Supporting information

-for-

Determination of the influence of water on the SO_3 + CH_3OH reaction in the gas phase and at the air-water interface

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‡ Chao Ding and Yang Cheng have contributed equally to this work.

S16	**Table S5** Coordinates stationary points for the SO_3 + CH_3OH → CH_3OSO_3H reaction without and with H_2O and CH_3OH as well as the hydrolysis reaction of SO_3 without and with H_2O and CH_3OH at the M06-2X/6-311+G(2*df*,2*pd*) level of theory

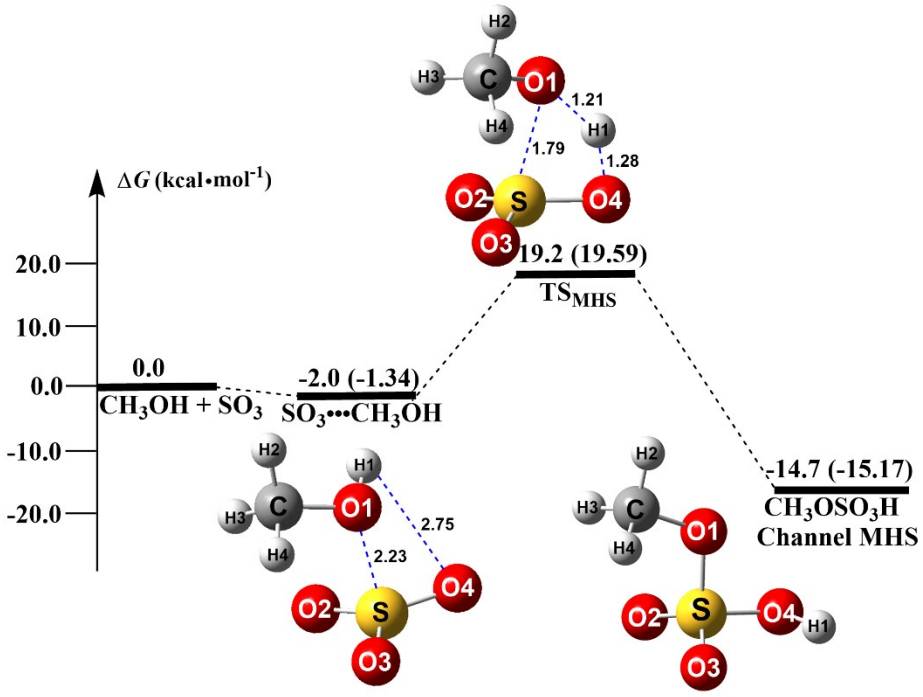

Fig. S1 Schematic potential energy surface for the SO_3 + CH_3OH → CH_3OSO_3H reaction (Distance are in angstroms at the M06-2X/6-311+G(2*df*,2*pd*) level of theory. The energy values correspond to calculations at the CCSD(T)-F12/cc-pVDZ-F12//M06-2X/6-311+G(2*df*,2*pd*) level; The values in parentheses are taken from reference 2)

The formation of CH_3OSO_3H (MHS) from the SO_3 + CH_3OH reaction has been studied theoretically before by several groups[1,2]. Herein, this reaction has been reinvestigated at the CCSD(T)-F12/cc-pVDZ-F12//M06-2X/6-311+G(2*df*,2*pd*) level to evaluate the catalytic effect of water molecule in the gas phase and at the air-water interface. As seen in Fig. S1, starting from the SO_3 + CH_3OH reactants, a four-membered ring SO_3•••CH_3OH complex was formed with a binding Gibbs free energy of 2.0 kcal·mol^{-1}, which was good agreement with complex R-a reported by Liu et al[2] geometrically and energetically. After SO_3•••CH_3OH complex, the reaction proceeded through transition state TS with the Gibbs free energy barrier of 21.2 kcal·mol^{-1}, and formed the product MHS, which was calculated to be 12.7 kcal·mol^{-1} more stable than SO_3•••CH_3OH. As for TS_{MHS} and MHS, their calculated geometries and relative free energies were consistent with previous studies reported by Shen et al.[1] and Liu et al.[2] Within the altitude range of 0-15 km, the rate coefficients for the SO_3 + CH_3OH → CH_3OSO_3H reaction listed in Table S4 were calculated to be 3.98 × 10^{-20} - 5.40 × 10^{-20} cm^3·molecules^{-1}·s^{-1} by using master equation. At 298 K, the calculated rate coefficient of the SO_3 + CH_3OH → CH_3OSO_3H reaction was 5.40 × 10^{-20} molecules·cm^{-3}·s^{-1}, which agreed with previously calculated value[2] (1.20 × 10^{-19} molecules·cm^{-3}·s^{-1}).

Reference

[1] G. Shen, M. Suto and L. C. Lee, *Int. J. Chem. Kinet.*, 1990, **22**, 633-639.
[2] L. Liu, J. Zhong, H. Vehkamäki, T. Kurtén, L. Du, X. Zhang, J. S. Francisco and X. C. Zeng, *Proc. Natl. Acad. Sci. U. S. A.*, 2019, **116**, 24966-24971.

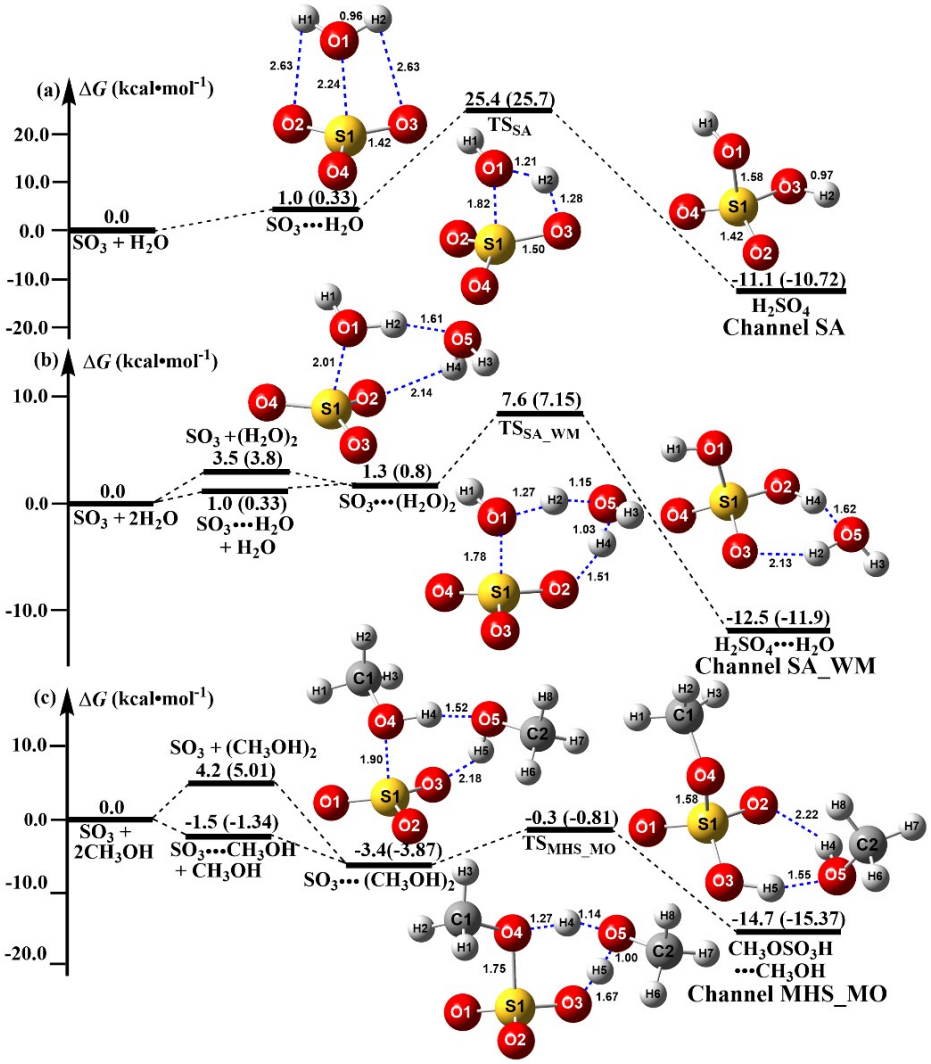

Fig. S2 Schematic energy diagrams for the hydrolysis of SO_3 without (a) and with H_2O (b), as well as CH_3OH-assisted $SO_3 + CH_3OH \rightarrow CH_3OSO_3H$ reaction (c) at the CCSD(T)-F12/cc-pVDZ-F12//M06-2X/6-311+G(2*df*,2*pd*) level of theory (The values in parentheses are reported from reference *Chem. Phys. Lett.*, 2013, **581**, 26-29, *J. Phys. Chem. A,* 2017, **121**, 3101-3108)

Table S1 Relative energies (ΔE and $\Delta(E + \mathrm{ZPE})$/(kcal·mol^{-1})), enthalpies (ΔH/(kcal·mol^{-1})), entropy (S(298 K)/(cal·mol^{-1}·K^{-1})) and free energies (ΔG(298 K)/(kcal·mol^{-1})) for the reactants, intermediates, transition states and products involved in the $SO_3 + CH_3OH \rightarrow CH_3OSO_3H$ reaction without and with H_2O and CH_3OH as well as the hydrolysis reaction of SO_3 without and with H_2O and CH_3OH

Species	ZPE	ΔE	S	ΔG	$\Delta(E + ZPE)$	ΔH
$SO_3 + CH_3OH$	40.6	0.0	121.4	0.0	0.0	0.0
SO_3•••CH_3OH	42.6	-13.6	87.2	-2.0 (-1.34)[a]	-11.6	-11.9
TS_{MHS}	40.2	9.0	79.4	19.2 (19.59)[a]	8.7	7.7
CH_3OSO_3H (MHS)	43.0	-27.4	80.9	-14.7 (15.17)[a]	-25.0	-25.7
$SO_3 + CH_3OH + H_2O$	54.2	0.0	166.5	0.0	0.0	0.0
SO_3•••$H_2O + CH_3OH$	56.5	-9.4	134.1	1.0 (0.33)[b]	-6.9	-7.6
SO_3•••$CH_3OH + H_2O$	56.2	-13.6	131.7	-1.5 (-1.34)[a]	-11.6	-11.9
CH_3OH•••$H_2O + SO_3$	56.0	-5.1	143.2	3.5 (3.68)[a]	-3.3	-3.4
SO_3•••CH_3OH•••H_2O	58.9	-27.3	94.8	-2.5 (-2.96)[a]	-22.6	-23.9
TS_{MHS_WM}	57.0	-20.3	86.9	3.8 (3.66)[a]	-17.5	-19.9
CH_3OSO_3H···H_2O (MHS···WM)	58.9	-39.7	94.3	-15.0 (-15.40)[a]	-35.0	-36.5
$SO_3 + CH_3OH + CH_3OH$	73.2	0.0	174.6	0.0	0.0	0.0
SO_3•••$CH_3OH + CH_3OH$	75.2	-13.6	143.6	-1.5 (-1.34)[a]	-11.6	-11.9
$(CH_3OH)_2 + SO_3$	74.7	-5.6	147.3	4.2 (5.01)[a]	-4.1	-4.0
SO_3••• $(CH_3OH)_2$	77.4	-29.7	101.1	-3.4 (-3.87)[a]	-25.5	-26.3
TS_{MHS_MO}	75.6	-25.8	95.3	-0.3 (-0.81)[a]	-23.4	-25.0
CH_3OSO_3H•••CH_3OH (MHS•••MO)	77.5	-41.0	100.8	-14.7 (-15.37)[a]	-36.7	-37.8
$SO_3 + H_2O$	21.6	0.0	106.2	0.0	0.0	0.0
SO_3•••H_2O	24.1	-9.4	78.1	1.0 (0.33)[b]	-6.9	-7.6
TS_{SA}	22.3	15.7	70.4	25.4 (25.7)[b]	16.4	14.7
H_2SO_4 (SA)	25.3	-23.6	71.6	-11.1 (-10.72)[b]	-20.0	-21.4
$SO_3 + H_2O + H_2O$	35.2	0.0	151.3	0.0	0.0	0.0
$SO_3 + (H_2O)_2$	37.4	-5.0	128.8	3.5 (3.8)[c]	-2.5	-3.2
SO_3•••$H_2O + H_2O$	37.5	-9.4	122.5	1.0 (0.33)[b]	-6.9	-7.6
SO_3•••$(H_2O)_2$	40.8	-21.5	87.1	1.3 (0.8)[c]	-15.9	-17.9
TS_{SA_WM}	39.1	-14.5	82.2	7.6 (7.15)[b]	-10.6	-13.6
H_2SO_4•••H_2O (SA•••WM)	41.1	-36.0	85.1	-12.5 (-11.9)[c]	-30.1	-32.3
$SO_3 + CH_3OH + H_2O$	54.2	0.0	166.5	0.0	0.0	0.0
SO_3•••$H_2O + CH_3OH$	56.5	-9.4	134.1	1.0 (0.33)[c]	-6.9	-7.6
SO_3•••$CH_3OH + H_2O$	56.2	-13.6	131.7	-1.5 (-1.34)[a]	-11.6	-11.9
CH_3OH•••$H_2O + SO_3$	56.0	-5.1	143.2	3.5 (3.68)[a]	-3.3	-3.4
SO_3•••H_2O•••CH_3OH	59.1	-22.9	95.1	0.8	-18.1	-19.5
TS_{SA_MO}	57.4	-19.5	89.5	3.5	-16.3	-18.4

H_2SO_4•••CH_3OH (SA•••MO)	59.1	-37.1	97.6	-14.2	-32.2	-33.7

[a] The values are reported from reference (*Proc. Natl. Acad. Sci. U. S. A.*, 2019, **116**, 24966-24971)

[b] The values are reported from reference (*Chem. Phys. Lett.*, 2013, **581**, 26-29)

[c] The values are reported from reference (*J. Phys. Chem. A,* 2017, **121**, 3101-3108)

Table S2 Equilibrium constants ($cm^3 \cdot molecule^{-1}$) for SO_3•••CH_3OH, SO_3•••H_2O, CH_3OH•••H_2O, $(H_2O)_2$ and SO_3···$(H_2O)_2$ within the altitude range of 0-15 km[a]

Altitude	*T*/K	SO_3•••CH_3OH	SO_3•••H_2O	CH_3OH•••H_2O	$(H_2O)_2$	SO_3••• $(H_2O)_2$
0 km	298.15	1.07×10^{-18}	2.69×10^{-21} (6.44×10^{-20})[b]	1.29×10^{-22}	2.00×10^{-22} (2.34×10^{-21})[c]	2.35×10^{-19} (6.83×10^{-19})[d]
5 km	259.30	1.86×10^{-17}	1.60×10^{-20}	2.71×10^{-22}	3.73×10^{-22}	2.69×10^{-18}
10 km	229.70	3.00×10^{-16}	9.19×10^{-20}	5.75×10^{-22}	7.03×10^{-22}	2.83×10^{-17}
15 km	212.60	2.21×10^{-15}	3.23×10^{-19}	9.98×10^{-22}	1.12×10^{-21}	1.51×10^{-16}

[a] The equilibrium constants ($cm^3 \cdot molecule^{-1}$) for the SO_3•••CH_3OH, SO_3•••H_2O, CH_3OH•••H_2O, $(H_2O)_2$ and SO_3•••$(H_2O)_2$ complexes involved in Table S2 were performed by ILT method in Mesmer code.

[b] The value was taken from reference (*Chemphyschem*., 2012, **13**, 323-329)

[c] The value was taken from reference (*J. Am. Chem. Soc.*, 2012, **134**, 20632-20644)

[d] The value was taken from reference (*J. Phys. Chem. A*, 2017, **121**, 3101-3108)

Table S3 The high-pressure limiting rate coefficient ($cm^3 \cdot molecules^{-1} \cdot s^{-1}$) for the reactants to pre-reactive complex process calculated by master equation within the temperature range of 213-320 K

T(K)	$SO_3 + CH_3OH \rightarrow SO_3 \bullet\bullet\bullet CH_3OH$	$SO_3 + CH_3OH \bullet\bullet\bullet H_2O \rightarrow SO_3 \bullet\bullet\bullet CH_3OH \bullet\bullet\bullet H_2O$	$SO_3 \bullet\bullet\bullet CH_3OH + CH_3OH \rightarrow SO_3 \bullet\bullet\bullet (CH_3OH)_2$
212.60	6.20×10^{-11}	5.09×10^{-11}	5.86×10^{-11}
215.50	6.24×10^{-11}	5.12×10^{-11}	5.90×10^{-11}
218.60	6.28×10^{-11}	5.16×10^{-11}	5.95×10^{-11}
223.70	6.36×10^{-11}	5.22×10^{-11}	6.01×10^{-11}
229.70	6.45×10^{-11}	5.29×10^{-11}	6.09×10^{-11}
235.10	6.52×10^{-11}	5.35×10^{-11}	6.17×10^{-11}
249.90	6.72×10^{-11}	5.52×10^{-11}	6.36×10^{-11}
259.30	6.84×10^{-11}	5.62×10^{-11}	6.48×10^{-11}
266.10	6.93×10^{-11}	5.69×10^{-11}	6.56×10^{-11}
271.00	7.00×10^{-11}	5.74×10^{-11}	6.62×10^{-11}
280.00	7.11×10^{-11}	5.84×10^{-11}	6.73×10^{-11}
290.00	7.24×10^{-11}	5.94×10^{-11}	6.85×10^{-11}
298.15	7.34×10^{-11}	6.02×10^{-11}	6.94×10^{-11}
300.00	7.36×10^{-11}	6.04×10^{-11}	6.96×10^{-11}
310.00	7.48×10^{-11}	6.14×10^{-11}	7.08×10^{-11}
320.00	7.60×10^{-11}	6.24×10^{-11}	7.19×10^{-11}
T(K)	$SO_3 + H_2O \rightarrow SO_3 \bullet\bullet\bullet H_2O$	$SO_3 \bullet\bullet\bullet H_2O + H_2O \rightarrow SO_3 \bullet\bullet\bullet (H_2O)_2$	$SO_3 + CH_3OH \bullet\bullet\bullet H_2O \rightarrow SO_3 \bullet\bullet\bullet H_2O \bullet\bullet\bullet CH_3OH$
212.60	1.13×10^{-10}	5.41×10^{-11}	7.48×10^{-11}
215.50	1.13×10^{-10}	5.45×10^{-11}	7.53×10^{-11}
218.60	1.14×10^{-10}	5.49×10^{-11}	7.59×10^{-11}
223.70	1.15×10^{-10}	5.55×10^{-11}	7.68×10^{-11}
229.70	1.17×10^{-10}	5.62×10^{-11}	7.78×10^{-11}
235.10	1.18×10^{-10}	5.69×10^{-11}	7.87×10^{-11}
249.90	1.22×10^{-10}	5.87×10^{-11}	8.11×10^{-11}
259.30	1.24×10^{-10}	5.97×10^{-11}	8.26×10^{-11}
266.10	1.26×10^{-10}	6.05×10^{-11}	8.37×10^{-11}
271.00	1.27×10^{-10}	6.11×10^{-11}	8.45×10^{-11}
280.00	1.29×10^{-10}	6.21×10^{-11}	8.59×10^{-11}
290.00	1.31×10^{-10}	6.32×10^{-11}	8.74×10^{-11}
298.15	1.33×10^{-10}	6.40×10^{-11}	8.86×10^{-11}
300.00	1.34×10^{-10}	6.43×10^{-11}	8.89×10^{-11}
310.00	1.36×10^{-10}	6.53×10^{-11}	9.04×10^{-11}
320.00	1.38×10^{-10}	6.64×10^{-11}	9.18×10^{-11}

Table S4 Rate coefficient ($cm^3 \cdot molecules^{-1} \cdot s^{-1}$) of $SO_3 + CH_3OH$, $SO_3 \bullet\bullet\bullet CH_3OH + CH_3OH$, $SO_3 \bullet\bullet\bullet CH_3OH + H_2O$ $SO_3 + H_2O$ and $SO_3 \bullet\bullet\bullet H_2O + H_2O$ reactions within the altitude range of 0-50 km[a]

H (km)	T (K)	p (Torr)	k_{MHS} (T, p)	k_{MHS_WM} (T, p)	k_{MHS_MO} (T, p)	k_{SA} (T, p)	k_{SA_WM} (T, p)	k_{SA_MO} (T, p)
0	280.00	760.00	4.70×10^{-20}	3.91×10^{-12}	2.54×10^{-11}	2.15×10^{-24}	1.42×10^{-12}	3.05×10^{-12}
	290.00		5.05×10^{-20}	3.41×10^{-12}	2.34×10^{-11}	2.79×10^{-24}	1.25×10^{-12}	2.67×10^{-12}
	298.15		5.40×10^{-20}	3.05×10^{-12}	2.19×10^{-11}	3.53×10^{-24} (1.50×10^{-23})[b]	1.14×10^{-12} (9.70×10^{-13})[c]	2.40×10^{-12}
	300.00		5.50×10^{-20}	2.96×10^{-12}	2.15×10^{-11}	3.75×10^{-24}	1.11×10^{-12}	2.34×10^{-12}
	310.00		6.09×10^{-20}	2.58×10^{-12}	1.97×10^{-11}	5.17×10^{-24}	9.78×10^{-13}	2.05×10^{-12}
	320.00		6.83×10^{-20}	2.25×10^{-12}	1.79×10^{-11}	7.31×10^{-24}	8.63×10^{-13}	1.80×10^{-12}
5	259.30	406.60	4.39×10^{-20}	5.21×10^{-12}	2.95×10^{-11}	1.39×10^{-24}	1.95×10^{-12}	4.04×10^{-12}
10	229.70	202.16	4.49×10^{-20}	7.70×10^{-12}	3.50×10^{-11}	9.70×10^{-25}	2.95×10^{-12}	6.06×10^{-12}
15	212.60	91.20	4.98×10^{-20}	9.47×10^{-12}	3.76×10^{-11}	8.82×10^{-25}	3.74×10^{-12}	7.64×10^{-12}
20	215.50	41.04	5.21×10^{-20}	8.25×10^{-12}	3.30×10^{-11}	9.01×10^{-25}	3.49×10^{-12}	7.32×10^{-12}
25	218.60	19.00	5.36×10^{-20}	7.82×10^{-12}	2.91×10^{-11}	9.21×10^{-25}	3.15×10^{-12}	6.97×10^{-12}
30	223.70	8.36	5.43×10^{-20}	7.10×10^{-12}	2.34×10^{-11}	9.56×10^{-25}	2.69×10^{-12}	6.34×10^{-12}
35	235.10	3.80	5.30×10^{-20}	4.44×10^{-12}	1.59×10^{-11}	1.05×10^{-24}	1.97×10^{-12}	4.52×10^{-12}
40	249.90	2.28	5.13×10^{-20}	2.26×10^{-12}	1.02×10^{-11}	1.24×10^{-24}	1.32×10^{-12}	2.30×10^{-12}
45	266.10	1.06	5.13×10^{-20}	8.21×10^{-13}	5.18×10^{-12}	1.61×10^{-24}	6.89×10^{-13}	8.99×10^{-13}
50	271.00	0.55	5.17×10^{-20}	4.14×10^{-13}	3.24×10^{-12}	1.78×10^{-24}	4.12×10^{-13}	4.44×10^{-13}

[a] k_{MHS}, k_{MHS_WM}, k_{MHS_MO}, k_{SA}, k_{SA_WM} and k_{SA_MO} are the rate coefficient of Channel MHS, Channel MHS_WM, Channel MHS_MO, Channel SA, Channel SA_WM, and Channel SA_MO, respectively.

[b] The value was taken from reference (*J. Am. Chem. Soc.*, **2012**, 134, 20632-20644)

[c] The value was taken from reference (*J. Phys. Chem. A,* **2019***,* 123, 3131-3141)

The collision energy transfer between the reactive complexes and bath gas (N_2) is approximated by a single exponential down model ($\langle \Delta E \rangle_{down}$ = 150 cm^{-1}) and

the one-dimensional asymmetric Eckart potential[1] was applied to tunneling correction in the rate constant calculations involving the typical addition reaction along with the hydrogen atom transfer. In addition, The Lennard-Jones parameters for the SO_3 (ε/k_B = 281.1 K and σ = 3.13 Å) and CH_3OH (ε/k_B = 481.8 K and σ =3.63 Å) were estimated by an empirical method,[2] while the parameters for N_2 was taken from the literature.[3]

Reference

[1] C, Eckart, *Phys. Rev.*, 1930, **35**, 1303-1309.

[2] R. G. Gilbert and S. C. Smith, *Theory of unimolecular and recombination reactions*, Publishers' Business Services, 1990.

[3] S. H. Robertson, M. J. Pilling, L. C. Jitariu and I. H. Hillier, *Phys. Chem. Chem. Phys.*, 2007, **9,** 4085-4097.

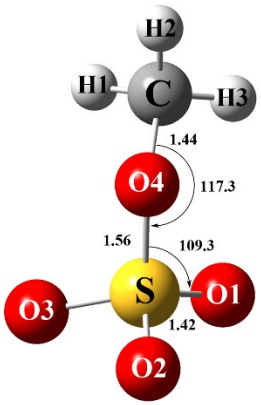

Fig. S3 The optimized geometrical structure for $CH_3OSO_3^-$ ion at the M06-2X/6-311+G(2*df*,2*pd*) level

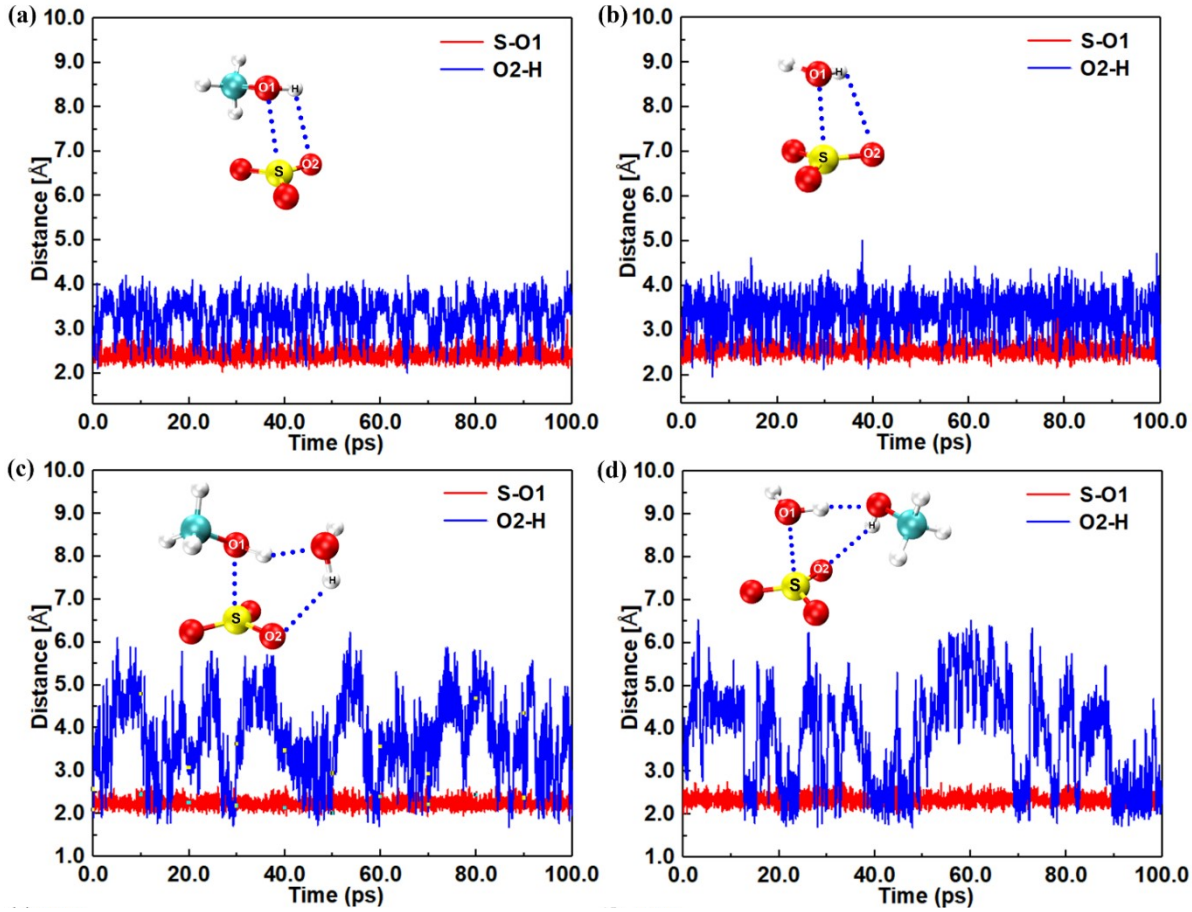

Fig. S4 The simulated trajectories of SO_3 + CH_3OH reaction (a), SO_3 + H_2O reaction (b), H_2O-assisted SO_3 + CH_3OH reaction (c) and CH_3OH-assisted SO_3 + H_2O reaction (d) in the gas phase

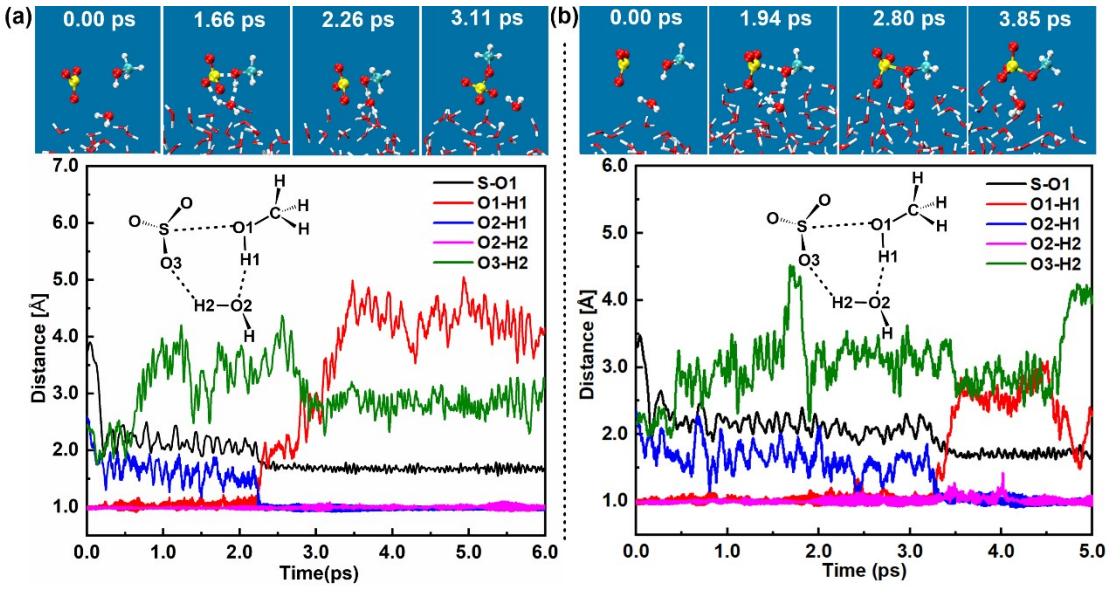

Fig. S5 The simulated trajectories of the $CH_3OSO_3^-$•••H_3O^+ ion pair formation from SO_3, CH_3OH and an interfacial water molecule at the air-water interface

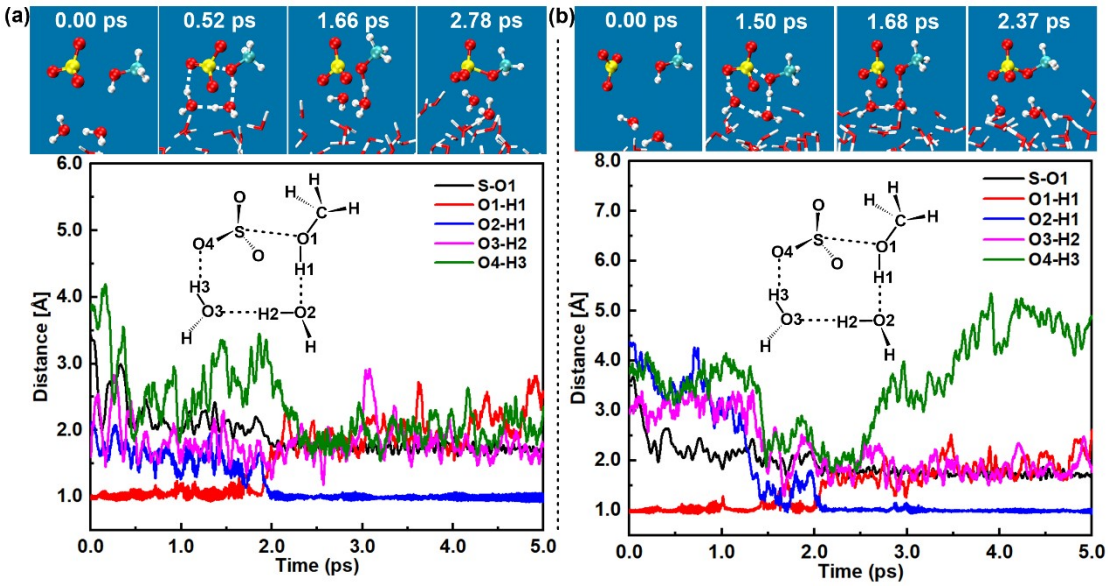

Fig. S6 The simulated trajectories of the $CH_3OSO_3^-$•••H_3O^+ ion pair formation from SO_3, CH_3OH and two interfacial water molecular at the air-water interface

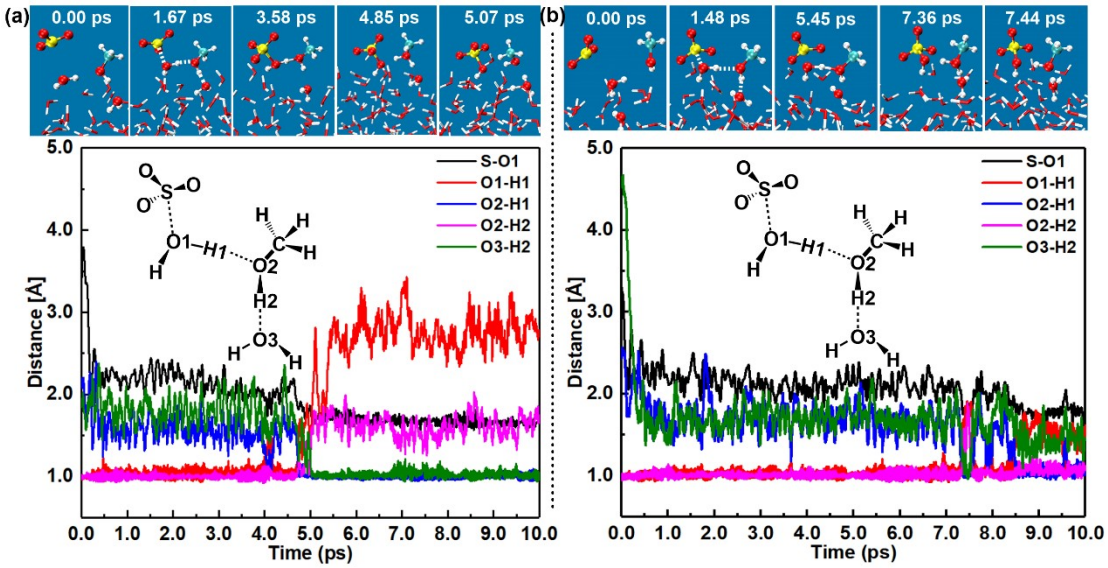

Fig. S7 The simulated trajectories of the HSO_4^- and H_3O^+ ions formation from SO_3, CH_3OH and an interfacial water molecule at the air-water interface

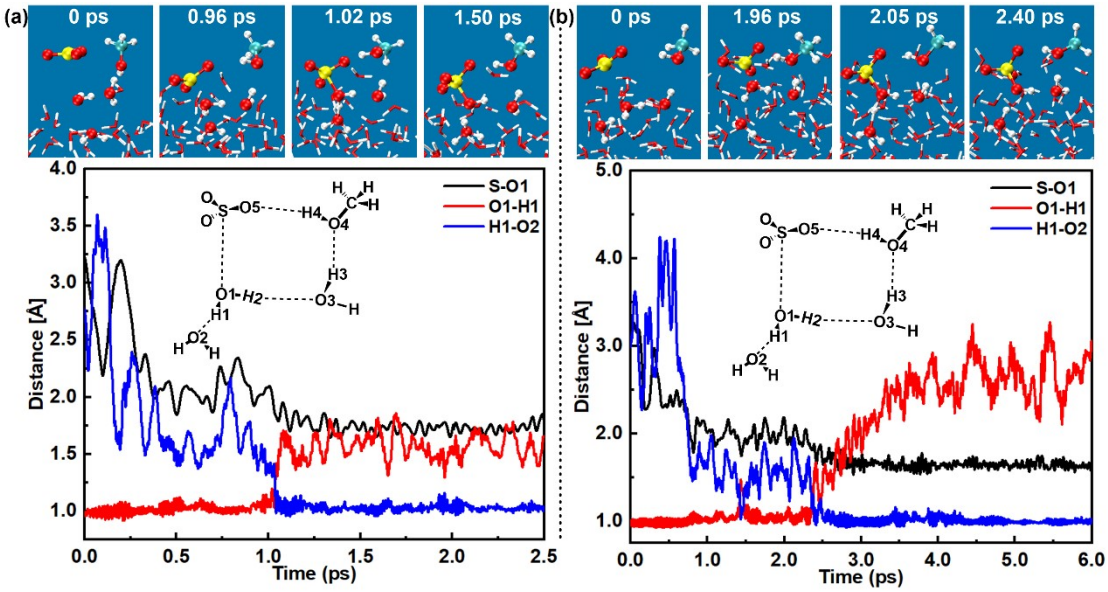

Fig. S8 The simulated trajectories of the HSO_4^- and H_3O^+ ions formation from SO_3, CH_3OH and two interfacial water molecules at the air-water interface

Table S5 Coordinates stationary points for the SO_3 + CH_3OH → CH_3OSO_3H reaction without and with H_2O and CH_3OH as well as the hydrolysis reaction of SO_3 without and with H_2O and CH_3OH at the M06-2X/6-311+G(2*df*,2*pd*) level of theory

	CH_3OH						
C	-0.66191500	-0.02063100	0.00000900				
H	-1.08247700	0.98201300	-0.00019900		**SO_3**		
H	-1.02028700	-0.54421200	0.88975100	S	0.00000000	0.00000000	0.00000000
H	-1.02028500	-0.54457800	-0.88951800	O	0.00000000	1.41906500	0.00000000
O	0.74345100	0.12214000	-0.00002000	O	1.22894600	-0.70953300	0.00000000
H	1.14692600	-0.74656100	0.00006900	O	-1.22894600	-0.70953300	0.00000000
	SO_3•••CH_3OH				**TS_{MHS}**		
S	-0.79785200	-0.08902400	0.01710600	S	-0.59725800	-0.09784400	-0.03361400
O	-0.74599200	-0.83876200	-1.15089800	O	-0.30038100	-1.25961100	-0.79838800
O	-0.57170000	-0.71514000	1.23934100	O	-1.38762100	-0.18829300	1.13841000
O	-1.32780200	1.19620800	-0.00286700	O	-0.70714300	1.18646300	-0.80498500
C	2.38024300	-0.20767100	0.01702800	C	2.16367000	-0.18934700	0.12980100
H	2.20265800	-1.07374300	-0.59873000	H	2.12509600	-1.12201900	0.68597800
H	2.44268300	-0.50667300	1.05370000	H	3.01620600	0.40349000	0.44693600
H	3.29945000	0.26923500	-0.29229800	H	2.20323700	-0.39408600	-0.93734800
O	1.28868900	0.67073600	-0.18867600	O	0.98976300	0.57102900	0.45112200
H	1.39381900	1.47725200	0.28627500	H	0.47263100	1.33749900	-0.32581900
	CH_3OSO_3H (MHS)						
S	-0.39118800	0.12680500	0.07222200				
O	-0.41048900	1.43740200	-0.47132100				
O	-1.47639700	-0.71757700	-0.68754800				
O	-0.51998500	-0.09225400	1.47607200		**H_2O**		
C	2.13819100	-0.08587600	-0.02263200	O	0.00000000	0.00000000	0.11651300
H	2.25015000	0.91898400	-0.42405500	H	0.00000000	0.76111400	-0.46605300
H	2.89714400	-0.74454500	-0.42932000	H	0.00000000	-0.76111400	-0.46605300
H	2.18829400	-0.07654000	1.06465100				
O	0.88259300	-0.64269000	-0.45139500				
H	-1.71148700	-1.49055500	-0.15749400				
	SO_3•••H_2O				**TS_{SA}**		
S	-0.41439700	0.00002000	-0.03540800	S	0.27132700	-0.00067200	0.06452500
O	-0.37795000	1.22800300	-0.75287900	O	0.66838000	1.36069300	0.13933400
O	-0.37800500	-1.22723400	-0.75411200	O	-0.55238000	-0.51043600	1.20835800
O	-0.75466100	-0.00066900	1.34052100	O	1.06391400	-0.95883200	-0.60803000
O	1.80323900	-0.00010700	0.28179800	O	-1.33699500	0.03116200	-0.78931900
H	2.14467900	0.77432100	-0.17810800	H	-1.59218200	0.94079100	-0.99582200
H	2.14468400	-0.77459300	-0.17799200	H	-1.49239800	-0.31073500	0.36068000
					CH_3OH•••H_2O		
	H_2SO_4			O	2.03948900	-0.22238600	0.00118500
S	-0.00000100	0.00002000	-0.15523400	H	2.52767100	0.12399700	-0.74864200
O	0.65946100	-1.06404600	-0.82199900	H	2.44588800	0.16951200	0.77722900
O	-1.02362400	-0.67886300	0.84002700	C	-1.65426300	-0.37813700	0.00204000
O	-0.65947500	1.06425200	-0.82172200	H	-2.64484300	0.06208400	0.09943200
O	1.02363900	0.67865200	0.84017800	H	-1.50026200	-1.06115600	0.84237300
H	-1.69535900	-0.03304900	1.09594400	H	-1.62746600	-0.95770000	-0.92530700
H	1.69536900	0.03276900	1.09593300	O	-0.72012700	0.67547500	-0.00342900
				H	0.16969100	0.30737300	-0.03937700
	SO_3•••CH_3OH•••H_2O				**TS_{MHS_WM}**		
S	0.79643400	0.42182200	-0.05172100	S	-0.58851400	-0.49176500	0.04309500
O	0.05261300	1.59408800	0.31229900	O	-1.77645900	-0.36631200	-0.73069300
O	1.85962600	-0.00102100	0.79205400	O	-0.66699900	-0.33530000	1.46532300
O	0.82936500	0.06370400	-1.43330900	O	0.37228100	-1.50341500	-0.40945100
C	-0.39749400	-2.14851200	-0.03612700	H	2.77094500	-0.19792400	0.82023400

H	0.61040000	-2.48058400	0.19482000	O	2.41978400	-0.18732500	-0.07695700
H	-0.54110600	-2.10266300	-1.11264000	H	1.76532000	-0.98749700	-0.18634400
H	-1.12502500	-2.80445700	0.43417200	H	1.54834300	0.55461300	-0.18848300
O	-0.54032700	-0.84004600	0.53607800	O	0.34766800	0.90847200	-0.42080800
H	-1.42162200	-0.40881900	0.31734500	C	-0.20440600	2.16187600	-0.00237700
O	-2.53724200	0.64154700	-0.10240400	H	0.44328200	2.94137500	-0.39292100
H	-1.94020200	1.40507500	-0.12339200	H	-1.19941100	2.25451000	-0.43076900
H	-3.25270300	0.86718700	0.49624900	H	-0.25602200	2.20295300	1.08371300
	CH_3OSO_3H•••H_2O				**SO_3•••H_2O•••CH_3OH**		
S	-0.21114000	-0.42161200	0.08936400	S	-1.05894900	-0.23644000	0.07385700
O	-1.06633600	-1.54529400	0.24532700	O	-2.38292900	0.24923200	-0.08523900
O	0.40288300	0.16671100	1.24991000	O	-0.47575200	-0.26340600	1.38135500
O	0.86937800	-0.72536500	-0.97007800	O	-0.52535200	-1.13372000	-0.90242400
H	2.37042000	0.76532000	0.81104200	H	1.62826300	0.13895600	1.18397700
O	2.86855300	0.61126600	-0.00385500	O	2.09123000	0.53802300	0.43484800
H	1.70470500	-0.21342100	-0.75113900	H	0.87304600	1.14983300	-0.25792800
H	3.15485900	1.46946500	-0.32373500	O	-0.08843600	1.37707500	-0.51908600
O	-0.98965500	0.71618200	-0.68360200	H	-0.16385400	1.44557400	-1.47821000
C	-2.18489900	1.17476000	-0.03282500	C	2.78880400	-0.48418100	-0.28220200
H	-2.59283900	1.93990700	-0.68395600	H	2.09481500	-1.23465900	-0.66014200
H	-2.88753400	0.35102400	0.07257600	H	3.29462900	0.00101100	-1.11227300
H	-1.94055400	1.59694000	0.94073300	H	3.53337300	-0.95020800	0.36043800
	TS_{SA_MO}				**H_2SO_4•••CH_3OH**		
S	0.98272900	0.14570100	0.11403100	S	-0.95927700	0.13443900	0.09243500
O	2.32852000	-0.28712200	-0.03645200	O	-1.86849600	1.22100900	-0.01799500
O	0.29624900	-0.23119400	1.33854400	O	-0.00129600	0.16808100	-1.12441800
O	0.60266200	1.41730500	-0.43408500	O	-0.19062000	-0.09118700	1.27769300
H	-1.37358300	-0.55024000	0.98780300	H	0.89870200	-0.22030500	-0.85002900
O	-1.96338600	-0.69453800	0.20112300	O	2.18935400	-0.68091900	-0.13150400
H	-1.09217300	-0.87180600	-0.52936600	H	1.78259000	-0.87986000	0.72153500
O	0.08894700	-0.95208900	-0.97645100	O	-1.77060100	-1.20813100	-0.13363300
H	0.25934700	-0.68295600	-1.88698500	H	-2.52534800	-1.02716300	-0.70842100
C	-2.64786900	0.54490100	-0.10140300	C	3.07126200	0.42948700	0.03524900
H	-1.92021400	1.34857400	-0.19780400	H	2.53776100	1.29156200	0.43659900
H	-3.18365100	0.39069400	-1.03184000	H	3.89499000	0.16487100	0.69566700
H	-3.35011700	0.74621100	0.70068000	H	3.46542600	0.67212100	-0.94694400
	SO_3•••$(CH_3OH)_2$				**TS_{MHS_MO}**		
S	0.89885600	-0.63470500	0.05547500	S	-0.87208200	-0.51786100	0.08659700
O	0.11449600	-1.51661200	-0.74699300	O	-0.51992300	-0.39841100	1.47515100
O	2.26804400	-0.41194900	-0.26190900	O	-0.07588100	-1.47996400	-0.66588700
O	0.48886900	-0.47028800	1.42537000	O	-2.24400100	-0.39107200	-0.27589800
C	0.79149500	2.16599200	-0.08475300	O	2.01569800	-0.03959900	-0.73117100
H	1.83424100	2.13904600	-0.38267700	H	1.47744500	-0.87925000	-0.82967500
H	0.70631400	2.16555800	1.00056400	H	1.08300300	0.61925200	-0.66463200
H	0.29377000	3.03086000	-0.51430300	O	-0.14978900	0.93295700	-0.57978700
O	0.17032800	0.98717900	-0.62440200	C	-0.59703000	2.15164300	0.02178900
H	-0.79473800	0.90095100	-0.29670600	H	-0.10872400	2.96760500	-0.50373800
O	-2.04837900	0.47149000	0.44810900	H	-1.67485300	2.21876600	-0.10535500
H	-1.63651600	-0.06563100	1.13922300	H	-0.34273000	2.16105500	1.08031100
C	-2.97406700	-0.32648900	-0.29656900	C	2.70857300	-0.07710400	0.53876400
H	-3.75911500	-0.69712700	0.35989100	H	3.47488200	-0.84329800	0.48089200
H	-3.41573700	0.32273300	-1.04681000	H	3.16825200	0.89579500	0.67898600
H	-2.46135600	-1.15668500	-0.78025800	H	1.99794400	-0.29267400	1.33508200
	CH_3OSO_3H•••CH_3OH				**SO_3•••$(H_2O)_2$**		
S	0.66600300	-0.49767100	0.05300700	S	-0.72655600	-0.21572400	-0.01563600
O	-0.34961500	-1.02126400	-0.97923900	O	0.02120300	-0.80276600	-1.09100900
O	1.85871900	-1.26836700	0.00340000	O	-1.89767500	0.52174300	-0.33607100

O	0.00677500	-0.29273700	1.31506300	O	-0.55376300	-0.76786200	1.28265300
C	1.98995400	1.67395400	0.05856600	H	2.05659400	-0.77081100	-0.53575300
H	2.93019200	1.13124300	-0.01135400	O	2.56888200	-0.09325700	-0.07175700
H	1.73134300	1.85735200	1.10050400	H	2.94629300	-0.51875200	0.70222000
H	2.05135800	2.61071700	-0.48437500	H	1.39094700	0.96571600	0.17856200
O	0.94646600	0.92561900	-0.58354500	O	0.47412400	1.36639800	0.26262700
H	-2.18149200	-0.49186100	1.01231500	H	0.32889200	1.98137700	-0.46639600
O	-2.55910500	-0.39310800	0.12879100				
H	-1.29146600	-0.82846700	-0.64506900				
C	-2.76511200	0.99917500	-0.11338900				
H	-3.15976200	1.09115400	-1.12093200				
H	-3.48711600	1.40607700	0.59252400				
H	-1.82407600	1.54660000	-0.03854200				
	TS_{SA_WM}				**H_2SO_4•••H_2O**		
S	-0.65233100	-0.14510200	-0.01916500	S	0.57588500	-0.07535900	0.12343300
O	-0.85657300	-0.74621700	1.25457600	O	1.74940700	-0.86585200	0.24755800
O	0.25182400	-0.88475000	-0.90835700	O	0.97143100	1.29314100	-0.56891300
O	-1.71014300	0.55338700	-0.66930800	H	1.72836900	1.14588600	-1.15045300
H	1.69307800	-0.64037300	-0.52213900	O	-0.21323400	0.29783800	1.25530000
O	2.40341600	-0.02626900	-0.08883100	O	-0.34398900	-0.74592400	-0.93380500
H	2.80197100	-0.47821400	0.66311400	H	-1.29425100	-0.47807300	-0.76000900
H	1.59301500	0.72374100	0.23889900	O	-2.65960000	0.10211100	-0.11057600
O	0.43244100	1.19840900	0.41778900	H	-2.27974800	0.36435100	0.73887300
H	0.18151000	1.95999800	-0.12018200	H	-3.40065300	-0.47694900	0.08014600