

# GAS-PHASE INTERACTION OF H<sub>2</sub>S WITH O<sub>2</sub>: A KINETIC AND QUANTUM CHEMISTRY STUDY OF THE POTENTIAL ENERGY SURFACE

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Supporting Information.

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**Table 1S.** Optimized geometrical parameters of reactants and products of reaction calculated using the MP2(full)/6-31G(d). Bond lengths are given in Å and bond angles are given in degrees.

Species	Geometrical parameters
H <sub>2</sub> S	H-S = 1.3395; >HSH=93.3
O <sub>2</sub>	O-O = 1.2460 (triplet) O-O = 1.2738 (singlet)
O <sub>2</sub> H	O-O = 1.3252; O-H = 0.9831; >OOH = 104.6
SH	S-H = 1.3444
HSO	O-S = 1.4900; H-S = 1.3689; >HSO = 106.6
OH	O-H = 0.9787
H <sub>2</sub> O	H-O = 0.9684; >HOH = 104.0
SO	S-O = 1.5240
SO <sub>2</sub>	S-O = 1.4760; >OSO = 119.8
H <sub>2</sub>	H-H = 0.7375

**Table 2S.** Optimized geometrical parameters of the [H<sub>2</sub>S,O<sub>2</sub>] isomers calculated using the MP2(full)/6-31G(d). The labelled of the oxygen and hydrogen atoms are shown in Figure 1 of the paper. Bond lengths are given in Å and bond angles are given in degrees.

Species	Geometrical parameters
Sulfoxyllic acid (C <sub>2</sub> )	H2-O2 = 0.9770; O2-S = 1.6670; >H1-O1-S = 107.4; >H1-O1-S-O2 = -82.7
Sulfoxyllic acid (C <sub>s</sub> )	H2-O2 = 0.9763; O2-S = 1.6661; >H1-O1-S = 108.1; >H1-O1-S-O2 = -88.9
Sulfinic Acid	H1-S = 1.3232; H2-O1 = 0.9774; O2-S = 1.4834; O1-S = 1.6910; >H1-S-O2 = 108.0; >H1-S-O1 = 86.0; >O2-S-O1 = 112.8; >H2-O1-S = 106.8; >H1-S-O1-H2 = -167.7; >O2-S-O1-H2 = 84.5
Dihydrogen sulfone	H1-S = H2-S = 1.3576; O1-S = O2-S = 1.4576; >H1-S-H2 = 99.1; >H1-S-O1 = 107.6; >O1-S-O2 = 124.4; >O1-S-H1-H2 = 111.9
Peroxide	H1-O1 = 0.9790; H2-S = 1.3457; O1-O2 = 1.4851; O2-S = 1.6771; >H1-O1-O2 = 98.9; >O1-O2-S = 109.4; >O2-S-H2 = 98.1; >H1-O1-O2-S = -100.1; >O1-O2-S-H2 = -80.6
Thiadioxirane	H1-S = 1.3702; O2-S = 1.7169; O1-O2 = 1.5823; >H1-S-H2 = 85.6; >H1-S-O1 = 90.3; >H1-S-O2 = 130.5; >O1-S1-O2 = 54.9; >H1-S-O1-O2 = 142.2; >H1-S-O2-O1 = -53.8;
Superoxide	H1-S = 1.3583; S-O2 = 1.5703; O2-O1 = 1.4715; >H1-S-H2 = 91.1; >H1-S-O2 = 100.6; >S-O2-O1 = 101.3; >H1-S-O2-O1 = -46.6

**Table 3S.** Optimized geometrical parameters of the transition states calculated using the MP2(full)/6-31G(d). The labelled of the oxygen and hydrogen atoms are shown in Figure 3 of the paper. Bond lengths are given in Å and bond angles are given in degrees.

TS	Geometrical parameters
a	H1-S = 1.3443; H2-S1 = 1.6977; H2-O2 = 1.1196; O2-O1=1.2679; >H1-S-H2 = 93.3; >S-H2-O2 = 172.9; >H2-O2-O1 = 109.2; >H1-S-H2-O2 = -29.6; >S-H2-O2-O1 = 81.1
b	H1-S = 1.3442; H2-S = 1.7028; H2-O1 = 1.1161; O1-O2 = 1.2680; >H1-S-H2 = 96.0; >S-H2-O1 = 117.9; >H2-O1-O2 = 108.1; >H1-S-H2-O1 = -179.6; >S-H2-O1-O2 = -0.4
c	H1-S = H2-S = 1.3522; S-O2 = 1.7224; O2-O1 = 1.3623; >H1-S-H2 = 92.4; >H1-S-O2 = 95.8; >H2-S-O2 = 95.8; >S-O2-O1 = 107.4; >H1-S-O2-O1 = -46.5
d	H1-S = 1.3581; H2-S = 1.3889; H2-O1 = 1.9235; O1-O2 = 1.4723; O2-S = 2.5850; >H1-S-H2 = 90.1; >H1-S-O2 = 103.2; >S-H2-O1 = 87.4; >S-O2-O1 = 98.7; >H2-O1-O2 = 74.2; >H1-S-O2-O1 = -59.1; >H1-S-H2-O1 = 80.5; >S-O2-O1-H2 = -22.4; >S-H2-O1-O2 = 25.5
e	H1-S = 1.7836; H1-O1= 1.1637; H2-O1 = 0.9924; O1-O2 = 1.6036; O2-S = 1.6989, >H1-O1-H2 = 104.6; H1-O1-O2 = 83.3; >H1-S-O2 = 64.8; >H1-O1-O2-S = 3.9; >H2-O1-O2-S= -100.0
f	H1-S = 1.3649; H2-O1 = 0.9916; S-O1 = 2.3576; S-O2 = 1.5315; O1-O2 = 2.1455; >H1-S-O2 = 105.0; >S-O2-O1 = 77.8; >O2-O1-H2 = 140.6; >O2-O1-S = 39.4; >H1-S-O2-O1 = -86.5;
g	H1-S = 1.3403; H2-S = 1.3776; S-O2 =1.7501; O2-O1 = 1.3746; H1-S-H2 = 94.17; >H1-S-O2 = 91.3; >H2-S-O2 = 115.0; >S-O2-O1 = 94.2; >H1-S-O2-O1 = 60.7; >H2-S-O2-O1 = 155.9
h	H1-S =1.3540; H2-S =1.4755; O1-S =1.6045; O2-S =1.6504; O1-O2 = 1.8647; >H1-S-O2 = 100.0; >H2-S-O1 = 76.2; O1-S-O2 = 70.0; >H1-S-H2 = 88.7; >H1-S-O2-O1 = -106.9; H2-S-O1-O2 = 117.6
i	H1-S = 1.5148; O1-S = 1.5100; S-O2 = 2.1128; H1-O2 = 1.2884; O2-H2 = 0.9836; >O1-S-H1 = 114.8; >O1-S-O2 = 111.8; >S-H1-O2 = 97.5; >H1-O2-H2 = 108.8; O1-S-H1-O2 = 94.0; S-H1-O2-H2 = 87.0
J	H1-S = 1.3996; H1-O1 = 1.4389; O1-S = 1.6213; S-O2 = 1.6813; O2-H2 = 0.9787; >H1-S-O1 = 56.3; >H1-S-O2 = 98.7; >O1-S-O2 = 111.2; >S-O2-H2 = 107.2; H1-S-O2-H2 = 151.8; O1-S-O2-H2 = 94.6
k	H1-S = 1.3649; H2-S = 1.4419; O1-S = 1.4693; O2-S = 1.5691; H2-O2 = 1.4534; >H1-S-H2 = 109.0; >H1-S-O1 = 106.4; >H2-S-O2 = 57.5; >O1-S-O2 = 120.0; H1-S-O1-O2 = -118.0; H2-S-O2-O1 = -137.4
l	H1-S = 1.3769; H2-S = 1.8375; O1-S = O2-S = 1.4700; H1-H1 = 1.3462; >O1-S-O2 = 125.6; >O1-S-H1 = 115.7; >O2-S-H2 = 101.8; >S-H1-H2 = 84.9; O1-S-H1-H2 = 81.0
m	H1-O1 = 1.3912; H1-O2 = 1.1788; H2-O2 = 0.9843; O2-S = 1.9129; O1-S = 1.5966; >H1-O1-S = 79.3; >O1-S-O2 = 81.6; >S-O2-H2 = 107.5; >H1-O1-S-O2 =1.8; >O1-S-O2-H2 = 100.4