**SUPPORTING INFORMATION**

**Reaction 1: SO2 + S2S2O + SO**

**SO2**

Single point energy (au): -549.578468

Geometry (Å)

S 0.000000 0.000000 0.000000

O 0.000000 0.000000 1.481272

O 1.312945 0.000000 -0.685816

Frequencies (cm-1)

1282.9635, 1117.7102, 496.2750

Electronic energy level

1

Rotational symmetry number

2

**S2**

Single point energy (au): -798.081825

Geometry (Å)

S 0.000000 0.000000 0.000000

S 0.000000 0.000000 1.932935

Frequencies (cm-1)

712.8571

Electronic energy level

3

Rotational symmetry number

2

**SP1**

Single point energy (au): -1347.622607

Geometry (Å)

S 0.000000 0.000000 0.000000

O 0.000000 0.000000 1.511380

O 1.482727 0.000000 -0.576975

S 2.378733 -1.849260 -0.707577

S 0.991078 -3.128411 -0.327663

Frequencies (cm-1)

1088.3608, 731.3000, 683.1132, 449.3341, 313.6681, 143.2955, 103.7032, 70.1918,

-552.6148

Electronic energy level

3

Rotational symmetry number

1

NS:SC scheme: 0:2

**Intermediate**

Single point energy (au): -1347.623254

Geometry (Å)

S 0.000000 0.000000 0.000000

O 0.000000 0.000000 1.513251

O 1.617852 0.000000 -0.547534

S 2.654693 -1.279636 0.031998

S 2.030396 -2.961726 -0.749721

Frequencies (cm-1)

1090.7403, 684.0586, 611.3006, 589.5814, 416.9929, 319.1841, 159.8422, 76.9631, 30.0465

Electronic energy level

3

Rotational symmetry number

1

NS:SC scheme: 0:2

**SP2**

Single point energy (au): -1347.600984

Geometry (Å)

S 0.000000 0.000000 0.000000

O 0.000000 0.000000 1.518096

O 2.185316 0.000000 -0.309434

S 2.907505 -0.104792 1.093575

S 3.116943 -1.973087 1.655713

Frequencies (cm-1)

1103.6820, 792.2405, 582.6971, 364.5554, 319.9940, 141.6376, 93.9551, 72.7098, -510.0754

Electronic energy level

3

Rotational symmetry number

1

NS:SC scheme: 0:2

**S2O**

Single point energy (au): -873.3513445

Geometry (Å)

O 0.000000 0.000000 0.000000

S 0.000000 0.000000 1.504861

S 1.723690 0.000000 2.370244

Frequencies (cm-1)

1125.9242 678.2489 368.6719

Electronic energy level

1

Rotational symmetry number

1

**SO**

Single point energy (au): -474.2635996

Geometry (Å)

O 0.000000 0.000000 -1.018610

S 0.000000 0.000000 0.509305

Frequencies (cm-1)

1115.0741

Electronic energy level

3

Rotational symmetry number

1

**Reaction 2: S2O + S2S3 + SO**

**S2O**

Single point energy (au): -873.3538085

Geometry (Å)

O 0.000000 0.000000 0.000000

S 0.000000 0.000000 1.472052

S 1.696571 0.000000 2.339722

Frequencies (cm-1)

1178.3257, 677.7944, 387.0252

Electronic energy level

1

Rotational symmetry number

1

**S2**

Single point energy (au): -798.0824642

Geometry (Å)

S 0.000000 0.000000 0.000000

S 0.000000 0.000000 1.913725

Frequencies (cm-1)

705.8582

Electronic energy level

3

Rotational symmetry number

2

**SP**

Single point energy (au): -1671.426557

Geometry (Å)

S 0.000000 0.000000 0.000000

O 0.000000 0.000000 1.500669

S 1.844717 0.000000 -0.756582

S 2.439081 -2.519882 -0.637872

S 1.067469 -3.416066 0.355368

Frequencies (cm-1)

1032.2129, 672.6298, 488.2885, 346.9167, 188.7146, 123.7255, 69.2862, 32.4247, - 237.05

Electronic energy level

3

Rotational symmetry number

1

NS:SC scheme: 2:0

**Intermediate 1**

Single point energy (au): -1671.439727

Geometry (Å)

S 0.000000 0.000000 0.000000

O 0.000000 0.000000 1.473065

S 1.700254 0.000000 -0.860511

S 2.578196 -4.226959 1.770776

S 1.604331 -2.692763 2.376772

Frequencies (cm-1)

1174.5805, 712.0835, 677.6385, 386.5666, 69.7865, 53.5307, 33.9054, 18.7774, 13.5208

Electronic energy level

3

Rotational symmetry number

1

NS:SC scheme: 0:2

**Intermediate 2**

Single point energy (au): -1671.432655

Geometry (Å)

S 0.000000 0.000000 0.000000

O 0.000000 0.000000 1.502120

S 2.024925 0.000000 -0.683801

S 2.765154 -1.785166 0.207201

S 3.470107 -1.355491 2.006902

Frequencies (cm-1)

1049.0187, 551.9299, 433.5714, 409.9067, 319.7585, 207.1634, 162.3159, 56.3719, 39.1350

Electronic energy level

3

Rotational symmetry number

1

NS:SC scheme: 0:2

**S3**

Single point energy (au): -1197.142632

Geometry (Å)

S 0.000000 0.000000 0.000000

S 0.000000 0.000000 1.938408

S 1.727479 0.000000 2.817752

Frequencies (cm-1)

671.5186, 579.9714, 268.0782

Electronic energy level

1

Rotational symmetry number

2

**SO**

Single point energy (au): -474.2650711

Geometry (Å)

O 0.000000 0.000000 0.000000

S 0.000000 0.000000 1.499807

Frequencies (cm-1)

1146.2939

Electronic energy level

3

Rotational symmetry number

1

**Reaction 3: SO + SHS2 + OH**

**SO**

Single point energy (au): -474.2652762

Geometry (Å)

O 0.000000 0.000000 0.000000

S 0.000000 0.000000 1.490051

Frequencies (cm-1)

1184.4788

Electronic energy level

3

Rotational symmetry number

1

**SH**

Single point energy (au): -399.5977893

Geometry (Å)

S 0.000000 0.000000 0.000000

H 0.000000 0.000000 1.343523

Frequencies (cm-1)

2710.2105

Electronic energy level

2 0

2 0.001717783

Rotational symmetry number

1

**SP**

Single point energy (au): -873.8985602

Geometry (Å)

S 0.000000 0.000000 0.000000

O 0.000000 0.000000 1.559018

S 2.014458 0.000000 -0.084042

H 1.351983 -0.000000 1.376852

Frequencies (cm-1)

1716.1004, 997.9457, 825.0698, 588.0819, 519.2389, -1924.74

Electronic energy level

2

Rotational symmetry number

1

**Intermediate 1**

Single point energy (au): -873.9371038

Geometry (Å)

S 0.000000 0.000000 0.000000

O 0.000000 0.000000 1.493472

S 1.987952 0.000000 -0.696629

H 2.203757 1.296917 -0.423093

Frequencies (cm-1)

2701.1741, 1092.5200, 802.4858, 483.7826, 306.2157, 146.7309

Electronic energy level

2

Rotational symmetry number

1

**Intermediate 2**

Single point energy (au): -873.9495397

Geometry (Å)

S 0.000000 0.000000 0.000000

O 0.000000 0.000000 2.912776

S 1.041733 0.000000 1.622838

H -0.899362 0.002212 2.559610

Frequencies (cm-1)

3797.3652 1157.3090 772.5760 660.5117 298.6143 80.1327

Electronic energy level

2

Rotational symmetry number

1

**S2**

Single point energy (au): -798.0826529

Geometry (Å)

S 0.000000 0.000000 0.000000

S 0.000000 0.000000 1.903536

Frequencies (cm-1)

738.8718

Electronic energy level

3

Rotational symmetry number

2

**OH**

Single point energy (au): -75.77671471

Geometry (Å)

O 0.000000 0.000000 0.000000

H 0.000000 0.000000 0.970399

Frequencies (cm-1)

3766.6510

Electronic energy level

2 0

2 0.000637887

Rotational symmetry number

1