Supporting information for

Explanation of the Unusual Temperature Dependence of the Atmospheric Important OH + H_2S → H_2O + SH Reaction and Prediction of the Rate Constant at Combustion Temperatures

Benjamin A. Ellingson and Donald G. Truhlar*

Department of Chemistry and Supercomputing Institute, University of Minnesota, 207 Pleasant St SE, Minneapolis, Minnesota 55455-0431

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Table S-1: M06-2X Forward Rate Constants (in cm^3 $molecule^{-1}$ sec^{-1}) with the Torsional Mode Treated at the RPG Level

T (K)	TST	CVT	CVT/SCT
200	5.60E-12	3.83E-12	4.38E-12
250	5.23E-12	3.97E-12	4.20E-12
298	5.22E-12	4.16E-12	4.23E-12
300	5.23E-12	4.17E-12	4.23E-12
350	5.45E-12	4.52E-12	4.49E-12
400	5.81E-12	4.96E-12	4.87E-12
500	6.87E-12	6.08E-12	5.90E-12
600	8.30E-12	7.50E-12	7.25E-12
700	1.00E-11	9.22E-12	8.91E-12
800	1.21E-11	1.12E-11	1.09E-11
1000	1.72E-11	1.62E-11	1.57E-11
1500	3.55E-11	3.24E-11	2.61E-11
2400	8.94E-11	7.78E-11	6.66E-11

Table S-2: CVT/CAG transmission coefficients

T(K)	$\kappa^{CVT/CAG}$
200.00	9.79E-01
250.00	9.58E-01
298.00	9.46E-01
300.00	9.46E-01
350.00	9.44E-01
400.00	9.43E-01
500.00	9.46E-01
600.00	9.49E-01
700.00	9.53E-01
800.00	9.56E-01
1000.00	9.62E-01
1500.00	8.04E-01
2400.00	8.56E-01

Complete references 15 and 25

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Absolute energies in hartrees and Cartesian coordinates in angstroms of all optimized structures

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Description of structure: H_2S molecule
Level of theory/basis: M06-2X/MG3S
Energy in hartrees: -399.383966
Cartesian coordinates in Å:

S	-0.039621	0.000000	-0.037973
H	-0.038590	0.000000	1.298146
H	1.295529	0.000000	-0.093487

Description of structure: OH radical
Level of theory/basis: M06-2X/MG3S
Energy in hartrees: -75.7291168
Cartesian coordinates in Å:

O	0.000000	0.000000	0.057545
H	0.000000	0.000000	-0.913287

Description of structure: SH radical
Level of theory/basis: M06-2X/MG3S
Energy in hartrees: -398.735221
Cartesian coordinates in Å:

H	0.000000	0.000000	-1.298992
S	0.000000	0.000000	0.040947

Description of structure: H_2O molecule
Level of theory/basis: M06-2X/MG3S
Energy in hartrees: -76.4248381
Cartesian coordinates in Å:

O	-0.051414	0.000000	-0.039954
H	-0.059344	0.000000	0.918305
H	0.875324	0.000000	-0.284209

Description of structure: H_2S-OH transition state
Level of theory/basis: M06-2X/MG3S
Energy in hartrees: -475.113463
Cartesian coordinates in Å:

S	-0.064125	0.008119	-0.929881
H	1.246857	0.267088	-0.880538
H	-0.060791	-0.515904	0.362098
O	0.078254	-0.050734	1.778232
H	-0.393724	0.796421	1.796001

Description of structure: H_2S molecule
Level of theory/basis: MPW1K/MG3S
Energy in hartrees: -399.428082
Cartesian coordinates in Å:

S	-0.039389	0.000000	-0.037759
H	-0.041866	0.000000	1.294358
H	1.291423	0.000000	-0.096505

Description of structure: OH radical
Level of theory/basis: MPW1K/MG3S
Energy in hartrees: -75.737005
Cartesian coordinates in Å:

O	0.000000	0.000000	0.057020
H	0.000000	0.000000	-0.904955

Description of structure: SH radical
Level of theory/basis: MPW1K/MG3S
Energy in hartrees: -398.776724
Cartesian coordinates in Å:

H	0.000000	0.000000	-1.295404
S	0.000000	0.000000	0.040834

Description of structure: H_2O molecule
Level of theory/basis: MPW1K/MG3S
Energy in hartrees: -76.4307179
Cartesian coordinates in Å:

O	-0.050819	0.000000	-0.039499
H	-0.060557	0.000000	0.910201
H	0.867096	0.000000	-0.283329

Description of structure: H_2S-OH transition state
Level of theory/basis: MPW1K/MG3S
Energy in hartrees: -475.163924
Cartesian coordinates in Å:

S	-0.059712	0.010810	-0.924269
H	1.248432	0.263939	-0.901409
H	-0.050695	-0.484589	0.384178
O	0.068629	-0.057167	1.767823
H	-0.392640	0.785012	1.781959

Description of structure: H_2S molecule
Level of theory/basis: BB1K/MG3S
Energy in hartrees: -399.450172
Cartesian coordinates in Å:

S	-0.039451	0.000000	-0.037821
H	-0.038777	0.000000	1.293168
H	1.290327	0.000000	-0.093348

Description of structure: OH radical
Level of theory/basis: BB1K/MG3S
Energy in hartrees: -75.7295085
Cartesian coordinates in Å:

O	0.000000	0.000000	0.057123
H	0.000000	0.000000	-0.906583

Description of structure: SH radical
Level of theory/basis: BB1K/MG3S
Energy in hartrees: -398.800415
Cartesian coordinates in Å:

H	0.000000	0.000000	-1.294571
S	0.000000	0.000000	0.040808

Description of structure: H_2O molecule
Level of theory/basis: BB1K/MG3S
Energy in hartrees: -76.4224266
Cartesian coordinates in Å:

O	-0.050882	0.000000	-0.039548
H	-0.060424	0.000000	0.911070
H	0.867963	0.000000	-0.283409

Description of structure: H_2S-OH transition state
Level of theory/basis: BB1K/MG3S
Energy in hartrees: -475.179101
Cartesian coordinates in Å:

S	-0.067432	0.014324	-0.916955
H	1.244186	0.241755	-0.889704
H	-0.056659	-0.527895	0.369090
O	0.085380	-0.059045	1.754396
H	-0.403374	0.768805	1.766415

Description of structure: H_2S molecule
Level of theory/basis: MPWB1K/MG3S
Energy in hartrees: -399.450371
Cartesian coordinates in Å:

S	-0.039415	0.000000	-0.037786
H	-0.039219	0.000000	1.292463
H	1.289604	0.000000	-0.093760

Description of structure: OH radical
Level of theory/basis: MPWB1K/MG3S
Energy in hartrees: -75.7288346
Cartesian coordinates in Å:

O	0.000000	0.000000	0.057072
H	0.000000	0.000000	-0.905770

Description of structure: SH radical
Level of theory/basis: MPWB1K/MG3S
Energy in hartrees: -398.800621
Cartesian coordinates in Å:

H	0.000000	0.000000	-1.293782
S	0.000000	0.000000	0.040783

Description of structure: H_2O molecule
Level of theory/basis: MPWB1K/MG3S
Energy in hartrees: -76.4215091
Cartesian coordinates in Å:

O	-0.050814	0.000000	-0.039495
H	-0.060726	0.000000	0.910342
H	0.867184	0.000000	-0.283521

Description of structure: H_2S-OH transition state
Level of theory/basis: MPWB1K/MG3S
Energy in hartrees: -475.178019
Cartesian coordinates in Å:

S	-0.064488	0.014029	-0.917756
H	1.244628	0.251557	-0.891291
H	-0.052148	-0.512043	0.377195
O	0.078659	-0.060477	1.755693
H	-0.395045	0.775239	1.764710

Description of structure: H_2S molecule
Level of theory/basis: MC-QCISD/3
Energy in hartrees: -398.9556552
Cartesian coordinates in Å:

S	-0.038680	-0.039756	0.000000
H	1.302533	-0.039756	0.000000
H	-0.075460	1.300971	0.000000

Description of structure: OH radical
Level of theory/basis: MC-QCISD/3
Energy in hartrees: -75.66464382
Cartesian coordinates in Å:

O	0.000000	0.000000	-0.057701
H	0.000000	0.000000	0.915763

Description of structure: SH radical
Level of theory/basis: MC-QCISD/3
Energy in hartrees: -398.3011599
Cartesian coordinates in Å:

H	0.000000	0.000000	0.041134
S	0.000000	0.000000	-1.304936

Description of structure: H_2O molecule
Level of theory/basis: MC-QCISD/3
Energy in hartrees: -76.36842014
Cartesian coordinates in Å:

O	-0.890140	-0.242064	0.000000
H	0.050769	-0.042627	0.000000
H	0.084394	0.918592	0.000000

Description of structure: H_2S-OH transition state
Level of theory/basis: MC-QCISD/3
Energy in hartrees: -474.6189966
Cartesian coordinates in Å:

S	-0.859731	-0.138550	-0.318710
H	0.543580	-0.138550	-0.318710
H	-0.891964	1.202902	-0.318710
O	1.655950	0.219697	0.587217
H	1.341213	-0.155766	1.428574

Description of structure: H_2S molecule
Level of theory/basis: MCG3/3//MC-QCISD/3
Energy in hartrees: -401.6246401
Cartesian coordinates in Å:

S	-0.038680	-0.039756	0.000000
H	1.302533	-0.039756	0.000000
H	-0.075460	1.300971	0.000000

Description of structure: OH radical
Level of theory/basis: MCG3/3//MC-QCISD/3
Energy in hartrees: -76.16286137
Cartesian coordinates in Å:

O	0.000000	0.000000	-0.057701
H	0.000000	0.000000	0.915763

Description of structure: SH radical
Level of theory/basis: MCG3/3//MC-QCISD/3
Energy in hartrees: -400.9676100
Cartesian coordinates in Å:

H	0.000000	0.000000	0.041134
S	0.000000	0.000000	-1.304936

Description of structure: H_2O molecule
Level of theory/basis: MCG3/3//MC-QCISD/3
Energy in hartrees: -76.8683636
Cartesian coordinates in Å:

O	-0.890140	-0.242064	0.000000
H	0.050769	-0.042627	0.000000
H	0.084394	0.918592	0.000000

Description of structure: H_2S-OH transition state
Level of theory/basis: MCG3/3//MC-QCISD/3
Energy in hartrees: -477.7868487
Cartesian coordinates in Å:

S	-0.859731	-0.138550	-0.318710
H	0.543580	-0.138550	-0.318710
H	-0.891964	1.202902	-0.318710
O	1.655950	0.219697	0.587217
H	1.341213	-0.155766	1.428574

Description of structure: H_2S-OH van der Waals complex
Level of theory/basis: M06-2X/MG3S
Energy in hartrees: -475.1207749
Cartesian coordinates in Å:

S	-0.008176	-0.063297	-0.007049
H	-0.006628	0.014736	1.326708
H	1.323016	0.022230	-0.072097
O	0.711485	2.500721	0.673819
H	0.036310	2.769957	0.033289

Description of structure: H_2S-HO van der Waals complex
Level of theory/basis: M06-2X/MG3S
Energy in hartrees: -475.1186610
Cartesian coordinates in Å:

S	0.000000	0.000000	0.000000
H	0.000000	0.000000	1.337486
H	1.336093	0.000000	-0.062030
O	-0.298963	3.429569	-0.284658
H	-0.243820	2.456654	-0.232721