Supporting Information (SI) for

Theoretical Investigation into Competing Unimolecular Reactions Encountered in the Pyrolysis of Acetamide

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TS1

Input orientation:

Atomic Type	Coordinates (Angstroms) X	Y	Z
O	0.000000	0.000000	0.000000
H	0.000000	0.000000	1.299148
H	0.756972	0.000000	-0.788435
H	-0.971779	0.164443	-0.478092
O	-0.004924	-1.446237	0.707442
C	0.002784	-2.486849	0.068420
S	-0.018975	-1.428712	2.157268
H	-0.133780	-0.579604	2.688497
H	-0.113019	-2.312218	2.638626

Frequencies

-1760.1694	270.5016	418.3934
783.2113	852.6581	929.9729
961.7628	1094.0983	1151.3577
1439.0398	1547.5484	1579.8044
1797.4027	1934.1270	3105.3656
3198.3868	3451.9041	3576.2075

Rotational constants (GHZ): 10.41755 8.98870 5.04355

Sum of electronic and zero-point Energies= -209.020919

TS2

Input orientation:

Atomic Type	Coordinates (Angstroms) X	Y	Z
O	-0.056477	0.032163	0.195149
H	0.100410	0.240728	1.258138
H	0.920561	-0.172089	-0.250177
H	-0.497590	0.906830	-0.295101
O	-0.847080	-1.366061	-0.655927
C	-0.709944	-1.454184	-1.866179
S	-1.548462	-2.142310	0.091514
H	-1.199766	-1.129234	1.061522
H	-2.145871	-2.892557	-0.226867

Frequencies

216.2154	301.5299	
410.8519	479.5490	584.2146
627.7452	707.5855	764.3328
1110.5552	1209.1560	1223.2155
1281.0123	1430.8221	1442.9607
1805.2828	2015.5808	2949.5824
3111.5999	3179.9564	3434.0723

Rotational constants (GHZ): 10.51229 7.71819 4.58279

Sum of electronic and zero-point Energies= -209.012280

TS3

Input orientation:

Atomic Type	Coordinates (Angstroms) X	Y	Z
O	0.049951	0.062373	0.014132
H	-0.023749	-0.019752	1.103114
H	1.103887	0.102924	-0.272594
H	-0.411985	1.004775	-0.299652
O	-0.613679	-1.085802	-0.734972
C	-0.472364	-1.318900	-1.988743
S	-1.387041	-1.894970	-0.050355
H	-1.686408	-1.778538	0.905255
H	-1.664604	-2.539614	-1.582276

Frequencies

-1931.7286	96.4372	387.5890
441.6306	512.5048	703.9373
1016.2209	1030.9743	1073.0848
1137.6055	1166.0136	1424.4597
1499.2033	1502.9017	1550.6780
1637.8428	2100.3628	3073.3079
3138.1562	3161.6797	3553.4000

Rotational constants (GHZ): 12.60702 8.45994 5.22668

Sum of electronic and zero-point Energies= -209.069829

TS4

Input orientation:

Atomic Type	Coordinates (Angstroms) X	Y	Z
O	-0.050256	-0.063256	0.249948
H	0.039067	-0.114432	1.339655
H	0.966129	-0.010189	-0.148526
H	-0.386737	0.813329	-1.304027
O	-0.764658	-1.054143	-0.450267
C	-0.717075	-1.027407	-1.727302
S	-1.460388	-1.978079	0.283912
H	-1.565518	-1.908537	1.284152
H	-2.044781	-2.634000	-0.215474

Frequencies

373.2950 429.2132

440.0496 529.8037 625.2576

732.8936 820.1998 986.8606

1058.8345 1094.2330 1160.9477

1420.0871 1508.5847 1511.7960

1646.5149 1975.0307 3095.1286

3164.0739 3598.8555 3727.8903

Rotational constants (GHZ): 11.98917 9.00926 5.27453

Sum of electronic and zero-point Energies= -209.031960

TS5

Input orientation:

Atomic Type	Coordinates (Angstroms) X	Y	Z
O	0.000000	0.000000	0.000000
H	0.000000	0.000000	1.092183
H	1.034645	0.000000	-0.359920
H	-0.468797	0.922369	-0.359804
O	-0.731386	-1.192193	-0.541988
C	-0.727249	-1.188922	-1.899828
S	-1.331118	-2.167857	0.094016
H	-0.738451	-1.143689	0.941777
H	-1.218488	-1.989256	-2.164213

Frequencies

	156.0418	255.7048
339.4277	380.3754	458.4030
529.5843	621.4164	813.6948
926.8018	981.7704	1197.5560
1273.5926	1430.7713	1451.9195
1923.1648	2242.4944	3023.8978
3150.8517	3217.2662	3716.1493

Rotational constants (GHZ): 10.23682 7.76138 4.55445

Sum of electronic and zero-point Energies= -208.950863

TS6

Input orientation:

Atomic Type	Coordinates (Angstroms) X	Y	Z
O	0.000000	0.000000	0.000000
H	0.000000	0.000000	1.092183
H	1.034645	0.000000	-0.359920
H	-0.468797	0.922369	-0.359804
O	-0.692379	-1.128609	-0.513082
C	-0.519285	-1.107852	-2.168953
S	-1.274998	-2.076432	0.104773
H	-1.387544	-2.111531	-1.850362
H	-0.488348	-0.621873	-3.014304

Frequencies

178.5518	268.3282	
380.4078	395.7126	481.0834
631.7571	781.2014	937.8910
1064.5326	1067.4807	1231.7263
1406.8922	1465.4074	1476.3886
1816.1068	2053.4393	3052.1734
3122.9861	3131.8984	3787.4093

Rotational constants (GHZ): 10.93641 7.37080 4.58861

Sum of electronic and zero-point Energies= -209.018962

TS7

Input orientation:

Atomic Type	Coordinates (Angstroms) X	Y	Z
O	0.000000	0.000000	0.000000
H	0.000000	0.000000	1.092183
H	1.034645	0.000000	-0.359920
H	-0.674755	0.463675	-1.601754
O	-0.682627	-1.112713	-0.505855
C	-0.704188	-1.151541	-1.965073
S	-1.265246	-2.060537	0.112000
H	-1.192556	-1.939665	1.122271
H	-1.195427	-1.951875	-2.229458

Frequencies

279.5765 451.6980

456.7011 505.1405 599.5854

705.5736 739.7765 814.2685

930.5160 1008.7061 1049.4778

1147.8890 1354.1251 1456.1703

1807.6302 1887.5297 3111.4857

3197.2252 3532.9125 3769.0164

Rotational constants (GHZ): 10.43408 8.82897 4.92936

Sum of electronic and zero-point Energies= -208.986296

TS8

Input orientation:

Atomic Type	Coordinates (Angstroms) X	Y	Z
O	0.000000	0.000000	0.000000
H	0.000000	0.000000	1.090716
H	1.059269	0.000000	-0.324307
H	-0.459841	0.898743	-0.412834
O	-1.403991	-1.329491	-0.367073
C	-0.751909	-2.167440	-1.065862
S	-2.529862	-1.124443	0.097952
H	-2.720178	-0.298749	0.648494
H	0.009655	-1.204713	-0.721571

Frequencies

213.9197 303.1561

460.4446 475.2797 560.9932

620.3769 650.4506 716.3524

950.2629 1102.7333 1186.6412

1263.8198 1431.9968 1442.2687

1768.7026 2000.4860 2954.8350

3116.4008 3187.8439 3656.7245

Rotational constants (GHZ): 10.59319 8.28545 4.79342

Sum of electronic and zero-point Energies= -208.967462