Supporting information for:

Prediction of mechanism and thermochemical properties of O_3+H_2S atmospheric reaction

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In this supporting information, we present:

Geometries of some the intermediates and the transition state optimized by B3LYP/6-311++G(3df, 3pd)

C1

S	1.85920700	-0.06212900	-0.10497800
H	1.81200400	1.12848200	0.51182600
H	1.41450700	-0.71214100	0.98109700
O	-1.61995800	0.04974800	-0.34883200
O	-1.34911500	-1.05782600	0.17894700
O	-1.15265400	1.08029300	0.19322600

C2

O	0.96484500	1.28701400	-0.22397900
O	0.49215900	0.31760000	0.40353700
O	1.07729200	-1.22993900	-0.16654100
H	1.78843300	-1.30534100	0.48709600
H	-1.64563900	1.10747600	0.13606500
S	-1.27607300	-0.17497100	-0.04545600

C3

O	-0.03305300	1.48117400	-0.24767400
O	-2.16364400	-0.52928800	0.00547400
O	0.78194300	0.69046800	0.37564700
S	0.98661600	-0.82670000	-0.08078000
H	-1.76470300	0.21306700	-0.46620300
H	-2.70311700	-0.12468900	0.69110600

SOO

O	1.26482200	0.89199100	0.00000000
S	-0.63241100	-0.79109400	0.00000000
O	0.00000000	0.69019600	0.00000000

TS1

O	-2.12409400	-0.61038800	-0.19470900
O	-1.13811200	-0.15916100	0.39025100
O	-0.71188300	1.08222400	-0.11708500
H	0.33169100	0.88724500	-0.03132400
H	2.51620600	0.25168800	0.94307700
S	1.80905100	-0.22752100	-0.09621300

TS2

O	0.52408700	1.62903100	-0.20930700
O	0.32160600	0.55496200	0.37916900
O	1.32162100	-1.17167100	-0.17427700
H	1.88808800	-1.35785600	0.58830400
H	-0.25444200	-1.39474600	-0.02343100
S	-1.18576000	-0.33412300	-0.03309700

TS3

O	1.21309700	-0.98446300	0.18495800
O	1.36252700	0.24893200	-0.32283300
O	0.51947200	1.05427400	0.21687700
H	-1.64100100	0.15018400	1.17820500
H	-0.18566400	-0.93338900	0.12933800
S	-1.43338100	-0.11042100	-0.12122200

TS4

O	0.91301900	0.85020400	0.30450900
O	1.49784400	-0.82107200	-0.21463000
O	-0.21727400	0.96739000	-0.31488400
S	-1.22922100	-0.37370000	0.07269500
H	0.17169400	-1.03692700	0.00567100
H	1.94712500	-0.95604600	0.63124900

TS5

O	2.16796800	-0.61069300	-0.25273000
O	1.49551500	0.15442300	0.45750200
O	0.42810300	0.79196500	-0.27458900
H	-0.27809700	0.93669500	0.42798800
H	-1.36554100	-1.29166900	0.38575500
S	-1.94306600	-0.14566200	-0.01595000

TS6

S	0.00000000	0.82047500	0.00000000
O	0.85249600	-0.36615700	0.00000000
O	-0.85249600	-1.27479200	0.00000000

HSOOOH

O	1.64423900	-0.64484200	0.18313100
O	1.17508400	0.56090600	-0.30943000

O	-0.19111300	0.84453900	0.33126000
H	-1.20282200	-1.11500800	0.88852300
H	1.33295500	-1.28499900	-0.47746100
S	-1.32223900	-0.23030100	-0.12817200

HOO

O	0.05528700	-0.60773400	0.00000000
O	0.05528700	0.71629500	0.00000000
H	-0.88458600	-0.86848500	0.00000000

HSO

O	0.05321800	1.03672300	0.00000000
H	-1.27724400	-0.81230500	0.00000000
S	0.05321800	-0.46759300	0.00000000

HSOH

O	-1.08665400	0.02283100	-0.11767200
H	-1.45062000	0.02588800	0.77439500
H	0.87014200	1.22840300	0.01247200
S	0.57960700	-0.08980900	0.00965700