

Electronic Supplementary Information (ESI)

Gas-phase and water-mediated mechanisms for the OCS + OH reaction

Joel Leitão Nascimento, and Tiago Vinicius Alves*

*Departamento de Físico-Química, Instituto de Química, Universidade Federal da Bahia,
Rua Barão de Jeremoabo, 147, Salvador, Bahia, 40170-115, Brazil*

*E-mail address: tiagova@ufba.br

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S.1. Gas-phase mechanism

S.1.1 Low- (LL) and high-level (HL) electronic energies, cartesian coordinates and non-scaled harmonic vibrational frequencies

LL = M06-2X/aug-cc-pVTZ

HL = CCSD(T)/aug-cc-pVTZ

COS

LL = -511.542710639 HL = -510.92974915

6	0.000000000	0.000000000	-0.528126000
8	0.000000000	0.000000000	-1.676733000
16	0.000000000	0.000000000	1.036414000

Frequencies -- 535.4970 535.4970 885.5288

Frequencies -- 2157.1138

OH

LL = -75.7338089766 HL = -75.64558487

8	0.000000000	0.000000000	-0.110321000
1	0.000000000	0.000000000	0.861756000

Frequencies -- 3764.3649

PRC

LL = -587.281124853 HL = -586.57791056

6	0.753441000	0.384736000	0.006957000
8	1.064742000	1.486772000	0.017229000
16	0.352917000	-1.133921000	-0.008903000
8	-2.038761000	0.504566000	-0.080306000
1	-2.375167000	-0.096384000	0.605318000

Frequencies --	62.2894	104.1798	134.7177
Frequencies --	362.6218	533.3290	536.9645
Frequencies --	875.7245	2170.0900	3769.0975

TS1

LL = -587.270941995 HL = -586.56970801

6	0.510114000	0.399936000	-0.003962000
8	1.623556000	0.665520000	-0.012416000
16	-1.097927000	0.425498000	0.001634000
8	0.194431000	-1.583938000	0.110772000
1	-0.037753000	-1.860233000	-0.789218000

Frequencies --	-429.0270	236.3487	350.9136
Frequencies --	443.9066	554.0574	759.4635
Frequencies --	815.5516	2139.6775	3788.6246

I1

LL = -587.327338696 HL = -586.62145862

6	-0.436999000	0.122444000	0.000018000
8	-0.974611000	1.190250000	-0.000003000
16	1.309559000	-0.056799000	-0.000003000
8	-1.064590000	-1.058311000	0.000005000
1	-2.017346000	-0.881389000	-0.000065000

Frequencies --	313.4671	478.6970	500.2445
Frequencies --	693.1089	739.9615	1156.5500
Frequencies --	1341.6097	1812.6639	3774.6767

TS2

LL = -587.312794795 HL = -586.60715708

6	0.450825000	0.151574000	-0.009268000
8	0.989452000	1.208489000	0.017067000

16	-1.292885000	-0.049321000	0.003362000
8	1.102594000	-1.044485000	-0.111790000
1	1.244845000	-1.432351000	0.759608000

Frequencies --	-483.9288	293.7312	481.0081
Frequencies --	614.4725	773.0255	1103.1479
Frequencies --	1168.0984	1851.4268	3841.7384

I2

LL = -587.321341856 HL = -585.53449146

6	0.000000000	0.486312000	0.000000000
8	-0.915158000	1.246541000	0.000000000
16	-0.298344000	-1.258067000	0.000000000
8	1.276409000	0.887584000	0.000000000
1	1.883500000	0.138211000	0.000000000

Frequencies --	308.0753	391.3234	471.2157
Frequencies --	658.0811	750.9707	1147.5627
Frequencies --	1295.3536	1841.1761	3832.1983

TS3

LL = -587.259810300 HL = -586.55603805

6	-0.834012000	-0.011535000	0.000172000
8	-1.510438000	-0.949321000	-0.000103000
16	1.413653000	-0.207183000	0.000027000
8	-0.752393000	1.229510000	0.000070000
1	0.488273000	1.142627000	-0.001201000

Frequencies --	-1673.9647	249.8989	463.6682
Frequencies --	570.8740	688.1609	740.0547
Frequencies --	1281.6800	1621.0210	2177.3570

HS

LL = -398.738845133 HL = -398.29133188

16	0.000000000	0.000000000	0.078952000
1	0.000000000	0.000000000	-1.263234000

Frequencies -- 2747.4754

C02

LL = -188.594208121 HL = -188.34004637

6	0.000000000	0.000000000	-0.000001000
8	0.000000000	0.000000000	-1.155241000
8	0.000000000	0.000000000	1.155241000

Frequencies -- 694.2549 694.2549 1411.4670

Frequencies -- 2445.0400

TS4

LL = -587.274486216 HL = -586.57207377

6	-1.034543000	-0.005385000	0.000567000
8	-2.030814000	0.567588000	-0.007423000
16	0.360476000	-0.734706000	0.010173000
8	1.852873000	0.773963000	-0.113968000
1	1.809738000	0.953084000	-1.065389000

Frequencies -- -221.8238 87.8830 201.8496

Frequencies -- 479.4715 533.6411 814.3160

Frequencies -- 859.2223 2135.0380 3791.9915

I3

LL = -587.278795227 HL = -586.57307902

6	0.122865000	-0.924610000	1.601201000
8	0.172713000	-0.501980000	2.690033000

16	0.549550000	-0.615823000	0.007463000
8	1.422889000	0.815282000	-0.121938000
1	0.805529000	1.555764000	-0.152902000

Frequencies --	82.3385	309.1011	425.0001
Frequencies --	456.5251	626.3383	711.0247
Frequencies --	1125.1925	1951.8078	3828.1038

TS5

LL = -587.271916623 HL = -586.56581538

6	-1.339643000	-0.517360000	0.056555000
8	-1.856316000	0.493757000	-0.051154000
16	0.772082000	-0.628735000	-0.013273000
8	1.185977000	0.954596000	-0.110032000
1	1.194200000	1.228472000	-1.034087000

Frequencies --	-306.1930	127.2491	172.8561
Frequencies --	378.0355	445.3964	850.5242
Frequencies --	1183.3909	2063.5985	3827.5412

H0S

LL = -473.961868133 HL = -473.41883024

16	0.036398000	-0.599473000	0.000000000
8	0.036398000	1.030276000	0.000000000
1	-0.873559000	1.349359000	0.000000000

Frequencies --	895.5899	1184.2235	3817.2191
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C0

LL = -113.320239086 HL = -113.16172486

6	0.000000000	0.000000000	-0.640789000
8	0.000000000	0.000000000	0.480592000

Frequencies -- 2269.5264

S.1.2 CVT-ISPE/SCT thermal rate constants

cos + oh --> i1

250.00	9.215E-17
260.00	1.349E-16
270.00	1.925E-16
280.00	2.683E-16
290.00	3.663E-16
300.00	4.905E-16
310.00	6.457E-16
320.00	8.368E-16
330.00	1.069E-15
340.00	1.348E-15
350.00	1.680E-15
360.00	2.070E-15
370.00	2.525E-15
380.00	3.052E-15
390.00	3.656E-15
400.00	4.345E-15
410.00	5.125E-15
420.00	6.004E-15
430.00	6.987E-15
440.00	8.081E-15
450.00	9.295E-15
460.00	1.063E-14
470.00	1.211E-14
480.00	1.372E-14
490.00	1.547E-14
500.00	1.739E-14
510.00	1.945E-14
520.00	2.169E-14
530.00	2.410E-14

540.00	2.668E-14
550.00	2.945E-14
i1 --> cos + oh	
250.00	8.484E-14
260.00	9.010E-13
270.00	8.057E-12
280.00	6.177E-11
290.00	4.125E-10
300.00	2.432E-09
310.00	1.282E-08
320.00	6.097E-08
330.00	2.643E-07
340.00	1.053E-06
350.00	3.880E-06
360.00	1.331E-05
370.00	4.279E-05
380.00	1.294E-04
390.00	3.703E-04
400.00	1.006E-03
410.00	2.605E-03
420.00	6.452E-03
430.00	1.533E-02
440.00	3.503E-02
450.00	7.723E-02
460.00	1.646E-01
470.00	3.398E-01
480.00	6.810E-01
490.00	1.327E+00
500.00	2.519E+00
510.00	4.665E+00
520.00	8.440E+00
530.00	1.494E+01
540.00	2.589E+01
550.00	4.399E+01

i1 --> i2

250.00	1.991E+06
260.00	3.636E+06
270.00	6.370E+06
280.00	1.075E+07
290.00	1.753E+07
300.00	2.772E+07
310.00	4.263E+07
320.00	6.390E+07
330.00	9.360E+07
340.00	1.342E+08
350.00	1.887E+08
360.00	2.605E+08
370.00	3.538E+08
380.00	4.732E+08
390.00	6.239E+08
400.00	8.117E+08
410.00	1.043E+09
420.00	1.326E+09
430.00	1.667E+09
440.00	2.074E+09
450.00	2.558E+09
460.00	3.127E+09
470.00	3.791E+09
480.00	4.561E+09
490.00	5.448E+09
500.00	6.462E+09
510.00	7.616E+09
520.00	8.922E+09
530.00	1.039E+10
540.00	1.204E+10
550.00	1.387E+10

i2 --> i1

250.00	1.251E+09
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260.00	1.769E+09
270.00	2.445E+09
280.00	3.310E+09
290.00	4.396E+09
300.00	5.738E+09
310.00	7.372E+09
320.00	9.337E+09
330.00	1.167E+10
340.00	1.441E+10
350.00	1.760E+10
360.00	2.127E+10
370.00	2.546E+10
380.00	3.021E+10
390.00	3.556E+10
400.00	4.153E+10
410.00	4.817E+10
420.00	5.549E+10
430.00	6.354E+10
440.00	7.233E+10
450.00	8.190E+10
460.00	9.226E+10
470.00	1.034E+11
480.00	1.154E+11
490.00	1.283E+11
500.00	1.420E+11
510.00	1.566E+11
520.00	1.721E+11
530.00	1.885E+11
540.00	2.057E+11
550.00	2.239E+11

i2 --> hs + co2

250.00	3.803E-13
260.00	2.049E-12
270.00	1.017E-11

280.00	4.675E-11
290.00	1.999E-10
300.00	8.002E-10
310.00	3.012E-09
320.00	1.071E-08
330.00	3.611E-08
340.00	1.158E-07
350.00	3.547E-07
360.00	1.039E-06
370.00	2.917E-06
380.00	7.870E-06
390.00	2.043E-05
400.00	5.116E-05
410.00	1.237E-04
420.00	2.892E-04
430.00	6.550E-04
440.00	1.439E-03
450.00	3.071E-03
460.00	6.376E-03
470.00	1.289E-02
480.00	2.542E-02
490.00	4.892E-02
500.00	9.204E-02
510.00	1.694E-01
520.00	3.054E-01
530.00	5.397E-01
540.00	9.358E-01
550.00	1.594E+00

cos + oh --> i3

250.00	1.630E-15
260.00	2.229E-15
270.00	2.985E-15
280.00	3.921E-15
290.00	5.064E-15
300.00	6.439E-15

310.00	8.074E-15
320.00	9.996E-15
330.00	1.223E-14
340.00	1.481E-14
350.00	1.776E-14
360.00	2.111E-14
370.00	2.489E-14
380.00	2.912E-14
390.00	3.383E-14
400.00	3.905E-14
410.00	4.480E-14
420.00	5.111E-14
430.00	5.800E-14
440.00	6.550E-14
450.00	7.364E-14
460.00	8.242E-14
470.00	9.188E-14
480.00	1.020E-13
490.00	1.129E-13
500.00	1.245E-13
510.00	1.369E-13
520.00	1.501E-13
530.00	1.640E-13
540.00	1.788E-13
550.00	1.944E-13

i3 --> cos + oh

250.00	2.418E+12
260.00	2.537E+12
270.00	2.654E+12
280.00	2.770E+12
290.00	2.885E+12
300.00	2.998E+12
310.00	3.110E+12
320.00	3.221E+12

330.00	3.330E+12
340.00	3.437E+12
350.00	3.543E+12
360.00	3.647E+12
370.00	3.750E+12
380.00	3.851E+12
390.00	3.950E+12
400.00	4.048E+12
410.00	4.144E+12
420.00	4.238E+12
430.00	4.331E+12
440.00	4.423E+12
450.00	4.512E+12
460.00	4.601E+12
470.00	4.687E+12
480.00	4.773E+12
490.00	4.856E+12
500.00	4.939E+12
510.00	5.020E+12
520.00	5.099E+12
530.00	5.177E+12
540.00	5.254E+12
550.00	5.330E+12

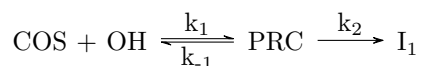
i3 --> hos + co

250.00	2.531E+09
260.00	3.507E+09
270.00	4.748E+09
280.00	6.298E+09
290.00	8.200E+09
300.00	1.050E+10
310.00	1.324E+10
320.00	1.646E+10
330.00	2.021E+10
340.00	2.452E+10

350.00	2.943E+10
360.00	3.497E+10
370.00	4.119E+10
380.00	4.810E+10
390.00	5.572E+10
400.00	6.409E+10
410.00	7.323E+10
420.00	8.313E+10
430.00	9.382E+10
440.00	1.053E+11
450.00	1.176E+11
460.00	1.307E+11
470.00	1.446E+11
480.00	1.594E+11
490.00	1.749E+11
500.00	1.912E+11
510.00	2.083E+11
520.00	2.262E+11
530.00	2.449E+11
540.00	2.643E+11
550.00	2.845E+11

S.1.3 Pre-equilibrium model (PEM)

The interaction between COS and OH forms a pre-reactive complex (PC_{OH}) thermodynamically more stable than the isolated reactants. After that, it produces the intermediate 1 (I1), passing by the TS1, i.e.,



Applying the pre-equilibrium model, the overall effective rate constant for the reaction pathway can be calculated as the product of the equilibrium constant for PRC formation and the subsequent unimolecular rate constant, i.e.,:

$$k_{\text{PEM}} = K_{\text{eq}} k_{\text{uni}}^{\text{CVT-ISPE/SCT}} \quad (1)$$

S.2. Water-mediated mechanism

S.2.1 Low- (LL) and high-level (HL) electronic energies, cartesian coordinates and non-scaled harmonic vibrational frequencies

H2O

LL = -76.4301040421 HL = -76.34228852

8	0.000000000	0.116357000	0.000000000
1	0.762603000	-0.465429000	0.000000000
1	-0.762603000	-0.465429000	0.000000000

Frequencies -- 1617.8382 3868.7250 3972.0575

OH-H2O

LL = -152.173547669 HL = -151.99724315

8	1.256589000	-0.000068000	-0.063815000
1	1.756940000	-0.767126000	0.223409000
1	1.754331000	0.768961000	0.222674000
1	-0.638136000	-0.002687000	-0.038385000
8	-1.615731000	0.000174000	0.012853000

Frequencies -- 112.3515 151.2774 196.1759

Frequencies -- 398.3763 608.1718 1615.8283

Frequencies -- 3637.2115 3862.4027 3964.5616

CPOH

LL = -587.281124853 HL = -586.57791056

6	0.753441000	0.384736000	0.006957000
8	1.064742000	1.486772000	0.017229000
16	0.352917000	-1.133921000	-0.008903000
8	-2.038761000	0.504566000	-0.080306000
1	-2.375167000	-0.096384000	0.605318000

Frequencies --	62.2894	104.1798	134.7177
Frequencies --	362.6218	533.3290	536.9645
Frequencies --	875.7245	2170.0900	3769.0975

CPW1

LL = -587.976195221 HL = -587.27534972

6	-0.010078000	-0.221710000	-0.486000000
8	-0.012906000	0.127509000	-1.582575000
16	-0.006989000	-0.722178000	0.992948000
8	0.062687000	2.676802000	-0.263182000
1	0.050374000	2.621959000	-1.221699000
1	0.084286000	3.612731000	-0.054525000

Frequencies --	55.9300	57.5862	125.8783
Frequencies --	155.3212	179.0444	537.8100
Frequencies --	541.5696	893.6569	1610.9697
Frequencies --	2148.1573	3861.3607	3966.7219

PRC1W1

LL = -663.714750308 HL = -662.92366692

6	0.026313000	0.311669000	-0.108703000
8	0.424745000	1.387020000	-0.139788000
16	-0.520897000	-1.157013000	-0.071956000
8	-2.766297000	0.650316000	0.079667000
1	-3.002253000	0.106548000	0.849460000
8	2.896339000	-0.046671000	0.152745000
1	2.899909000	0.908269000	0.052217000
1	3.817069000	-0.315085000	0.137877000

Frequencies --	5.9243	48.4109	64.8927
Frequencies --	70.2469	109.0741	134.8031
Frequencies --	136.0381	168.9628	186.9321

Frequencies --	375.8185	530.5559	540.6104
Frequencies --	880.9167	1613.5844	2159.7932
Frequencies --	3770.7742	3860.5893	3965.7991

PRC1W2

LL = -663.722553413 HL = -662.93115367

6	0.919356000	0.636202000	-0.188812000
8	0.475686000	1.689016000	-0.338806000
16	1.519354000	-0.787891000	0.024601000
8	-1.137941000	-1.089894000	-1.347453000
1	-1.511397000	-0.664951000	-0.547866000
8	-1.912024000	0.537648000	0.876915000
1	-2.695671000	0.588217000	1.428283000
1	-1.695671000	1.438682000	0.620110000

Frequencies --	44.1420	59.0704	96.1554
Frequencies --	123.6457	140.3139	197.9109
Frequencies --	212.8296	246.4706	503.0794
Frequencies --	532.5101	542.6088	633.7770
Frequencies --	895.9357	1607.5011	2137.6504
Frequencies --	3628.8154	3849.1197	3955.6240

PRC1W3

LL = -663.721682910 HL = -662.93004107

6	0.851329000	-0.223128000	-0.189690000
8	1.026222000	-0.505709000	0.906170000
16	0.630833000	0.149366000	-1.700020000
8	-0.828909000	2.116265000	0.040046000
1	-1.448855000	1.361516000	0.103737000
8	-2.233576000	-0.389976000	-0.067114000
1	-3.072820000	-0.739088000	0.241555000
1	-2.121796000	-0.702099000	-0.969188000

Frequencies --	37.5523	66.7195	92.5128
Frequencies --	98.8965	125.2020	173.4623
Frequencies --	193.9449	222.8645	500.5116
Frequencies --	535.8217	546.3678	589.4631
Frequencies --	875.3619	1605.8148	2171.0602
Frequencies --	3642.3636	3849.7284	3954.4506

TS1W1

LL = -663.705237886 HL = -662.91601054

6	0.490743000	-0.398491000	0.082894000
8	1.606460000	-0.663320000	0.099563000
16	-1.111207000	-0.390912000	0.090351000
8	0.197702000	1.595485000	-0.180048000
1	-0.030918000	1.935612000	0.698191000
8	0.533041000	-3.326263000	0.403007000
1	0.483257000	-4.283731000	0.373263000
1	1.463054000	-3.108471000	0.303091000

Frequencies --	-413.8974	18.9107	72.6728
Frequencies --	91.8793	120.8431	195.0208
Frequencies --	220.9501	243.2896	347.5998
Frequencies --	443.5727	553.8203	756.4366
Frequencies --	822.5441	1616.7685	2127.9842
Frequencies --	3793.6332	3860.2281	3964.8349

TS1W2

LL = -663.710710470 HL = -662.92123206

6	-0.815809000	0.781459000	0.375460000
8	-0.444423000	1.695991000	0.965598000
16	-1.604849000	-0.232852000	-0.577244000
8	0.357114000	-0.839667000	0.689729000
1	0.989315000	-0.650683000	-0.028113000
8	1.886528000	0.945306000	-0.901674000

1	2.505644000	1.254668000	-1.565946000
1	1.883787000	1.607351000	-0.204501000

Frequencies --	-476.4973	53.4279	73.5098
Frequencies --	99.0623	164.3573	197.3624
Frequencies --	208.4603	239.2548	449.8387
Frequencies --	523.6050	611.6243	825.9177
Frequencies --	863.4242	1613.4591	2108.0370
Frequencies --	3704.5641	3850.9997	3957.8867

TS1W3

LL = -663.710660363 HL = -662.92171957

6	0.867510000	-0.365732000	-0.281139000
8	1.222898000	-1.380058000	-0.678295000
16	0.597383000	1.203632000	-0.056040000
8	-0.220450000	-0.560412000	1.405365000
1	-1.123628000	-0.489406000	1.037140000
8	-2.550986000	-0.120026000	-0.195410000
1	-2.368860000	0.727542000	-0.609573000
1	-3.504704000	-0.179125000	-0.105518000

Frequencies --	-492.0601	23.8923	64.4935
Frequencies --	99.1699	158.3101	182.8872
Frequencies --	232.2604	247.9007	447.6753
Frequencies --	528.2661	628.9928	814.2016
Frequencies --	916.7226	1607.3209	2130.9674
Frequencies --	3639.4277	3853.8100	3957.6612

TS1W4

LL = -663.710742875 HL = -662.92177452

6	0.941793000	0.040150000	0.176640000
8	2.006568000	0.378624000	-0.082101000
16	-0.345916000	-0.791368000	0.658399000

8	-0.419346000	1.457195000	-0.272999000
1	-0.561926000	1.851860000	0.610823000
8	-0.531927000	2.161900000	2.510458000
1	-0.488103000	1.312398000	2.957251000
1	0.083215000	2.738535000	2.969394000

Frequencies --	-496.5579	30.5123	59.1395
Frequencies --	112.4365	171.6411	184.6258
Frequencies --	229.5191	247.8973	448.0825
Frequencies --	533.1126	650.3257	816.4251
Frequencies --	905.4709	1612.3420	2124.3269
Frequencies --	3631.7604	3853.1358	3955.5178

I1W1

LL = -663.768242405 HL = -662.97228643

6	-0.324484000	0.557060000	-0.057459000
8	0.454815000	1.474521000	-0.063692000
16	0.097526000	-1.135343000	0.125630000
8	-1.646211000	0.710565000	-0.191697000
1	-1.819499000	1.659258000	-0.283072000
8	2.714987000	-0.145477000	0.331226000
1	3.215572000	-0.289297000	-0.475084000
1	2.229875000	0.680798000	0.196135000

Frequencies --	64.6326	114.2780	172.3225
Frequencies --	219.1903	282.9758	353.3723
Frequencies --	497.8857	504.0318	580.6329
Frequencies --	705.1312	750.3333	1160.9692
Frequencies --	1346.6724	1623.8159	1776.8061
Frequencies --	3751.1598	3777.9347	3924.5531

I1W2

LL = -663.775968115 HL = -662.98150763

6	0.819479000	-0.632414000	0.535986000
8	1.844101000	-0.953326000	1.086671000
16	0.666929000	0.932455000	-0.250253000
8	-0.275208000	-1.361806000	0.443525000
1	-0.111633000	-2.222460000	0.906054000
8	0.729611000	-3.396196000	1.857039000
1	1.528290000	-2.848218000	1.851218000
1	0.990249000	-4.283110000	1.600138000

Frequencies --	67.0280	149.1644	194.4617
Frequencies --	224.8518	324.7023	351.5074
Frequencies --	495.4661	567.3123	677.3746
Frequencies --	788.0228	862.4342	1247.3483
Frequencies --	1448.7453	1608.1016	1767.4556
Frequencies --	3316.7612	3752.6330	3931.4594

I1W3

LL = -663.768124364 HL = -662.97354597

6	1.002240000	-0.640799000	-0.075825000
8	2.129869000	-0.924604000	0.189878000
16	0.700009000	0.410344000	-1.483259000
8	-0.051568000	-1.055470000	0.607547000
1	-0.886196000	-0.713116000	0.229368000
8	-2.316316000	-0.024295000	-0.561799000
1	-2.486853000	0.920799000	-0.530318000
1	-2.579818000	-0.321589000	-1.436720000

Frequencies --	61.1542	82.1336	97.8881
Frequencies --	172.2442	208.5570	276.4306
Frequencies --	326.0465	476.1004	666.3264
Frequencies --	761.7915	815.3266	1207.5408
Frequencies --	1381.4620	1617.4265	1834.8275
Frequencies --	3535.4911	3849.8795	3949.3904

TS4W1

LL = -663.708889110 HL = -662.91841356

6	0.940440000	0.166111000	0.293729000
8	1.892210000	0.811322000	0.293797000
16	-0.407193000	-0.644936000	0.277363000
8	-1.942254000	0.734578000	-0.264741000
1	-2.055883000	1.170942000	0.592543000
8	2.843138000	-1.941064000	0.071297000
1	3.600272000	-1.356954000	-0.014379000
1	3.159699000	-2.814662000	-0.167454000

Frequencies --	-196.4248	10.6652	47.4553
Frequencies --	89.1147	94.6215	113.3222
Frequencies --	147.0211	164.6103	203.7155
Frequencies --	482.4340	537.8643	808.8276
Frequencies --	864.1723	1614.4882	2134.2924
Frequencies --	3796.7687	3861.1773	3965.6060

TS4W2

LL = -663.713850047 HL = -662.92322062

6	-0.012994000	-0.724754000	1.563018000
8	0.452047000	-0.536584000	2.604117000
16	-0.686403000	-0.879266000	0.157708000
8	-1.583506000	0.972906000	-0.336049000
1	-1.886921000	1.202207000	0.560791000
8	-2.058211000	1.195717000	2.576191000
1	-1.322512000	1.244752000	3.192380000
1	-2.841498000	1.437723000	3.074967000

Frequencies --	-275.8463	33.8502	55.4040
Frequencies --	92.3341	114.9692	151.6241
Frequencies --	171.3427	188.1492	471.7089
Frequencies --	503.6779	530.8544	873.2487

Frequencies --	942.4560	1616.5750	2108.2484
Frequencies --	3708.5206	3854.5601	3957.2740

I3W1

LL = -663.712725945 HL = -662.91980258

6	-0.094908000	-0.409582000	-0.367221000
8	0.718591000	0.419145000	-0.202065000
16	-1.752646000	-0.675736000	-0.343170000
8	-2.567964000	0.746898000	-0.002987000
1	-2.590526000	0.876491000	0.952770000
8	3.566483000	-0.636154000	0.091552000
1	2.750202000	-0.143548000	-0.034069000
1	4.259752000	-0.074966000	-0.259998000

Frequencies --	10.4517	14.6824	48.7869
Frequencies --	75.7371	140.1747	202.2277
Frequencies --	309.8038	321.0054	447.2847
Frequencies --	457.2587	627.7643	729.3166
Frequencies --	1132.8459	1624.6461	1935.4764
Frequencies --	3825.5523	3847.6293	3955.2984

I3W2

LL = -663.725412289 HL = -662.93109408

6	0.425869000	1.266473000	-0.022212000
8	-0.593937000	1.595424000	-0.516857000
16	1.231091000	-0.201222000	0.265692000
8	0.380878000	-1.407570000	-0.465494000
1	-0.527483000	-1.407543000	-0.095389000
8	-2.069757000	-0.693910000	0.448964000
1	-2.055100000	0.182867000	0.044754000
1	-2.948273000	-1.052520000	0.307315000

Frequencies --	82.1635	126.1259	161.0184
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Frequencies --	186.1335	229.6038	321.4880
Frequencies --	387.8712	415.8439	537.1769
Frequencies --	596.7005	711.6484	802.0769
Frequencies --	1317.8748	1612.1447	1882.8054
Frequencies --	3499.3301	3797.9927	3937.6142

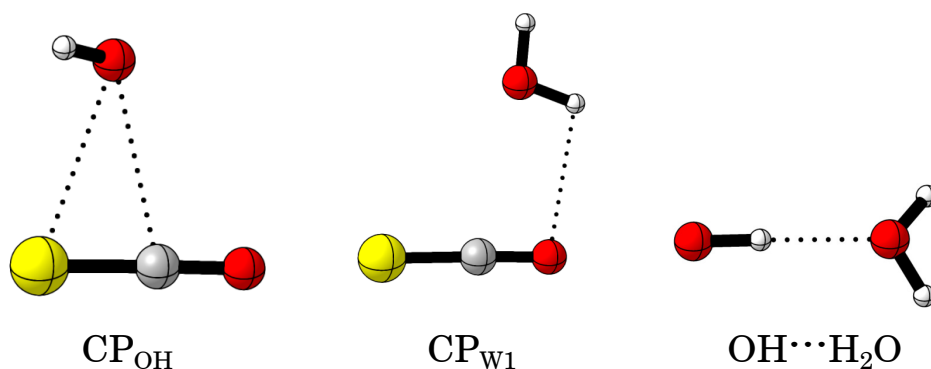


Fig. S.1.: Complexes from the long-range interactions between OH radicals, OCS and water monomer.

S.2.2 Two- and three-body equilibrium constants, unimolecular, and bimolecular rate constants

3B Equilibrium Constants

	K(3B)_1		K(3B)_2		K(3B)_3
250	5.24E-47		3.26E-44		1.84E-44
250	5.24E-47		3.26E-44		1.84E-44
260	4.68E-47		2.17E-44		1.29E-44
270	4.23E-47		1.50E-44		9.29E-45
280	3.88E-47		1.06E-44		6.90E-45
290	3.59E-47		7.79E-45		5.25E-45
300	3.35E-47		5.84E-45		4.09E-45
310	3.15E-47		4.48E-45		3.25E-45
320	2.99E-47		3.51E-45		2.63E-45
330	2.86E-47		2.80E-45		2.17E-45
340	2.74E-47		2.27E-45		1.81E-45
350	2.65E-47		1.87E-45		1.53E-45

360	2.57E-47		1.56E-45		1.32E-45
370	2.50E-47		1.32E-45		1.14E-45
380	2.45E-47		1.13E-45		1.00E-45
390	2.41E-47		9.80E-46		8.87E-46
400	2.37E-47		8.56E-46		7.92E-46
410	2.34E-47		7.56E-46		7.14E-46
420	2.32E-47		6.72E-46		6.48E-46
430	2.31E-47		6.03E-46		5.92E-46
440	2.30E-47		5.44E-46		5.44E-46
450	2.29E-47		4.95E-46		5.03E-46
460	2.29E-47		4.53E-46		4.68E-46
470	2.30E-47		4.17E-46		4.38E-46
480	2.30E-47		3.86E-46		4.11E-46
490	2.31E-47		3.59E-46		3.88E-46
500	2.33E-47		3.35E-46		3.68E-46
510	2.35E-47		3.15E-46		3.50E-46
520	2.37E-47		2.96E-46		3.34E-46
530	2.39E-47		2.80E-46		3.20E-46
540	2.41E-47		2.66E-46		3.08E-46
550	2.44E-47		2.54E-46		2.97E-46

Unimolecular Rate Constants (CVT-ISPE/SCT)

	k_uni_1		k_uni_2		k_uni_3		k_uni_4
250	2.67E+07		5.71E+06		3.56E+07		3.46E+07
250	2.67E+07		5.71E+06		3.56E+07		3.46E+07
260	4.08E+07		8.61E+06		5.07E+07		4.94E+07
270	6.05E+07		1.28E+07		7.11E+07		6.93E+07
280	8.73E+07		1.86E+07		9.80E+07		9.56E+07
290	1.23E+08		2.65E+07		1.33E+08		1.30E+08
300	1.70E+08		3.72E+07		1.77E+08		1.73E+08
310	2.29E+08		5.11E+07		2.32E+08		2.27E+08
320	3.04E+08		6.92E+07		3.00E+08		2.93E+08
330	3.96E+08		9.21E+07		3.83E+08		3.74E+08
340	5.09E+08		1.21E+08		4.82E+08		4.70E+08
350	6.45E+08		1.56E+08		5.99E+08		5.84E+08

360	8.08E+08		1.99E+08		7.35E+08		7.18E+08
370	9.99E+08		2.50E+08		8.94E+08		8.73E+08
380	1.22E+09		3.12E+08		1.08E+09		1.05E+09
390	1.48E+09		3.84E+08		1.28E+09		1.25E+09
400	1.78E+09		4.67E+08		1.52E+09		1.48E+09
410	2.12E+09		5.65E+08		1.78E+09		1.74E+09
420	2.50E+09		6.76E+08		2.07E+09		2.02E+09
430	2.94E+09		8.02E+08		2.39E+09		2.34E+09
440	3.42E+09		9.45E+08		2.75E+09		2.69E+09
450	3.96E+09		1.11E+09		3.13E+09		3.07E+09
460	4.55E+09		1.29E+09		3.56E+09		3.49E+09
470	5.20E+09		1.48E+09		4.01E+09		3.94E+09
480	5.92E+09		1.70E+09		4.51E+09		4.42E+09
490	6.70E+09		1.94E+09		5.04E+09		4.95E+09
500	7.55E+09		2.21E+09		5.60E+09		5.51E+09
510	8.47E+09		2.49E+09		6.21E+09		5.65E+09
520	9.46E+09		2.81E+09		6.85E+09		6.21E+09
530	1.05E+10		3.14E+09		7.53E+09		6.81E+09
540	1.17E+10		3.50E+09		8.25E+09		7.43E+09
550	1.29E+10		3.89E+09		9.00E+09		8.09E+09

2B Equilibrium Constants Bimolecular Rate Constants (CVT-ISPE/SCT)

	K(2B)_1		K(2B)_2		k_bi_1		k_bi_2
250	7.90E-23		1.93E-20		1.49E-15		1.25E-16
250	7.90E-23		1.93E-20		1.49E-15		1.25E-16
260	7.46E-23		1.40E-20		2.02E-15		1.73E-16
270	7.10E-23		1.04E-20		2.68E-15		2.35E-16
280	6.80E-23		7.95E-21		3.49E-15		3.13E-16
290	6.56E-23		6.19E-21		4.48E-15		4.10E-16
300	6.35E-23		4.91E-21		5.66E-15		5.29E-16
310	6.18E-23		3.96E-21		7.07E-15		6.73E-16
320	6.04E-23		3.24E-21		8.72E-15		8.46E-16
330	5.93E-23		2.69E-21		1.06E-14		1.05E-15

340	5.83E-23		2.26E-21	1.29E-14		1.29E-15
350	5.75E-23		1.92E-21	1.54E-14		1.57E-15
360	5.69E-23		1.65E-21	1.83E-14		1.90E-15
370	5.65E-23		1.43E-21	2.15E-14		2.27E-15
380	5.61E-23		1.25E-21	2.52E-14		2.69E-15
390	5.59E-23		1.11E-21	2.93E-14		3.17E-15
400	5.57E-23		9.84E-22	3.38E-14		3.71E-15
410	5.57E-23		8.81E-22	3.89E-14		4.32E-15
420	5.57E-23		7.93E-22	4.44E-14		4.99E-15
430	5.58E-23		7.19E-22	5.05E-14		5.74E-15
440	5.60E-23		6.55E-22	5.71E-14		6.56E-15
450	5.62E-23		6.00E-22	6.43E-14		7.47E-15
460	5.65E-23		5.53E-22	7.22E-14		8.47E-15
470	5.69E-23		5.11E-22	8.07E-14		9.56E-15
480	5.73E-23		4.75E-22	8.98E-14		1.07E-14
490	5.77E-23		4.42E-22	9.97E-14		1.20E-14
500	5.82E-23		4.14E-22	1.10E-13		1.34E-14
510	5.87E-23		3.89E-22	1.22E-13		1.49E-14
520	5.93E-23		3.66E-22	1.34E-13		1.66E-14
530	5.99E-23		3.46E-22	1.47E-13		1.83E-14
540	6.05E-23		3.28E-22	1.60E-13		2.02E-14
550	6.12E-23		3.11E-22	1.75E-13		2.21E-14

S.2.3 Termolecular rate constants

Termolecular Rate Constants [$K(3B)*k_{uni_j}$]

	k_ter_1		k_ter_2		k_ter_3		k_ter_4
250	1.40E-39		1.86E-37		6.56E-37		6.37E-37
250	1.40E-39		1.86E-37		6.56E-37		6.37E-37
260	1.91E-39		1.87E-37		6.53E-37		6.36E-37
270	2.56E-39		1.91E-37		6.61E-37		6.44E-37
280	3.38E-39		1.98E-37		6.76E-37		6.59E-37
290	4.41E-39		2.06E-37		6.98E-37		6.80E-37
300	5.68E-39		2.17E-37		7.24E-37		7.07E-37
310	7.21E-39		2.29E-37		7.56E-37		7.37E-37
320	9.08E-39		2.43E-37		7.91E-37		7.72E-37

330	1.13E-38		2.58E-37		8.30E-37		8.10E-37
340	1.40E-38		2.74E-37		8.72E-37		8.51E-37
350	1.71E-38		2.92E-37		9.19E-37		8.96E-37
360	2.08E-38		3.11E-37		9.68E-37		9.45E-37
370	2.50E-38		3.31E-37		1.02E-36		9.97E-37
380	3.00E-38		3.53E-37		1.08E-36		1.05E-36
390	3.57E-38		3.76E-37		1.14E-36		1.11E-36
400	4.22E-38		4.00E-37		1.20E-36		1.17E-36
410	4.97E-38		4.26E-37		1.27E-36		1.24E-36
420	5.82E-38		4.54E-37		1.34E-36		1.31E-36
430	6.77E-38		4.84E-37		1.42E-36		1.38E-36
440	7.86E-38		5.15E-37		1.49E-36		1.46E-36
450	9.07E-38		5.47E-37		1.58E-36		1.55E-36
460	1.04E-37		5.82E-37		1.67E-36		1.63E-36
470	1.19E-37		6.18E-37		1.76E-36		1.72E-36
480	1.36E-37		6.57E-37		1.85E-36		1.82E-36
490	1.55E-37		6.97E-37		1.95E-36		1.92E-36
500	1.76E-37		7.40E-37		2.06E-36		2.03E-36
510	1.99E-37		7.84E-37		2.17E-36		1.98E-36
520	2.24E-37		8.31E-37		2.29E-36		2.08E-36
530	2.51E-37		8.81E-37		2.41E-36		2.18E-36
540	2.81E-37		9.33E-37		2.54E-36		2.29E-36
550	3.14E-37		9.87E-37		2.67E-36		2.40E-36

Termolecular Rate Constants [K(2B)*k_uni_j]

	k_ter_1		k_ter_2
250	1.18E-37		2.41E-36
250	1.18E-37		2.41E-36
260	1.51E-37		2.42E-36
270	1.90E-37		2.45E-36
280	2.37E-37		2.49E-36
290	2.94E-37		2.54E-36
300	3.60E-37		2.60E-36
310	4.37E-37		2.67E-36
320	5.27E-37		2.74E-36

330	6.30E-37		2.83E-36
340	7.49E-37		2.92E-36
350	8.85E-37		3.02E-36
360	1.04E-36		3.13E-36
370	1.22E-36		3.25E-36
380	1.41E-36		3.37E-36
390	1.64E-36		3.51E-36
400	1.89E-36		3.65E-36
410	2.16E-36		3.80E-36
420	2.47E-36		3.96E-36
430	2.82E-36		4.13E-36
440	3.20E-36		4.30E-36
450	3.62E-36		4.49E-36
460	4.08E-36		4.68E-36
470	4.59E-36		4.88E-36
480	5.14E-36		5.10E-36
490	5.75E-36		5.32E-36
500	6.41E-36		5.55E-36
510	7.14E-36		5.80E-36
520	7.92E-36		6.06E-36
530	8.78E-36		6.32E-36
540	9.70E-36		6.60E-36
550	1.07E-35		6.89E-36

Table S.1.: Branching ratios (in percentage) for the formation of gas-phase and water-assisted mechanism products for RH=20% and RH=100%.

T/K	20%		100%	
	gas-phase	water-mediated	gas-phase	water-mediated
280	99.9	0.1	99.6	0.4
290	99.9	0.1	99.6	0.4
300	99.8	0.2	99.2	0.8
310	99.8	0.2	99.0	1.0
320	99.7	0.3	98.7	1.3

Analytical expressions proposed by Zheng et al. (see text)

$$k = A \left(\frac{T}{300} \right)^n \exp \left(-\frac{B(T + T_0)}{T^2 + T_0^2} \right)$$