS7	22.2	20.7
TS8	22.2	20.5
6	-7.8	0.1
TS9a	21.9	30.6
TS9b	22.2	30.9
TS10	19.9	24.9
TS11	20.9	24.2
TS12a	21.3	24.4
TS12b	18.1	22.7
TS13a	21.8	25.2
TS13b	17.2	21.3

Table S2. Method A-calculated solvation-energy-included $E(0)$ ($E(0)_{\text{Asol}}$), Method A-calculated uncorrected solution-phase Gibbs free energies (ΔG_{sol}) and Method A-calculated corrected solution-phase Gibbs free energies ($\Delta G_{\text{sol}}'$) of intermediates and transition states (in Hartree).

species	$E(0)_{\text{Asol}}$	ΔG_{sol}	$\Delta G_{\text{sol}}'$
1	-1529.422404	-1529.393868	-1529.386697
2	-551.834523	-551.807089	-551.807089
3	-930.072751	-930.032427	-930.0252558
4	-1151.179932	-1151.165732	-1151.158561
TS1	-1481.895893	-1481.807492	-1481.800321
5	-1481.911927	-1481.818067	-1481.810896
TS2	-1597.537793	-1597.400071	-1597.3929
MeOH	-115.642350	-115.614014	-115.6068428
TS3	-2033.731007	-2033.592893	-2033.585722
TS4	-2411.961307	-2411.813859	-2411.806688
6	-1082.621655	-1082.547052	-1082.539881
H ₂ S	-399.288708	-399.293421	-399.2862498
TS5	-1481.883790	-1481.795513	-1481.788342
7	-1481.890425	-1481.800249	-1481.793078
TS6	-2033.722687	-2033.590184	-2033.583013
TS7	-2411.954014	-2411.810645	-2411.803474
TS8	-1597.522834	-1597.392282	-1597.385111
CS ₂	-834.252748	-834.268775	-834.2616038
8a	-248.371165	-248.299459	-248.2922878
8b	-248.368405	-248.296045	-248.2888738
TS9a	-1082.575794	-1082.499631	-1082.49246
TS9b	-1082.575069	-1082.499196	-1082.492025
TS10	-1198.232918	-1198.109724	-1198.102553
TS11	-1481.873589	-1481.787500	-1481.780329

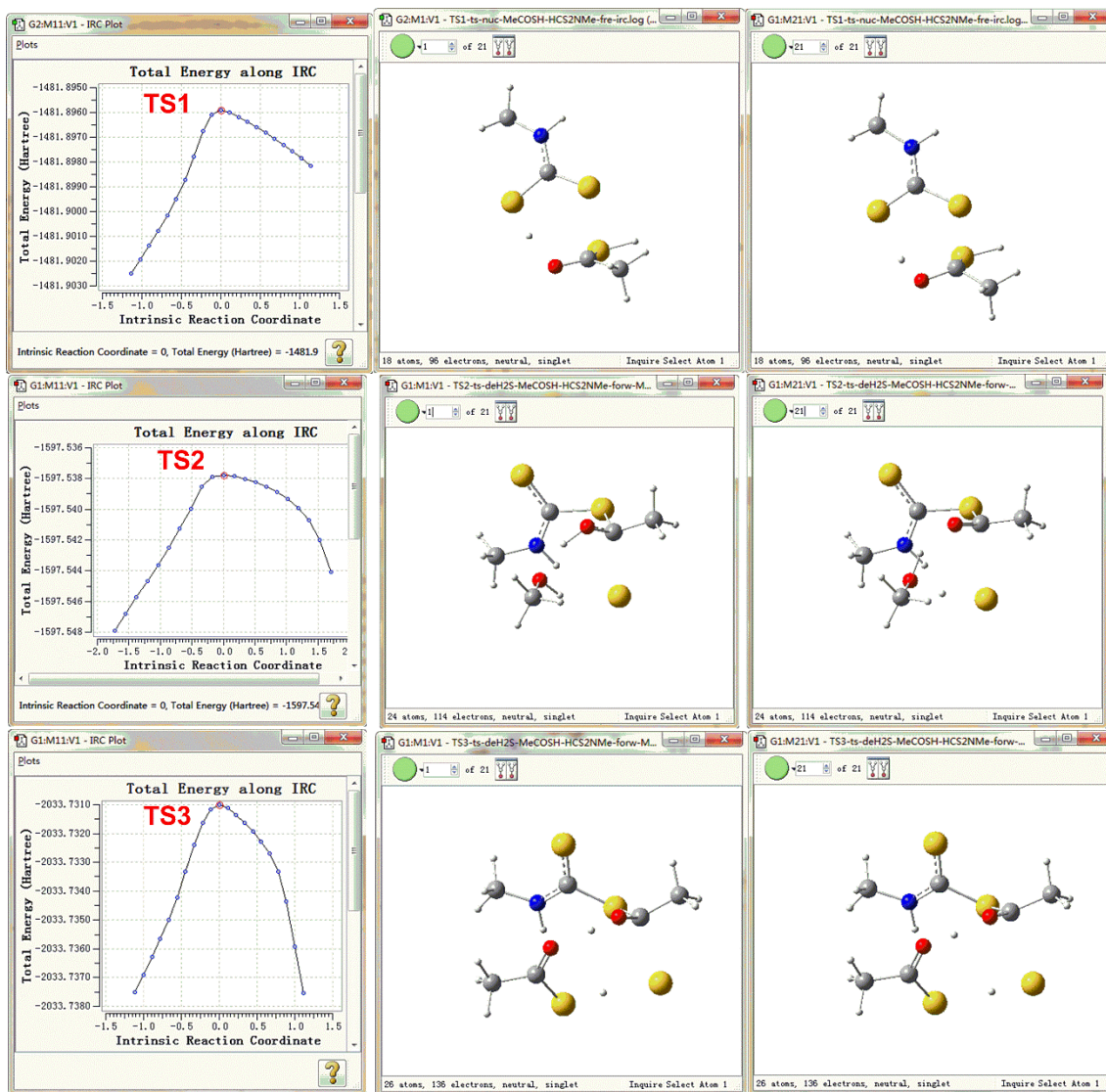
TS12a	-1634.421884	-1634.300573	-1634.293402
TS12b	-1634.429097	-1634.305615	-1634.298444
TS13a	-2012.660680	-2012.525039	-2012.517868
TS13b	-2012.667550	-2012.532486	-2012.525315
9	-1121.896576	-1121.797338	-1121.790167
TS14	-1121.862491	-1121.759482	-1121.752311
TS15	-1237.519507	-1237.369338	-1237.362167
TS16	-1521.160904	-1521.047512	-1521.040341
TS17	-1673.710048	-1673.562355	-1673.555184
TS18	-2051.946892	-2051.784296	-2051.777125
10	-1274.247460	-1274.125172	-1274.118001
TS19	-1274.199327	-1274.075948	-1274.068777
TS20	-1389.856816	-1389.684754	-1389.677583
TS21	-1673.498617	-1673.363319	-1673.356148
TS22	-1826.052785	-1825.882058	-1825.874887
TS23	-2204.291529	-2204.106854	-2204.099683
11	-1274.247190	-1274.126995	-1274.119824
TS24	-1274.202729	-1274.078404	-1274.071233
TS25	-1389.859272	-1389.688221	-1389.68105
TS26	-1673.501089	-1673.366395	-1673.359224
TS27	-1826.055688	-1825.883650	-1825.876479
TS28	-2204.293818	-2204.108881	-2204.10171
12	-436.808030	-436.727757	-436.7205858
CO₂	-188.439412	-188.448519	-188.4413478
TS29a	-436.762572	-436.679837	-436.6726658
TS29b	-436.761194	-436.678383	-436.6712118
TS30	-552.419977	-552.289340	-552.2821688

TS31	-836.060818	-835.966599	-835.9594278
TS32	-988.614066	-988.483749	-988.4765778
TS33	-1366.852603	-1366.708964	-1366.701793
H ₂ O	-76.370612	-76.367259	-76.3600878
CH ₃ COOH	-228.934059	-228.899735	-228.8925638
CH ₃ NHCOOH	-284.264451	-284.214441	-284.2072698
13	-1082.591680	-1082.516855	-1082.509684
TS34	-1082.591522	-1082.516176	-1082.509005
14	-2012.681590	-2012.544509	-2012.537338
TS35	-2012.678854	-2012.542351	-2012.53518

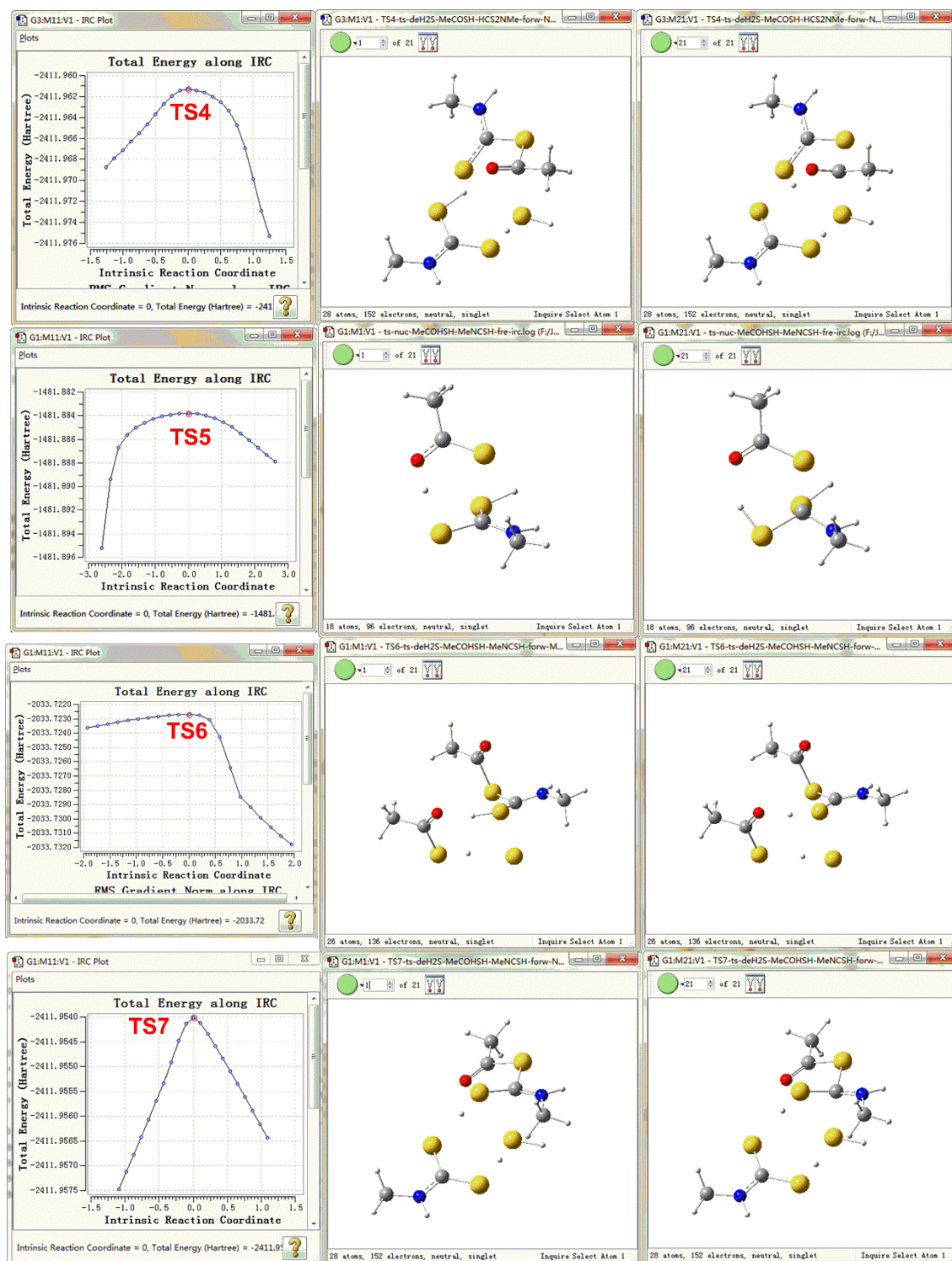
Table S3. Method A-calculated vibrational entropies (S_v in $\text{cal}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$), rotational entropies (S_r in $\text{cal}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$) and thermodynamic corrections for enthalpy (H_c in hartree), Method-B calculated solvation-energy-included $E(0)$ ($E(0)_{\text{Bsol}}$ in hartree), and corrected solution-phase Gibbs free energies of method B (G_{Bsol}' in hartree).

species	S_v	S_r	H_c	$E(0)_{\text{Bsol}}$	G_{Bsol}'
1	21.914	29.323	0.072278	-1529.927065	-1529.876103
2	8.016	25.104	0.061653	-552.1540181	-552.1050736
TS1	34.342	30.735	0.139049	-1482.637588	-1482.526431
TS2	51.817	31.781	0.197397	-1598.415568	-1598.254863
TS3	60.229	32.72	0.202496	-2034.783504	-2034.622143
TS4	70.207	33.81	0.217249	-2413.126581	-2412.955726
TS5	37.465	30.683	0.140383	-1482.626742	-1482.51571
TS6	69.533	32.917	0.2014	-2034.782915	-2034.627164
TS7	78.698	33.721	0.217161	-2413.119636	-2412.952861
TS8	61.263	31.88	0.194763	-1598.404895	-1598.25136
6	27.194	29.698	0.12107	-1083.226633	-1083.129567
H_2S	0.046	12.65	0.018661	-399.4320297	-399.4163731
TS9a	22.028	29.343	0.120008	-1083.179554	-1083.080926
TS9b	22.468	29.371	0.11994	-1083.178928	-1083.08059
TS10	42.847	31.122	0.178051	-1198.973899	-1198.827965
TS11	42.493	31.117	0.140791	-1482.616471	-1482.507626
TS12a	56.755	32.549	0.183762	-1635.340245	-1635.195886
TS12b	52.128	32.25	0.183592	-1635.345172	-1635.198643
TS13a	61.689	33.382	0.201015	-2013.688266	-2013.529395
TS13b	62.154	33.08	0.200515	-2013.693849	-2013.535555

IRC analysis were performed by using G09 program with 10 points along the reverse and forward reaction paths to examine, respectively. Thereafter, the 1st and 21st points obtained in IRC analysis were further optimized as minima and they can transform into the corresponding intermediates. The IRC plots and the structures of the related 1st and 21st points were shown in Figure S4.



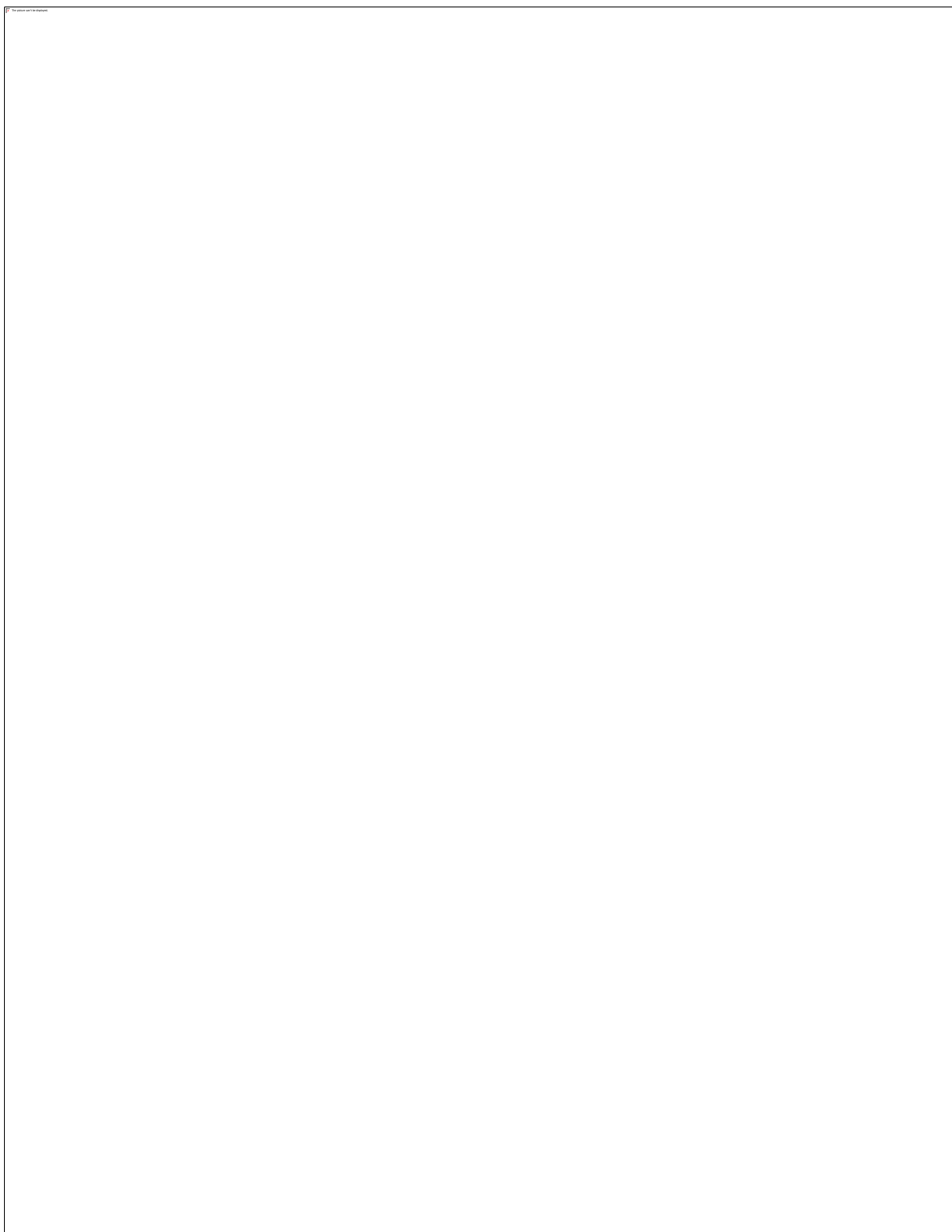
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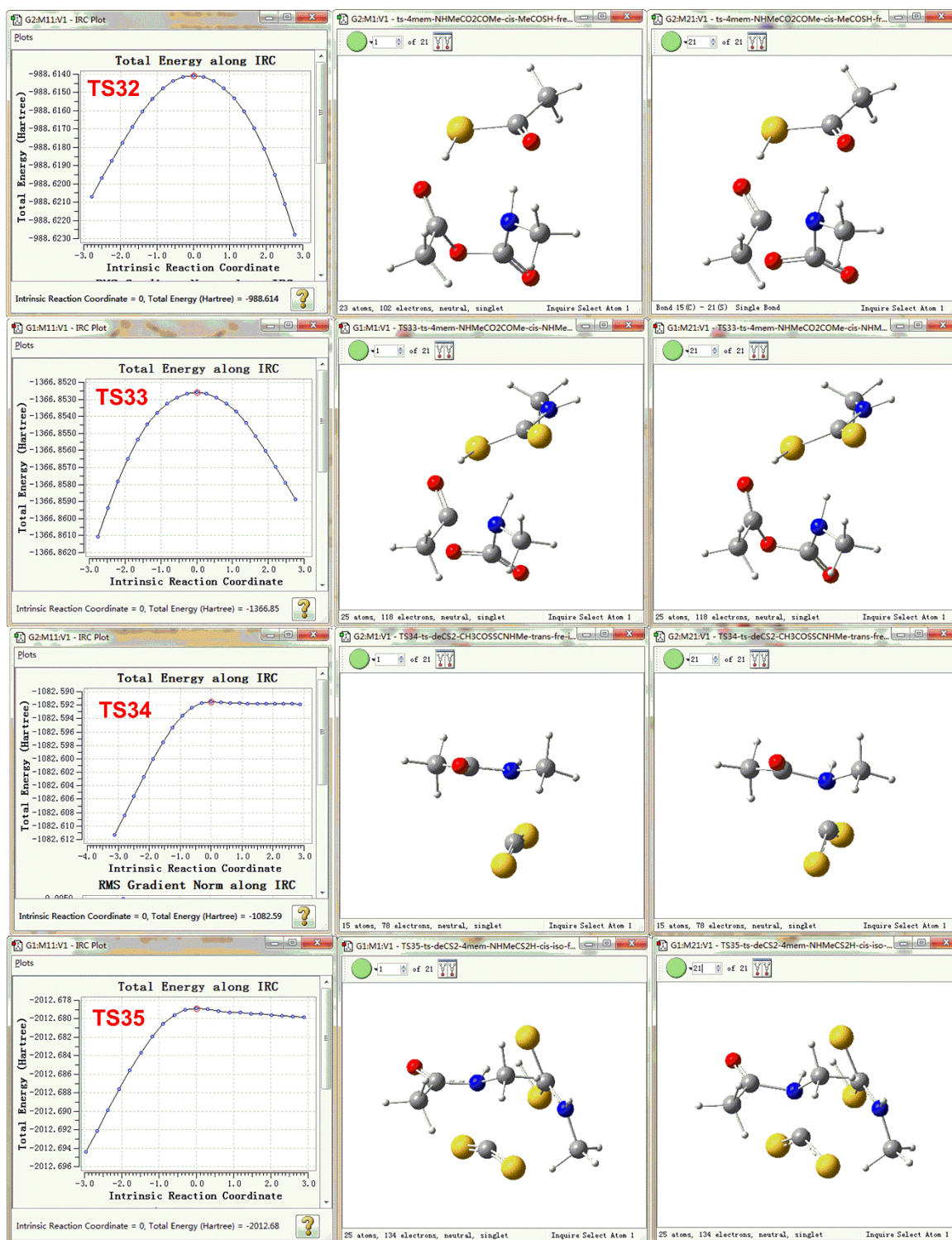


Fig. S4 IRC plots of all transition states.

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

1

C	0.75947100	0.26230200	-0.01426000
S	0.25690300	-1.38812200	-0.04793000
S	-0.28638100	1.64669600	-0.02930500
N	2.08163900	0.52456800	0.02713600
H	2.33853500	1.50781700	0.03657200
C	3.14834000	-0.45336100	0.04635000
H	3.03704400	-1.15165500	0.89161300
H	3.16712900	-1.05562800	-0.87781500
H	4.10434900	0.07962500	0.14298900
K	-2.64177600	-0.31805100	0.03473200

2

H	1.75688700	1.00564300	0.01834500
S	1.28554000	-0.26509100	-0.00100400
C	-0.45158000	0.23075900	-0.00322800
O	-0.78703900	1.39254500	-0.00042800
C	-1.40288500	-0.93434500	0.00025700
H	-1.18813200	-1.61129900	-0.84167500
H	-1.28119600	-1.51134500	0.93161600
H	-2.43309500	-0.56038600	-0.07098000

3

C	0.10511200	-0.01735500	-0.00007500
S	-0.30045100	1.60088700	0.00000400
S	1.79986000	-0.60641300	0.00015600
N	-0.77902300	-1.02058100	-0.00010800
H	-0.44130400	-1.98050400	-0.00110100
C	-2.21592200	-0.82824000	0.00011400
H	-2.53804900	-0.26681300	0.89179400
H	-2.53772500	-0.26339400	-0.88949500
H	-2.69712100	-1.81470500	-0.00193000
H	2.34166800	0.63147000	-0.00131100

4

C	1.02151700	-0.32386100	-0.00118800
O	0.22369600	-1.28551800	-0.00043800
C	2.51133500	-0.62525000	0.00011400
H	2.68178400	-1.71257200	-0.02142200
H	2.99725600	-0.15752200	-0.87056900
H	2.98352100	-0.19785400	0.89907200
S	0.55257700	1.34660100	-0.00007300
K	-2.13107700	-0.18415000	0.00021300

TS1

imaginary frequency = -780.6821 cm⁻¹

C	-1.90977500	-0.05077600	-0.31501200
O	-1.49253600	-0.77326500	-1.27971600
C	-2.90198300	1.03314800	-0.59777600
H	-2.64188700	1.52498500	-1.54482800
H	-3.89714200	0.56509000	-0.70153200
H	-2.94993100	1.77212900	0.21300100
S	-1.94260000	-0.84078700	1.29145100
H	-2.38311200	0.24088000	1.97759500
C	1.36151800	0.34403700	-0.05928500
S	1.18296400	-1.30048400	-0.58369400
S	0.09084600	1.50080200	-0.03031000
N	2.57471600	0.73565600	0.34650700
H	2.65029300	1.69462800	0.67869600
C	3.77617400	-0.07754700	0.35605100
H	3.70188300	-0.90312600	1.08311400
H	3.96843800	-0.51222300	-0.63759100
H	4.62213200	0.56422500	0.63433200
H	-0.40835000	-1.15573800	-1.03363200

5

C	-1.63552900	0.08804600	-0.23976600
O	-1.60537700	-0.88536100	-1.20892800
C	-2.85563000	0.96804700	-0.44773100
H	-2.81254700	1.42960400	-1.44688200
H	-3.75565300	0.33828700	-0.38890900

H	-2.92424100	1.75698800	0.31425800
S	-1.66224200	-0.73831100	1.43653200
H	-1.75610800	0.40362300	2.15889100
C	1.25930600	0.22295900	-0.15498200
S	1.33364100	-1.39745900	-0.59667300
S	-0.16186700	1.27804500	-0.36367600
N	2.30460200	0.88485300	0.34377500
H	2.16393300	1.84353700	0.65737500
C	3.63489300	0.32460000	0.49387500
H	3.63446200	-0.50433000	1.21978000
H	4.00620300	-0.06303200	-0.46782800
H	4.30378300	1.11761900	0.85113200
H	-0.71977900	-1.33168500	-1.16012200

TS2

imaginary frequency = -374.9431 cm⁻¹

C	1.12536000	-1.04107600	-0.47604000
O	0.85971300	-0.20082400	-1.38221900
C	2.19744000	-2.07383100	-0.72253000
H	1.83544100	-2.75195000	-1.51585200
H	3.11000000	-1.57501500	-1.07720400
H	2.42537400	-2.66087000	0.17678900
S	2.26128200	0.29635600	1.21741500
H	1.45120400	-0.06037400	2.23995900
C	-1.54300300	-0.54177900	0.25112600

S	-2.59960900	-0.58501400	-1.02567100
S	-0.26260400	-1.80957300	0.49182800
N	-1.53125900	0.38875700	1.20849100
H	-0.83887500	0.30618500	1.94861400
C	-2.40196200	1.54609400	1.22073500
H	-3.45979400	1.23893300	1.24293900
H	-2.17313200	2.14531200	2.11127100
H	-2.24526400	2.15519800	0.31616200
H	0.52222100	1.01397800	-0.97525300
H	1.10321600	1.66578400	0.36080700
O	0.51749600	1.98403300	-0.43425500
C	1.20514200	3.00122200	-1.19614600
H	2.23885200	2.69178000	-1.40938900
H	0.65108800	3.14037500	-2.13293200
H	1.19784600	3.93159100	-0.61357100

TS3

imaginary frequency = -744.1560 cm⁻¹

C	-1.80624900	-0.69449000	0.36568500
O	-1.22962200	-0.40923800	1.47309200
C	-3.06154000	-1.50325300	0.45228700
H	-2.75018000	-2.53075500	0.71549800
H	-3.71437300	-1.11178600	1.24421300
H	-3.59739700	-1.53799700	-0.50440700
S	-2.75325300	1.45189200	-0.25782700

H	-2.82511200	1.24261000	-1.59504600
C	0.79735300	-1.47520000	-0.47929700
S	0.99977400	-2.67901500	0.63905300
S	-0.82819000	-0.98057100	-1.14268900
N	1.77155600	-0.80743200	-1.09969200
H	1.51435700	0.00477600	-1.65903400
C	3.18118900	-1.05067100	-0.86786100
H	3.44625500	-0.84245500	0.18142000
H	3.42910800	-2.10287300	-1.07830800
H	3.76146900	-0.39689000	-1.53082300
H	-0.32901700	0.15935700	1.41415000
C	1.28823700	1.75622900	0.69304000
C	2.70966700	2.22808200	0.87423400
H	3.19122100	1.66288400	1.68432500
H	3.27631800	2.09791200	-0.06038800
H	2.72098400	3.30284900	1.11506000
H	-1.23755300	1.93080300	-0.34599200
O	0.86157800	0.87707700	1.47189600
S	0.39450900	2.48686200	-0.59299000

TS4

imaginary frequency = -626.3050 cm⁻¹

C	0.88115800	1.52610200	-0.56180700
O	0.25091000	0.68780700	-1.25678000
C	0.82963900	2.99191000	-0.96450400

H	1.27598100	3.08236600	-1.96902700
H	-0.22147000	3.30933000	-1.02903000
H	1.37342700	3.64668900	-0.26926000
S	0.01357400	1.55509900	1.46556300
H	-0.15628300	2.90127600	1.51316500
C	2.73667100	-0.61211600	0.07192700
S	1.57181600	-1.44747800	0.92635200
S	2.72303700	1.15051300	-0.21103700
N	3.83934900	-1.18587900	-0.43076700
H	4.45844400	-0.61520000	-1.00188500
C	4.19177100	-2.57870300	-0.24475700
H	4.21728800	-2.83717400	0.82586000
H	3.45915400	-3.24360100	-0.73140000
H	5.18294200	-2.74723600	-0.68568000
H	-0.69354200	-0.32465700	-0.67898800
C	-3.03722000	-0.32804800	-0.13172500
S	-1.63641200	-1.33717300	-0.29114900
S	-2.96603800	1.39261600	0.01494000
N	-4.22584300	-0.91318200	-0.09822900
H	-5.02788500	-0.31485000	0.09508300
C	-4.47769100	-2.33533400	-0.26469000
H	-3.97767500	-2.71259700	-1.16972800
H	-4.11459200	-2.90712500	0.60478400
H	-5.55999200	-2.48473900	-0.36096400
H	-1.55921700	1.43839800	0.71291700

TS5

imaginary frequency = -173.0565 cm⁻¹

C	1.12245300	-0.22453200	-0.14184100
S	1.03595200	-0.51265900	1.61674700
S	0.76759900	-1.69081800	-1.10521000
N	2.10963400	0.57864600	-0.57152500
H	2.32518400	0.53587600	-1.56575600
C	2.46413800	1.81627100	0.10461200
H	1.56032400	2.41380800	0.31780900
H	2.98832300	1.62262000	1.05192500
H	3.12934500	2.39051200	-0.55247400
H	0.63198000	-1.06012000	-2.30070800
C	-2.13201300	0.14613300	0.18564200
O	-1.92613300	-0.78043900	0.98426200
C	-3.55461500	0.47725300	-0.20349800
H	-4.23624700	0.20173900	0.61583800
H	-3.67578300	1.53818200	-0.46312300
H	-3.82206300	-0.12114700	-1.09183800
S	-0.88731700	1.09094100	-0.58003000
H	-0.31896100	-0.81865500	1.54130900

7

C	0.86700800	-0.11424700	-0.16292300
S	1.04947800	-0.68017100	1.58441700

S	0.65561600	-1.62066500	-1.19694600
N	2.04082600	0.58631200	-0.53129400
H	2.14448500	0.63187600	-1.54391800
C	2.34744100	1.85795500	0.11201600
H	1.62918000	2.66589400	-0.12432200
H	2.36980200	1.73639500	1.20432400
H	3.34611300	2.18311500	-0.21436800
H	0.37019900	-0.96299400	-2.35163400
C	-2.07426000	0.11352400	0.18462900
O	-2.00982800	-0.94551700	0.77881000
C	-3.37820500	0.77668200	-0.16967900
H	-4.13898800	0.49051400	0.57112200
H	-3.29035200	1.87137500	-0.22538000
H	-3.69598900	0.40797400	-1.16031300
S	-0.65957000	1.03330000	-0.39616000
H	-0.24190500	-1.08709600	1.68782900

MeOH

O	-0.74870000	0.12391400	0.00000900
H	-1.13564100	-0.76397700	-0.00003100
C	0.65922800	-0.01901200	0.00000500
H	1.10168200	0.99004700	-0.00069900
H	1.03416000	-0.55109000	0.89603800
H	1.03403400	-0.55221700	-0.89540400

H₂S

S	0.00000000	0.00000000	0.10400100
H	0.00000000	0.97926200	-0.83200900
H	0.00000000	-0.97926200	-0.83200900

6

C	1.97946500	0.27739700	-0.01799800
C	3.36086600	-0.30502100	0.05258100
H	3.60052600	-0.49936800	1.11245000
H	3.43883100	-1.25566200	-0.49482800
H	4.07919900	0.42652200	-0.34406400
O	1.74859000	1.46988900	-0.03397000
S	0.70276000	-1.00471200	-0.03501500
C	-0.91343100	-0.20413200	-0.00470300
N	-0.95722400	1.12134400	-0.00231900
H	-0.06570300	1.62879800	-0.01998900
S	-2.21389700	-1.24484300	0.01386400
C	-2.19568300	1.87500900	0.01962700
H	-1.94833000	2.94431800	0.02188900
H	-2.81366700	1.64507500	-0.86318400
H	-2.78811600	1.63516600	0.91709000

TS6

imaginary frequency = -220.0632 cm⁻¹

C	1.65063000	0.05416100	0.02508700
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S	1.27810100	-0.22978100	1.69354600
S	0.73872500	-2.54119700	-0.76853800
N	2.90291200	0.09136300	-0.36499200
H	3.07733500	0.31725000	-1.34421000
C	4.02731800	-0.37071900	0.43091400
H	4.08947500	0.19164000	1.37503600
H	3.91507400	-1.44532700	0.65177500
H	4.94763300	-0.21138600	-0.14256300
H	0.44850700	-2.50654600	-2.09277000
C	0.17403200	2.30898600	-0.51417900
O	0.88253800	2.80374200	0.32560900
C	-1.03364200	2.95361600	-1.12730700
H	-0.89468200	4.04380800	-1.14862200
H	-1.24749100	2.57077900	-2.13584000
H	-1.89588000	2.71766500	-0.47963800
S	0.40720200	0.60230700	-1.13319200
H	-0.10163400	-0.13078600	1.51716200
C	-2.62659800	-0.23419400	0.64977800
C	-3.98134100	0.43190500	0.61729500
H	-4.03833900	1.05797900	-0.28972100
H	-4.79994000	-0.30013900	0.56930900
H	-4.09466100	1.07809800	1.49969200
H	-1.02173100	-1.97393200	-0.36606000
O	-1.71890600	0.26722800	1.31794600
S	-2.50374700	-1.67376200	-0.33535200

TS7

imaginary frequency = -725.6718 cm⁻¹

C	1.73444500	0.92992000	-0.38287800
S	0.55814100	0.49352000	-1.63737900
S	0.47355600	0.36056300	1.76125400
N	2.00617400	2.22956300	-0.26183400
H	2.82935300	2.48817500	0.28188800
C	1.06311000	3.30460300	-0.53731400
H	1.37430700	4.18428600	0.04057800
H	1.05375800	3.56698800	-1.60646800
H	0.04761500	3.00578500	-0.24018800
H	0.89837200	1.56751600	2.21179000
C	2.61933400	-1.77631900	0.01810300
O	1.47200200	-2.10019300	-0.12485500
C	3.75420200	-2.70878700	0.33495000
H	3.77187000	-2.86589000	1.42717800
H	3.56605700	-3.67699000	-0.15136400
H	4.73021400	-2.30925700	0.02392100
S	3.20818300	-0.06237300	-0.08042300
H	-0.26276300	-0.39145700	-0.90105700
C	-2.93394600	-0.13465200	0.12134400
S	-1.86803900	-1.44059100	-0.13474000
S	-2.44253100	1.44996100	0.66843200
N	-4.25045900	-0.28455300	-0.08756500

H	-4.84917200	0.50573500	0.13975000
C	-4.88908300	-1.48991000	-0.57569600
H	-4.41025000	-1.83705500	-1.50445400
H	-4.82734200	-2.30901300	0.16034100
H	-5.94619600	-1.26611400	-0.77180500
H	-0.99916100	0.95735500	1.22916000

TS8

imaginary frequency = -285.0270 cm⁻¹

C	-0.09834400	0.95329600	0.03513500
S	0.45697200	0.45540600	1.61497100
S	0.53720500	-1.33634500	-1.52500700
N	0.58558300	1.79677600	-0.72938500
H	0.16091300	2.04148100	-1.62452900
C	1.99754700	2.08871900	-0.60797000
H	2.27411000	2.16776800	0.45178400
H	2.60235100	1.29852000	-1.08227100
H	2.20074200	3.04192900	-1.11349100
H	-0.24514600	-2.12527200	-0.75695600
C	-2.56993400	-0.54798000	0.27730600
O	-1.94754300	-1.44265200	0.77560200
C	-4.03814300	-0.57599500	-0.03684000
H	-4.50136900	0.41809900	0.04656000
H	-4.16184300	-0.92787700	-1.07560300
H	-4.53298600	-1.28789800	0.63865800

S	-1.85597600	1.05347100	-0.25517500
H	1.64330000	-0.30519400	1.17738200
O	2.55624800	-1.30902500	0.65952600
H	1.95833800	-1.47492900	-0.16158800
C	3.84639700	-0.89047100	0.23251600
H	3.84636300	-0.61562100	-0.83530300
H	4.17193500	-0.01793900	0.82143200
H	4.57821000	-1.70299400	0.38110000

CS₂

C	0.00000000	0.00000000	0.00000000
S	0.00000000	0.00000000	1.56136400
S	0.00000000	0.00000000	-1.56136400

8a

C	0.48246500	0.15898400	-0.00578600
N	-0.62095900	-0.61898200	-0.00648300
H	-0.49510800	-1.62597300	-0.00293300
C	-1.97299000	-0.10296200	0.00403500
H	-2.53806300	-0.45579200	-0.87432000
H	-2.51358400	-0.41734100	0.91234300
H	-1.93096800	0.99321700	-0.01929800
O	0.43610200	1.39477600	-0.00044500
C	1.80391800	-0.57493600	0.00189000
H	2.44807700	-0.15367300	-0.78489700

H 2.30561900 -0.39341500 0.96651800

H 1.70156000 -1.65886600 -0.14930500

8b

C -0.61233400 -0.15547900 0.00016800

N 0.63376700 -0.67932600 0.00114700

H 0.67713800 -1.69509700 -0.00074000

C 1.88117400 0.06134500 -0.00048700

H 2.71169300 -0.65671000 0.00303100

H 1.98500700 0.69653100 -0.89566500

H 1.98321200 0.70291400 0.89024700

O -1.61484000 -0.88015900 -0.00047900

C -0.71303300 1.35236200 0.00010000

H -0.21879500 1.78040000 0.88704700

H -0.21848600 1.78043400 -0.88665600

H -1.77226200 1.63871800 -0.00014300

TS9a

imaginary frequency = -224.3316 cm⁻¹

C 1.58481300 -0.08002000 0.02231200

C 1.98706600 -0.65401500 1.35179800

H 1.13265300 -1.01756700 1.93480900

H 2.67755300 -1.49208500 1.16513000

H 2.52525600 0.12742300 1.91214100

O 2.28786400 0.51848000 -0.74713200

S 0.08256800 -1.31623000 -0.78164100

C -0.92247500 -0.16701000 0.00882600

N -0.03415500 0.90229600 0.44225000

H -0.18554100 1.12676800 1.43234700

S -2.53728000 -0.17170600 0.28804800

C -0.09074600 2.12183400 -0.37277300

H -1.09954500 2.56044900 -0.34080100

H 0.63876000 2.84066500 0.02411200

H 0.17048600 1.87267200 -1.40992700

TS9b

imaginary frequency = -251.8190 cm⁻¹

C -1.60785600 -0.05530600 -0.09475200

S -0.14124000 -1.64208800 -0.01427200

C 0.88596600 -0.27116100 -0.14506700

N 0.01153900 0.83118800 -0.52596900

H -0.10248500 0.82290700 -1.54691900

S 2.49481900 -0.11485900 0.13260400

C 0.31715200 2.18498200 -0.05658700

H 1.28406100 2.52658600 -0.45490300

H -0.48073800 2.85517300 -0.40425200

H 0.35751700 2.19286200 1.04008000

O -2.38260000 -0.05299500 -1.01156300

C -1.89006900 0.32227900 1.33192200

H -2.58893300 -0.42339200 1.74215800

H	-0.99029200	0.35237500	1.95670300
H	-2.38752400	1.30551700	1.33502200

TS10

imaginary frequency = -202.0871 cm⁻¹

C	0.24657900	1.40646300	0.14896200
O	1.45390000	1.25055600	0.12527800
C	-1.47463300	-0.36104700	-0.09799000
C	-0.44114800	2.63296600	0.68418600
H	-1.52793200	2.50925500	0.76814600
H	-0.00893800	2.87103300	1.66897800
H	-0.22784900	3.46766200	-0.00302600
N	-0.65569400	-0.02922200	1.06036000
H	2.25183500	-0.12874500	-0.70585800
C	0.29800800	-1.07042800	1.46727900
H	0.90312300	-0.67614100	2.29432500
H	-0.23929700	-1.97199500	1.79768600
H	0.94417900	-1.31381200	0.61520900
H	-1.24165200	0.25296500	1.85478100
S	-0.83834600	0.61492200	-1.36898700
S	-2.70049200	-1.43967400	-0.08791100
O	2.74911500	-0.93915600	-0.94017400
C	3.78489800	-1.06630300	0.01314800
H	3.40081400	-1.18764000	1.04460700
H	4.37683500	-1.96375000	-0.23017100

H	4.47379600	-0.19936500	0.00883200
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TS11

imaginary frequency = -209.7064 cm⁻¹

C	0.14629000	1.54655300	-0.02279300
O	1.27408200	1.60418800	0.41614300
C	-1.29195700	-0.47960000	-0.15268900
C	-0.74968100	2.73013400	-0.26773300
H	-1.77703000	2.44286300	-0.52234500
H	-0.74568100	3.36074000	0.63570700
H	-0.32230100	3.30945900	-1.10186400
N	-0.96794500	0.35454000	0.99634500
H	2.46443800	-0.00438600	0.02264000
C	-0.18590800	-0.30885500	2.04797900
H	0.09898400	0.44458800	2.79451900
H	-0.78168000	-1.10070800	2.52626200
H	0.71752700	-0.74779500	1.60481200
H	-1.81531900	0.77843800	1.39213500
S	3.13787100	-1.16333600	-0.20005700
S	-0.27128600	0.09164900	-1.41723500
S	-2.41613400	-1.66603400	-0.13770900
H	4.02432700	-0.92434400	0.79599100

TS12a

imaginary frequency = -217.0680 cm⁻¹

C	-1.07662500	1.55718900	0.12566600
O	0.08767300	1.87900000	0.24945700
C	-2.02657600	-0.72350500	-0.07661200
C	-2.24948800	2.45345000	0.41976500
H	-3.20790800	1.92005500	0.40705900
H	-2.08903400	2.91994700	1.40481800
H	-2.26965700	3.24688600	-0.34451600
N	-1.50164400	-0.04060000	1.09657300
H	1.42985700	0.87405000	-0.68471400
C	-0.27994000	-0.63386800	1.65946600
H	0.17105000	0.08771200	2.35307200
H	-0.51793700	-1.56809900	2.18911800
H	0.42301400	-0.84864200	0.84607600
H	-2.22104100	0.06241800	1.82179900
S	2.36368400	0.05987600	-1.25980300
C	3.30130100	-0.18299400	0.25808000
O	2.97834400	0.32769600	1.30874100
C	4.50147700	-1.07551600	0.08759700
H	4.18914400	-2.06496700	-0.28344700
H	5.19299300	-0.64604700	-0.65508600
H	5.01367200	-1.18541300	1.05324100
S	-1.57687700	0.28514400	-1.40097300
S	-2.85878700	-2.12850700	-0.03252300

imaginary frequency = -250.9338 cm⁻¹

C	1.03900500	-1.57838700	0.13911400
O	0.05584200	-2.19584900	0.50924200
C	1.35725700	0.78758900	-0.42160300
C	2.44810600	-2.09973100	0.25180300
H	3.20552500	-1.35315800	-0.01499500
H	2.60918600	-2.44875100	1.28392900
H	2.54141200	-2.96285000	-0.42601400
N	1.12315400	0.15767200	0.85741300
H	0.11079200	0.26914800	1.07156400
C	1.94537700	0.52200700	2.01074300
H	3.00769300	0.37462100	1.77695400
H	1.77885000	1.57412600	2.28712500
H	1.65544000	-0.12345900	2.85123100
H	-1.60524600	-1.55691300	-0.05071100
C	-2.60174200	0.53383500	0.35443200
O	-1.60767000	0.83585600	0.99444900
C	-3.78713600	1.45099400	0.23016700
H	-4.32453100	1.31238200	-0.71861600
H	-4.48522000	1.22478400	1.05480100
H	-3.45156300	2.49252200	0.33436800
S	0.90456000	-0.43095200	-1.55968900
S	1.96366100	2.28918100	-0.64777600
S	-2.79915800	-1.02848300	-0.47184700

TS12b

TS13a

imaginary frequency = -201.2802 cm⁻¹

C	-1.75321600	1.52829100	-0.19399500
O	-0.60779300	1.92350300	-0.13754100
C	-2.52001600	-0.81983100	0.10075400
C	-2.97316000	2.40309400	-0.10710000
H	-3.90340400	1.82828000	-0.02122800
H	-2.85836500	3.07331000	0.75954400
H	-3.01392500	3.01680100	-1.02153600
N	-2.10848700	0.14916900	1.10656900
H	0.77242600	0.74337100	-0.79690600
C	-0.88198500	-0.19503000	1.83774200
H	-0.60906900	0.65516600	2.47623300
H	-1.04418400	-1.09129800	2.45511200
H	-0.07214400	-0.38461400	1.12320400
H	-2.87416000	0.34735300	1.76152200
S	1.56782100	-0.19067500	-1.38843700
S	-2.15518200	-0.07330300	-1.40869700
S	-3.18342800	-2.27437700	0.43870100
C	2.91201800	-0.05810800	-0.21534900
S	2.83831300	0.86112100	1.17840900
N	3.97301200	-0.79085100	-0.57395400
H	3.94330600	-1.30062900	-1.45422300
C	5.19197900	-0.89033500	0.20403900
H	5.67607200	0.09401400	0.31109000

H	4.98373200	-1.27460500	1.21519300
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H	5.87628000	-1.57615200	-0.31213000
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TS13b

imaginary frequency = -254.0172 cm⁻¹

C	1.74334300	-1.37304700	0.52591700
O	0.81218400	-2.07813700	0.87709400
C	1.77453400	0.81592800	-0.57575500
C	3.15623400	-1.54657100	1.01829800
H	3.82778200	-0.74473400	0.68892700
H	3.13919700	-1.59626400	2.11840500
H	3.53034900	-2.50803500	0.63231000
N	1.38540300	0.46020100	0.76247300
H	0.33558300	0.39069400	0.80742600
C	1.86335200	1.24881100	1.89702700
H	2.96001700	1.29359700	1.88957000
H	1.45980900	2.27204400	1.85460400
H	1.51584100	0.76006700	2.81768200
H	-0.79288600	-1.79826500	-0.00322800
C	-2.57649200	-0.25557700	-0.05280500
S	1.79664900	-0.70279500	-1.40568600
S	2.14704700	2.32190600	-1.09438700
S	-1.91277100	-1.72061100	-0.78750400
S	-1.80255000	0.65597100	1.14403400
N	-3.77858400	0.09228500	-0.51295600

H -4.16988900 0.94675500 -0.12136300

C -4.56454100 -0.61884500 -1.50653000

H -4.76438400 -1.65527800 -1.18951900

H -5.52205400 -0.09701700 -1.62481700

H -4.05286500 -0.63975600 -2.48269100

9

C -1.90633600 0.14395900 -0.37843700

C -3.37176500 -0.12065500 -0.17096500

H -3.62211300 -1.08708200 -0.64104400

H -3.63487500 -0.18098600 0.89504500

H -3.95195700 0.67198300 -0.66411100

O -1.44233200 0.78421600 -1.29181300

S -0.87892400 -0.67373100 0.86724700

C 0.78917700 -0.39924900 0.20111800

N 1.25642400 0.85477300 0.17703800

S 1.63876300 -1.74831100 -0.28771100

C 2.57293200 1.09790600 -0.40903500

H 2.74934600 2.17939700 -0.44990400

H 3.36050300 0.61801700 0.19317100

H 2.62131700 0.67760400 -1.42480100

C 0.56283500 2.03930000 0.67387600

H 0.24127900 2.67494900 -0.16541300

H -0.31048900 1.75938100 1.27058800

H 1.25220500 2.61469800 1.30978300

TS14

imaginary frequency = -199.8432 cm⁻¹

C 1.60501300 -0.17835200 -0.00640100

C 1.98163900 -0.22420800 1.44843500

H 1.13228400 -0.40792400 2.11451700

H 2.70890400 -1.04295400 1.56776500

H 2.47785500 0.72286400 1.71330400

O 2.34030700 0.07431700 -0.92292100

S 0.13042600 -1.70428200 -0.29429700

C -0.89560800 -0.35494400 -0.04196800

N -0.02838300 0.82997500 -0.09306600

S -2.51458600 -0.28492900 0.21033300

C -0.04042100 1.44804300 -1.43264800

H -1.02851300 1.89067300 -1.62813700

H 0.73174600 2.22805600 -1.46096000

H 0.18140700 0.68796400 -2.19087300

C -0.25825100 1.82694200 0.96374600

H 0.56266400 2.55617900 0.93267000

H -1.21451200 2.34642600 0.79954900

H -0.28327300 1.33686100 1.94344900

TS15

imaginary frequency = -179.6061 cm⁻¹

C 0.29689800 1.36057200 -0.16850500

O	1.49768400	1.31047000	0.04817500
C	-1.29113900	-0.50842200	-0.34495700
C	-0.49124200	2.64404900	-0.14540200
H	-1.56701500	2.50085300	-0.29353100
H	-0.30325900	3.16238700	0.80788700
H	-0.10317900	3.27240000	-0.96259400
N	-0.66243200	0.11429700	0.83337100
C	-1.60129800	0.64113500	1.84066000
H	-2.36161700	1.26504800	1.35818700
H	-2.09534700	-0.19032800	2.36415100
H	-1.02829700	1.23908500	2.56151900
H	2.46573300	-0.07529800	-0.49798000
S	-0.45945400	0.17745700	-1.68047300
S	-2.49450000	-1.61038800	-0.27507400
C	0.32922600	-0.79540800	1.44713900
H	1.00861000	-1.17217600	0.67521800
H	0.89642000	-0.22875800	2.19662900
H	-0.19653100	-1.63335200	1.92631400
O	2.97039400	-0.90026800	-0.65676700
C	3.90765300	-1.02193600	0.39399300
H	3.42599000	-1.13363600	1.38524200
H	4.51631500	-1.92360200	0.21612500
H	4.59725300	-0.15735700	0.44914700

TS16

imaginary frequency = -193.6194 cm⁻¹

C	0.21762400	1.42498700	-0.31408900
O	1.25623000	1.67369300	0.25515200
C	-1.07120200	-0.70269700	-0.29286500
C	-0.65239700	2.44774300	-0.99325900
H	-1.58442700	2.03525100	-1.39315000
H	-0.86822800	3.25819100	-0.27938900
H	-0.06465100	2.86635500	-1.82543300
N	-0.93443200	0.34559700	0.73063400
C	-2.19826600	0.95913200	1.17295900
H	-2.79702800	1.25372300	0.30422200
H	-2.77432100	0.24551500	1.78054400
H	-1.95697000	1.84305000	1.77819800
H	2.74761800	0.26150100	0.31502000
S	0.11332100	-0.33423600	-1.47885400
S	-2.16605400	-1.91602200	-0.21793500
S	3.54652200	-0.83748600	0.29475800
C	-0.13494900	-0.12768500	1.87854100
H	0.80021200	-0.57472400	1.52310600
H	0.09388400	0.73337800	2.52018800
H	-0.71065300	-0.87633800	2.44200500
H	2.74026500	-1.45960000	-0.59619100

TS17

imaginary frequency = -166.7289 cm⁻¹

C	0.95919800	-1.55908500	-0.13270100
O	0.14420200	-2.04808700	0.62543800
C	1.35833700	0.87462700	-0.41790900
C	2.02941400	-2.34872700	-0.83673100
H	2.71146400	-1.73129400	-1.43020700
H	2.59130900	-2.93359200	-0.09182900
H	1.51318900	-3.05135800	-1.51039100
N	1.81387800	-0.04600800	0.63665800
C	3.27645000	-0.10937100	0.80055700
H	3.75897300	-0.26415100	-0.17104800
H	3.64644300	0.82962900	1.23903300
H	3.51098800	-0.94487800	1.47313500
H	-1.72655600	-1.48714000	0.41311200
C	-2.94268900	0.53850000	0.36376700
O	-2.06660900	1.03603800	1.03847500
C	-4.10177600	1.31655900	-0.19814300
H	-3.88046000	1.55774500	-1.25206000
H	-5.03553500	0.73531400	-0.17535500
H	-4.21820400	2.25359200	0.36388800
S	0.31496500	-0.05771700	-1.40719400
S	1.80761400	2.44433000	-0.52198300
S	-2.95989800	-1.19627800	-0.09137100
C	1.13562800	0.21642400	1.92049800
H	0.05511600	0.28982300	1.75826800
H	1.35742500	-0.61450800	2.60305400

H	1.50766900	1.16033800	2.34523300
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TS18

imaginary frequency = -166.2489 cm⁻¹

C	-1.34231700	1.56078300	0.03800700
O	-0.58905600	1.90375400	0.93008500
C	-1.90262100	-0.76668900	-0.58888400
C	-2.27484700	2.50101100	-0.67899600
H	-2.93083300	2.00143100	-1.39975200
H	-2.87219700	3.05041000	0.06525600
H	-1.64359700	3.22529100	-1.21839300
N	-2.38195200	0.05238200	0.53507700
C	-3.84281100	0.22507300	0.59438600
H	-4.22643700	0.53095100	-0.38537500
H	-4.32345000	-0.71949800	0.89012200
H	-4.06762100	0.99817300	1.34109300
H	1.27245700	1.35877900	0.66532500
C	2.82845800	-0.37389500	0.35220500
S	-0.66360900	0.16273200	-1.31869300
S	-2.48852600	-2.24889900	-0.96196700
S	2.48329600	1.34479200	0.04674800
C	-1.83563500	-0.42072700	1.82138400
H	-0.74762300	-0.53728600	1.73888600
H	-2.07098400	0.32607700	2.59125900
H	-2.29406400	-1.38626900	2.08123800

N	3.97191400	-0.79592900	-0.20228800
C	4.89213900	-0.00754300	-1.00213300
H	4.41607300	0.35339700	-1.92916800
H	5.27190200	0.86175800	-0.44022800
H	5.74481900	-0.64250600	-1.27351600
S	1.83893200	-1.38234900	1.25439000
H	4.19860000	-1.77439600	-0.04039800

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C	0.43091200	0.55470500	-0.01692600
O	0.04570900	1.71103900	-0.07426200
S	-0.69913600	-0.85569600	0.12105200
C	-2.39020400	-0.23514200	0.03004200
N	-2.58866500	1.07216000	-0.05925300
H	-1.76058600	1.67767000	-0.07276800
S	-3.55904300	-1.42134700	0.07212900
C	-3.90694400	1.67033600	-0.14524400
H	-3.78717200	2.75908600	-0.21549800
H	-4.44814000	1.30232700	-1.03149100
H	-4.51006900	1.42608500	0.74394600
C	1.87095100	0.19071800	-0.02097400
C	2.33023100	-1.12798500	-0.18801000
C	2.80046300	1.23440700	0.14510400
C	3.69887100	-1.39542100	-0.18237200
H	1.62980000	-1.95159700	-0.33835400

C	4.16604900	0.96054800	0.15364600
H	2.43578700	2.25500400	0.27211500
C	4.61710100	-0.35442800	-0.00965200
H	4.04978900	-2.42090800	-0.31739600
H	4.88310300	1.77374100	0.28826800
H	5.68875000	-0.56857700	-0.00454800

TS19

imaginary frequency = -236.5528 cm⁻¹

C	0.10197200	1.04230800	-0.41591400
O	0.06486900	2.24405300	-0.54046100
S	-1.23971700	-0.05399100	-1.60277100
C	-1.93683500	-0.36306200	-0.06533100
N	-1.14554200	0.42961000	0.87534700
H	-0.73254000	-0.17197000	1.59786100
S	-3.18727200	-1.31895200	0.37976900
C	-1.84481900	1.56273700	1.49206300
H	-1.14891600	2.06850700	2.17435100
H	-2.15825200	2.25961900	0.70370400
H	-2.72516500	1.21044200	2.04952900
C	1.34996400	0.25046800	-0.15518000
C	2.53654600	0.98596800	-0.00872200
C	1.38389200	-1.14733300	-0.03199100
C	3.74124200	0.33210500	0.25784000
H	2.50340900	2.07252500	-0.10490000

C	2.58833200	-1.79552600	0.24183900
H	0.47554200	-1.73903300	-0.15497800
C	3.76978800	-1.05923600	0.38527500
H	4.66035000	0.91298400	0.36768600
H	2.60487200	-2.88377900	0.33796900
H	4.71186900	-1.57247000	0.59380400

TS20

imaginary frequency = -215.5277 cm⁻¹

C	-0.11026300	0.49116000	-0.36332300
O	0.47887400	1.56162800	-0.40834400
C	1.06499300	-1.66174400	-0.03910100
N	0.63226300	-0.66589300	0.93998200
H	2.24121300	1.82158300	-0.67221300
S	0.60470900	-0.97958000	-1.55187400
S	1.80212700	-3.06788500	0.33051100
C	1.70041800	-0.01808600	1.71130500
H	2.39565700	0.47022800	1.01722700
H	1.23925100	0.73055200	2.36890000
H	2.23720500	-0.76295800	2.31713300
O	3.17528500	2.09256600	-0.56312200
C	3.16058500	3.25732200	0.23915300
H	2.72600200	3.07917200	1.24186500
H	4.19932300	3.59814300	0.37967700
H	2.59591900	4.08529900	-0.23158600

C	-1.59421400	0.39360200	-0.15240400
C	-2.28431500	1.59845500	0.05086500
C	-2.29951000	-0.81973300	-0.12898200
C	-3.66254900	1.59028900	0.27447200
H	-1.72950400	2.53781800	0.03037800
C	-3.67547500	-0.82379100	0.10237000
H	-1.78282600	-1.76705200	-0.29466300
C	-4.36069300	0.37983800	0.30250100
H	-4.19202000	2.53392700	0.42779700
H	-4.21659800	-1.77276500	0.12136400
H	-5.43923100	0.37260600	0.47871100
H	-0.07674800	-1.06328800	1.56792100

TS21

imaginary frequency = -230.4880 cm⁻¹

C	-0.35540600	0.61840700	-0.09198300
O	0.11185800	1.71750700	0.13379900
C	1.31607800	-1.20722600	-0.04570700
N	0.44471500	-0.68703200	1.00849400
H	2.14267700	2.00593900	-0.24833400
S	0.69271100	-0.51235500	-1.48829500
S	2.59877800	-2.18790300	0.20533100
S	3.49621900	2.06849100	-0.34733700
C	1.07923000	-0.14537900	2.21175500
H	1.74264200	0.68032000	1.92184600

H	0.28887500	0.22572200	2.87775300
H	1.66303700	-0.92326900	2.72463500
H	3.59440700	0.75019600	-0.63557900
H	-0.25901400	-1.39464200	1.25377300
C	-1.82244900	0.31873800	-0.09569500
C	-2.68213700	1.36178600	0.28316500
C	-2.35762100	-0.93143100	-0.43977600
C	-4.06216200	1.15471900	0.31783700
H	-2.25679200	2.33135400	0.54740800
C	-3.73713500	-1.13542100	-0.39869400
H	-1.69956300	-1.74651300	-0.74797100
C	-4.59209700	-0.09360200	-0.02180000
H	-4.72549500	1.97224400	0.61079700
H	-4.14727700	-2.11150500	-0.66826800
H	-5.67248600	-0.25595000	0.00429900

TS22

imaginary frequency = -241.8876 cm⁻¹

C	0.61444400	-0.74082300	-0.23963500
O	0.01257400	-1.79042600	-0.04357300
C	-0.27850900	1.53754500	-0.30826700
N	-0.04503900	0.64176000	0.80756200
H	-0.96838300	0.22462700	1.05559300
C	0.63148400	1.13565600	2.00773700
H	1.59530700	1.58508800	1.73826500

H	0.00649700	1.88357800	2.51772100
H	0.79652800	0.27982500	2.67649100
H	-1.81205600	-1.84766200	-0.42259800
C	-3.57557200	-0.57564200	0.47577300
O	-2.74901600	0.00543400	1.16069200
C	-5.04812600	-0.29343900	0.58211400
H	-5.56485700	-0.41794200	-0.38024100
H	-5.48699800	-1.00882400	1.29914600
H	-5.19452100	0.72469800	0.96941500
S	-0.10873500	0.49893800	-1.67791900
S	-0.58519000	3.13632200	-0.19991300
S	-3.15744700	-1.84806300	-0.69318300
C	2.11416500	-0.65070900	-0.12631400
C	2.86857800	0.47769200	-0.48292900
C	2.76828600	-1.77710100	0.39659500
C	4.25377200	0.47762200	-0.31030500
H	2.38547600	1.36086300	-0.90124600
C	4.15454100	-1.77572500	0.56225100
H	2.17840700	-2.65304500	0.67043300
C	4.90096000	-0.64767800	0.21069700
H	4.83101000	1.36204600	-0.59043400
H	4.65199100	-2.66016000	0.96800200
H	5.98621200	-0.64500600	0.33949000

TS23

imaginary frequency = -233.1228 cm⁻¹

C	1.01048400	-0.62059300	-0.47535800
O	0.27943400	-1.60643800	-0.46115200
C	0.34189200	1.72283700	-0.27696500
N	0.43300500	0.67738600	0.71617200
H	-0.53205200	0.29667000	0.91592500
C	1.09485000	0.95049600	1.99255800
H	2.10731700	1.33511800	1.81729900
H	0.51770800	1.68606900	2.57272900
H	1.15043700	0.00607900	2.55096200
H	-1.49244500	-1.28681100	-0.78880100
C	-3.38834900	-0.58925600	0.42429600
S	0.53258100	0.86284800	-1.76456600
S	0.14090900	3.31386400	0.02659000
S	-2.78822700	-1.05232600	-1.17264200
S	-2.40844400	-0.36140600	1.78565000
N	-4.70963300	-0.42785600	0.49252400
H	-5.06889000	-0.11942800	1.39395600
C	-5.66635300	-0.63294500	-0.58183500
H	-5.57215100	-1.64460500	-1.00775600
H	-6.67628400	-0.51864100	-0.16900000
H	-5.53261000	0.10547700	-1.38978400
C	2.49547000	-0.73115500	-0.25463600
C	2.97079100	-1.97766300	0.18134700
C	3.39941500	0.32786100	-0.42753500

C	4.32964200	-2.16255400	0.44305800
H	2.26325000	-2.79786700	0.31178800
C	4.75682300	0.14059000	-0.16050600
H	3.05346200	1.30191700	-0.77430400
C	5.22588300	-1.10329300	0.27448000
H	4.68833500	-3.13820600	0.78036100
H	5.45259700	0.97168000	-0.29809200
H	6.28986700	-1.24631100	0.47913000

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C	-2.76786300	-1.11200200	-0.00939400
O	-1.87928700	-1.94313000	-0.02596500
S	-2.48862700	0.66990700	-0.00685300
C	-0.70523100	0.99554100	-0.00365200
N	0.08649400	-0.08194400	-0.01462900
H	-0.41536200	-0.98392400	-0.02375200
S	-0.33836600	2.61497300	0.01511000
C	1.48895000	-0.22921000	-0.00750100
C	1.95299900	-1.55967700	0.00985600
C	2.41655300	0.82502600	-0.01783300
C	3.31826300	-1.83077300	0.01834400
H	1.22855500	-2.37817900	0.01766300
C	3.78469800	0.53641000	-0.00910300
H	2.07114200	1.85535200	-0.03263100
C	4.24537500	-0.78188100	0.00941100

H	3.65956700	-2.86880900	0.03248400
H	4.49845700	1.36422900	-0.01715400
H	5.31735900	-0.99287600	0.01644900
C	-4.22574300	-1.46102500	0.02218400
H	-4.43103400	-1.98387700	0.97134700
H	-4.88142500	-0.58345900	-0.05893900
H	-4.43454600	-2.16233900	-0.80132700

TS24

imaginary frequency = -211.7047 cm⁻¹

C	1.26368100	-1.56688500	0.06649300
O	0.61269800	-2.13838400	0.88901400
S	2.47608000	0.16817400	0.82342000
C	1.27846400	0.96438000	-0.09112100
N	0.38642800	-0.08390700	-0.64828300
H	0.48621200	-0.10687000	-1.66980500
S	1.02936000	2.55419900	-0.41016900
C	-1.00028800	-0.03766800	-0.29096800
C	-1.96748500	-0.24286500	-1.27913500
C	-1.36687000	0.14533300	1.04706300
C	-3.31786700	-0.25842600	-0.92510100
H	-1.65902700	-0.38268600	-2.31832800
C	-2.71988700	0.12892900	1.38938200
H	-0.60500600	0.30359400	1.81138600
C	-3.69633300	-0.07264900	0.40836300

H	-4.07619200	-0.41093300	-1.69669800
H	-3.01161700	0.27506000	2.43209500
H	-4.75379200	-0.08138200	0.68307500
C	2.05771900	-2.14652000	-1.06375300
H	1.37744600	-2.77355900	-1.66457500
H	2.51955500	-1.37975400	-1.69619000
H	2.84199700	-2.78879600	-0.63445500

TS25

imaginary frequency = -173.4032 cm⁻¹

C	-1.24803000	0.50306300	1.30899100
O	-0.53740400	1.48553900	1.28594700
C	-1.40963500	-1.04310000	-0.61672900
N	-0.51578400	-0.93063800	0.57448900
H	-0.40860400	2.43723300	-0.25347500
S	-2.52621600	0.23590800	-0.46057300
S	-1.23084600	-2.22732300	-1.72766500
O	-0.15524800	2.97190800	-1.03058200
C	0.98060600	3.72176800	-0.64582200
H	1.83073700	3.08187700	-0.34115400
H	1.30663400	4.32664200	-1.50746900
H	0.76296400	4.41476200	0.19023100
H	-0.69955300	-1.72868200	1.19685800
C	0.90253000	-0.82910500	0.34062700
C	1.76986700	-1.60193900	1.11582300

C	1.38752600	0.06589300	-0.61712200
C	3.14785500	-1.48160000	0.92569000
H	1.36406800	-2.29523600	1.85689100
C	2.76724500	0.17726300	-0.79830800
H	0.70474100	0.68228400	-1.20161000
C	3.64772600	-0.59351800	-0.03168200
H	3.83054100	-2.08802300	1.52531500
H	3.15529100	0.87270900	-1.54587300
H	4.72605800	-0.50294400	-0.18254600
C	-2.04694800	0.03206700	2.48964100
H	-2.74453300	0.83439600	2.77294400
H	-2.60994000	-0.88687600	2.28563000
H	-1.34615100	-0.13536900	3.32506800

TS26

imaginary frequency = -213.0687 cm⁻¹

C	-0.98257600	-0.50668200	1.56001700
O	-0.72976800	0.62826600	1.85681800
C	-0.84523300	-1.19368400	-0.86203700
N	0.13207700	-1.17289500	0.25892100
H	-1.38129900	2.31034800	0.70731500
S	-2.35343200	-0.75241600	-0.19651200
S	-0.40856800	-1.61223800	-2.38332800
S	-1.86193500	3.11873900	-0.26938500
H	-2.45740000	2.07524000	-0.89234800

H	0.35261900	-2.14339900	0.51495200
C	1.34448000	-0.42155200	0.10811600
C	2.53896000	-0.95749400	0.59860100
C	1.30703400	0.86013600	-0.44982900
C	3.71203900	-0.20479000	0.51948800
H	2.54572400	-1.95930700	1.03520800
C	2.48559400	1.60426000	-0.52288100
H	0.37196400	1.27896000	-0.82195500
C	3.68795100	1.07608300	-0.04181000
H	4.64812300	-0.62365300	0.89608800
H	2.45976000	2.60613900	-0.95787400
H	4.60759400	1.66260400	-0.10510000
C	-1.28086800	-1.64866900	2.48273600
H	-1.45323400	-2.59043500	1.94889900
H	-0.42612300	-1.75501100	3.17195600
H	-2.17546700	-1.38833400	3.06906600

TS27

imaginary frequency = -211.6088 cm⁻¹

C	0.04010000	-1.34694600	-1.35474900
O	0.83274300	-0.83151800	-2.12120600
C	-0.08245500	-1.09523600	1.09534100
N	-0.46403400	-0.22834200	-0.03095600
H	0.30007500	0.48171100	-0.11105400
H	2.47355000	-0.22258800	-1.43497000

C	2.83676600	1.46101500	0.15882300
O	1.62382100	1.58598000	0.23387200
C	3.78064800	2.28139000	0.99146200
H	4.69501700	2.54499200	0.44084500
H	3.26422000	3.18734400	1.33764300
H	4.07496100	1.68425300	1.87198400
S	0.83387000	-2.34273800	0.35767900
S	-0.45419600	-0.79654000	2.65839600
S	3.63261100	0.27901000	-0.90357200
C	-1.73601300	0.43365700	-0.08548200
C	-1.77879900	1.72403100	-0.62488100
C	-2.90993000	-0.21259400	0.31737800
C	-3.00790900	2.37177900	-0.76370600
H	-0.85177900	2.21440500	-0.92925000
C	-4.13240100	0.44590600	0.17797800
H	-2.87109800	-1.21775400	0.73752500
C	-4.18625600	1.73556000	-0.36228600
H	-3.04134100	3.38001100	-1.18317300
H	-5.05040700	-0.05527300	0.49378700
H	-5.14710000	2.24481500	-0.46818600
C	-1.17045500	-2.12470300	-1.79226300
H	-0.80896600	-2.98618900	-2.37430700
H	-1.78061700	-2.48706100	-0.95848300
H	-1.77712900	-1.48482500	-2.45274300

TS28

imaginary frequency = -221.9155 cm⁻¹

C	0.71709500	1.68222600	-1.24569800
O	-0.12022900	1.49512900	-2.10444800
C	0.22147400	0.97084200	1.07927500
N	0.79106900	0.26430800	-0.07403400
H	0.05777500	-0.38443500	-0.46613000
H	-1.86486900	0.89453600	-1.42438000
C	-2.73967300	-1.02711200	-0.40357300
S	0.01486600	2.58838000	0.55588300
S	-0.16766700	0.23054200	2.48549900
S	-3.00218300	0.69841600	-0.69984100
S	-1.41081100	-1.89636900	-0.98791300
N	-3.69567300	-1.61234300	0.31411300
H	-3.55546200	-2.60151400	0.51086800
C	-4.86987500	-0.96670500	0.87570300
H	-5.48790100	-0.50595900	0.08816600
H	-5.46883600	-1.72802800	1.39010500
H	-4.58459100	-0.18987900	1.60422500
C	2.02608700	-0.45624800	0.05398500
C	2.29761300	-1.44839200	-0.89646500
C	2.97070500	-0.13013200	1.03314800
C	3.51719500	-2.12577600	-0.85592400
H	1.56067000	-1.67693700	-1.66853100
C	4.18690900	-0.81541000	1.06402500

H	2.76388900	0.65016100	1.76590200
C	4.46374800	-1.81417200	0.12530400
H	3.72661500	-2.90153100	-1.59623600
H	4.92362900	-0.56285500	1.83029500
H	5.41665000	-2.34754800	0.15758200
C	2.12198400	2.14513700	-1.49053500
H	2.06183700	3.15324500	-1.92944100
H	2.72615600	2.18573100	-0.57822300
H	2.59164500	1.46918200	-2.22267600

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C	-1.53094100	-0.28007300	-0.00243300
C	-2.92153800	0.26654400	0.00532600
H	-3.06127200	0.90048600	0.89496600
H	-3.06841900	0.90509400	-0.88002500
H	-3.64652500	-0.55614200	0.00534600
O	-1.23309800	-1.45283100	-0.01750800
C	0.77809900	0.63620400	0.00182700
N	1.29966700	-0.59016500	0.02019300
H	0.65924200	-1.38278600	0.00886400
C	2.73766900	-0.78418000	-0.00056400
H	2.94577400	-1.85595400	0.11022600
H	3.17950500	-0.43345500	-0.94779800
H	3.22259300	-0.24227000	0.82637900
O	-0.62127700	0.73766200	0.00897000

O	1.39083700	1.68582100	-0.01449300
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CO₂

C	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.16276100
O	0.00000000	0.00000000	-1.16276100

TS29a

imaginary frequency = -272.8958 cm⁻¹

C	1.09327900	0.01449000	-0.20078500
O	1.41755800	0.72258300	-1.12122700
O	0.05930000	-1.19396700	-0.60635800
C	-0.99394700	-0.68679100	-0.03905700
O	-2.13029900	-1.07964300	-0.02142900
C	1.97185900	-0.49998500	0.89873900
H	1.41759900	-1.07986100	1.64745900
H	2.46837600	0.35677400	1.37835900
H	2.74329800	-1.14159000	0.44419300
N	-0.48084900	0.53387900	0.59284100
H	-0.50592100	0.45255400	1.61615000
C	-1.06073100	1.79695700	0.12866900
H	-0.61749400	2.62167900	0.70157100
H	-2.15234500	1.79343400	0.26653200
H	-0.82280100	1.92005900	-0.93743900

TS29b

imaginary frequency = -301.7689 cm⁻¹

C	-1.15504700	-0.13340300	-0.14191000
O	-1.82775900	-0.36656700	-1.11140000
O	-0.09192800	-1.36672900	0.27568700
C	0.98752400	-0.69440900	0.02839200
O	2.14251100	-0.95940600	0.24269200
C	-1.60124100	0.49292400	1.14485400
H	-0.79888400	0.57121800	1.88838600
H	-2.00748300	1.49157000	0.92447600
H	-2.41053200	-0.13164800	1.55407100
N	0.48179600	0.55585600	-0.55039400
H	0.50673900	0.49141600	-1.57601000
C	1.08034300	1.81068300	-0.08126800
H	2.14072100	1.85479400	-0.37306700
H	0.53914600	2.65185200	-0.53364300
H	1.00565700	1.86665900	1.01230400

TS30

imaginary frequency = -212.5243 cm⁻¹

C	-0.65237400	1.07853900	-0.05219800
O	0.53333500	1.36586400	-0.10387500
C	-1.35781200	-0.94401600	-0.42984900
C	-1.75084300	2.05209900	0.26162400

H	-2.73589100	1.57264800	0.33108400
H	-1.51283400	2.56128200	1.20692300
H	-1.77260100	2.80290300	-0.54404400
N	-1.00268500	-0.42778200	0.89464100
H	1.72998300	0.20169500	-0.70389100
O	-1.14793200	0.09921700	-1.19037200
O	-1.72666200	-2.04742000	-0.71497200
C	0.13439600	-1.07918700	1.55928200
H	0.39259200	-0.50077500	2.45609900
H	-0.13248500	-2.10721000	1.84458700
H	0.98400800	-1.09606100	0.86563000
H	-1.82437200	-0.37292200	1.50910500
O	2.49649400	-0.40230100	-0.80441300
C	3.50263600	0.08738700	0.05927700
H	4.39632700	-0.54911700	-0.04682300
H	3.79863500	1.12610100	-0.18469800
H	3.19752700	0.06411700	1.12379400

TS31

imaginary frequency = -245.8529 cm⁻¹

C	1.00264600	-0.96515600	-0.03056100
O	0.17534700	-1.62537100	0.56248400
C	0.54683200	1.09150400	-0.63948300
C	2.37257400	-1.42549800	-0.43010500
H	2.96069900	-0.63303400	-0.91020900

H	2.89478200	-1.79253200	0.46580300
H	2.25378000	-2.26376600	-1.13467500
N	1.19265200	0.72645000	0.62532300
H	-1.80656800	-1.03373400	0.22635900
S	-2.99122400	-0.41484600	-0.01901200
O	0.40733800	-0.06252500	-1.22939900
O	0.21802100	2.18872400	-0.99746700
H	-2.46411000	0.29511600	-1.04429400
C	0.45785700	1.05294900	1.85236600
H	1.02231800	0.66840500	2.71169800
H	0.33306200	2.14197800	1.94512600
H	-0.52962800	0.57439600	1.81137600
H	2.16158900	1.06614400	0.65750700

C	-2.00335600	1.69206400	-1.23176100
H	-3.06054300	1.67149300	-0.93793700
H	-1.59715000	2.70053800	-1.05928800
H	-1.90947900	1.44168000	-2.29665000
H	1.06603000	-1.50436600	0.02576400
C	2.49094200	0.34035700	-0.30593800
O	1.54635700	0.92122500	-0.81601900
C	3.84055700	0.98185500	-0.14433700
H	3.92188000	1.36630600	0.88716700
H	4.65857200	0.26425300	-0.30188700
H	3.92858300	1.82551000	-0.84279500
S	2.38822700	-1.31379100	0.34341900
O	-1.48461100	-0.51326700	1.29734200
O	-1.35288000	1.72121400	1.70962100

TS32

imaginary frequency = -230.4614 cm⁻¹

C	-1.60202100	-1.03902300	-0.19873400
O	-0.70347400	-1.78456700	-0.55718400
C	-1.35139900	0.75456800	0.99831600
C	-3.05454900	-1.25766800	-0.51421600
H	-3.70524700	-0.46955200	-0.11559900
H	-3.17359800	-1.32303300	-1.60559800
H	-3.34816900	-2.22233500	-0.07148100
N	-1.24595000	0.70890500	-0.45104500
H	-0.23504600	0.71805200	-0.70914300

TS33

imaginary frequency = -220.2762 cm⁻¹

C	-2.10728200	-0.79596000	-0.66368600
O	-1.25210000	-1.20393500	-1.43724100
C	-1.70092000	-0.02570800	1.32279800
C	-3.57828300	-0.78148600	-0.96452700
H	-4.17902400	-0.37127300	-0.14328600
H	-3.74485700	-0.19493800	-1.87982400
H	-3.89040700	-1.82047300	-1.15353900
N	-1.68405800	0.77053600	0.10891900

H	-0.69466900	0.94193500	-0.21028300
C	-2.43556000	2.02969000	0.09980100
H	-3.48067700	1.84631700	0.38027200
H	-1.98425500	2.73572000	0.81387300
H	-2.39056900	2.45464500	-0.91151000
H	0.45766300	-1.22302800	-0.71660800
C	2.21815200	0.29274700	-0.28654600
S	1.64911000	-1.36820200	-0.05227000
S	1.28344900	1.53849000	-0.94783600
N	3.47410500	0.50288900	0.10582500
H	3.80695000	1.46091300	0.01726100
C	4.39039100	-0.48339500	0.65274900
H	4.49989600	-1.34277700	-0.02763500
H	5.37114300	-0.00842800	0.77938000
H	4.04962300	-0.85029600	1.63516900
O	-1.89943100	-1.23127500	0.84843100
O	-1.59735400	0.34993100	2.45777000

CH₃COOH

C	-0.09025800	0.11690000	-0.00166000
O	-0.78761500	-1.02854900	-0.00032900
C	1.39072900	-0.12030900	-0.00059900
H	1.92527600	0.83579200	-0.05217900
H	1.67579200	-0.66026900	0.91659900
H	1.66798500	-0.75803600	-0.85439700

H	-1.73951800	-0.81259200	0.00409400
O	-0.62893000	1.20549400	0.00025900

H₂O

O	0.00000000	0.00000000	0.12123600
H	0.00000000	0.75642700	-0.48494400
H	0.00000000	-0.75642700	-0.48494400

CH₃NHCOOH

C	0.52230600	0.09250300	0.00003900
N	-0.61362600	-0.62771300	0.00025100
H	-0.54517500	-1.63995900	0.00001400
C	-1.91414100	0.01000900	-0.00011200
H	-2.68854400	-0.76779400	0.00080600
H	-2.05296600	0.64418800	0.89124400
H	-2.05343700	0.64253000	-0.89259500
O	1.62346000	-0.69179300	-0.00015300
O	0.57460700	1.31786100	0.00002800
H	2.40198300	-0.10859600	0.00021400

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C	1.58489200	-0.32953100	-0.21500800
C	1.51048600	-1.17819600	-1.43599800
H	0.48974300	-1.25996600	-1.83145100
H	2.19902800	-0.78464300	-2.19434200

H	1.84281000	-2.19252800	-1.14997200
O	2.49373900	0.35654900	0.14407300
S	-0.65114800	1.66243500	-0.66434500
C	-0.90824200	0.14432900	-0.04051100
N	0.37027900	-0.44824000	0.68580600
H	0.16845200	-1.45245600	0.80529100
S	-2.20029900	-0.89625600	0.00219400
C	0.57083100	0.16385600	2.02475500
H	-0.34478700	-0.00713200	2.60340200
H	1.42710400	-0.31564100	2.51385500
H	0.75113400	1.23604400	1.89498500

TS34

imaginary frequency = -284.7881 cm⁻¹

C	-1.58911700	0.36312400	-0.18279900
C	-1.55234000	1.67374800	-0.89250800
H	-0.56038000	1.84548700	-1.33840400
H	-2.32976400	1.69147100	-1.66565400
H	-1.72720300	2.48551600	-0.16636100
O	-2.38607400	-0.52094900	-0.34047800
S	0.91512600	-1.50806600	-0.93665900
C	0.97414700	-0.12348300	-0.06182100
N	-0.49665000	0.16913400	0.79149800
H	-0.29132400	1.06152500	1.25726900
S	2.04549000	1.08434300	0.25763100

C	-0.74761200	-0.89369900	1.78572500
H	0.11732700	-0.93499700	2.45929000
H	-1.65861600	-0.65751500	2.35150400
H	-0.86523400	-1.84639800	1.25856300

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C	2.24792200	-1.26169200	-0.44397600
O	1.77828900	-2.35156300	-0.60565300
C	1.11327000	0.98004300	-0.19861600
C	3.57425900	-0.77532300	-0.92876800
H	3.66172600	0.31727600	-0.92427200
H	4.34062300	-1.19527800	-0.25361400
H	3.75531700	-1.17489800	-1.93522800
N	1.53615100	-0.32605600	0.51813400
H	0.62066400	-0.80507700	0.74259500
C	2.27829900	-0.21074100	1.80289200
H	3.19695500	0.36674000	1.65420800
H	1.63289800	0.29674500	2.52729500
H	2.50520000	-1.22820100	2.14863300
H	-3.10534300	-2.19016600	-0.63746700
C	-2.14868400	-0.38825800	0.43608700
S	0.67720700	0.67906700	-1.78378400
S	1.11469500	2.37055300	0.70938900
S	-3.29392400	-0.86491900	-0.83190300
S	-1.32457100	-1.52442800	1.38348200

N	-2.00811800	0.92278900	0.58929600
H	-1.31539300	1.21708700	1.27736900
C	-2.55254000	1.95239200	-0.27718400
H	-2.11991400	1.88033200	-1.28920800
H	-3.64965200	1.87702500	-0.33968200
H	-2.29527900	2.93088100	0.14504100

S	-1.41797200	2.35197300	-0.40942700
S	3.38479000	-0.45357200	0.85117100
S	1.45259100	-1.87773500	-1.00851700
N	1.91086400	0.74404900	-0.95443800
H	1.21466700	0.77019300	-1.69626100
C	2.38573700	2.01438600	-0.43419700
H	2.00129200	2.18868300	0.58476200
H	3.48692200	2.04856100	-0.41795400
H	2.02523000	2.81507000	-1.09049400

TS35

imaginary frequency = -290.8988 cm⁻¹

C	-2.50427000	-1.17560200	0.33960700
O	-2.16523600	-2.12590300	0.99648200
C	-1.03417000	0.98779300	0.41221300
C	-3.88430000	-0.61227200	0.25969800
H	-3.87067100	0.48742700	0.27163000
H	-4.34909900	-0.93004300	-0.68870200
H	-4.47915500	-1.00605600	1.09300400
N	-1.48514800	-0.47919100	-0.45066300
H	-0.60923400	-1.03887400	-0.38852800
C	-1.82182000	-0.29780600	-1.87649700
H	-2.63451900	0.42686600	-1.98839600
H	-0.93133800	0.07281600	-2.39689700
H	-2.11099800	-1.27101300	-2.29885500
H	3.31563500	-1.78963100	1.04749700
C	2.17731900	-0.45909000	-0.45171800
S	-0.33364800	0.58150800	1.83792300