

Supporting information

-for-

A novel formation mechanism of $\text{NH}_2\text{SO}_3\text{H}$ and its enhancing effect on methanesulfonic acid-methylamine aerosol particle formation in agriculture-developed and coastal industrial areas

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S. NO	Caption
S1	Fig. S1 (a) The z coordinates of HNSO_2 molecule as the function of simulation time; (b) the density profile of water; (c) the pie chart with the occurrence percentages of HNSO_2 molecule at the air-water interface and in water phase
S2-S3	Fig. S2 Optimized geometries of HNSO_2 , H_2O , $\text{CH}_3\text{SO}_3\text{H}$, $(\text{H}_2\text{O})_2$, $\text{HNSO}_2\cdots\text{H}_2\text{O}$ and $\text{CH}_3\text{SO}_3\text{H}\cdots\text{H}_2\text{O}$ at the M06-2X/6-311++G(2df,2pd) level (bond distances in Angstroms and angles in degrees) along with the stabilization energies of $(\text{H}_2\text{O})_2$, $\text{HNSO}_2\cdots\text{H}_2\text{O}$ and $\text{CH}_3\text{SO}_3\text{H}\cdots\text{H}_2\text{O}$ at the CCSD(T)-F12/cc-pVDZ-F12//M06-2X/6-311++G(2df,2pd) level of theory
S4-S5	Fig. S3 The optimized geometries and electric energies (in Hartree-Fock) for the complexes of $\text{HNSO}_2\cdots\text{H}_2\text{O}\cdots\text{CH}_3\text{SO}_3\text{H}$ at the M06-2X/6-311++G(2df,2pd) level of theory
S6	Fig. S4 The potential energy profile (ΔG) for the hydrolysis reaction of HNSO_2 without (a) and with (b) H_2O at the CCSD(T)-F12/cc-pVDZ-F12//M06-2X/6-311++G(2df,2pd) level of theory
S7	Table S1 Zero point energy (ZPE/(kcal·mol ⁻¹)), entropies (S/(cal·mol ⁻¹ ·K ⁻¹)), relative energies (ΔE and $\Delta(E + \text{ZPE})$ /(kcal·mol ⁻¹)), enthalpies ($\Delta H(298)$ /(kcal·mol ⁻¹)), and free energies ($\Delta G(298)$ /(kcal·mol ⁻¹)) for the hydrolysis reaction of HNSO_2 without and with H_2O and $\text{CH}_3\text{SO}_3\text{H}$
S8	Table S2 Equilibrium constants (cm ³ ·molecule ⁻¹) for the $\text{HNSO}_2\cdots\text{H}_2\text{O}$, $\text{H}_2\text{O}\cdots\text{H}_2\text{O}$, and $\text{CH}_3\text{SO}_3\text{H}\cdots\text{H}_2\text{O}$ complexes within the temperature range of 212.6-320.0 K
S9	Table S3 The high-pressure limiting rate constant (cm ³ ·molecule ⁻¹ ·s ⁻¹) for the hydrolysis reaction of HNSO_2 with H_2O and $\text{CH}_3\text{SO}_3\text{H}$ within the temperature range of 212.6-320.0 K
S10	Part 1. Calculations of reaction rate coefficients

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S11	Table S4 Rate coefficients (k , $\text{cm}^3 \cdot \text{molecule}^{-1} \cdot \text{s}^{-1}$) for the hydrolysis of HNSO_2 by master equation within the temperature range of 212.6-320.0 K
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S22-S24	Fig. S11 BOMD simulation trajectories and snapshots of $\text{CH}_3\text{SO}_3\text{H}^-$ and H_3O^+ ions forming mechanism via loop structure routes in $\text{CH}_3\text{SO}_3\text{H}$ -mediated hydration HNSO_2 at the air-water interface
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S37	Fig. S16 (a) The $J(\text{cm}^{-3} \text{s}^{-1})$ and (b) R as a function of $[\text{MSA}]$ with $[\text{SFA}] = 10^8 \text{ molecules cm}^{-3}$ and three different $[\text{MA}]$ (black line: $[\text{MA}] = 2.5 \times 10^7 \text{ molecules cm}^{-3}$, red line: $[\text{MA}] = 2.5 \times 10^8 \text{ molecules cm}^{-3}$, blue line: $[\text{MA}] = 2.5 \times 10^9 \text{ molecules cm}^{-3}$) at 238.15 K
S38	Fig. S17 (a) The $J(\text{cm}^{-3} \text{s}^{-1})$ and (b) R as a function of $[\text{MSA}]$ with $[\text{SFA}] = 10^8 \text{ molecules cm}^{-3}$ and three different $[\text{MA}]$ (black line: $[\text{MA}] = 2.5 \times 10^7 \text{ molecules cm}^{-3}$, red line: $[\text{MA}] = 2.5 \times 10^8 \text{ molecules cm}^{-3}$, blue line: $[\text{MA}] = 2.5 \times 10^9 \text{ molecules cm}^{-3}$) at 258.15 K
S39	Fig. S18 (a) The $J(\text{cm}^{-3} \text{s}^{-1})$ and (b) R as a function of $[\text{MSA}]$ with $[\text{SFA}] = 10^8 \text{ molecules cm}^{-3}$ and three different $[\text{MA}]$ (black line: $[\text{MA}] = 2.5 \times 10^7 \text{ molecules cm}^{-3}$, red line: $[\text{MA}] = 2.5 \times 10^8 \text{ molecules cm}^{-3}$, blue line: $[\text{MA}] = 2.5 \times 10^9 \text{ molecules cm}^{-3}$) at 298.15 K
S40	Fig. S19 Main cluster formation mechanism of MSA-MA-SFA-based system at 238.15 K, $[\text{MSA}] = 10^7 \text{ molecules} \cdot \text{cm}^{-3}$, $[\text{MA}] = 2.5 \times 10^8 \text{ molecules} \cdot \text{cm}^{-3}$, and $[\text{SFA}] = 10^6 \text{ molecules} \cdot \text{cm}^{-3}$. The black arrows indicate the pure MSA-MA-based growth pathways. Blue arrows represent the pathways containing SFA
S41	Fig. S20 Main cluster formation mechanism of MSA-MA-SFA-based system at 258.15 K, $[\text{MSA}] = 10^7 \text{ molecules} \cdot \text{cm}^{-3}$, $[\text{MA}] = 2.5 \times 10^8 \text{ molecules} \cdot \text{cm}^{-3}$, and $[\text{SFA}] = 10^6$

	molecules·cm ⁻³ . The black arrows indicate the pure MSA-MA-based growth pathways. Blue arrows represent the pathways containing SFA
S42	Fig. S21 Main cluster formation mechanism of MSA-MA-SFA-based system at 298.15 K, [MSA] = 10 ⁷ molecules·cm ⁻³ , [MA] = 2.5 × 10 ⁸ molecules·cm ⁻³ , and [SFA] = 10 ⁶ molecules·cm ⁻³ . The black arrows indicate the pure MSA-MA-based growth pathways. Blue arrows represent the pathways containing SFA
S43	Table S6 The Gibbs free energy for the formation of (SFA) _x (MSA) _y (MA) _z ($z \leq x + y \leq 3$) clusters ΔG (kcal·mol ⁻¹) at pressure of 1 atm and temperatures of 298.15, 278.15, 258.15, 238.15 and 218.15 K
S44-S45	Table S7 Evaporation rates γ (s ⁻¹) for the studied clusters at different temperatures of 298.15, 278.15, 258.15, 238.15 and 218.15 K
S46-S47	Table S8 Collision coefficients (β , cm ³ ·s ⁻¹) for each cluster in the present study
S48	Table S9 Total evaporation coefficients ($\sum \gamma$, s ⁻¹) for each cluster in the present study
S49-S50	Table S10 Ratios ($\beta \cdot C / \sum \gamma$) between monomer molecule collisions and evaporation coefficients for each cluster involving SFA in the present study ([MSA] = 1.0 × 10 ⁷ molecules·cm ⁻³ , [MA] = 2.5 × 10 ⁷ molecules·cm ⁻³ , [SFA] = 1.0 × 10 ⁷ molecules·cm ⁻³)
S51	Table S11 The formation rate J of MSA at the conditions of $T = 238.15$ K, [MSA] = 10 ⁶ -10 ⁸ molecules·cm ⁻³ , [MA] = 10 ⁷ -10 ¹¹ molecules·cm ⁻³ , and [SFA] = 0, 10 ⁸ -10 ¹² molecules·cm ⁻³ . MSA, MA and SFA represent sulfuric acid, ammonia and formic acid, respectively
S52	Table S12 The formation rate J of MSA at the conditions of $T = 258.15$ K, [MSA] = 10 ⁶ -10 ⁸ molecules·cm ⁻³ , [MA] = 10 ⁷ -10 ¹¹ molecules·cm ⁻³ , and [SFA] = 0, 10 ⁸ -10 ¹² molecules·cm ⁻³ . MSA, MA and SFA represent sulfuric acid, ammonia and formic acid, respectively
S53	Table S13 The formation rate J of MSA at the conditions of $T = 278.15$ K, [MSA] = 10 ⁶ -10 ⁸ molecules·cm ⁻³ , [MA] = 10 ⁷ -10 ¹¹ molecules·cm ⁻³ , and [SFA] = 0, 10 ⁸ -10 ¹² molecules·cm ⁻³ . MSA, MA and SFA represent sulfuric acid, ammonia and formic acid, respectively
S54	Table S14 The formation rate J of MSA at the conditions of $T = 298.15$ K, [MSA] = 10 ⁶ -10 ⁸ molecules·cm ⁻³ , [MA] = 10 ⁷ -10 ¹¹ molecules·cm ⁻³ , and [SFA] = 0, 10 ⁸ -10 ¹² molecules·cm ⁻³ . MSA, MA and SFA represent sulfuric acid, ammonia and formic acid, respectively
S55-S76	Table S15 Cartesian coordinates of all molecules and clusters in the studied system

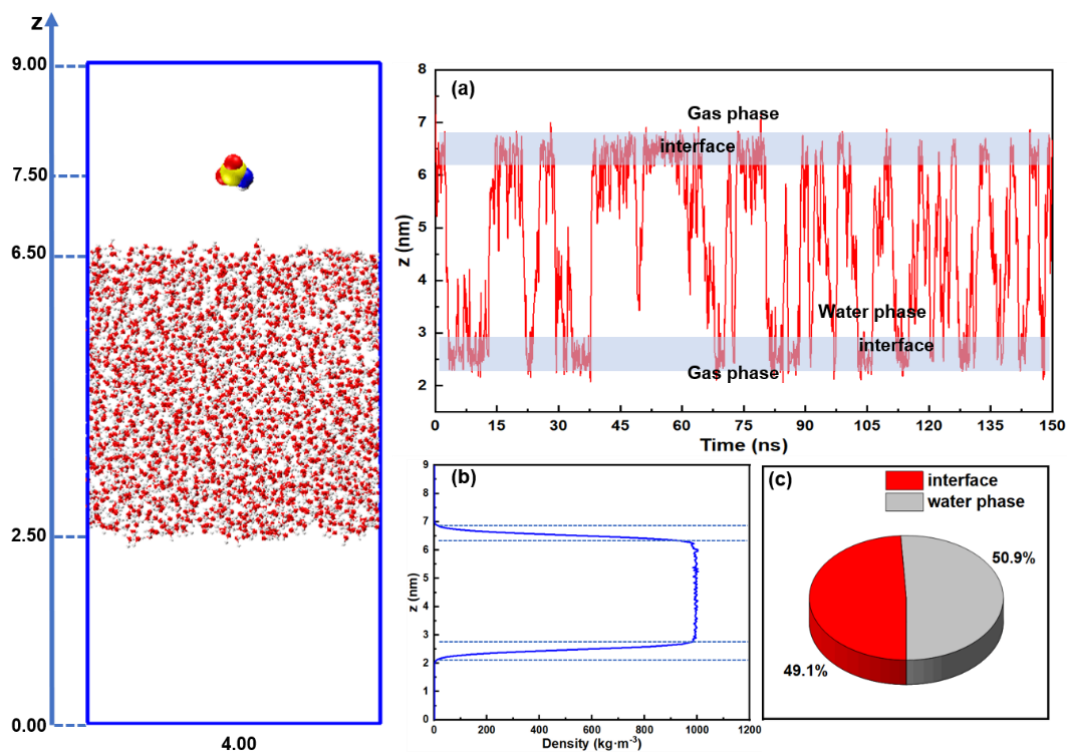


Fig. S1 (a) The z coordinates of HNSO₂ molecule as the function of simulation time; (b) the density profile of water; (c) the pie chart with the occurrence percentages of HNSO₂ molecule at the air-water interface and in water phase

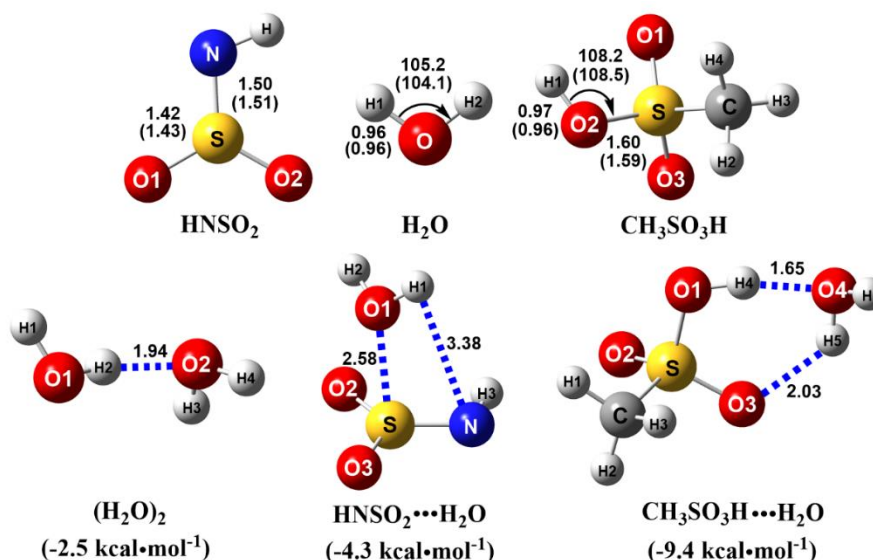


Fig. S2 Optimized geometries of HNSO_2 , H_2O , $\text{CH}_3\text{SO}_3\text{H}$, $(\text{H}_2\text{O})_2$, $\text{HNSO}_2 \cdots \text{H}_2\text{O}$ and $\text{CH}_3\text{SO}_3\text{H} \cdots \text{H}_2\text{O}$ at the M06-2X/6-311++G(2df,2pd) level (bond distances in Angstroms and angles in degrees) along with the stabilization energies of $(\text{H}_2\text{O})_2$, $\text{HNSO}_2 \cdots \text{H}_2\text{O}$ and $\text{CH}_3\text{SO}_3\text{H} \cdots \text{H}_2\text{O}$ at the CCSD(T)-F12/cc-pVDZ-F12//M06-2X/6-311++G(2df,2pd) level of theory

Fig. S2 illustrated the optimized geometries of monomer reactants of HNSO_2 , H_2O and $\text{CH}_3\text{SO}_3\text{H}$, which were consistent with the available experimental bond lengths (Å) and bond angles. The mean absolute deviation of bond lengths (Å) and bond angles ($^\circ$) between the calculations at the M06-2X/6-311++G(2df,2pd) level and the experimental values^{1, 2, 3} were less than 0.01 Å and 1.1° , respectively. As for the dimer reactant of $(\text{H}_2\text{O})_2$, single hydrogen bond geometry has been obtained, which was in good agreement with the previous reports^{4, 5} $\text{HNSO}_2 \cdots \text{H}_2\text{O}$ and $\text{CH}_3\text{SO}_3\text{H} \cdots \text{H}_2\text{O}$ displayed cage-like structures, and these geometrical structures were in good agreement with earlier findings⁶. The stabilization energies of $(\text{H}_2\text{O})_2$, $\text{CH}_3\text{SO}_3\text{H} \cdots \text{H}_2\text{O}$ with respect to the isolated reactants were in the range of -2.5 to -9.4 kcal·mol⁻¹, and these energy values matched well with the earlier findings⁷.

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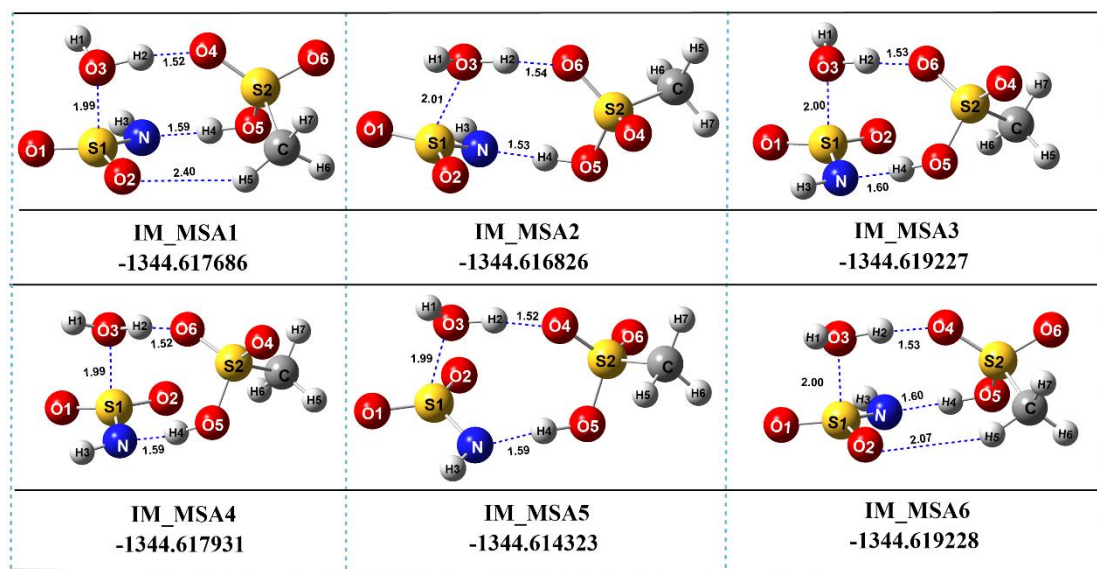


Fig. S3 The optimized geometries and electric energies (in Hartree-Fock) for the complexes of $\text{HNSO}_2 \cdots \text{H}_2\text{O} \cdots \text{CH}_3\text{SO}_3\text{H}$ at the M06-2X/6-311++G(2df,2pd) level of theory

To obtain the most stable configurations of $\text{HNSO}_2 \cdots \text{H}_2\text{O} \cdots \text{CH}_3\text{SO}_3\text{H}$, 500 auto-generated structures were produced by ABCcluster^{1,2} software with TIP4P model^{3,4} for H_2O and CHARMM force field⁵ for HNSO_2 and $\text{CH}_3\text{SO}_3\text{H}$. The generated structures were firstly optimized at the semi-empirical PM7 level by using MOPAC 2016^{6,7}. Then, only structures with the following characteristics were selected and were optimized at the M06-2X/6-311++G(*d,p*) level: (i) the structures contains the $\text{S}(\text{HNSO}_2) \cdots \text{O}(\text{H}_2\text{O})$ interaction of electron donor-acceptor (EDA); (ii) the structures facilitate the transfer of hydrogen atom from H_2O to HNSO_2 . Subsequently, more than 50 isomers with an order of electronic energies were selected for geometry optimization by a relatively high level of M06-2X/6-311G(2*d*,2*p*). Finally, the global minimum isomers within 6.0 kcal·mol⁻¹ were re-optimized by the M06-2X/6-311++G(2*df*,2*pd*) level. As for the reactant complex $\text{HNSO}_2 \cdots \text{H}_2\text{O} \cdots \text{CH}_3\text{SO}_3\text{H}$ its optimized geometries and stabilization energies have been illustrated in Fig. S2. As seen in Fig. S2, seven geometric isomers of $\text{HNSO}_2 \cdots \text{H}_2\text{O} \cdots \text{CH}_3\text{SO}_3\text{H}$ (labeled as IM_MSA*n*, *n* = 1-6) have been optimized at the M06-2X/6-311++G(2*df*,2*pd*) level, where complex IM_MSA1 is the most favorable complex with its binding energy larger by 0.8-3.1 kcal·mol⁻¹ than the other isomers. Based on the stable complex IM_MSA1, Fig. 1 shows the favorable PES profile for the the hydrolysis reaction of HNSO_2 with $\text{CH}_3\text{SO}_3\text{H}$.

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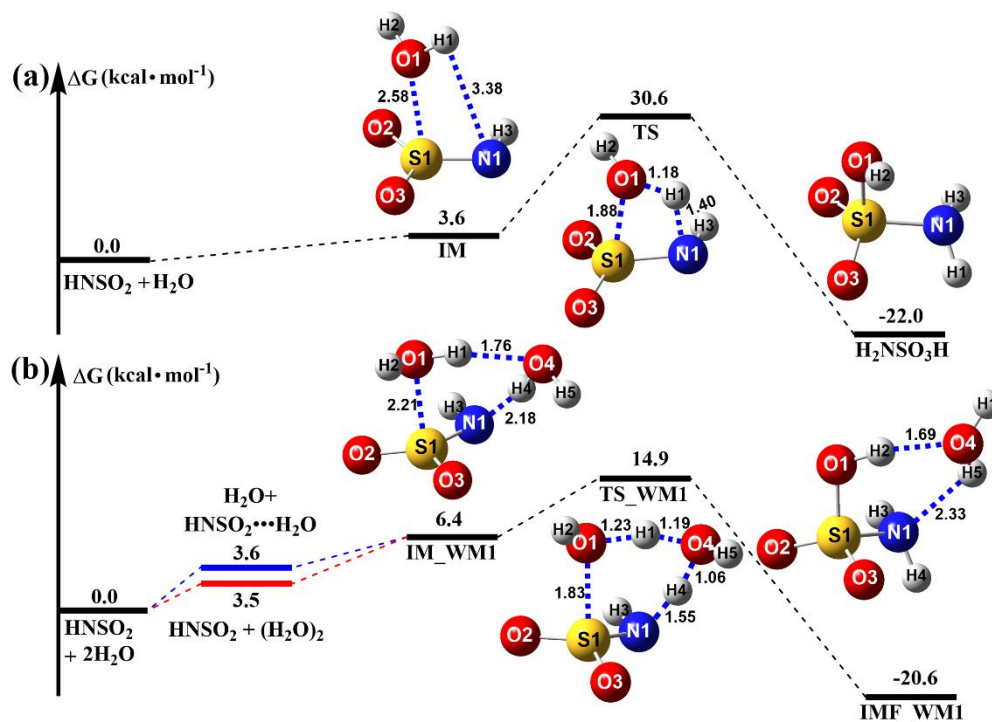


Fig. S4 The potential energy profile (ΔG) for the hydrolysis reaction of HNSO_2 without (a) and with (b) H_2O at the CCSD(T)-F12/cc-pVDZ-F12//M06-2X/6-311++G(2df,2pd) level of theory

92 **Table S1** Zero point energy (ZPE/(kcal·mol⁻¹)), entropies (S/(cal·mol⁻¹·K⁻¹)), relative energies (ΔE
93 and $\Delta(E + \text{ZPE})$ /(kcal·mol⁻¹)), enthalpies ($\Delta H(298)$ /(kcal·mol⁻¹)), and free energies
94 ($\Delta G(298)$ /(kcal·mol⁻¹)) for the hydrolysis reaction of HNSO₂ without and with H₂O and CH₃SO₃H

<i>Species</i>	ZPE	ΔE	S	ΔG	$\Delta(E + \text{ZPE})$	ΔH
HNSO ₂ + H ₂ O	28.7	0.0	110.6	0.0	0.0	0.0
IM	30.3	-6.0	83.2	3.6	-4.4	-4.5
TS	29.2	20.2	71.9	30.6	20.6	19.1
IMF	32.8	-35.9	73.2	-22.0	-31.8	-33.2
HNSO ₂ + 2H ₂ O	42.3	0.0	155.7	0.0	0.0	0.0
HNSO ₂ + (H ₂ O) ₂	44.8	-5.0	133.2	3.5	-2.5	-3.2
HNSO ₂ ···H ₂ O + H ₂ O	43.9	-6.0	128.3	3.6	-4.4	-4.5
IM_WM1	47.5	-17.1 (-20.3) ^a	89.1	6.4	-11.9	-13.5
TS_WM1	45.8	-8.2 (-12.1) ^a	79.8	14.9	-4.7	-7.7
IMF_WM1	48.7	-45.4 (-42.9) ^a	87.1	-20.6	-39.0	-41.0
HNSO ₂ + H ₂ O + CH ₃ SO ₃ H	68.2	0.0	185.4	0.0	0.0	0.0
HNSO ₂ + CH ₃ SO ₃ H···H ₂ O	70.5	-11.7	154.1	-0.9	-9.4	-10.2
HNSO ₂ ···H ₂ O + CH ₃ SO ₃ H	69.7	-6.0	158.0	3.6	-4.4	-4.5
IM_MSA1	72.4	-25.2	107.3	0.8	-21.0	-22.5
TS_MSA1	70.1	-22.9	102.6	1.6	-20.9	-23.1
IMF_MSA1	73.5	-49.3	109.5	-22.6	-44.0	-45.3

95 ^a The value was taken from reference (Manonmani, G., Sandhiya, L., and Senthilkumar, K.: Hydrolysis of HNSO₂:
96 A potential route for atmospheric production of H₂SO₄ and NH₃, Int J Quantum Chem, 120, e26182, 2020.)

Table S2 Equilibrium constants ($\text{cm}^3 \cdot \text{molecule}^{-1}$) for the $\text{HNSO}_2 \cdots \text{H}_2\text{O}$, $\text{H}_2\text{O} \cdots \text{H}_2\text{O}$, and $\text{CH}_3\text{SO}_3\text{H} \cdots \text{H}_2\text{O}$ complexes within the temperature range of 212.6-320.0 K

T/K	$\text{HNSO}_2 \cdots \text{H}_2\text{O}$	$\text{H}_2\text{O} \cdots \text{H}_2\text{O}$	$\text{CH}_3\text{SO}_3\text{H} \cdots \text{H}_2\text{O}$
212.6	7.34×10^{-21}	7.04×10^{-22}	3.71×10^{-16}
229.7	3.55×10^{-21}	4.32×10^{-22}	6.80×10^{-17}
259.3	1.32×10^{-21}	2.22×10^{-22}	5.90×10^{-18}
280.0	7.43×10^{-22}	1.51×10^{-22}	1.56×10^{-18}
290.0	5.85×10^{-22}	1.29×10^{-22}	8.61×10^{-19}
298.15	4.90×10^{-22}	1.14×10^{-22} (2.34×10^{-21}) ^a	5.52×10^{-19}
300.0	4.70×10^{-22}	1.11×10^{-22}	4.95×10^{-19}
310.0	3.84×10^{-22}	9.69×10^{-23}	2.96×10^{-19}
320.0	3.18×10^{-22}	8.56×10^{-23}	1.83×10^{-19}

^a The value was taken from reference (Torrent-Sucarrat, M., Francisco, J. S., and Anglada, J. M.: Sulfuric acid as autocatalyst in the formation of sulfuric acid, J. Am. Chem. Soc., 134, 20632-20644, 2012.)

Table S3 The high-pressure limiting rate constant ($\text{cm}^3 \cdot \text{molecule}^{-1} \cdot \text{s}^{-1}$) for the hydrolysis reaction of HNSO_2 with H_2O and $\text{CH}_3\text{SO}_3\text{H}$ within the temperature range of 212.6-320.0 K

$T(\text{K})$	$\text{HNSO}_2 + \text{H}_2\text{O}$ $\rightarrow \text{HNSO}_2 \cdots \text{H}_2\text{O}$	$\text{HNSO}_2 + \text{H}_2\text{O} \cdots \text{H}_2\text{O}$ $\rightarrow \text{HNSO}_2 \cdots \text{H}_2\text{O} \cdots \text{H}_2\text{O}$	$\text{HNSO}_2 + \text{CH}_3\text{SO}_3\text{H} \cdots \text{H}_2\text{O}$ $\rightarrow \text{HNSO}_2 \cdots \text{CH}_3\text{SO}_3\text{H} \cdots \text{H}_2\text{O}$
212.6	2.06×10^{-10}	1.96×10^{-10}	4.04×10^{-11}
229.7	2.14×10^{-10}	2.03×10^{-10}	4.20×10^{-11}
259.3	2.27×10^{-10}	2.16×10^{-10}	4.46×10^{-11}
280.0	2.36×10^{-10}	2.24×10^{-10}	4.63×10^{-11}
290.0	2.41×10^{-10}	2.28×10^{-10}	4.71×10^{-11}
298.15	2.44×10^{-10}	2.31×10^{-10}	4.78×10^{-11}
300.0	2.45×10^{-10}	2.32×10^{-10}	4.79×10^{-11}
310.0	2.49×10^{-10}	2.36×10^{-10}	4.87×10^{-11}
320.0	2.53×10^{-10}	2.40×10^{-10}	4.95×10^{-11}

Part 1. Calculations of reaction rate coefficients

The rate coefficients for the hydrolysis of HNSO₂ with CH₃SO₃H were calculated through a two-step process. Initially, the high-pressure-limit (HPL) rate coefficients were computed applying VRC-VTST methods within the Polyrate package¹. Subsequently, on the basis of the HPL rate coefficients, the rate coefficients for the hydrolysis of HNSO₂ with CH₃SO₃H were calculated within the temperature range of 212.6-320.0 K and pressures applying the Master Equation Solver for Multi-Energy Well Reactions (MESMER) program². The rate coefficients for the barrierless steps transitioning between reactants and pre-reactive complexes were assessed applying the Inverse Laplace Transform (ILT) method within MESMER calculations³, while the step transitioning between pre-reactive complexes and post-reactive complexes via transition states were evaluated using the RRKM theory⁴ in combination with the asymmetric Eckart model.

The ILT methods and RRKM theory can be respectively expressed in Eq. (S1)-Eq. (S2).

$$k(E) = \frac{W(E-E_0)}{h\rho(E)} \quad (\text{S1})$$

$$k^\infty(\beta) = \frac{1}{Q(\beta)} \int_0^\infty k(E)\rho(E)\exp(-\beta E)dE \quad (\text{S2})$$

In Eq (S1) and Eq (S2), the equation $W(E-E_0)$ represents the rovibrational sum of states (SOS) at the optimized transition state (TS) geometry, where E_0 signifies the reaction threshold energy; h represents Planck's constant, $\rho(E)$ denotes the density of rovibrational states of the reactant and $Q(\beta)$ is the corresponding canonical partition function. Additionally, electronic geometries, vibrational frequencies, and rotational constants were computed at the M06-2X/6-311++G(2df,2pd) level, while single-point energy calculations were refined at the CCSD(T)-F12/cc-pVDZ-F12 level.

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2. Glowacki, D. R., Liang, C.-H., Morley, C., Pilling, M. J., and Robertson, S. H.: MESMER: an open-source master equation solver for multi-energy well reactions, *J. Phys. Chem. A*, 116, 9545-9560, 2012.
3. Horváth, G., Horváth, I., Almousa, S. A. D., and Telek, M.: Numerical inverse Laplace transformation using concentrated matrix exponential distributions, *Perform. Evaluation.*, 137, 102067, 2020.
4. Mai, T. V. T., Duong, M. V., Nguyen, H. T., and Huynh, L. K.: Ab initio kinetics of the HOSO₂ + ³O₂ → SO₃ + HO₂ reaction, *Phys. Chem. Chem. Phys.*, 20, 6677-6687, 2018.

Table S4 Rate coefficients (k , $\text{cm}^3 \cdot \text{molecule}^{-1} \cdot \text{s}^{-1}$) for the hydrolysis of HNSO_2 by master equation within the temperature range of 212.6-320.0 K

T/K	k_{R}
212.6	2.55×10^{-28}
229.7	3.78×10^{-28}
259.3	1.04×10^{-27}
280.0	2.70×10^{-27}
290.0	4.53×10^{-27}
298.0	7.02×10^{-27}
300.0	7.86×10^{-27}
310.0	1.39×10^{-26}
320.0	2.50×10^{-26}

k_{R} is the bimolecular rate constant for the hydrolysis of HNSO_2 .

136 **Table S5** Concentrations (molecules·cm⁻³) of H₂O and CH₃SO₃H within the temperature range of 213-320 K and altitude range of 0-15 km

Altitude		0 km						5 km	10 km	15 km
T/K	RH	280.0	290.0	298.0	300.0	310.0	320.0	259.3	229.7	212.6
[H ₂ O]	20%RH ^a	5.16 × 10 ¹⁶	9.60 × 10 ¹⁶	1.50 × 10 ¹⁷	1.72 × 10 ¹⁷	2.92 × 10 ¹⁷	4.70 × 10 ¹⁷			
	40%RH ^a	1.03 × 10 ¹⁷	1.91 × 10 ¹⁷	3.10 × 10 ¹⁷	3.43 × 10 ¹⁷	5.84 × 10 ¹⁷	9.40 × 10 ¹⁷			
	60%RH ^a	1.55 × 10 ¹⁷	2.87 × 10 ¹⁷	4.50 × 10 ¹⁷	5.15 × 10 ¹⁷	8.77 × 10 ¹⁷	1.41 × 10 ¹⁸	2.70 × 10 ¹²	2.30 × 10 ¹¹	6.30 × 10 ⁶
	80%RH ^a	2.07 × 10 ¹⁷	3.82 × 10 ¹⁷	6.20 × 10 ¹⁷	6.86 × 10 ¹⁷	1.17 × 10 ¹⁸	1.88 × 10 ¹⁸			
	100%RH ^a	2.58 × 10 ¹⁷	4.78 × 10 ¹⁷	7.70 × 10 ¹⁷	8.58 × 10 ¹⁷	1.46 × 10 ¹⁸	2.35 × 10 ¹⁸			
[MSA] ^b = 10 ⁴ -10 ⁹										

137 ^a The value was taken from reference (Anglada, J.M., Hoffman, G.J., Slipchenko, L.V., M. Costa, M., Ruiz-Lopez, M.F., and Francisco, J.S., Atmospheric significance of water clusters and ozone-
138 water complexes. J. Phys. Chem. A 117, 10381-10396, 2013.)
139 ^b The value was taken from reference (Shen, J., Elm, J., Xie, H.-B., Chen, J., Niu, J., and Vehkamäki, H.: Structural effects of amines in enhancing methanesulfonic acid-driven new particle
140 formation, Environ. Sci. Technol., 54, 13498-13508, 2020.)

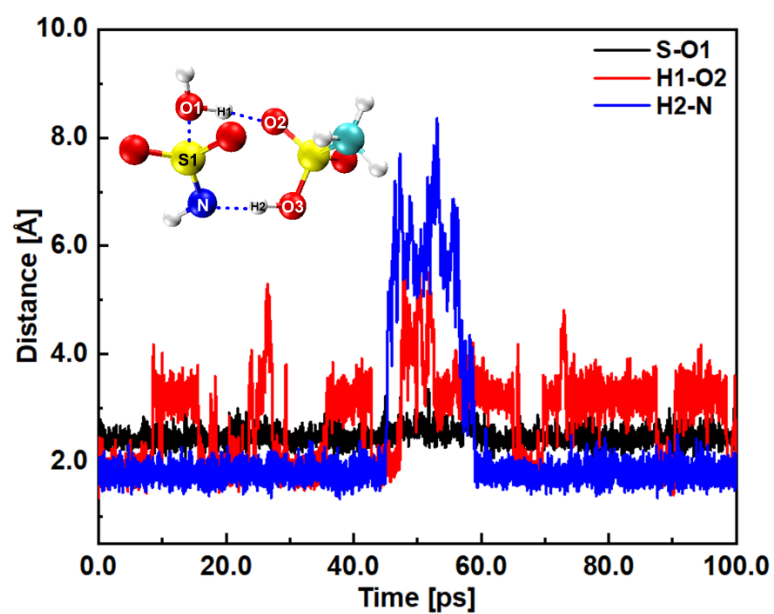


Fig. S5 The dynamic trajectories of CH₃SO₃H-assisted gaseous hydrolysis of HNSO₂

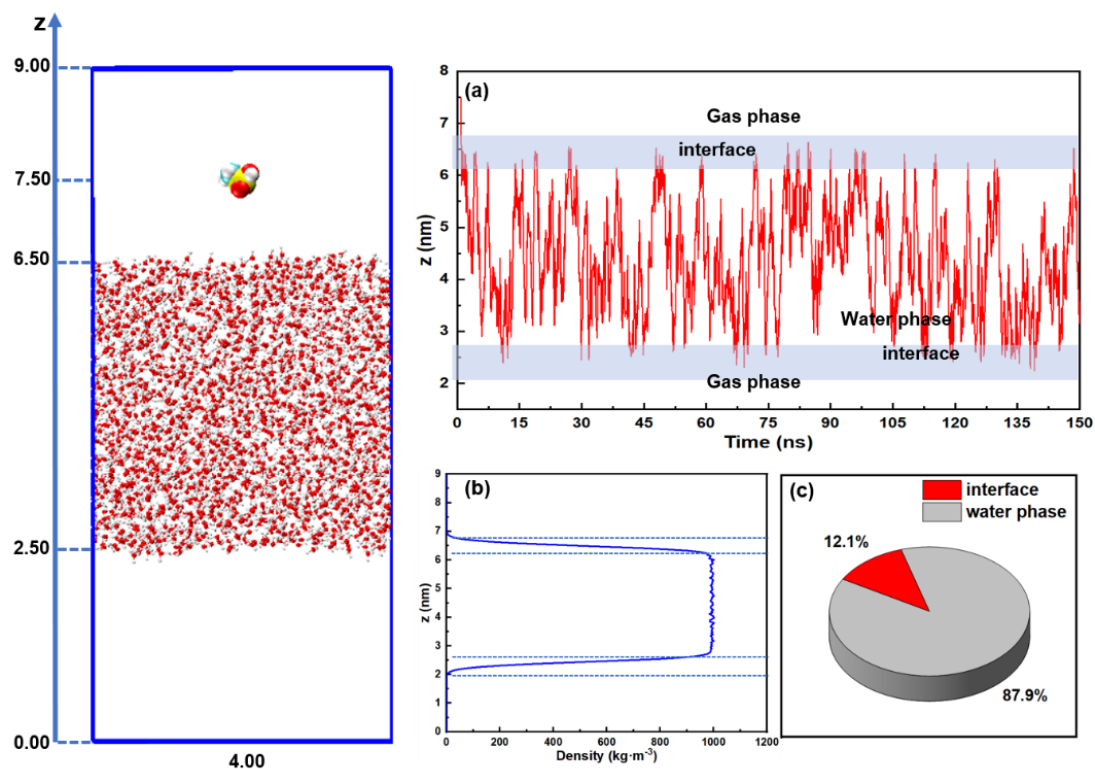


Fig. S6 (a) The z coordinates of MSA molecule as the function of simulation time; (b) the density profile of water; (c) the pie chart with the occurrence percentages of MSA molecule at the air-water interface and in water phase

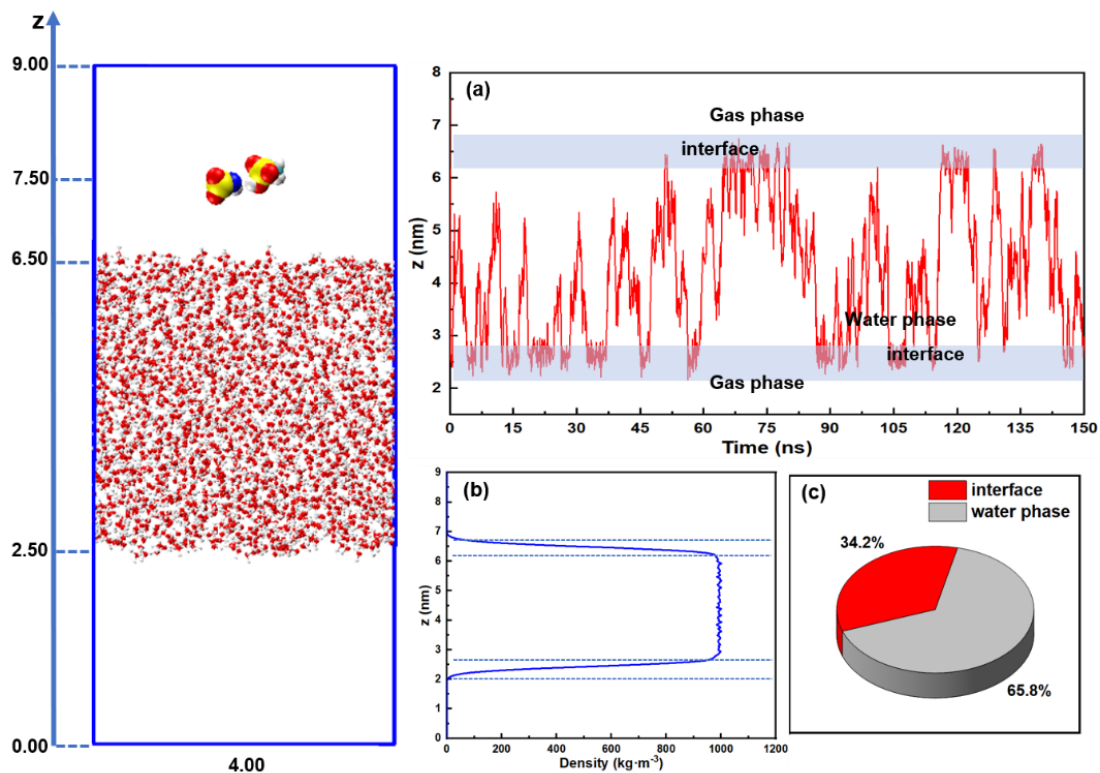


Fig. S7 (a) The z coordinates of complex $\text{HNSO}_2 \cdots \text{CH}_3\text{SO}_3\text{H}$ as the function of simulation time; (b) the density profile of water; (c) the pie chart with the occurrence percentages of complex $\text{HNSO}_2 \cdots \text{CH}_3\text{SO}_3\text{H}$ at the air-water interface and in water phase

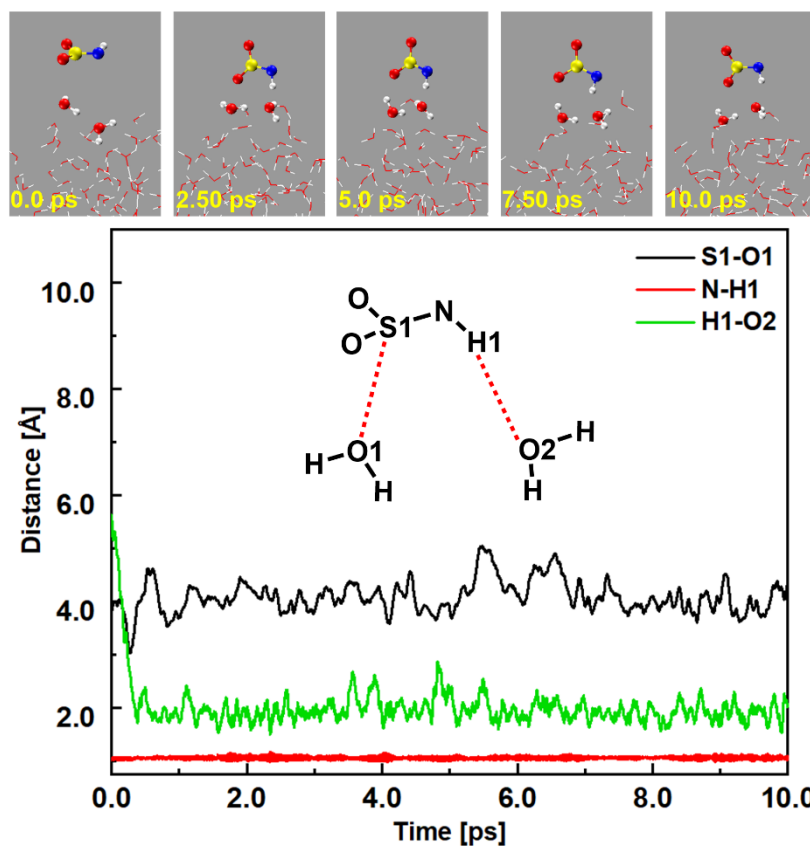


Fig. S8 Snapshot structures taken from the BOMD simulations of HNSO₂ reaction at the air-water interface

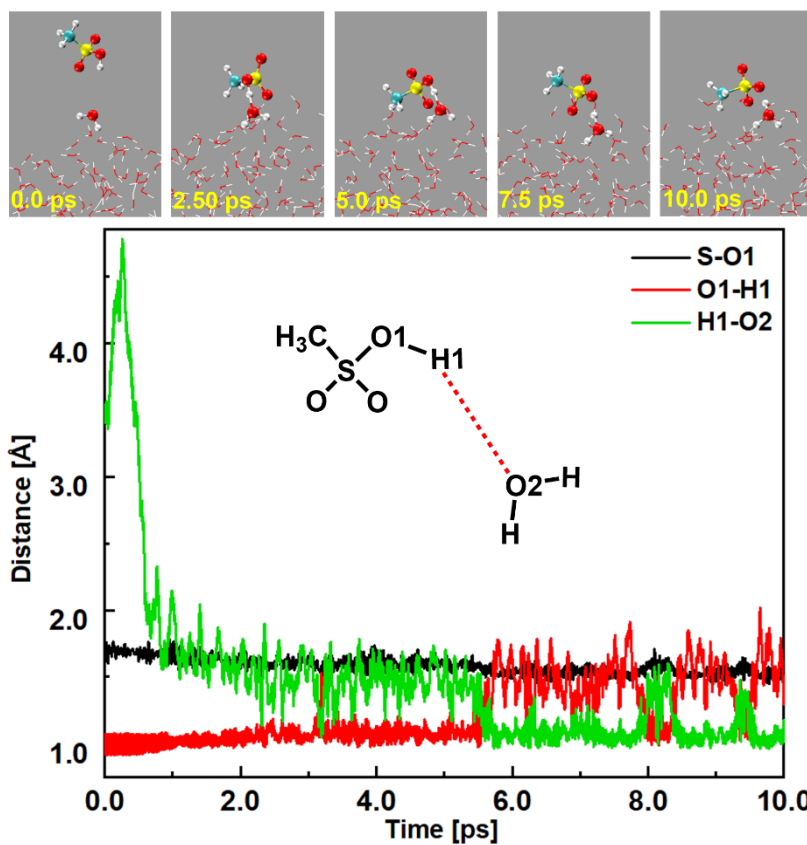
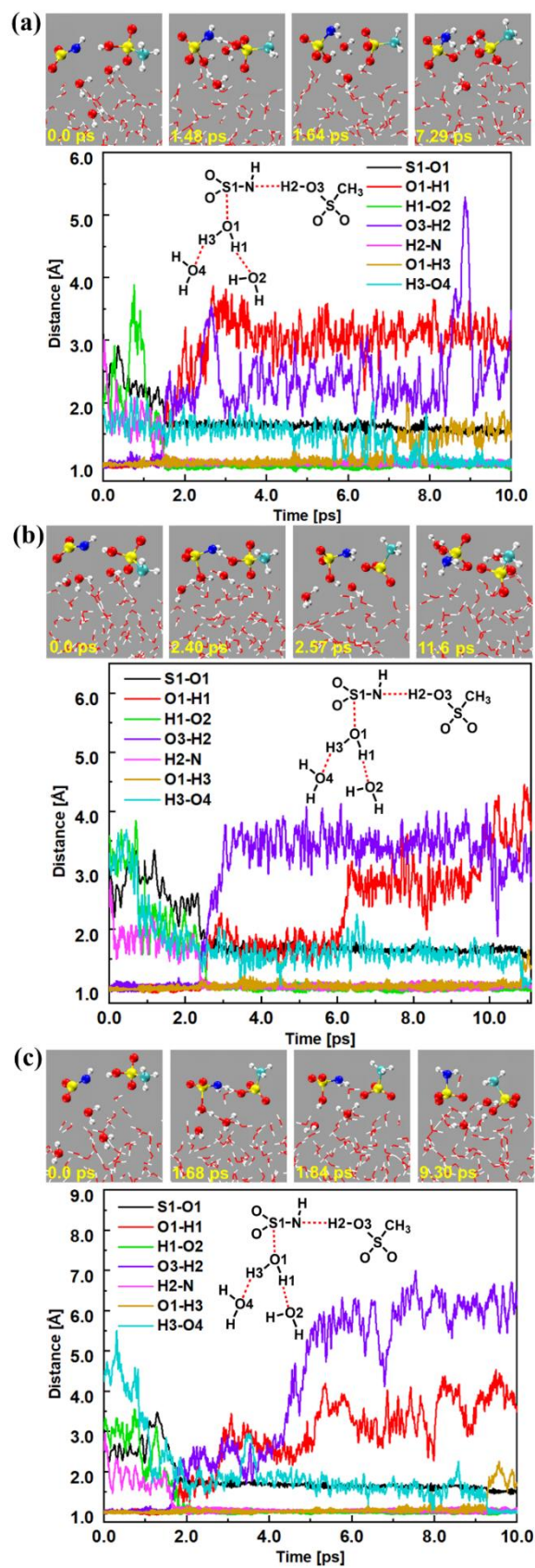
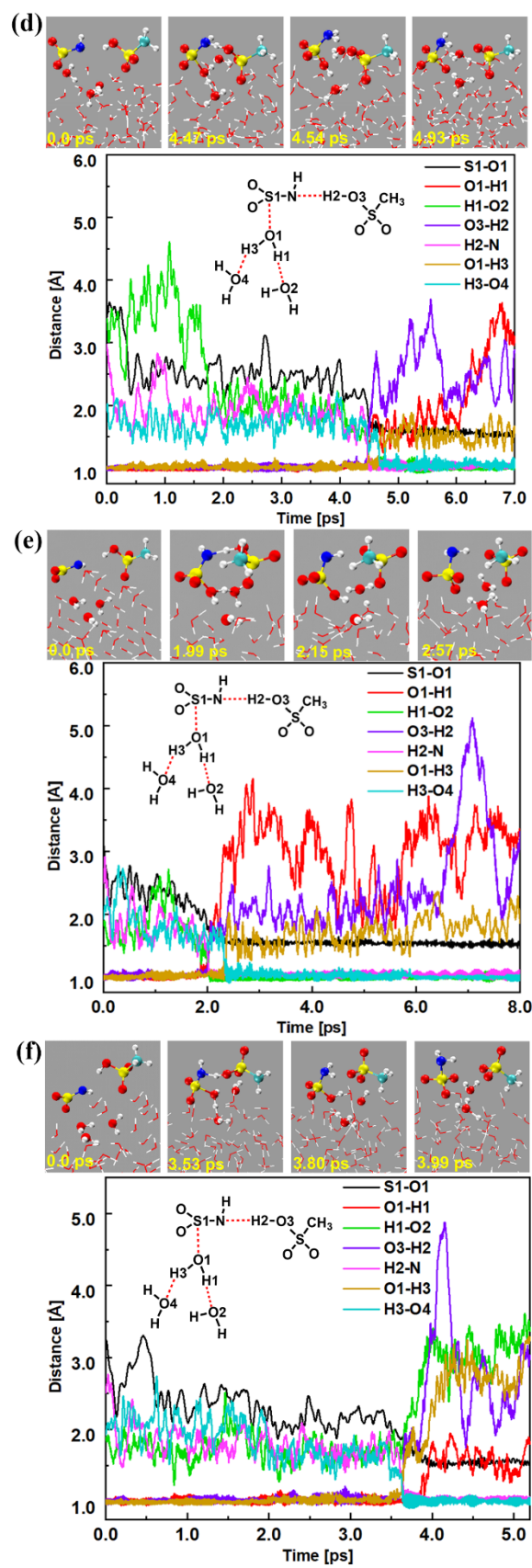
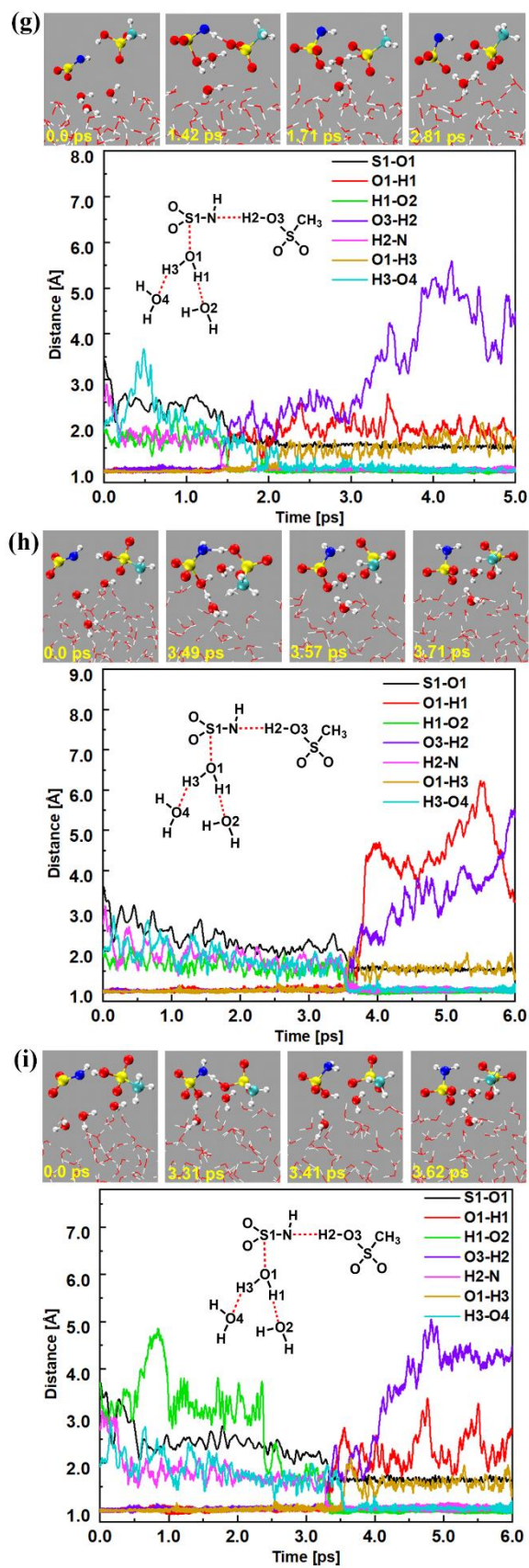


Fig. S9 Snapshot structures taken from the BOMD simulations of $\text{CH}_3\text{SO}_3\text{H}$ reaction at the air-water interface







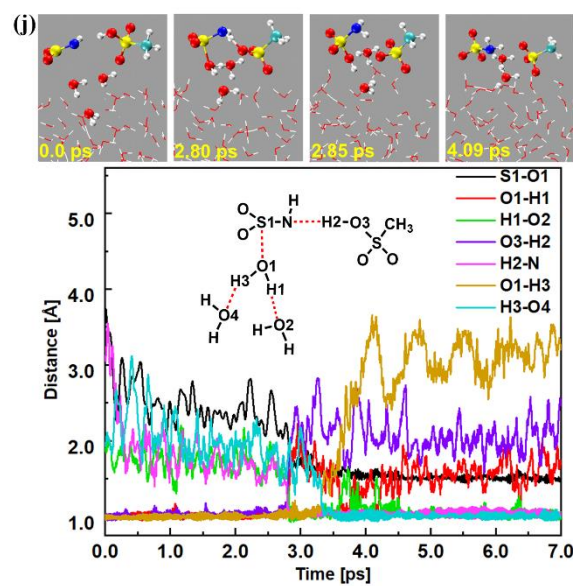
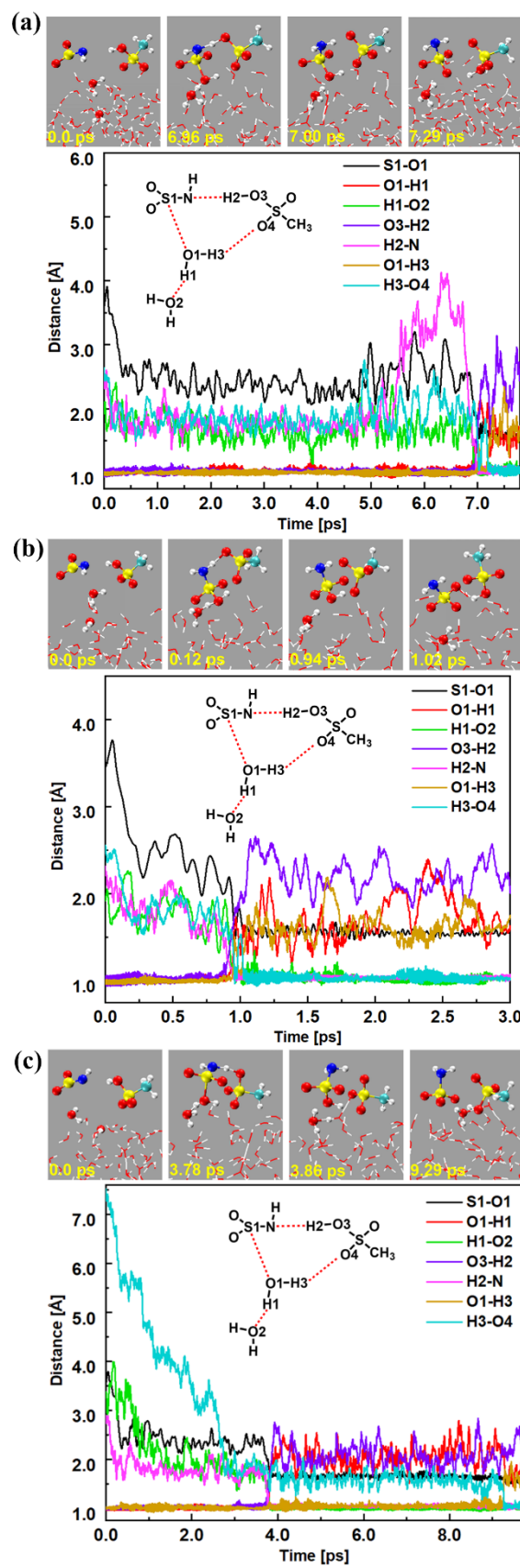
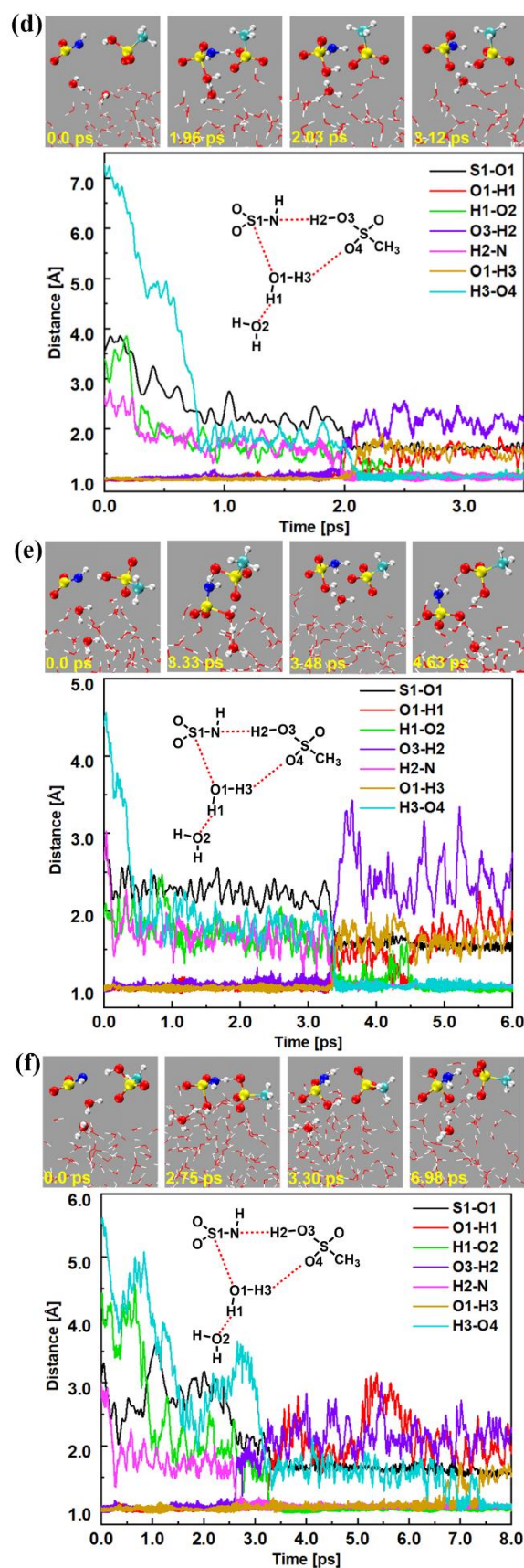


Fig. S10 BOMD simulation trajectories and snapshots of $\text{CH}_3\text{SO}_3\text{H}^-$ and H_3O^+ ions forming mechanism via the chain structure routes in $\text{CH}_3\text{SO}_3\text{H}$ -mediated hydration HNSO_2 at the air-water interface





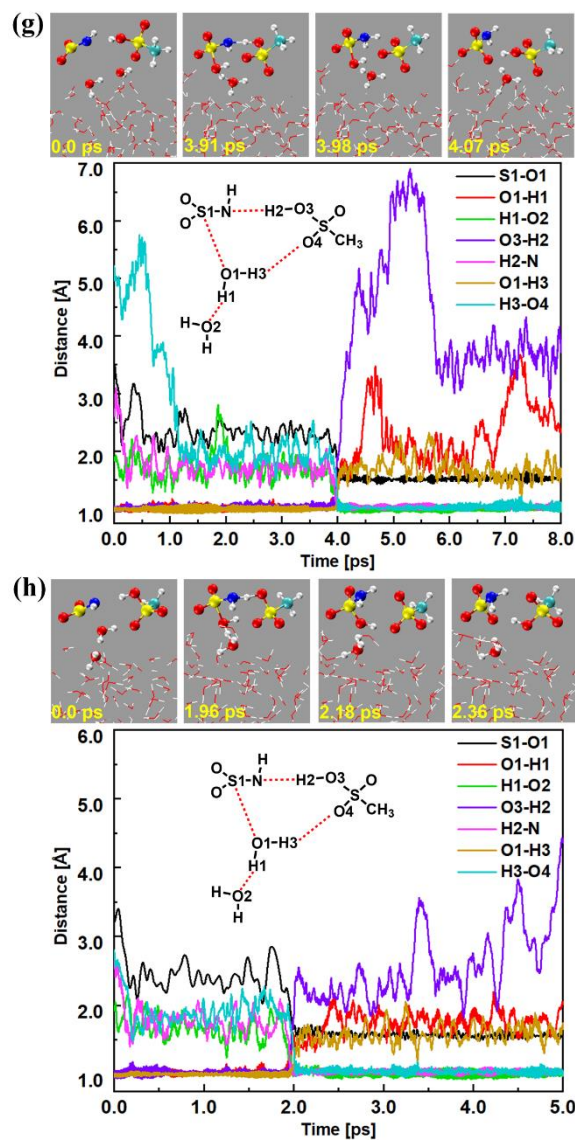
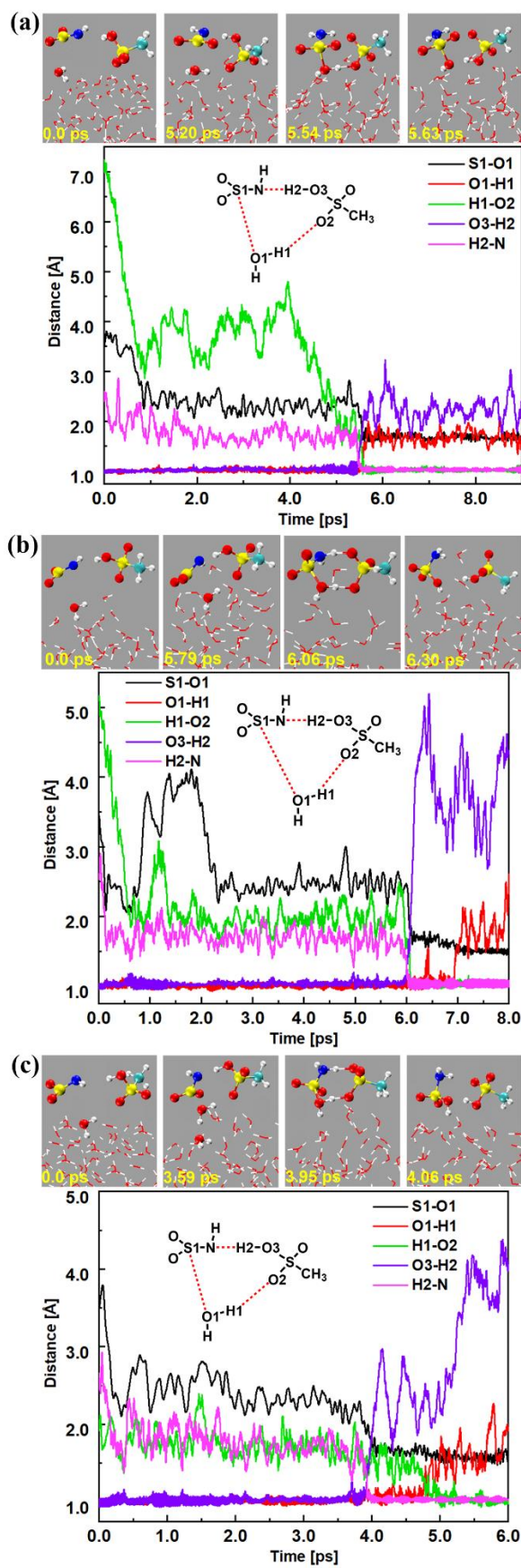


Fig. S11 BOMD simulation trajectories and snapshots of $\text{CH}_3\text{SO}_3\text{H}^-$ and H_3O^+ ions forming mechanism via loop structure routes in $\text{CH}_3\text{SO}_3\text{H}$ -mediated hydration HNSO_2 at the air-water interface



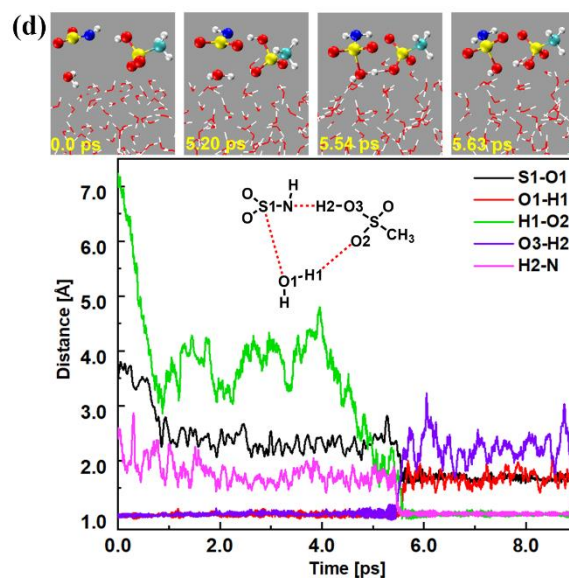
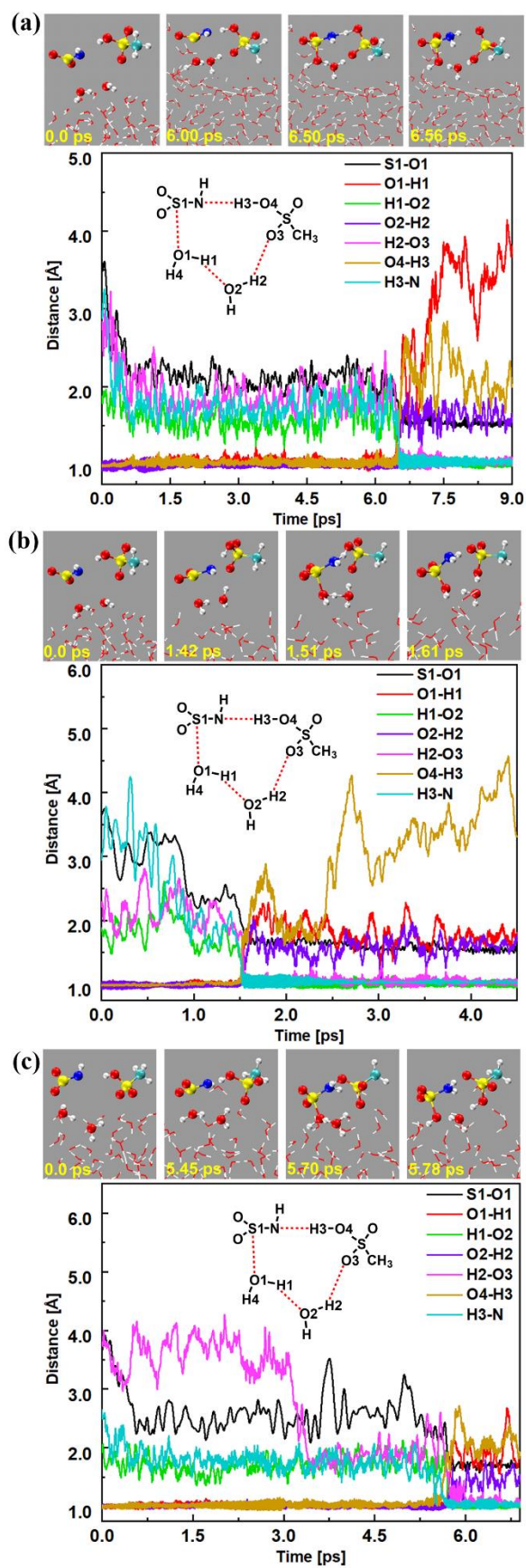
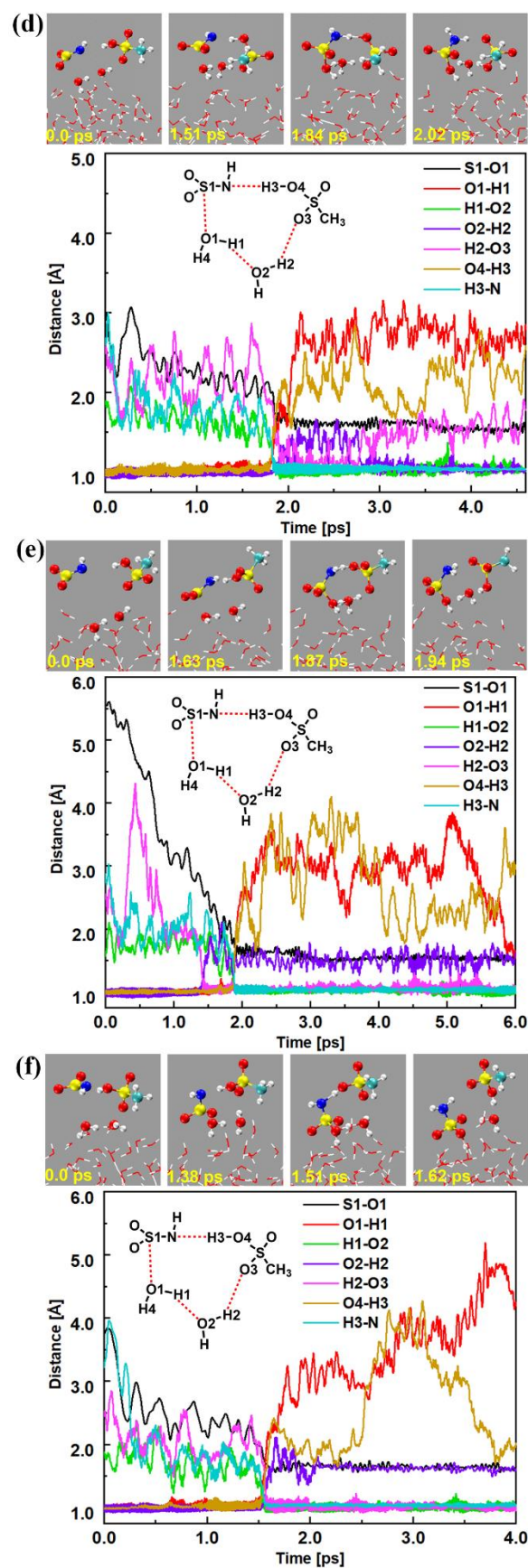
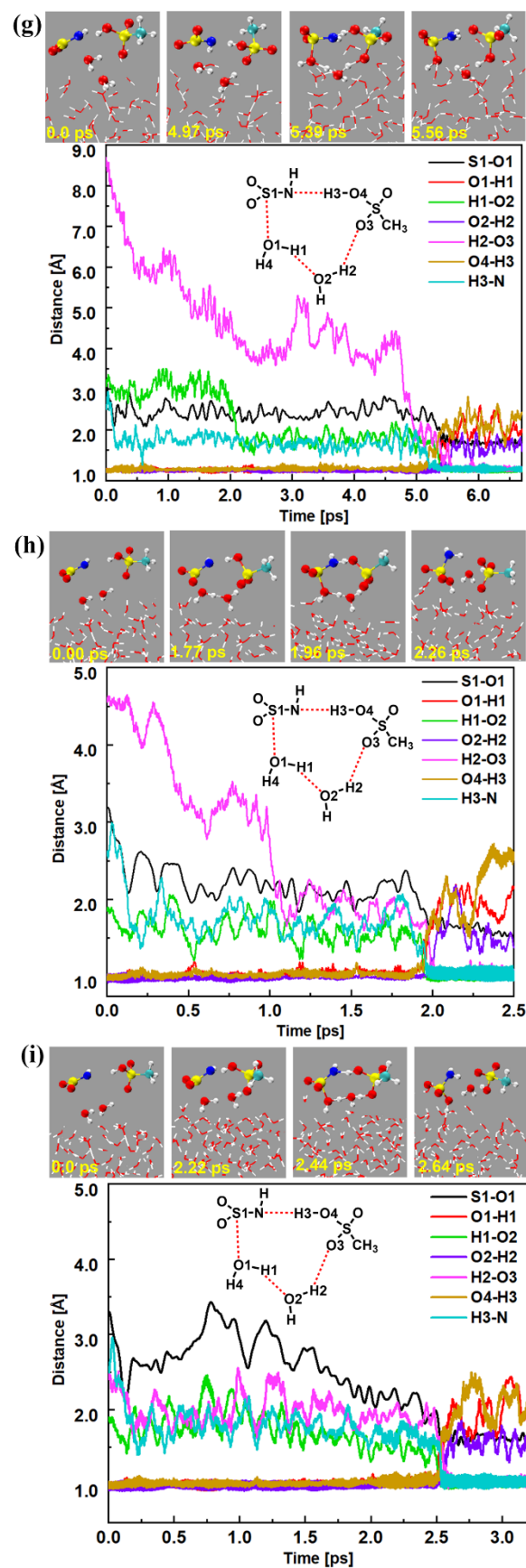
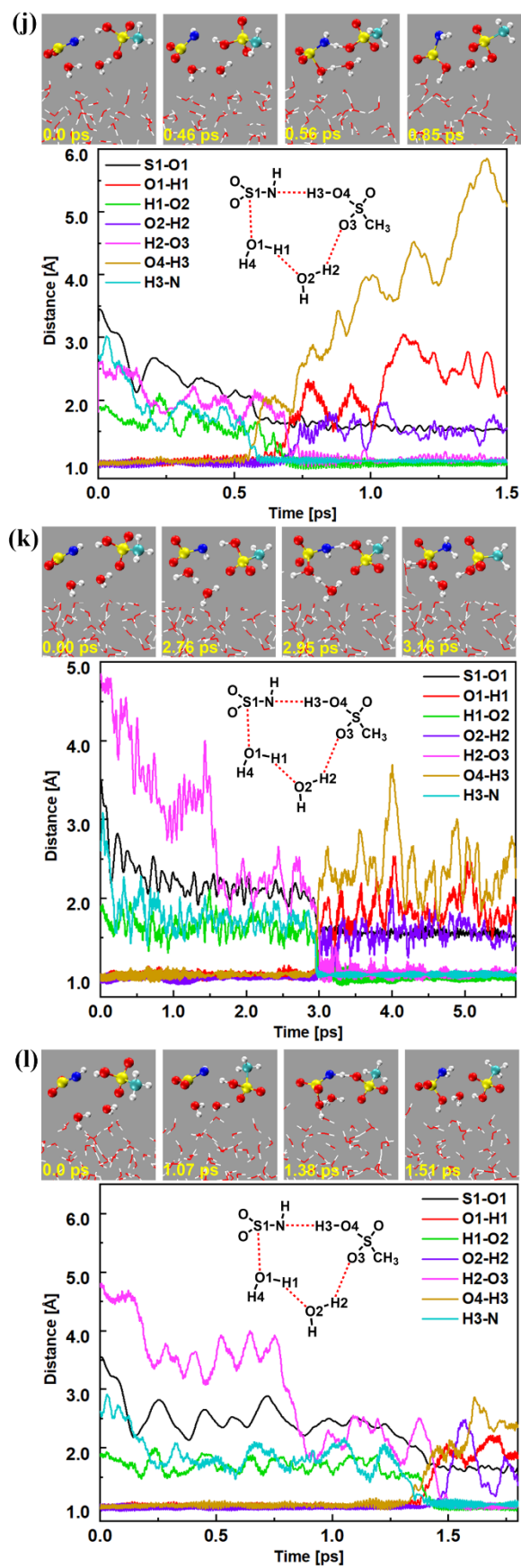


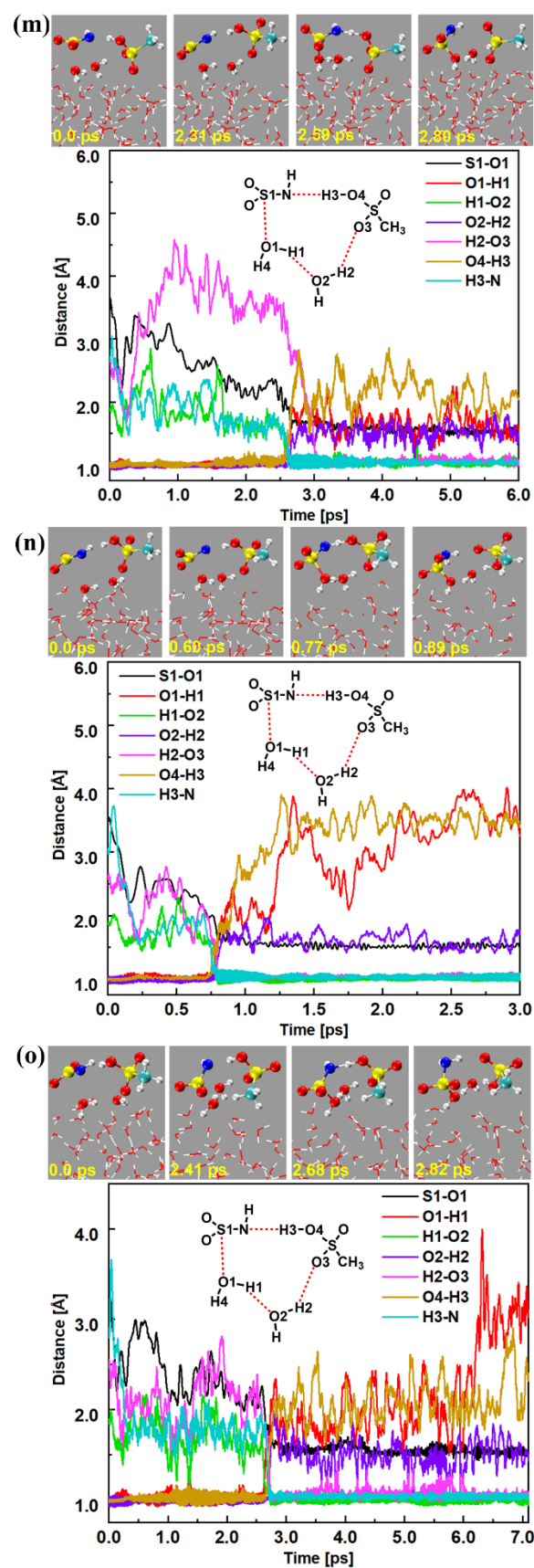
Fig. S12 BOMD simulation trajectories and snapshots of proton exchange mechanism in $\text{CH}_3\text{SO}_3\text{H}$ -mediated hydration HNSO_2 with a water molecule at the air-water interface

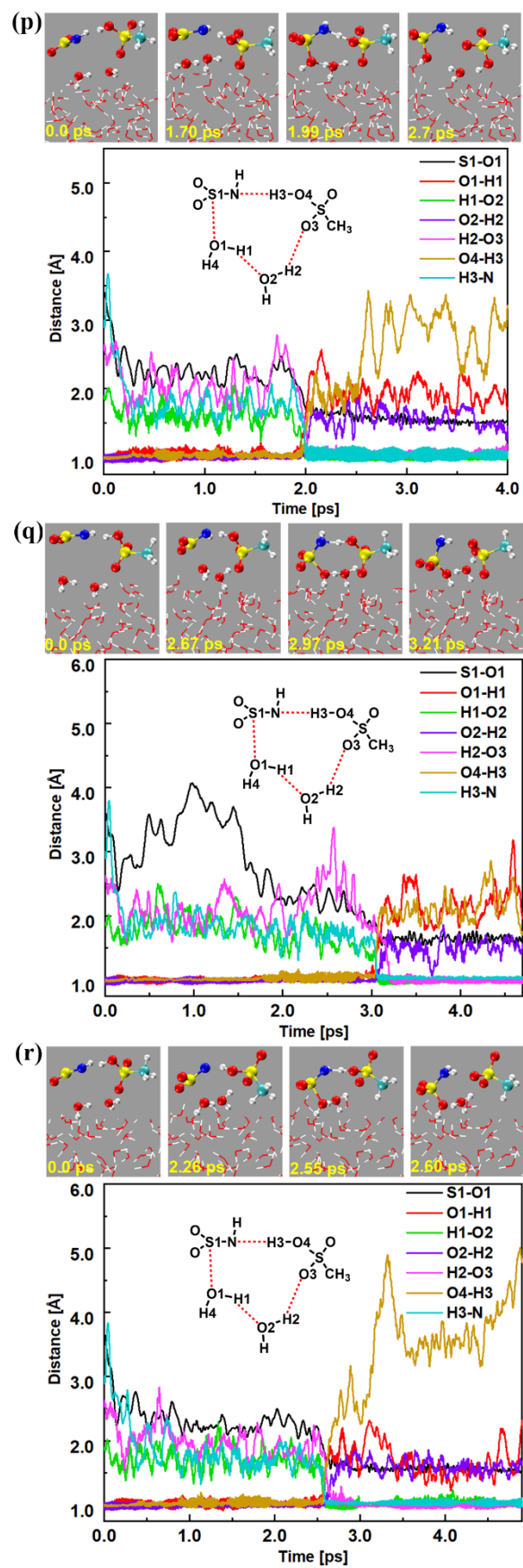












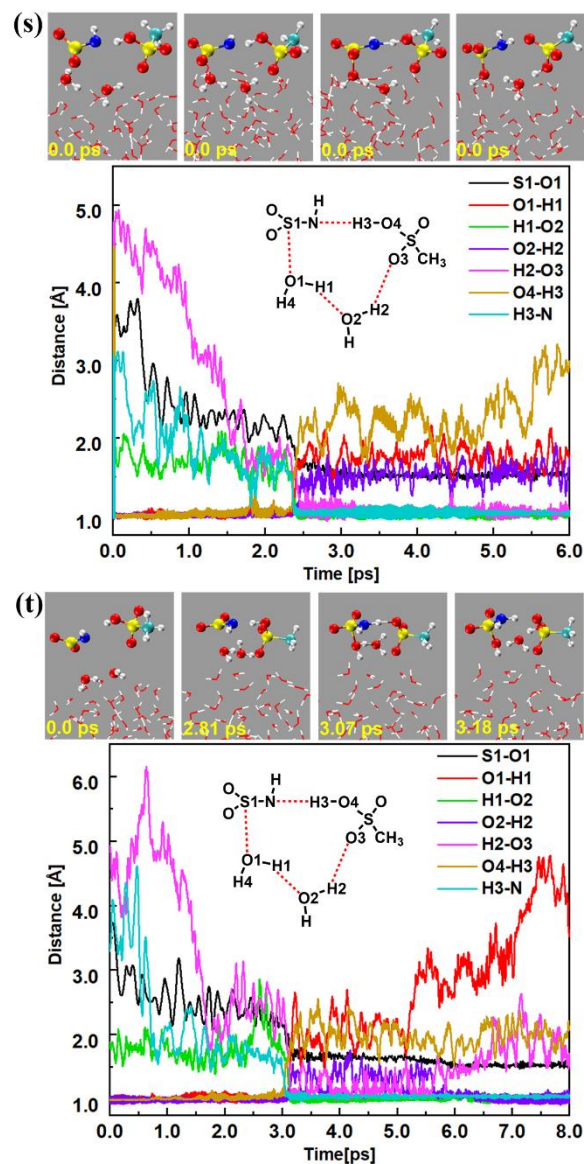
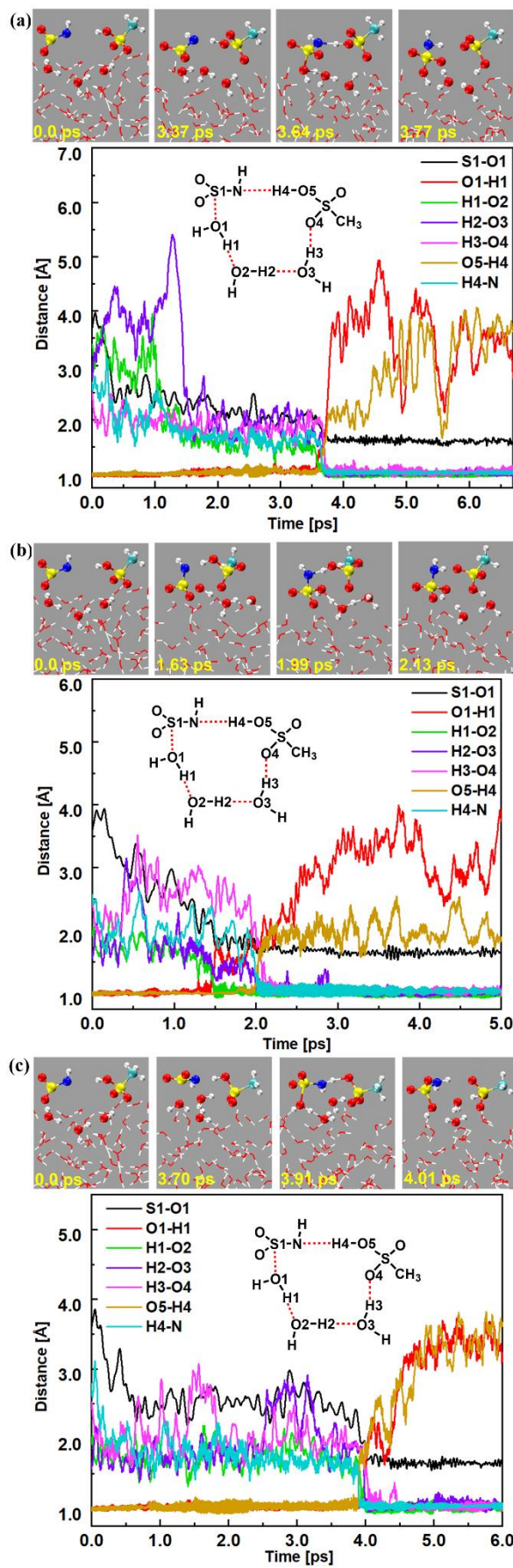


Fig.S13 BOMD simulation trajectories and snapshots of proton exchange mechanism in $\text{CH}_3\text{SO}_3\text{H}$ -mediated hydration HNSO_2 with two water molecules at the air-water interface



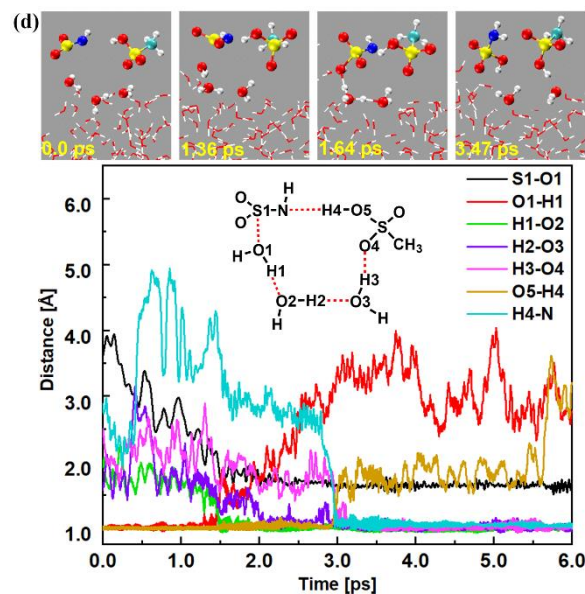


Fig. S14 BOMD simulation trajectories and snapshots of proton exchange mechanism in $\text{CH}_3\text{SO}_3\text{H}$ -mediated hydration HNSO_2 with three water molecules at the air-water interface

SFA · MSA	SFA · MA	SFA · MSA · MA	(SFA) ₂ · MSA
SFA · (MSA) ₂	(SFA) ₂ · MA	(SFA) ₂ · MSA · MA	SFA · (MSA) ₂ · MA
(SFA) ₃ · MA	SFA · MSA · (MA) ₂	(SFA) ₂ · (MA) ₂	(SFA) ₂ · MSA · (MA) ₂
SFA · (MSA) ₂ · (MA) ₂	(SFA) ₃ · (MA) ₂	(SFA) ₂ · MSA · (MA) ₃	(SFA) ₃ · (MA) ₃

Fig. S15 The most stable configurations of the SFA-MSA-MA-based clusters identified at the M06-2X/6-311++G(2df,2pd) level of theory. The lengths of hydrogen bonds are given in Å (Color code: blue = nitrogen, yellow = sulfur, red = oxygen, gray = carbon, and white = hydrogen)

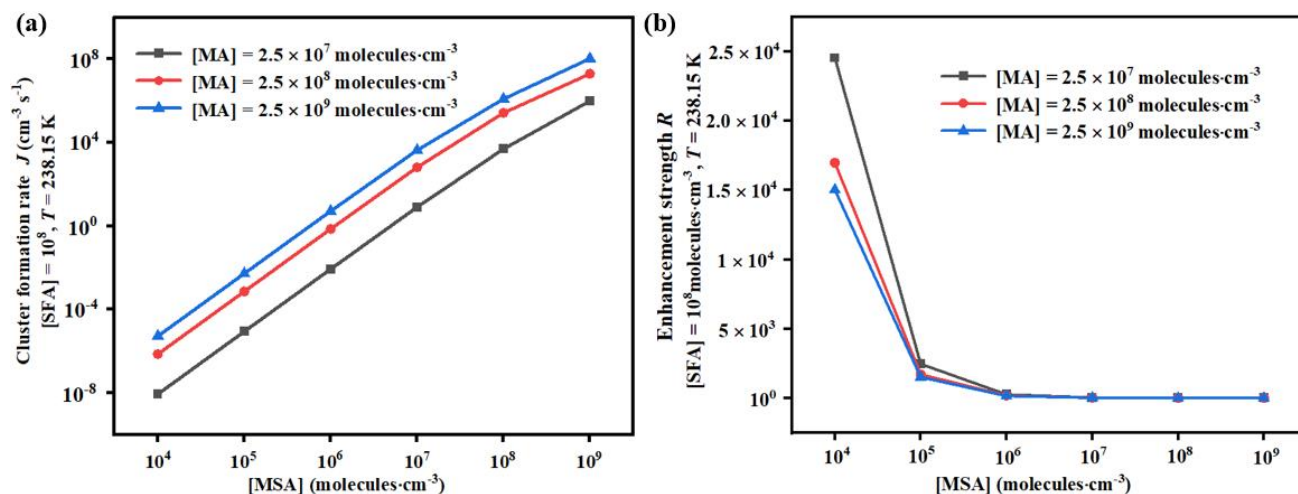


Fig. S16 (a) The J ($\text{cm}^{-3} \text{s}^{-1}$) and (b) R as a function of $[\text{MSA}]$ with $[\text{SFA}] = 10^8$ molecules cm^{-3} and three different $[\text{MA}]$ (black line: $[\text{MA}] = 2.5 \times 10^7$ molecules cm^{-3} , red line: $[\text{MA}] = 2.5 \times 10^8$ molecules cm^{-3} , blue line: $[\text{MA}] = 2.5 \times 10^9$ molecules cm^{-3}) at 238.15 K

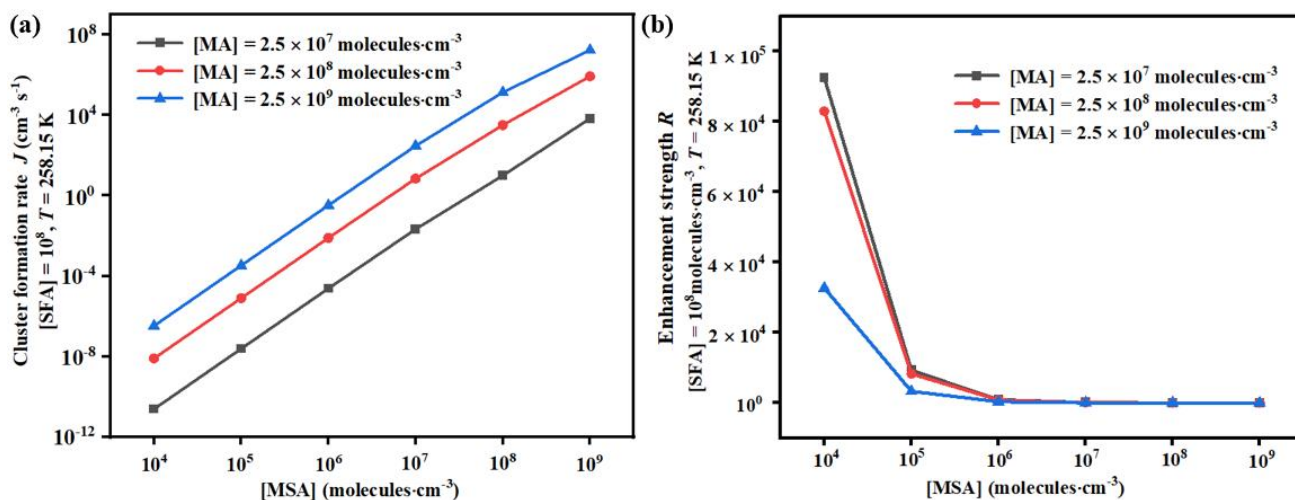


Fig. S17 (a) The J ($\text{cm}^{-3} \text{s}^{-1}$) and (b) R as a function of $[\text{MSA}]$ with $[\text{SFA}] = 10^8$ molecules cm^{-3} and three different $[\text{MA}]$ (black line: $[\text{MA}] = 2.5 \times 10^7$ molecules cm^{-3} , red line: $[\text{MA}] = 2.5 \times 10^8$ molecules cm^{-3} , blue line: $[\text{MA}] = 2.5 \times 10^9$ molecules cm^{-3}) at 258.15 K

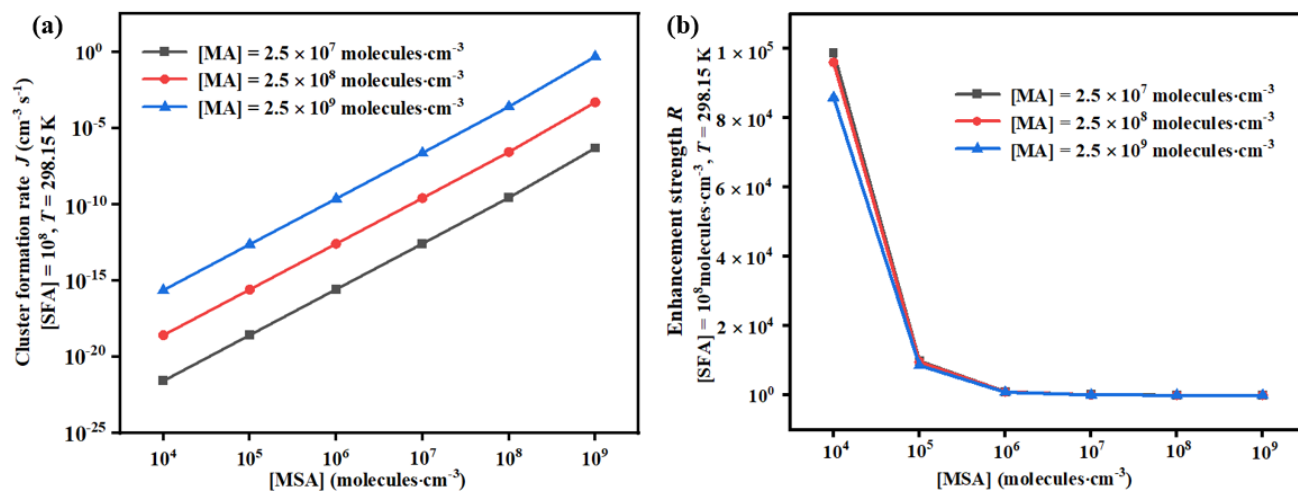


Fig. S18 (a) The J ($\text{cm}^{-3} \text{s}^{-1}$) and (b) R as a function of $[MSA]$ with $[SFA] = 10^8$ molecules cm^{-3} and three different $[MA]$ (black line: $[MA] = 2.5 \times 10^7$ molecules cm^{-3} , red line: $[MA] = 2.5 \times 10^8$ molecules cm^{-3} , blue line: $[MA] = 2.5 \times 10^9$ molecules cm^{-3}) at 298.15 K

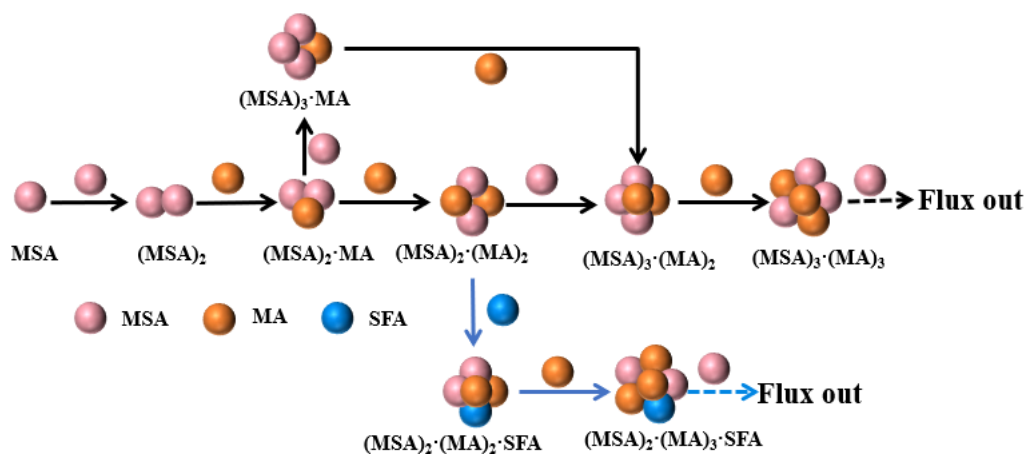


Fig. S19 Main cluster formation mechanism of MSA-MA-SFA-based system at 238.15 K, $[\text{MSA}] = 10^7$ molecules $\cdot\text{cm}^{-3}$, $[\text{MA}] = 2.5 \times 10^8$ molecules $\cdot\text{cm}^{-3}$, and $[\text{SFA}] = 10^6$ molecules $\cdot\text{cm}^{-3}$. The black arrows indicate the pure MSA-MA-based growth pathways. Blue arrows represent the pathways containing SFA

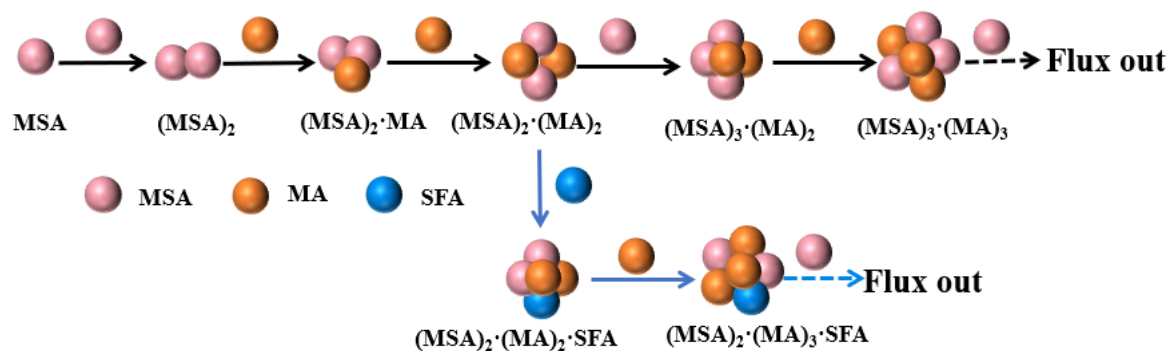


Fig. S20 Main cluster formation mechanism of MSA-MA-SFA-based system at 258.15 K, $[\text{MSA}] = 10^7$ molecules $\cdot\text{cm}^{-3}$, $[\text{MA}] = 2.5 \times 10^8$ molecules $\cdot\text{cm}^{-3}$, and $[\text{SFA}] = 10^6$ molecules $\cdot\text{cm}^{-3}$. The black arrows indicate the pure MSA-MA-based growth pathways. Blue arrows represent the pathways containing SFA

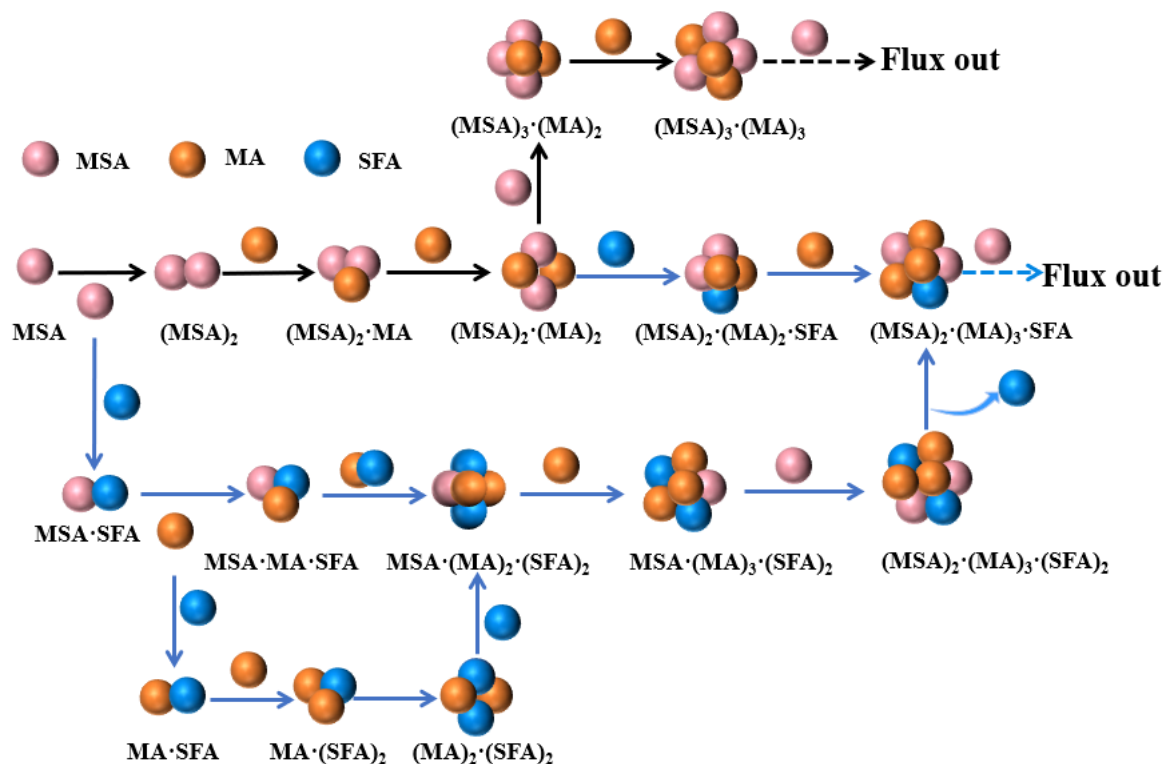


Fig. S21 Main cluster formation mechanism of MSA-MA-SFA-based system at 298.15 K, $[\text{MSA}] = 10^7$ molecules $\cdot\text{cm}^{-3}$, $[\text{MA}] = 2.5 \times 10^8$ molecules $\cdot\text{cm}^{-3}$, and $[\text{SFA}] = 10^6$ molecules $\cdot\text{cm}^{-3}$. The black arrows indicate the pure MSA-MA-based growth pathways. Blue arrows represent the pathways containing SFA

Table S6 The Gibbs free energy for the formation of $(\text{SFA})_x(\text{MSA})_y(\text{MA})_z$ ($z \leq x + y \leq 3$) clusters ΔG (kcal·mol⁻¹) at pressure of 1 atm and temperatures of 298.15, 278.15, 258.15, 238.15 and 218.15 K

Clusters	$T = 298.15$ K	$T = 278.15$ K	$T = 258.15$ K	$T = 238.15$ K
MSA·MA	-6.19 (-5.32) ^a	-6.87	-7.56	-8.25
(MSA) ₂	-8.51 (-6.76) ^a	-9.27	-10.03	-10.79
(MSA) ₂ ·MA	-21.17 (-20.36) ^a	-22.74	-24.31	-25.89
(MSA) ₂ ·(MA) ₂	-34.05 (-34.97) ^a	-36.31	-38.59	-40.86
(MSA) ₃	-11.44 (-11.31) ^a	-13.06	-14.69	-16.32
(MSA) ₃ ·MA	-30.29 (-31.68) ^a	-32.67	-35.06	-37.46
(MSA) ₃ ·(MA) ₂	-46.76 (-46.45) ^a	-49.82	-52.90	-55.98
(MSA) ₃ ·(MA) ₃	-59.17 (-59.33) ^a	-63.17	-67.19	-71.22
(SFA) ₂	-5.74(-5.76) ^b	-6.53	-7.32	-8.11
MA·SFA	-6.01	-6.73	-7.45	-8.17
(MA) ₂ ·(SFA) ₂	-31.26	-33.53	-35.81	-38.09
MA·(SFA) ₂	-23.85	-25.37	-26.90	-28.48
MSA·SFA	-9.33	-10.13	-10.93	-11.73
MSA·MA·SFA	-21.96	-23.57	-25.18	-26.79
MSA·(MA) ₂ ·SFA	-26.08	-28.48	-30.89	-33.31
(SFA) ₃	-11.87	-13.56	-15.27	-16.97
MSA ₂ ·MA·SFA	-24.29	-26.66	-29.05	-31.44
(MSA) ₂ ·(MA) ₂ ·SFA	-44.62	-47.82	-51.03	-54.25
(MSA) ₂ ·(MA) ₃ ·SFA	-57.46	-61.43	-65.42	-69.41
MSA·(SFA) ₂	-12.26	-13.89	-15.52	-17.15
MA·(SFA) ₃	-29.46	-32.01	-34.57	-37.13
MSA·(MA) ₂ ·(SFA) ₂	-45.12	-48.25	-51.39	-54.53
(MSA) ₂ ·SFA	-9.11	-10.75	-12.40	-14.06
MSA·MA·(SFA) ₂	-31.11	-33.56	-36.01	-38.47
(MA) ₂ ·(SFA) ₃	-44.04	-47.11	-50.19	-53.28
MSA·(MA) ₃ ·(SFA) ₂	-62.91	-66.77	-70.63	-74.52
(MA) ₃ ·(SFA) ₃	-53.82	-57.87	-61.94	-66.01

^a The value was taken from reference (Liu, L., Yu, F., Tu, K., Yang, Z., and Zhang, X.: Influence of atmospheric conditions on the role of trifluoroacetic acid in atmospheric sulfuric acid-dimethylamine nucleation, *Atmos. Chem. Phys.*, 21, 6221-6230, <https://doi.org/10.5194/acp-21-6221-2021>, 2021.)

^b The value was taken from reference (Shen, J., Elm, J., Xie, H. B., Chen, J., Niu, J., and Vehkamäki, H.: Structural effects of amines in enhancing methanesulfonic acid-driven new particle formation, *Environ. Sci. Technol.*, 54, 13498-13508, <https://doi.org/10.1021/acs.est.0c05358>, 2020.)

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Table S7 Evaporation rates γ (s^{-1}) for the studied clusters at different temperatures of 298.15, 278.15, 258.15, 238.15 and 218.15 K

Evaporation pathways	298.15 K	278.15 K	258.15 K	238.15 K
$\text{MSA} \cdot \text{MA} \rightarrow \text{MSA} + \text{MA}$	1.05×10^5	1.44×10^4	1.43×10^3	9.62×10^1
$\text{MSA} \cdot \text{SFA} \rightarrow \text{MSA} + \text{SFA}$	2.75×10^2	2.09×10^1	1.06×10^0	3.25×10^{-2}
$\text{MA} \cdot \text{SFA} \rightarrow \text{MA} + \text{SFA}$	1.26×10^5	1.66×10^4	1.59×10^3	1.03×10^2
$(\text{MSA})_2 \rightarrow \text{MSA} + \text{MSA}$	1.23×10^3	1.11×10^2	6.85×10^0	2.65×10^{-1}
$(\text{SFA})_2 \rightarrow \text{SFA} + \text{SFA}$	1.05×10^5	1.26×10^4	1.08×10^3	6.08×10^1
$(\text{MSA})_2 \cdot \text{MA} \rightarrow (\text{MSA})_2 + \text{MA}$	2.90×10^0	1.43×10^{-1}	4.43×10^{-3}	7.64×10^{-5}
$(\text{MSA})_2 \cdot \text{MA} \rightarrow \text{MSA} \cdot \text{MA} + \text{MSA}$	2.84×10^{-2}	9.29×10^{-4}	1.79×10^{-5}	1.77×10^{-7}
$(\text{MSA})_2 \cdot (\text{MA})_2 \rightarrow (\text{MSA})_2 \cdot \text{MA} + \text{MA}$	1.96×10^0	1.17×10^{-1}	4.48×10^{-3}	9.83×10^{-5}
$\text{MA} \cdot (\text{SFA})_2 \rightarrow (\text{SFA})_2 + \text{MA}$	2.82×10^{-4}	8.28×10^{-6}	1.41×10^{-7}	1.21×10^{-9}
$\text{MA} \cdot (\text{SFA})_2 \rightarrow \text{MA} \cdot \text{SFA} + \text{SFA}$	1.95×10^{-4}	5.22×10^{-6}	7.93×10^{-8}	5.96×10^{-10}
$(\text{MA})_2 \cdot (\text{SFA})_2 \rightarrow \text{MA} \cdot (\text{SFA})_2 + \text{MA}$	1.93×10^4	2.04×10^3	1.50×10^2	7.06×10^0
$(\text{MSA})_2 \cdot \text{SFA} \rightarrow (\text{MSA})_2 + \text{SFA}$	8.88×10^8	1.66×10^8	2.37×10^7	2.43×10^6
$(\text{MSA})_2 \cdot \text{SFA} \rightarrow \text{MSA} \cdot \text{SFA} + \text{MSA}$	3.81×10^9	8.44×10^8	1.48×10^8	1.91×10^7
$\text{MSA} \cdot (\text{SFA})_2 \rightarrow (\text{SFA})_2 + \text{MSA}$	4.27×10^4	4.24×10^3	2.94×10^2	1.30×10^1
$\text{MSA} \cdot (\text{SFA})_2 \rightarrow \text{MSA} \cdot \text{SFA} + \text{SFA}$	1.69×10^7	2.66×10^6	3.11×10^5	2.53×10^4
$(\text{MSA})_3 \rightarrow (\text{MSA})_2 + \text{MSA}$	1.89×10^7	2.78×10^6	3.01×10^5	2.23×10^4
$(\text{SFA})_3 \rightarrow (\text{SFA})_2 + \text{SFA}$	7.60×10^4	6.96×10^3	4.38×10^2	1.74×10^1
$(\text{MSA})_3 \cdot \text{MA} \rightarrow (\text{MSA})_2 \cdot \text{MA} + \text{MSA}$	5.28×10^2	4.00×10^1	2.01×10^0	6.10×10^{-2}
$(\text{MSA})_3 \cdot \text{MA} \rightarrow (\text{MSA})_3 + \text{MA}$	7.77×10^{-5}	1.98×10^{-6}	2.85×10^{-8}	2.01×10^{-10}
$(\text{MSA})_3 \cdot (\text{MA})_2 \rightarrow (\text{MSA})_2 \cdot (\text{MA})_2 + \text{MSA}$	1.44×10^0	7.28×10^{-2}	2.30×10^{-3}	4.04×10^{-5}
$(\text{MSA})_3 \cdot (\text{MA})_2 \rightarrow (\text{MSA})_3 \cdot \text{MA} + \text{MA}$	4.74×10^{-3}	1.88×10^{-4}	4.50×10^{-6}	5.73×10^{-8}
$(\text{MSA})_3 \cdot (\text{MA})_3 \rightarrow (\text{MSA})_3 \cdot (\text{MA})_2 + \text{MA}$	8.39×10^2	4.86×10^1	1.81×10^0	3.82×10^{-2}
$\text{MA} \cdot (\text{SFA})_3 \rightarrow \text{MA} \cdot (\text{SFA})_2 + \text{SFA}$	1.74×10^5	1.36×10^4	7.16×10^2	2.28×10^1
$\text{MA} \cdot (\text{SFA})_3 \rightarrow (\text{SFA})_3 + \text{MA}$	7.03×10^{-4}	1.76×10^{-5}	2.50×10^{-7}	1.73×10^{-9}
$(\text{MA})_2 \cdot (\text{SFA})_3 \rightarrow (\text{MA})_2 \cdot (\text{SFA})_2 + \text{SFA}$	1.09×10^0	5.40×10^{-2}	1.67×10^{-3}	2.87×10^{-5}
$(\text{MA})_2 \cdot (\text{SFA})_3 \rightarrow \text{MA} \cdot (\text{SFA})_3 + \text{MA}$	1.35×10^{-1}	9.04×10^{-3}	3.92×10^{-4}	9.95×10^{-6}
$(\text{MA})_3 \cdot (\text{SFA})_3 \rightarrow (\text{MA})_2 \cdot (\text{SFA})_3 + \text{MA}$	3.03×10^6	3.94×10^5	3.71×10^4	2.33×10^3
$\text{MSA} \cdot \text{SFA} \cdot \text{MA} \rightarrow \text{MA} \cdot \text{SFA} + \text{MSA}$	5.18×10^{-3}	1.50×10^{-4}	2.50×10^{-6}	2.09×10^{-8}

Evaporation pathways	298.15 K	278.15 K	258.15 K	238.15 K
$\text{MSA} \cdot \text{MA} \cdot \text{SFA} \rightarrow \text{MSA} \cdot \text{MA} + \text{SFA}$	6.71×10^{-3}	1.88×10^{-4}	3.01×10^{-6}	2.41×10^{-8}
$\text{MSA} \cdot \text{MA} \cdot \text{SFA} \rightarrow \text{MSA} \cdot \text{SFA} + \text{MA}$	2.95×10^0	1.48×10^{-1}	4.67×10^{-3}	8.22×10^{-5}
$\text{MSA} \cdot (\text{MA})_2 \cdot \text{SFA} \rightarrow \text{MSA} \cdot \text{MA} \cdot \text{SFA} + \text{MA}$	5.20×10^6	7.41×10^5	7.78×10^4	5.55×10^3
$(\text{MSA})_2 \cdot \text{MA} \cdot \text{SFA} \rightarrow \text{MSA} \cdot \text{MA} \cdot \text{SFA} + \text{MSA}$	5.01×10^7	9.32×10^6	1.32×10^6	1.33×10^5
$(\text{MSA})_2 \cdot \text{MA} \cdot \text{SFA} \rightarrow (\text{MSA})_2 \cdot \text{MA} + \text{SFA}$	1.22×10^7	1.93×10^6	2.28×10^5	1.86×10^4
$(\text{MSA})_2 \cdot \text{MA} \cdot \text{SFA} \rightarrow (\text{MSA})_2 \cdot \text{SFA} + \text{MA}$	3.96×10^{-2}	1.67×10^{-3}	4.26×10^{-5}	5.85×10^{-7}
$(\text{MSA})_2 \cdot (\text{MA})_2 \cdot \text{SFA} \rightarrow \text{MSA} \cdot (\text{MA})_2 \cdot \text{SFA} + \text{MSA}$	7.15×10^{-5}	1.78×10^{-6}	2.48×10^{-8}	1.68×10^{-10}
$(\text{MSA})_2 \cdot (\text{MA})_2 \cdot \text{SFA} \rightarrow (\text{MSA})_2 \cdot (\text{MA})_2 + \text{SFA}$	4.97×10^1	2.53×10^0	8.06×10^{-2}	1.43×10^{-3}
$(\text{MSA})_2 \cdot (\text{MA})_2 \cdot \text{SFA} \rightarrow (\text{MSA})_2 \cdot \text{MA} \cdot \text{SFA} + \text{MA}$	8.46×10^{-6}	1.62×10^{-7}	1.67×10^{-9}	7.97×10^{-12}
$(\text{MSA})_2 \cdot (\text{MA})_3 \cdot \text{SFA} \rightarrow (\text{MSA})_2 \cdot (\text{MA})_2 \cdot \text{SFA} + \text{MA}$	2.58×10^0	1.35×10^{-1}	4.42×10^{-3}	8.09×10^{-5}
$\text{MSA} \cdot \text{MA} \cdot (\text{SFA})_2 \rightarrow \text{MA} \cdot (\text{SFA})_2 + \text{MSA}$	1.17×10^4	9.09×10^2	4.72×10^1	1.48×10^0
$\text{MSA} \cdot \text{MA} \cdot (\text{SFA})_2 \rightarrow \text{MSA} \cdot \text{MA} \cdot \text{SFA} + \text{SFA}$	4.54×10^2	3.26×10^1	1.54×10^0	4.35×10^{-2}
$\text{MSA} \cdot \text{MA} \cdot (\text{SFA})_2 \rightarrow \text{MSA} \cdot (\text{SFA})_2 + \text{MA}$	8.61×10^{-5}	1.98×10^{-6}	2.52×10^{-8}	1.54×10^{-10}
$\text{MSA} \cdot (\text{MA})_2 \cdot (\text{SFA})_2 \rightarrow (\text{MA})_2 \cdot (\text{SFA})_2 + \text{MSA}$	1.90×10^{-1}	7.44×10^{-3}	1.76×10^{-4}	2.21×10^{-6}
$\text{MSA} \cdot (\text{MA})_2 \cdot (\text{SFA})_2 \rightarrow \text{MSA} \cdot (\text{MA})_2 \cdot \text{SFA} + \text{SFA}$	2.81×10^{-5}	7.52×10^{-7}	1.14×10^{-8}	8.49×10^{-11}
$\text{MSA} \cdot (\text{MA})_2 \cdot (\text{SFA})_2 \rightarrow \text{MSA} \cdot \text{MA} \cdot (\text{SFA})_2 + \text{MA}$	2.85×10^{-1}	1.51×10^{-2}	5.07×10^{-4}	9.58×10^{-6}
$\text{MSA} \cdot (\text{MA})_3 \cdot (\text{SFA})_2 \rightarrow \text{MSA} \cdot (\text{MA})_2 \cdot (\text{SFA})_2 + \text{MA}$	2.24×10^5	2.99×10^4	2.91×10^3	1.91×10^2

Collisions	β (cm ³ ·s ⁻¹)			
	298.15 K	278.15 K	258.15 K	238.15 K
MSA + MA	1.48×10^{-10}	1.38×10^{-10}	1.28×10^{-10}	1.18×10^{-10}
MSA + SFA	7.78×10^{-11}	7.26×10^{-11}	6.73×10^{-11}	6.21×10^{-11}
MA + SFA	1.31×10^{-10}	1.22×10^{-10}	1.14×10^{-10}	1.05×10^{-10}
MSA + MSA	8.68×10^{-11}	8.10×10^{-11}	7.52×10^{-11}	6.94×10^{-11}
SFA + SFA	6.93×10^{-11}	6.46×10^{-11}	6.00×10^{-11}	5.53×10^{-11}
(MSA) ₂ + MA	2.23×10^{-10}	2.08×10^{-10}	1.93×10^{-10}	1.78×10^{-10}
MSA·MA + MSA	1.11×10^{-10}	1.03×10^{-10}	9.58×10^{-11}	8.84×10^{-11}
(MSA) ₂ ·MA + MA	2.24×10^{-10}	2.09×10^{-10}	1.94×10^{-10}	1.79×10^{-10}
(SFA) ₂ + MA	2.17×10^{-10}	2.02×10^{-10}	1.88×10^{-10}	1.73×10^{-10}
MA·SFA + SFA	9.54×10^{-11}	8.90×10^{-11}	8.26×10^{-11}	7.62×10^{-11}
MA·(SFA) ₂ + MA	2.14×10^{-10}	1.99×10^{-10}	1.85×10^{-10}	1.71×10^{-10}
(MSA) ₂ + SFA	9.84×10^{-11}	9.18×10^{-11}	8.52×10^{-11}	7.86×10^{-11}
MSA·SFA + MSA	1.06×10^{-10}	9.89×10^{-11}	9.18×10^{-11}	8.47×10^{-11}
(SFA) ₂ + MSA	1.04×10^{-10}	9.73×10^{-11}	9.03×10^{-11}	8.33×10^{-11}
MSA·SFA + SFA	9.70×10^{-11}	9.05×10^{-11}	8.40×10^{-11}	7.75×10^{-11}
(MSA) ₂ + MSA	1.07×10^{-10}	1.00×10^{-10}	9.30×10^{-11}	8.58×10^{-11}
(SFA) ₂ + SFA	9.54×10^{-11}	8.90×10^{-11}	8.26×10^{-11}	7.62×10^{-11}
(MSA) ₂ ·MA + MSA	1.05×10^{-10}	9.77×10^{-11}	9.07×10^{-11}	8.36×10^{-11}
(MSA) ₃ + MA	2.09×10^{-10}	1.95×10^{-10}	1.81×10^{-10}	1.67×10^{-10}
(MSA) ₂ ·(MA) ₂ + MSA	1.23×10^{-10}	1.15×10^{-10}	1.07×10^{-10}	9.83×10^{-11}
(MSA) ₃ ·MA + MA	2.32×10^{-10}	2.16×10^{-10}	2.01×10^{-10}	1.85×10^{-10}
(MSA) ₃ ·(MA) ₂ + MA	2.72×10^{-10}	2.53×10^{-10}	2.35×10^{-10}	2.17×10^{-10}
MA·(SFA) ₂ + SFA	9.15×10^{-11}	8.54×10^{-11}	7.92×10^{-11}	7.31×10^{-11}
(SFA) ₃ + MA	2.26×10^{-10}	2.11×10^{-10}	1.96×10^{-10}	1.81×10^{-10}
(MA) ₂ ·(SFA) ₂ + SFA	1.03×10^{-10}	9.64×10^{-11}	8.94×10^{-11}	8.25×10^{-11}
MA·(SFA) ₃ + MA	2.70×10^{-10}	2.52×10^{-10}	2.34×10^{-10}	2.16×10^{-10}
(MA) ₂ ·(SFA) ₃ + MA	2.48×10^{-10}	2.31×10^{-10}	2.14×10^{-10}	1.98×10^{-10}
MA·SFA + MSA	1.05×10^{-10}	9.78×10^{-11}	9.08×10^{-11}	8.38×10^{-11}
MSA·MA + SFA	1.01×10^{-10}	9.41×10^{-11}	8.74×10^{-11}	8.06×10^{-11}
MSA·SFA + MA	2.20×10^{-10}	2.05×10^{-10}	1.91×10^{-10}	1.76×10^{-10}
MSA·MA·SFA + MA	2.19×10^{-10}	2.05×10^{-10}	1.90×10^{-10}	1.75×10^{-10}
MSA·MA·SFA + MSA	1.03×10^{-10}	9.57×10^{-11}	8.88×10^{-11}	8.19×10^{-11}

Collisions	β (cm ³ ·s ⁻¹)			
	298.15 K	278.15 K	258.15 K	238.15 K
(MSA) ₂ ·MA + SFA	9.59×10^{-11}	8.95×10^{-11}	8.31×10^{-11}	7.66×10^{-11}
(MSA) ₂ ·SFA + MA	2.17×10^{-10}	2.03×10^{-10}	1.88×10^{-10}	1.73×10^{-10}
MSA·(MA) ₂ ·SFA + MSA	1.14×10^{-10}	1.07×10^{-10}	9.91×10^{-11}	9.14×10^{-11}
(MSA) ₂ ·(MA) ₂ + SFA	1.14×10^{-10}	1.06×10^{-10}	9.83×10^{-11}	9.07×10^{-11}
(MSA) ₂ ·MA·SFA + MA	2.80×10^{-10}	2.61×10^{-10}	2.42×10^{-10}	2.23×10^{-10}
(MSA) ₂ ·(MA) ₂ ·SFA + MA	2.73×10^{-10}	2.55×10^{-10}	2.37×10^{-10}	2.18×10^{-10}
MA·(SFA) ₂ + MSA	1.00×10^{-10}	9.34×10^{-11}	8.67×10^{-11}	7.99×10^{-11}
MSA·MA·SFA + SFA	9.39×10^{-11}	8.76×10^{-11}	8.13×10^{-11}	7.50×10^{-11}
MSA·(SFA) ₂ + MA	2.32×10^{-10}	2.16×10^{-10}	2.01×10^{-10}	1.85×10^{-10}
(MA) ₂ ·(SFA) ₂ + MSA	1.12×10^{-10}	1.05×10^{-10}	9.72×10^{-11}	8.97×10^{-11}
MSA·(MA) ₂ ·SFA + SFA	1.05×10^{-10}	9.83×10^{-11}	9.12×10^{-11}	8.42×10^{-11}
MSA·MA·(SFA) ₂ + MA	6.02×10^{-10}	5.61×10^{-10}	5.21×10^{-10}	4.81×10^{-10}
MSA·(MA) ₂ ·(SFA) ₂ + MA	2.80×10^{-10}	2.61×10^{-10}	2.43×10^{-10}	2.24×10^{-10}

229 **Table S9** Total evaporation coefficients ($\sum \gamma$, s⁻¹) for each cluster in the present study

Clusters	$\sum \gamma$, (s ⁻¹)			
	298.15 K	278.15 K	258.15 K	238.15 K
MSA·MA	1.05×10^5	1.43×10^4	1.43×10^3	9.62×10^1
MSA·SFA	8.03×10^4	1.02×10^4	9.35×10^2	5.72×10^1
MA·SFA	9.48×10^5	1.59×10^5	2.00×10^4	1.77×10^3
(MSA) ₂	1.22×10^3	1.10×10^2	6.82×10^0	2.64×10^{-1}
(SFA) ₂	1.41×10^5	1.84×10^4	1.73×10^3	1.09×10^2
(MSA) ₂ ·MA	2.93×10^0	1.44×10^{-1}	4.45×10^{-3}	7.66×10^{-5}
(MSA) ₂ ·(MA) ₂	1.90×10^0	1.13×10^{-1}	4.33×10^{-3}	9.50×10^{-5}
MA·(SFA) ₂	4.77×10^{-4}	1.35×10^{-5}	2.20×10^{-7}	1.80×10^{-9}
(MA) ₂ ·(SFA) ₂	1.72×10^8	4.27×10^7	8.45×10^6	1.26×10^6
(MSA) ₂ ·SFA	4.70×10^9	1.01×10^9	1.71×10^8	2.15×10^7
MSA·(SFA) ₂	1.70×10^7	2.66×10^6	3.12×10^5	2.54×10^4
(MSA) ₃	1.89×10^7	2.77×10^6	3.01×10^5	2.23×10^4
(SFA) ₃	2.37×10^{11}	8.47×10^{10}	2.55×10^{10}	6.20×10^9
(MSA) ₃ ·MA	5.28×10^2	4.00×10^1	2.01×10^0	6.10×10^{-2}
(MSA) ₃ ·(MA) ₂	1.45×10^0	7.30×10^{-2}	2.30×10^{-3}	4.04×10^{-5}
(MSA) ₃ ·(MA) ₃	5.41×10^0	2.18×10^{-1}	5.32×10^{-3}	6.89×10^{-5}
MA·(SFA) ₃	1.74×10^5	1.36×10^4	7.16×10^2	2.28×10^1
(MA) ₂ ·(SFA) ₃	1.22×10^0	6.30×10^{-2}	2.06×10^{-3}	3.87×10^{-5}
(MA) ₃ ·(SFA) ₃	2.61×10^9	3.62×10^8	3.69×10^7	2.55×10^6
MSA·MA·SFA	2.96×10^0	1.49×10^{-1}	4.68×10^{-3}	8.23×10^{-5}
MSA·(MA) ₂ ·SFA	3.32×10^3	2.77×10^2	1.56×10^1	5.39×10^{-1}
MSA ₂ ·MA·SFA	6.23×10^7	1.12×10^7	1.55×10^6	1.52×10^5
(MSA) ₂ ·(MA) ₂ ·SFA	4.97×10^1	2.53×10^0	8.06×10^{-2}	1.43×10^{-3}
(MSA) ₂ ·(MA) ₃ ·SFA	1.43×10^2	1.42×10^1	9.83×10^{-1}	4.29×10^{-2}
MSA·MA·(SFA) ₂	1.21×10^4	9.41×10^2	4.88×10^1	1.52×10^0
MSA·(MA) ₂ ·(SFA) ₂	9.77×10^{-1}	4.92×10^{-2}	1.58×10^{-3}	2.87×10^{-5}
MSA·(MA) ₃ ·(SFA) ₂	5.53×10^2	5.38×10^1	3.67×10^0	1.60×10^{-1}

Table S10 Ratios ($\beta \cdot C / \Sigma \gamma$) between monomer molecule collisions and evaporation coefficients for each cluster involving SFA in the present study ($[\text{MSA}] = 1.0 \times 10^7 \text{ molecules} \cdot \text{cm}^{-3}$, $[\text{MA}] = 2.5 \times 10^7 \text{ molecules} \cdot \text{cm}^{-3}$, $[\text{SFA}] = 1.0 \times 10^7 \text{ molecules} \cdot \text{cm}^{-3}$)

		$(\beta \cdot C / \Sigma \gamma)$			
Clusters		298.15 K	278.15 K	258.15 K	238.15 K
Collision with MSA monomer: $C = [\text{MSA}]$					
MSA·MA		1.05×10^{-14}	7.21×10^{-14}	6.72×10^{-13}	9.19×10^{-12}
MSA·SFA		1.32×10^{-14}	9.71×10^{-14}	9.81×10^{-13}	1.48×10^{-11}
MA·SFA		1.11×10^{-15}	6.17×10^{-15}	4.54×10^{-14}	4.73×10^{-13}
$(\text{MSA})_2$		8.82×10^{-13}	9.11×10^{-12}	1.36×10^{-10}	3.25×10^{-9}
$(\text{SFA})_2$		7.38×10^{-15}	5.30×10^{-14}	5.22×10^{-13}	7.65×10^{-12}
$(\text{MSA})_2 \cdot \text{MA}$		3.58×10^{-10}	6.77×10^{-9}	2.04×10^{-7}	1.09×10^{-5}
$(\text{MSA})_2 \cdot (\text{MA})_2$		6.48×10^{-10}	1.01×10^{-8}	2.46×10^{-7}	1.03×10^{-5}
$\text{MA} \cdot (\text{SFA})_2$		2.10×10^{-6}	6.92×10^{-5}	3.94×10^{-3}	4.43×10^{-1}
$(\text{MA})_2 \cdot (\text{SFA})_2$		6.52×10^{-18}	2.45×10^{-17}	1.15×10^{-16}	7.09×10^{-16}
MSA·MA·SFA		3.46×10^{-10}	6.44×10^{-9}	1.90×10^{-7}	9.96×10^{-6}
MSA· $(\text{MA})_2 \cdot \text{SFA}$		3.45×10^{-13}	3.86×10^{-12}	6.36×10^{-11}	1.69×10^{-9}
Collision with MA monomer: $C = [\text{MA}]$					
MSA·SFA		6.85×10^{-13}	5.04×10^{-12}	5.09×10^{-11}	7.69×10^{-10}
$(\text{MSA})_2$		4.58×10^{-11}	4.73×10^{-10}	7.08×10^{-9}	1.69×10^{-7}
$(\text{SFA})_2$		3.83×10^{-13}	2.75×10^{-12}	2.71×10^{-11}	3.97×10^{-10}
$(\text{MSA})_2 \cdot \text{MA}$		1.91×10^{-8}	3.62×10^{-7}	1.09×10^{-5}	5.84×10^{-4}
$\text{MA} \cdot (\text{SFA})_2$		1.12×10^{-4}	3.69×10^{-3}	2.10×10^{-1}	2.37×10^1
$(\text{MSA})_2 \cdot \text{SFA}$		1.16×10^{-17}	5.02×10^{-17}	2.75×10^{-16}	2.01×10^{-15}
MSA· $(\text{SFA})_2$		3.41×10^{-15}	2.03×10^{-14}	1.61×10^{-13}	1.82×10^{-12}
$(\text{MSA})_3$		2.76×10^{-15}	1.76×10^{-14}	1.50×10^{-13}	1.87×10^{-12}
$(\text{SFA})_3$		2.38×10^{-19}	6.23×10^{-19}	1.92×10^{-18}	7.28×10^{-18}
$(\text{MSA})_3 \cdot \text{MA}$		1.10×10^{-10}	1.35×10^{-9}	2.49×10^{-8}	7.59×10^{-7}
$(\text{MSA})_3 \cdot (\text{MA})_2$		4.69×10^{-8}	8.68×10^{-7}	2.55×10^{-5}	1.34×10^{-3}
$\text{MA} \cdot (\text{SFA})_3$		3.88×10^{-13}	4.63×10^{-12}	8.16×10^{-11}	2.36×10^{-9}
$(\text{MA})_2 \cdot (\text{SFA})_3$		5.06×10^{-8}	9.16×10^{-7}	2.60×10^{-5}	1.28×10^{-3}
MSA·MA·SFA		1.85×10^{-8}	3.44×10^{-7}	1.01×10^{-5}	5.32×10^{-4}
$(\text{MSA})_2 \cdot \text{MA} \cdot \text{SFA}$		1.12×10^{-15}	5.80×10^{-15}	3.91×10^{-14}	3.67×10^{-13}
$(\text{MSA})_2 \cdot (\text{MA})_2 \cdot \text{SFA}$		1.38×10^{-9}	2.52×10^{-8}	7.34×10^{-7}	3.81×10^{-5}
MSA·MA· $(\text{SFA})_2$		4.49×10^{-12}	5.40×10^{-11}	9.67×10^{-10}	2.85×10^{-8}
MSA· $(\text{MA})_2 \cdot (\text{SFA})_2$		7.17×10^{-8}	1.33×10^{-6}	3.85×10^{-5}	1.95×10^{-3}
Collision with SFA monomer: $C = [\text{SFA}]$					
MSA·MA		9.60×10^{-15}	6.58×10^{-14}	6.13×10^{-13}	8.38×10^{-12}
MSA·SFA		1.21×10^{-14}	8.89×10^{-14}	8.98×10^{-13}	1.36×10^{-11}

Clusters	$(\beta \cdot C / \Sigma \gamma)$			
	298.15 K	278.15 K	258.15 K	238.15 K
MA·SFA	1.01×10^{-15}	5.61×10^{-15}	4.13×10^{-14}	4.30×10^{-13}
(MSA) ₂	8.07×10^{-13}	8.34×10^{-12}	1.25×10^{-10}	2.98×10^{-9}
(SFA) ₂	6.75×10^{-15}	4.84×10^{-14}	4.78×10^{-13}	6.99×10^{-12}
(MSA) ₂ ·MA	3.28×10^{-10}	6.21×10^{-9}	1.87×10^{-7}	1.00×10^{-5}
(MSA) ₂ ·(MA) ₂	5.98×10^{-10}	9.35×10^{-9}	2.27×10^{-7}	9.55×10^{-6}
MA·(SFA) ₂	1.92×10^{-6}	6.33×10^{-5}	3.60×10^{-3}	4.05×10^{-1}
(MA) ₂ ·(SFA) ₂	6.00×10^{-18}	2.26×10^{-17}	1.06×10^{-16}	6.53×10^{-16}
MSA·MA·SFA	3.17×10^{-10}	5.90×10^{-9}	1.74×10^{-7}	9.12×10^{-6}
MSA·(MA) ₂ ·SFA	3.18×10^{-13}	3.55×10^{-12}	5.85×10^{-11}	1.56×10^{-9}

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Table S11 The formation rate J of MSA at the conditions of $T = 238.15$ K, $[\text{MSA}] = 10^6$ - 10^8 molecules $\cdot\text{cm}^{-3}$, $[\text{MA}] = 10^7$ - 10^{11} molecules $\cdot\text{cm}^{-3}$, and $[\text{SFA}] = 0, 10^8$ - 10^{12} molecules $\cdot\text{cm}^{-3}$. MSA, MA and SFA represent sulfuric acid, ammonia and formic acid, respectively

[MSA]	[MA]	[SFA] = 0	[SFA] = 10^4	[SFA] = 10^5	[SFA] = 10^6	[SFA] = 10^7	[SFA] = 10^8
[MSA] = 10^5	[MA] = 2.5×10^7	3.54×10^{-9}	4.80×10^{-9}	1.62×10^{-8}	1.30×10^{-7}	1.22×10^{-6}	8.69×10^{-6}
[MSA] = 10^5	[MA] = 2.5×10^8	4.27×10^{-7}	5.34×10^{-7}	1.49×10^{-6}	1.10×10^{-5}	1.02×10^{-4}	7.26×10^{-4}
[MSA] = 10^5	[MA] = 2.5×10^9	3.47×10^{-6}	4.21×10^{-6}	1.08×10^{-5}	7.60×10^{-5}	6.78×10^{-4}	5.23×10^{-3}
[MSA] = 10^6	[MA] = 2.5×10^7	3.48×10^{-5}	3.61×10^{-5}	4.71×10^{-5}	1.58×10^{-4}	1.22×10^{-3}	8.64×10^{-3}
[MSA] = 10^6	[MA] = 2.5×10^8	4.19×10^{-3}	4.29×10^{-3}	5.22×10^{-3}	1.45×10^{-2}	1.04×10^{-1}	7.20×10^{-1}
[MSA] = 10^6	[MA] = 2.5×10^9	3.40×10^{-2}	3.47×10^{-2}	4.11×10^{-2}	1.04×10^{-1}	6.90×10^{-1}	5.14×10^0
[MSA] = 10^7	[MA] = 2.5×10^7	3.01×10^{-1}	3.02×10^{-1}	3.11×10^{-1}	3.97×10^{-1}	1.24×10^0	8.08×10^0
[MSA] = 10^7	[MA] = 2.5×10^8	3.47×10^1	3.48×10^1	3.55×10^1	4.28×10^1	1.14×10^2	6.53×10^2
[MSA] = 10^7	[MA] = 2.5×10^9	2.72×10^2	2.73×10^2	2.78×10^2	3.26×10^2	7.74×10^2	4.31×10^3
[MSA] = 10^8	[MA] = 2.5×10^7	1.14×10^3	1.14×10^3	1.14×10^3	1.17×10^3	1.44×10^3	4.98×10^3
[MSA] = 10^8	[MA] = 2.5×10^8	9.01×10^4	9.01×10^4	9.02×10^4	9.19×10^4	1.08×10^5	2.64×10^5
[MSA] = 10^8	[MA] = 2.5×10^9	5.34×10^5	5.34×10^5	5.35×10^5	5.42×10^5	6.12×10^5	1.23×10^6
[MSA] = 10^9	[MA] = 2.5×10^7	6.99×10^5	6.99×10^5	7.00×10^5	7.02×10^5	7.30×10^5	9.89×10^5
[MSA] = 10^9	[MA] = 2.5×10^8	1.66×10^7	1.66×10^7	1.66×10^7	1.67×10^7	1.69×10^7	1.97×10^7
[MSA] = 10^9	[MA] = 2.5×10^9	9.54×10^7	9.54×10^7	9.54×10^7	9.55×10^7	9.65×10^7	1.06×10^8

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Table S12 The formation rate J of MSA at the conditions of $T = 258.15$ K, $[\text{MSA}] = 10^6$ - 10^8 molecules $\cdot\text{cm}^{-3}$, $[\text{MA}] = 10^7$ - 10^{11} molecules $\cdot\text{cm}^{-3}$, and $[\text{SFA}] = 0, 10^8$ - 10^{12} molecules $\cdot\text{cm}^{-3}$. MSA, MA and SFA represent sulfuric acid, ammonia and formic acid, respectively

[MSA]	[MA]	[SFA] = 0	[SFA] = 10^4	[SFA] = 10^5	[SFA] = 10^6	[SFA] = 10^7	[SFA] = 10^8
[MSA] = 10^5	[MA] = 2.5×10^7	2.63×10^{-12}	5.59×10^{-12}	3.22×10^{-11}	2.98×10^{-10}	2.96×10^{-9}	2.43×10^{-8}
[MSA] = 10^5	[MA] = 2.5×10^8	9.62×10^{-10}	1.87×10^{-9}	1.00×10^{-8}	9.19×10^{-8}	9.18×10^{-7}	7.97×10^{-6}
[MSA] = 10^5	[MA] = 2.5×10^9	1.02×10^{-7}	1.47×10^{-7}	5.60×10^{-7}	4.68×10^{-6}	4.48×10^{-5}	3.31×10^{-4}
[MSA] = 10^6	[MA] = 2.5×10^7	2.61×10^{-8}	2.90×10^{-8}	5.52×10^{-8}	3.17×10^{-7}	2.93×10^{-6}	2.40×10^{-5}
[MSA] = 10^6	[MA] = 2.5×10^8	9.54×10^{-6}	1.04×10^{-5}	1.84×10^{-5}	9.88×10^{-5}	9.10×10^{-4}	7.86×10^{-3}
[MSA] = 10^6	[MA] = 2.5×10^9	1.00×10^{-3}	1.05×10^{-3}	1.45×10^{-3}	5.49×10^{-3}	4.48×10^{-2}	3.28×10^{-1}
[MSA] = 10^7	[MA] = 2.5×10^7	2.44×10^{-4}	2.47×10^{-4}	2.69×10^{-4}	4.93×10^{-4}	2.73×10^{-3}	2.12×10^{-2}
[MSA] = 10^7	[MA] = 2.5×10^8	8.75×10^{-2}	8.83×10^{-2}	9.50×10^{-2}	1.63×10^{-1}	8.47×10^{-1}	6.90×10^0
[MSA] = 10^7	[MA] = 2.5×10^9	8.89×10^0	8.92×10^0	9.26×10^0	1.26×10^1	4.53×10^1	2.94×10^2
[MSA] = 10^8	[MA] = 2.5×10^7	1.52×10^0	1.52×10^0	1.53×10^0	1.61×10^0	2.41×10^0	9.90×10^0
[MSA] = 10^8	[MA] = 2.5×10^8	4.80×10^2	4.80×10^2	4.83×10^2	5.06×10^2	7.41×10^2	3.17×10^3
[MSA] = 10^8	[MA] = 2.5×10^9	3.46×10^4	3.46×10^4	3.47×10^4	3.57×10^4	4.52×10^4	1.35×10^5
[MSA] = 10^9	[MA] = 2.5×10^7	4.61×10^3	4.61×10^3	4.61×10^3	4.63×10^3	4.83×10^3	6.79×10^3
[MSA] = 10^9	[MA] = 2.5×10^8	6.06×10^5	6.06×10^5	6.06×10^5	6.09×10^5	6.32×10^5	8.51×10^5
[MSA] = 10^9	[MA] = 2.5×10^9	1.32×10^7	1.32×10^7	1.32×10^7	1.33×10^7	1.36×10^7	1.69×10^7

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241 **Table S13** The formation rate J of MSA at the conditions of $T = 278.15$ K, $[\text{MSA}] = 10^6$ - 10^8 molecules $\cdot\text{cm}^{-3}$, $[\text{MA}] = 10^7$ - 10^{11} molecules $\cdot\text{cm}^{-3}$, and $[\text{SFA}] = 0, 10^8$ - 10^{12}
 242 molecules $\cdot\text{cm}^{-3}$. MSA, MA and SFA represent sulfuric acid, ammonia and formic acid, respectively

[MSA]	[MA]	[SFA] = 0	[SFA] = 10^4	[SFA] = 10^5	[SFA] = 10^6	[SFA] = 10^7	[SFA] = 10^8
[MSA] = 10^5	[MA] = 2.5×10^7	1.68×10^{-17}	3.26×10^{-17}	1.75×10^{-16}	1.60×10^{-15}	1.59×10^{-14}	1.65×10^{-13}
[MSA] = 10^5	[MA] = 2.5×10^8	1.67×10^{-14}	3.21×10^{-14}	1.71×10^{-13}	1.56×10^{-12}	1.54×10^{-11}	1.56×10^{-10}
[MSA] = 10^5	[MA] = 2.5×10^9	1.53×10^{-11}	2.74×10^{-11}	1.36×10^{-10}	1.22×10^{-9}	1.21×10^{-8}	1.22×10^{-7}
[MSA] = 10^6	[MA] = 2.5×10^7	1.68×10^{-13}	1.84×10^{-13}	3.26×10^{-13}	1.75×10^{-12}	1.60×10^{-11}	1.65×10^{-10}
[MSA] = 10^6	[MA] = 2.5×10^8	1.67×10^{-10}	1.82×10^{-10}	3.21×10^{-10}	1.71×10^{-9}	1.56×10^{-8}	1.57×10^{-7}
[MSA] = 10^6	[MA] = 2.5×10^9	1.53×10^{-7}	1.65×10^{-7}	2.74×10^{-7}	1.36×10^{-6}	1.22×10^{-5}	1.22×10^{-4}
[MSA] = 10^7	[MA] = 2.5×10^7	1.68×10^{-9}	1.70×10^{-9}	1.84×10^{-9}	3.25×10^{-9}	1.74×10^{-8}	1.67×10^{-7}
[MSA] = 10^7	[MA] = 2.5×10^8	1.67×10^{-6}	1.69×10^{-6}	1.82×10^{-6}	3.19×10^{-6}	1.69×10^{-5}	1.57×10^{-4}
[MSA] = 10^7	[MA] = 2.5×10^9	1.53×10^{-3}	1.54×10^{-3}	1.65×10^{-3}	2.72×10^{-3}	1.34×10^{-2}	1.22×10^{-1}
[MSA] = 10^8	[MA] = 2.5×10^7	1.69×10^{-5}	1.69×10^{-5}	1.70×10^{-5}	1.83×10^{-5}	3.12×10^{-5}	1.72×10^{-4}
[MSA] = 10^8	[MA] = 2.5×10^8	1.68×10^{-2}	1.68×10^{-2}	1.69×10^{-2}	1.82×10^{-2}	3.07×10^{-2}	1.62×10^{-1}
[MSA] = 10^8	[MA] = 2.5×10^9	1.54×10^1	1.54×10^1	1.55×10^1	1.64×10^1	2.59×10^1	1.22×10^2
[MSA] = 10^9	[MA] = 2.5×10^7	1.75×10^{-1}	1.75×10^{-1}	1.75×10^{-1}	1.76×10^{-1}	1.84×10^{-1}	2.72×10^{-1}
[MSA] = 10^9	[MA] = 2.5×10^8	1.78×10^2	1.78×10^2	1.78×10^2	1.79×10^2	1.86×10^2	2.68×10^2
[MSA] = 10^9	[MA] = 2.5×10^9	1.30×10^5	1.30×10^5	1.30×10^5	1.31×10^5	1.34×10^5	1.73×10^5

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Table S14 The formation rate J of MSA at the conditions of $T = 298.15$ K, $[\text{MSA}] = 10^6$ - 10^8 molecules $\cdot\text{cm}^{-3}$, $[\text{MA}] = 10^7$ - 10^{11} molecules $\cdot\text{cm}^{-3}$, and $[\text{SFA}] = 0, 10^8$ - 10^{12} molecules $\cdot\text{cm}^{-3}$. MSA, MA and SFA represent sulfuric acid, ammonia and formic acid, respectively

[MSA]	[MA]	[SFA] = 0	[SFA] = 10^4	[SFA] = 10^5	[SFA] = 10^6	[SFA] = 10^7	[SFA] = 10^8
[MSA] = 10^5	[MA] = 2.5×10^7	2.62×10^{-23}	4.79×10^{-23}	2.43×10^{-22}	2.20×10^{-21}	2.21×10^{-20}	2.58×10^{-19}
[MSA] = 10^5	[MA] = 2.5×10^8	2.62×10^{-20}	4.79×10^{-20}	2.43×10^{-19}	2.20×10^{-18}	2.20×10^{-17}	2.52×10^{-16}
[MSA] = 10^5	[MA] = 2.5×10^9	2.68×10^{-17}	4.85×10^{-17}	2.44×10^{-16}	2.20×10^{-15}	2.18×10^{-14}	2.31×10^{-13}
[MSA] = 10^6	[MA] = 2.5×10^7	2.62×10^{-19}	2.83×10^{-19}	4.79×10^{-19}	2.44×10^{-18}	2.23×10^{-17}	2.58×10^{-16}
[MSA] = 10^6	[MA] = 2.5×10^8	2.62×10^{-16}	2.84×10^{-16}	4.79×10^{-16}	2.44×10^{-15}	2.23×10^{-14}	2.52×10^{-13}
[MSA] = 10^6	[MA] = 2.5×10^9	2.68×10^{-13}	2.90×10^{-13}	4.85×10^{-13}	2.44×10^{-12}	2.21×10^{-11}	2.31×10^{-10}
[MSA] = 10^7	[MA] = 2.5×10^7	2.62×10^{-15}	2.64×10^{-15}	2.83×10^{-15}	4.79×10^{-15}	2.46×10^{-14}	2.58×10^{-13}
[MSA] = 10^7	[MA] = 2.5×10^8	2.62×10^{-12}	2.64×10^{-12}	2.84×10^{-12}	4.79×10^{-12}	2.46×10^{-11}	2.52×10^{-10}
[MSA] = 10^7	[MA] = 2.5×10^9	2.68×10^{-9}	2.71×10^{-9}	2.90×10^{-9}	4.85×10^{-9}	2.45×10^{-8}	2.32×10^{-7}
[MSA] = 10^8	[MA] = 2.5×10^7	2.62×10^{-11}	2.62×10^{-11}	2.64×10^{-11}	2.84×10^{-11}	4.80×10^{-11}	2.71×10^{-10}
[MSA] = 10^8	[MA] = 2.5×10^8	2.63×10^{-8}	2.63×10^{-8}	2.65×10^{-8}	2.84×10^{-8}	4.81×10^{-8}	2.66×10^{-7}
[MSA] = 10^8	[MA] = 2.5×10^9	2.69×10^{-5}	2.69×10^{-5}	2.71×10^{-5}	2.90×10^{-5}	4.85×10^{-5}	2.52×10^{-4}
[MSA] = 10^9	[MA] = 2.5×10^7	2.65×10^{-7}	2.65×10^{-7}	2.65×10^{-7}	2.67×10^{-7}	2.86×10^{-7}	4.84×10^{-7}
[MSA] = 10^9	[MA] = 2.5×10^8	2.66×10^{-4}	2.66×10^{-4}	2.66×10^{-4}	2.68×10^{-4}	2.87×10^{-4}	4.83×10^{-4}
[MSA] = 10^9	[MA] = 2.5×10^9	2.73×10^{-1}	2.73×10^{-1}	2.73×10^{-1}	2.75×10^{-1}	2.94×10^{-1}	4.85×10^{-1}

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Table S15 Cartesian coordinates of all molecules and clusters in the studied system

MSA:

Atoms	X	Y	Z
S	0.08625500	0.13875900	0.06729200
O	0.20786800	1.40372500	-0.58037200
O	0.60516400	-0.08599700	1.38677800
O	0.76916500	-0.95690500	-0.88879000
H	1.34875900	-1.50079600	-0.34066100
C	-1.60359500	-0.37243200	-0.00520600
H	-2.16873100	0.34875600	0.57873100
H	-1.91343000	-0.35301000	-1.04542600
H	-1.68268700	-1.36709600	0.42100400

MA:

Atoms	X	Y	Z
H	-0.44173500	-1.10950800	0.81057800
N	0.04994100	-0.75699600	0.00000000
C	0.04994100	0.70512600	0.00000000
H	-0.44173500	-1.10950800	-0.81057800
H	0.58870300	1.06082400	0.87680200
H	-0.94317000	1.16558700	0.00000000
H	0.58870300	1.06082400	-0.87680200

SFA:

Atoms	X	Y	Z
S	-0.04565300	0.04592600	-0.14447900
O	-1.08453900	-0.21880200	1.02805600
O	-0.12674900	-1.02547100	-1.08448500
O	-0.25134700	1.40779700	-0.49883900
N	1.39184100	-0.14902500	0.64833400
H	-1.09734200	-1.16493200	1.21837500
H	1.73213500	0.74411300	0.98246800
H	2.05384700	-0.57901100	0.01463600

(MSA)₁·(MA)₁:

Atoms	X	Y	Z
N	2.26374800	-0.78481100	-0.01141900
H	2.96027900	-1.43769100	-0.34749300
H	1.99700800	-1.05454400	0.93010200
C	2.77584800	0.59667400	-0.00964200
H	3.65756200	0.71837100	0.61835700
H	3.01894400	0.88490500	-1.02947200
H	1.98571500	1.24970800	0.35497300

Atoms	X	Y	Z
S	-0.86242000	0.15986100	0.05001700
O	-1.17602700	1.51047400	-0.31989200
O	-0.19896900	-0.06953900	1.31801900
O	-0.02782800	-0.52825500	-1.06719700
H	0.95971700	-0.72449400	-0.68816500
C	-2.35647500	-0.78577200	0.00743500
H	-3.02354100	-0.35409900	0.74801700
H	-2.77867400	-0.69647000	-0.98871700
H	-2.11818100	-1.81663800	0.24786100

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256 (MSA)₁·(SFA)₁:

Atoms	X	Y	Z
S	-1.77748800	0.04604700	-0.07120300
O	-1.22918800	-0.85281400	-1.06384500
O	-1.32031800	1.41045800	-0.10465000
O	-1.56889500	-0.56176700	1.35823500
H	-0.59123500	-0.64199300	1.48903100
C	-3.53295000	-0.00784900	-0.14465900
H	-3.81229100	0.39613900	-1.11339900
H	-3.84182900	-1.04355300	-0.04700300
H	-3.91905800	0.60698000	0.66216100
S	1.97318100	-0.07149400	0.09330200
O	1.51298400	-0.71650300	-1.26885100
O	1.07624500	-0.54448900	1.12270100
O	3.37096500	-0.29041400	0.18255700
N	1.71047900	1.53251800	-0.02108100
H	0.53725400	-0.83045300	-1.27027300
H	2.26719600	1.93923800	-0.76145500
H	0.71887500	1.74449700	-0.10629100

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258 (MSA)₁·(SFA)₁·(MA)₁:

Atoms	X	Y	Z
N	-0.21536000	2.31867300	-0.59293600
H	0.02058800	2.92148800	-1.37513900
H	0.63521800	1.77768600	-0.31819000
C	-0.68847200	3.08312900	0.58713000
H	0.10158900	3.74723600	0.92315800
H	-1.57442300	3.64980800	0.31794400
H	-0.92541700	2.35573500	1.35670200
S	-1.77778500	-0.56718400	-0.05684400
O	-1.14332400	0.00216000	1.13500800
O	-0.94772100	-1.63107500	-0.66057800
O	-2.15682700	0.47273400	-1.02387400

Atoms	X	Y	Z
H	-0.95555800	1.63525400	-0.88860200
C	-3.27491900	-1.36478700	0.44118100
H	-3.01906900	-2.13700900	1.15989000
H	-3.91774700	-0.61298700	0.88832500
H	-3.73215900	-1.79269500	-0.44552800
S	2.15157100	-0.31648400	0.02569900
O	1.25256200	-0.51816100	-1.24299000
O	3.46702300	-0.76189600	-0.28056700
O	1.95313800	1.05735600	0.45141300
N	1.53243100	-1.24554200	1.21076000
H	0.38218900	-1.01765600	-1.03629700
H	0.57843800	-0.95260000	1.42765100
H	1.58780800	-2.22649700	0.96647500

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260

(MSA)₁·(SFA)₁·(MA)₂:

Atoms	X	Y	Z
N	1.27888700	-2.30583600	-0.66569200
H	1.19878900	-2.84808800	-1.52088500
H	0.38221900	-2.42320700	-0.14388800
C	2.45985600	-2.68742300	0.13748200
H	2.39242400	-3.73455500	0.41680600
H	3.35719800	-2.50652500	-0.44665200
H	2.46478500	-2.05103100	1.01606600
S	1.67356000	1.02413300	0.01852200
O	1.45804300	0.11610300	1.15279500
O	0.56880300	1.97192600	-0.18837500
O	2.07526200	0.29617600	-1.19110300
H	1.34965400	-1.29969500	-0.93475100
C	3.06362200	2.04008900	0.45521600
H	2.80659300	2.59203400	1.35410800
H	3.91400400	1.38854900	0.63161200
H	3.25896600	2.71502500	-0.37253500
S	-1.69300900	-1.13177300	0.08360500
O	-0.83990800	-0.60911600	-0.98542600
O	-3.11364900	-0.98109400	-0.18632400
O	-1.25860600	-2.47045000	0.49979600
N	-1.43811000	-0.06056900	1.35541300
H	-1.06401100	1.52094200	-0.67766100
H	-0.43272600	-0.00846700	1.53443800
H	-1.91718600	-0.42981600	2.16922400
H	-2.16526000	2.12914900	-1.76900800
N	-2.05847200	1.82271200	-0.80639800
C	-2.35099600	2.89614100	0.16836300
H	-2.64657000	0.98908300	-0.66086300

Atoms	X	Y	Z
H	-3.36232300	3.26467400	0.02649400
H	-1.62389900	3.68945800	0.02900700
H	-2.23206600	2.45934200	1.15392600

261

262 (MSA)₁·(SFA)₂:

Atoms	X	Y	Z
S	1.84587300	-1.37363300	0.01983300
O	0.82780400	-1.89814200	-1.03564800
O	1.14243600	-0.89837700	1.18182500
O	2.76540000	-0.47344900	-0.63927300
H	2.40713200	1.16989400	-0.35497800
C	2.74137900	-2.83499100	0.42853100
H	2.04522000	-3.53876600	0.87405100
H	3.17390500	-3.22702300	-0.48694200
H	3.51507000	-2.54579500	1.13376800
S	0.58551600	2.19630600	-0.07855500
O	0.18854100	3.52007200	-0.40434800
O	0.12606600	1.10580700	-0.94150600
O	2.13469200	2.07628400	-0.06369300
N	0.20880500	1.92428700	1.48472600
H	-1.33843000	0.70234600	-1.15752700
H	0.35035600	0.93806200	1.69885900
H	-0.76606600	2.16444000	1.63096500
S	-2.40116100	-0.62812300	0.08025100
O	-1.62759200	-1.83246500	-0.13077300
O	-2.19564100	0.13966200	1.26700900
O	-2.26344000	0.28523600	-1.17460800
N	-3.96036400	-1.09565500	0.03257400
H	-0.10440200	-1.84085300	-0.68126200
H	-4.16069100	-1.62025300	-0.80979000
H	-4.57921800	-0.30235900	0.14422500

263

264 (MSA)₁·(SFA)₂·(MA)₁:

Atoms	X	Y	Z
N	0.23257300	-0.52840400	2.39574300
H	1.21152400	-0.66898100	2.63475800
H	0.01112800	-1.19521700	1.64303300
C	-0.68315600	-0.66547000	3.55091100
H	-0.56883600	-1.65389700	3.98483200
H	-0.44166900	0.09553900	4.28629000
H	-1.69386900	-0.53083100	3.18288700
S	0.76799600	2.15687300	-0.09040900
O	-0.08450300	1.54985600	-1.12777000

Atoms	X	Y	Z
O	2.16321200	1.68497100	-0.22405000
O	0.23694800	1.99373900	1.26054900
H	0.15178000	0.41426600	1.95761100
C	0.82343100	3.89052700	-0.41754800
H	1.21592900	4.02777900	-1.42013000
H	-0.18951000	4.27318700	-0.33643400
H	1.47308000	4.34549500	0.32359800
S	1.86078300	-1.72046800	-0.44214200
O	2.40579100	-0.66505900	0.58670100
O	2.88747200	-2.67118800	-0.69637700
O	0.58972600	-2.17404000	0.08847700
N	1.52714600	-0.92708700	-1.82133800
H	2.34303500	0.30560000	0.23554700
H	0.82041200	-0.19896500	-1.70505000
H	2.37196700	-0.57737600	-2.25581600
S	-2.64042200	-0.48130300	-0.40953800
O	-2.64252900	0.99415900	-0.91427400
O	-1.91019200	-0.55293300	0.83190200
O	-3.99234000	-0.92709800	-0.47422200
N	-1.69822000	-1.23932300	-1.52212700
H	-1.69787600	1.30089700	-0.97474200
H	-2.26392500	-1.68280700	-2.23291600
H	-1.05770000	-1.88221900	-1.06367600

265

266

(MSA)₁·(SFA)₂·(MA)₂:

Atoms	X	Y	Z
N	-0.09812500	2.46508100	-0.25975000
H	0.75026800	1.97240800	-0.59721300
H	-0.08194000	2.40727000	0.76137900
C	-0.17601900	3.84842700	-0.76224500
H	0.69786300	4.40692900	-0.44101100
H	-0.21194400	3.81786500	-1.84669600
H	-1.07974800	4.31653600	-0.38451800
S	-2.94281200	0.07123800	-0.58150400
O	-2.97593100	0.19676500	0.87569200
O	-2.43886300	-1.23509600	-1.04062900
O	-2.29442200	1.20978400	-1.24819800
H	-0.92456100	1.90058100	-0.57714300
C	-4.63240300	0.11893400	-1.12083500
H	-5.15574800	-0.70815400	-0.65108700
H	-5.05373600	1.06953400	-0.80859200
H	-4.64481200	0.02406600	-2.20216200
S	0.14179900	-0.09466600	1.86164800
O	0.03944200	-0.02252900	0.42313000

Atoms	X	Y	Z
O	1.43440900	-0.83702300	2.24680100
O	0.03402800	1.16205100	2.55761800
N	-0.98083400	-1.20394000	2.32499600
H	-0.93490100	-1.84879500	-0.76670500
H	-1.87033600	-0.85974800	1.93137300
H	-1.03090500	-1.24341100	3.33754300
H	0.75755800	-1.85328000	-0.75254800
N	-0.08245200	-2.43092900	-0.56324400
C	-0.07889700	-3.68128200	-1.34437300
H	-0.10453600	-2.59521800	0.44373000
H	0.80447900	-4.26306300	-1.09930500
H	-0.06474700	-3.42503900	-2.39894300
H	-0.97843400	-4.24690200	-1.12114200
S	2.90904900	0.08404400	-0.70742400
O	3.09377500	0.20145900	0.75536600
O	2.33912400	-1.18414500	-1.13796700
O	2.25554800	1.26313900	-1.26809600
N	4.48011100	0.02599900	-1.25863600
H	2.20359800	-0.43995800	1.63006200
H	4.45138400	-0.03899700	-2.27036400
H	4.93875000	0.89232600	-0.99875300

267

268 (MSA)₁·(SFA)₂·(MA)₃:

Atoms	X	Y	Z
N	-0.77975000	-0.58328900	-1.95741600
H	-0.22778000	-0.99069200	-1.18931900
H	-0.80656700	0.44014900	-1.80813700
C	-0.12581100	-0.91739500	-3.23735500
H	0.89725200	-0.55624500	-3.19710800
H	-0.12671100	-1.99565600	-3.36473700
H	-0.66334000	-0.44265500	-4.05232300
S	-3.33828400	-0.59555300	0.20086000
O	-2.38789700	0.52780300	0.12727600
O	-3.15719300	-1.37216500	1.43438700
O	-3.32099200	-1.40296700	-1.01962200
H	-1.74243200	-0.94447900	-1.86074100
C	-4.96047200	0.11612100	0.30399000
H	-5.00187200	0.73274500	1.19665200
H	-5.12235200	0.71101400	-0.58971500
H	-5.67714700	-0.69742500	0.36301700
S	0.23443800	2.32340000	-0.40277100
O	0.63758700	1.01609600	0.14519000
O	1.34504600	3.28055600	-0.38530400
O	-0.39655500	2.19120700	-1.71119500

Atoms	X	Y	Z
N	-0.85646400	2.91624000	0.70383100
H	-1.48609400	-1.06306000	1.88226900
H	-1.69454300	2.33782400	0.62379700
H	-1.07641000	3.87054900	0.43977900
H	0.04627300	-1.61072200	1.46686000
N	-0.47329400	-0.82787500	1.87648300
C	0.05872300	-0.43881700	3.19631900
H	-0.34102400	-0.05238700	1.20316700
H	1.12973900	-0.29450000	3.09752100
H	-0.14511700	-1.22419300	3.91779700
H	-0.42343100	0.48320600	3.50705400
S	2.19832200	-1.77842300	-0.10278300
O	2.61940500	-0.89787100	-1.19287000
O	2.44642600	-1.25790700	1.23288000
O	0.80749000	-2.23920300	-0.26601000
N	3.21296800	-3.09899900	-0.24099500
H	2.72218100	2.28235300	-0.33429700
H	2.95376600	-3.77317500	0.47082500
H	3.06751500	-3.51710100	-1.15352100
H	4.29968400	1.67422700	-0.44166600
N	3.38372800	1.53147900	-0.02800500
C	3.43584100	1.54664000	1.45451400
H	3.00642900	0.62788200	-0.38432200
H	3.87264800	2.48591600	1.78076700
H	4.01002000	0.69555700	1.80247100
H	2.41116600	1.46350300	1.79906200

269

270 (SFA)₁·(MA)₁:

Atoms	X	Y	Z
H	0.90531600	-0.78686000	-0.69834300
N	2.22367900	-0.72567300	-0.04736400
C	2.62380200	0.69000000	0.01175900
H	2.96005900	-1.30434900	-0.43091400
H	1.80632200	1.25001300	0.45875800
H	2.77623100	1.05743800	-1.00033800
H	3.53313900	0.84761800	0.59107500
S	-0.95621000	-0.09556200	0.08123100
O	-0.27297500	-0.19486100	1.34537000
O	-0.11638600	-0.75074400	-1.02985600
O	-2.30679000	-0.54518400	-0.03856600
N	-0.83071900	1.52080100	-0.33668300
H	2.00684800	-1.06191100	0.88535600
H	-1.19511800	2.05747000	0.44388800
H	-1.41775700	1.69000200	-1.14698700

271

272 (MSA)₂:

Atoms	X	Y	Z
S	-2.01703200	-0.12116800	-0.07554800
O	-3.38279900	-0.51870000	-0.15695700
O	-1.08526100	-0.58726700	-1.08778600
O	-1.47968700	-0.56725800	1.33259400
H	-0.49471800	-0.63142600	1.32106200
C	-1.90839400	1.63907100	-0.00788700
H	-2.29408700	2.01082200	-0.95333000
H	-2.52434700	1.97225200	0.82154800
H	-0.86386000	1.91150700	0.12239100
S	1.83810800	0.07678800	0.05760300
O	1.22156500	-0.65720800	1.14747700
O	1.49707400	1.46543100	-0.07088500
O	1.56577000	-0.68493700	-1.28834900
H	0.58261500	-0.74670300	-1.38965200
C	3.58316300	-0.12754000	0.14798100
H	3.90252300	0.38176000	1.05269800
H	3.79580100	-1.19039300	0.19726700
H	4.01694800	0.33258200	-0.73418000

273

274 (MSA)₂·(MA)₁:

Atoms	X	Y	Z
N	0.77377400	2.33273000	-0.72007100
H	-0.12344400	1.81205000	-0.63298100
H	0.70873400	2.94627200	-1.52667500
C	1.06893900	3.07984700	0.52553600
H	1.13538400	2.35191400	1.32733100
H	2.01515300	3.60039600	0.41425300
H	0.27040300	3.78865900	0.72150900
S	1.78237900	-0.73183800	-0.07931400
O	0.97900500	-1.71451000	-0.77475000
O	1.01601400	-0.01631700	0.98562700
O	2.44644400	0.26163400	-0.94456300
H	1.51030900	1.59290300	-0.89430700
C	3.08399800	-1.58801200	0.75961300
H	2.62704200	-2.30585300	1.43378300
H	3.68115500	-2.08983700	0.00417700
H	3.67476800	-0.85808300	1.30364400
S	-2.27077600	-0.11980600	0.07022900
O	-1.57166900	0.93570200	-0.65631500
O	-3.60267000	0.14925300	0.51545600
O	-1.41644100	-0.53601400	1.29484500
H	-0.40953900	-0.36815500	1.14170600

Atoms	X	Y	Z
C	-2.26653000	-1.55293800	-0.95696300
H	-1.23194700	-1.78749300	-1.19475900
H	-2.74328900	-2.35259800	-0.39828600
H	-2.84069900	-1.30434100	-1.84505300

275

276 (MSA)₂·(SFA)₁:

Atoms	X	Y	Z
S	2.52743000	-0.71148500	-0.14183400
O	2.90820300	0.51136000	-0.78330500
O	1.58584300	-1.59151500	-0.79223900
O	2.00351900	-0.40970500	1.31578000
H	1.45015800	0.41335400	1.30413800
C	3.96223800	-1.64977700	0.27302000
H	4.40002500	-1.97384500	-0.66693100
H	4.64130000	-1.00442000	0.82042800
H	3.65124500	-2.50269700	0.86790500
S	-0.42701700	1.98282900	0.13143100
O	-0.07121400	1.02086100	-1.02683400
O	0.49235900	1.78270300	1.22916800
O	-1.84240000	1.90386800	0.42456100
H	-2.81091600	0.47366600	0.73318600
C	-0.06840500	3.54794800	-0.58635900
H	0.96705300	3.51572000	-0.91411500
H	-0.74762400	3.69812200	-1.41922100
H	-0.21389100	4.29656500	0.18684600
S	-2.27646000	-1.36500200	-0.10543000
O	-1.91443900	-0.69864200	-1.34619700
O	-3.20210000	-0.43026000	0.73613800
O	-2.92055400	-2.62841400	-0.16503600
N	-0.89922500	-1.33250300	0.77900000
H	-0.81598800	0.34628600	-1.20558800
H	-0.09723000	-1.62350500	0.21396600
H	-0.98954000	-1.88427000	1.62345200

277

278 (MSA)₂·(SFA)₁·(MA)₁:

Atoms	X	Y	Z
N	-0.01836400	-1.95799700	-0.00643000
H	-0.82136400	-2.22276500	-0.57918200
H	-0.11511600	-0.94337600	0.14944200
C	0.03307900	-2.69035900	1.27720000
H	-0.86421200	-2.45747000	1.84147700
H	0.09492300	-3.75638400	1.08121000
H	0.91601500	-2.35127600	1.80909200

Atoms	X	Y	Z
S	2.97123300	-0.56608400	-0.28750300
O	2.25698800	-0.46957300	0.99329500
O	2.99724300	0.71745400	-1.01351900
O	2.49667100	-1.68850200	-1.09859500
H	0.87130000	-2.04901900	-0.53861800
C	4.66585900	-0.91077800	0.09276000
H	5.04325800	-0.09693000	0.70394400
H	4.70286500	-1.85323700	0.63015300
H	5.20891400	-0.97681000	-0.84508400
S	0.07030500	1.93796800	0.17680600
O	1.40644000	2.52636300	-0.32630200
O	-0.91243800	2.97549800	0.17751000
O	-0.19621500	0.72820600	-0.57722300
N	0.29262100	1.47013200	1.73228300
H	2.05193800	1.76743200	-0.62180400
H	1.10741000	0.85573300	1.77787900
H	0.40617500	2.29165600	2.31348500
S	-3.10874900	-0.56855500	-0.21106800
O	-2.67194700	-1.50952400	-1.20438000
O	-2.42560900	-0.52378200	1.05427500
O	-4.64133900	-0.90950600	0.11020400
H	-4.73989900	-0.92357100	1.07033900
C	-3.25821200	1.02610400	-0.94045500
H	-2.28890600	1.26274000	-1.36740600
H	-4.03181800	0.95696000	-1.69938100
H	-3.50859100	1.73522300	-0.15742500

279

280

(MSA)₂·(SFA)₁·(MA)₂:

Atoms	X	Y	Z
N	0.16668400	-1.40622000	-1.81642600
H	0.86192800	-0.69087000	-2.05986400
H	-0.78549300	-1.02199400	-1.88877200
C	0.35827100	-2.66087900	-2.56378000
H	1.37414600	-3.00545500	-2.39632800
H	-0.35034400	-3.39620200	-2.19518800
H	0.19375200	-2.48504000	-3.62212600
N	0.14550400	0.06960000	2.07231900
H	-0.31587700	-0.54726600	1.37989300
H	-0.48282800	0.85332800	2.23774500
C	0.44922800	-0.71262300	3.28645700
H	1.11551600	-1.51632700	2.98892900
H	0.92981300	-0.07580000	4.02279600
H	-0.47375300	-1.12221000	3.68542400
S	2.74583800	-0.45661500	0.03157100

Atoms	X	Y	Z
O	2.70448800	-0.22950000	-1.40734800
O	1.82610400	-1.51935100	0.47658500
O	2.57029000	0.76370100	0.84975900
H	1.01581300	0.42577900	1.63236700
C	4.38486300	-1.02761700	0.40480400
H	4.55312500	-1.94687400	-0.14769800
H	5.08297200	-0.25638100	0.09368400
H	4.44775000	-1.20017900	1.47477200
S	-2.55764800	-0.92111400	0.15404000
O	-2.64544500	0.34721600	0.92258200
O	-1.41174900	-1.72750200	0.60766300
O	-2.59912800	-0.74169800	-1.29006800
H	0.33447000	-1.56054300	-0.81153700
C	-4.01354200	-1.82084300	0.60958000
H	-4.87399000	-1.23157800	0.30753900
H	-3.99139700	-2.77200200	0.08661200
H	-3.99880000	-1.96705300	1.68498000
S	-0.39653100	2.31080400	-0.59342100
O	-1.85940200	2.50548300	-0.13307900
O	-0.10578800	0.89943600	-0.66751000
O	-0.17161600	3.15349600	-1.72134300
N	0.46783300	2.82352500	0.72990500
H	-2.21323500	1.63108600	0.26944500
H	0.50622100	3.83670100	0.73300400
H	1.40856800	2.43286300	0.62842300

281

282 (MSA)₂·(SFA)₁·(MA)₃:

Atoms	X	Y	Z
N	0.12925400	-0.14997600	-2.00791100
H	0.32017300	0.85426700	-1.85972900
H	-0.88374800	-0.29910000	-1.93395900
C	0.71810800	-0.66402300	-3.25714400
H	1.78521900	-0.46746400	-3.21954900
H	0.53850500	-1.73351700	-3.31030400
H	0.27081300	-0.16243500	-4.11010200
N	0.39547900	-1.22532500	1.92241200
H	0.77753200	-1.63266600	1.05003800
H	-0.62760700	-1.31653200	1.87995200
C	1.01508200	-1.82868200	3.11670100
H	2.08324400	-1.64811800	3.05886200
H	0.60371100	-1.36800700	4.00977000
H	0.80706900	-2.89429600	3.12468800
S	2.93349500	-0.54632900	-0.10204700
O	2.74640900	0.61091600	-0.97869400

Atoms	X	Y	Z
O	1.94722300	-1.61572000	-0.39364500
O	2.97581600	-0.21469100	1.31858000
H	0.60681200	-0.22513000	1.83081200
C	4.51517300	-1.24260800	-0.51574900
H	4.49502400	-1.52895100	-1.56306300
H	5.26876400	-0.48158800	-0.33689000
H	4.67937000	-2.10801900	0.11896800
S	-2.31210500	-1.67165000	-0.13856400
O	-2.45423000	-1.13647000	1.23803200
O	-1.01955500	-2.30323000	-0.36207000
O	-2.65302100	-0.65405100	-1.14148800
H	0.55701700	-0.65439100	-1.21702900
C	-3.54289100	-2.94304500	-0.28129000
H	-4.51851100	-2.49164500	-0.12872000
H	-3.46425400	-3.36817000	-1.27733700
H	-3.33962100	-3.69451700	0.47553700
S	0.05968500	2.38321900	0.20389000
O	-0.86065400	3.30360400	0.88197600
O	-0.24651900	0.97607100	0.51831900
O	0.11125400	2.59243600	-1.24389200
N	1.53311300	2.66502200	0.89716500
H	-2.21031900	2.26085600	1.19122300
H	1.76797500	3.64060000	0.75171800
H	2.21641800	2.07053100	0.42426500
H	-3.78445300	1.71378900	1.49472200
N	-2.99215200	1.65107600	0.86359400
H	-2.65421900	0.67020500	0.86970200
C	-3.34075000	2.10196800	-0.50856500
H	-4.08520000	1.43524200	-0.92685700
H	-3.69541200	3.12662700	-0.45361900
H	-2.43346600	2.06042400	-1.10304100

283

284 (MSA)₂·(MA)₂:

Atoms	X	Y	Z
N	0.11192700	-2.09657100	0.01406700
H	0.88599900	-1.72297100	-0.57703400
H	-0.69082900	-2.37208200	-0.55919700
C	0.63550000	-3.16287400	0.88977300
H	1.44362000	-2.73873300	1.47811600
H	-0.15595000	-3.51655400	1.54308900
H	1.01051100	-3.97914600	0.28048900
N	-0.11192300	2.09657300	0.01402900
H	0.24452800	1.30262100	0.57021500
H	-0.88599500	1.72295200	-0.57705800

Atoms	X	Y	Z
C	-0.63551500	3.16286000	0.88974300
H	0.15593300	3.51656500	1.54304800
H	-1.01056100	3.97912000	0.28046500
H	-1.44361300	2.73869200	1.47809700
S	2.55170800	0.17194000	-0.22445200
O	2.38340100	-1.01980300	-1.07173500
O	1.65768900	0.10853800	0.95327600
O	2.43510000	1.43813200	-0.94524300
H	0.69081300	2.37210700	-0.55925000
C	4.21080900	0.09765900	0.39822800
H	4.32519500	-0.83359800	0.94431900
H	4.88201500	0.13222100	-0.45454200
H	4.36384300	0.95349200	1.04822000
S	-2.55170700	-0.17193900	-0.22441200
O	-2.38340600	1.01978100	-1.07172700
O	-1.65767400	-0.10851100	0.95330200
O	-2.43511300	-1.43815000	-0.94517500
H	-0.24448900	-1.30260900	0.57025800
C	-4.21080000	-0.09763700	0.39828400
H	-4.88201600	-0.13222300	-0.45447700
H	-4.36382800	-0.95345100	1.04830400
H	-4.32517800	0.83363600	0.94434900

285

286 (SFA)₂:

Atoms	X	Y	Z
S	1.94099500	-0.03812100	0.08938100
O	1.63046500	-1.04323800	-1.07511700
O	1.04729800	-0.35013200	1.18230000
O	3.34887100	-0.05958700	0.27474000
N	1.49427800	1.41063700	-0.52020200
H	0.66552400	-1.03200800	-1.23859600
H	2.26943500	2.05706800	-0.51766900
H	0.64845500	1.76287600	-0.08507300
S	-1.77388000	0.05080700	-0.03323800
O	-1.58921400	-0.81218800	1.25792500
O	-1.44539400	1.41799300	0.24642600
O	-1.11402100	-0.61602500	-1.12949300
N	-3.38451100	-0.08175900	-0.23469000
H	-0.62312900	-0.80874100	1.45154100
H	-3.82181100	0.82871500	-0.20954800
H	-3.604734000	-0.60761700	-1.06893400

287 (SFA)₂·(MA)₁:

Atoms	X	Y	Z
H	-1.55598100	1.64215800	-0.82412500
N	-0.75339900	2.31448400	-0.70620500
C	-0.86366600	3.06419700	0.56761200
H	-0.70215000	2.93064900	-1.51176300
H	-0.96187800	2.33044600	1.36011700
H	-1.74007700	3.70407000	0.53557700
H	0.03260800	3.65947600	0.71215000
S	2.18332300	-0.21522100	-0.06969500
O	1.46037100	0.74981100	-0.87374900
O	1.59510000	-1.62287500	-0.36720700
O	3.59809200	-0.30427200	-0.18149900
N	1.82945000	0.13521800	1.49394200
H	0.10097800	1.71690000	-0.70099900
H	2.39872200	-0.44695700	2.09651700
H	0.83355000	-0.01815700	1.65367100
S	-1.73988300	-0.68039800	-0.03031400
O	-0.93075900	-1.56916800	-0.86169100
O	-0.98739200	0.00111800	1.01975400
O	-2.52334600	0.28531900	-0.81585100
N	-2.77835100	-1.71004000	0.75583900
H	0.60346700	-1.58335200	-0.56820200
H	-3.20110500	-2.32122400	0.06612600
H	-3.50160500v	-1.16640100	1.21230600

288

289

(SFA)₂·(MA)₂:

Atoms	X	Y	Z
H	0.76020400	1.28556600	0.89213400
S	-2.35222000	0.21155500	-0.28299200
O	-1.80732900	1.29217100	-1.09680500
O	-2.36089700	-1.09653400	-0.91469700
O	-1.72908500	0.14382700	1.05856500
N	0.14628500	2.10390900	0.68572400
H	-0.34751800	1.88761700	-0.19979300
C	0.91480000	3.36288200	0.61782300
H	1.38284800	3.54800200	1.58014700
H	0.24642600	4.18073500	0.36656000
H	1.67517800	3.23817600	-0.14530500
H	-0.76023900	-1.28573200	0.89189800
S	2.35222300	-0.21150500	-0.28298500
O	1.72906200	-0.14399900	1.05857100
O	1.80735900	-1.29199800	-1.09697900
O	2.36089700	1.09668400	-0.91448000
N	-0.14630300	-2.10402700	0.68535500
H	0.34751600	-1.88757300	-0.20011400

Atoms	X	Y	Z
C	-0.91479500	-3.36300100	0.61721500
H	-1.38286700	-3.54829500	1.57949400
H	-0.24640000	-4.18080000	0.36583000
H	-1.67515500	-3.23817900	-0.14591200
N	-3.92072900	0.70686800	0.02811700
H	-4.34639200	0.93071600	-0.86510000
H	-4.42428200	-0.07201300	0.43792400
N	3.92073200	-0.70685000	0.02807300
H	4.34640900	-0.93056100	-0.86517100
H	4.42427300	0.07197600	0.43800300
H	-0.59422900	2.09959700	1.38544100
H	0.59419800	-2.09982700	1.38508600

290

291 (MSA)₃:

Atoms	X	Y	Z
S	-0.99750600	1.99166100	0.10351800
O	-0.04095400	1.87612400	1.16639600
O	-2.30343300	1.37811400	0.27254600
O	-0.39749100	1.45690400	-1.23071000
S	2.78804600	-0.28282000	-0.12524000
O	2.21335000	-1.73915200	-0.24575500
H	1.23319900	-1.70421500	-0.13827500
O	1.99242800	0.60087800	-0.96504600
O	4.18743500	-0.35911600	-0.38173400
H	0.52793000	1.07692500	-1.08118500
C	-1.27984700	3.68991700	-0.27640800
H	-1.76574500	4.13077500	0.58920300
H	-0.31541900	4.15133800	-0.46434600
H	-1.92194700	3.73555700	-1.15043700
C	2.48310300	0.13032500	1.56122300
H	3.06616000	-0.55422300	2.16932700
H	2.80623600	1.15849700	1.69716500
H	1.41537000	0.04494300	1.74310600
S	-1.61543300	-1.86135800	0.08338200
O	-1.66525400	-3.25982300	0.35366400
O	-0.34477700	-1.15975000	0.20769400
O	-2.63988700	-1.15345000	1.03310400
H	-2.54164900	-0.17445500	0.92431600
C	-2.24555400	-1.51715200	-1.52926300
H	-3.23400200	-1.96009400	-1.60074400
H	-2.26993200	-0.43718300	-1.65052400
H	-1.55945100	-1.97198800	-2.23874600

292 (MSA)₃·(MA)₁:

Atoms	X	Y	Z
N	0.33303400	-0.03735500	2.17339700
H	-0.17968800	-0.56037900	1.44510100
H	0.77822400	0.77905100	1.71222800
C	-0.61861200	0.39570100	3.22100400
H	-1.34169600	1.05274100	2.74793900
H	-1.12506600	-0.47648400	3.62071500
H	-0.07948200	0.92217200	4.00232700
S	0.10369400	2.14871500	-0.34584400
O	0.41741600	1.23576600	-1.47065300
O	1.16165500	2.15939600	0.66265600
O	-1.21374600	1.86024900	0.24056700
H	1.08876900	-0.63288300	2.50781900
C	0.01365700	3.77136600	-1.04087100
H	0.98656400	4.00291400	-1.46335500
H	-0.75514200	3.76197200	-1.80754000
H	-0.23994700	4.45836100	-0.23956100
S	-2.64975500	-1.20520500	-0.25443700
O	-3.81370900	-2.03234000	-0.30032000
O	-1.85157100	-1.19092400	0.95707200
O	-3.10368600	0.26332200	-0.56351800
H	-2.38182300	0.90011000	-0.29319700
C	-1.59171500	-1.57980000	-1.61551600
H	-1.16680600	-2.56171800	-1.42967300
H	-2.20691500	-1.57154300	-2.51002900
H	-0.80903400	-0.82610800	-1.64898400
S	2.44299900	-1.12526600	-0.12023000
O	1.08596500	-1.63099700	-0.11938300
O	2.95637500	-0.68703500	1.15571400
O	2.58509100	-0.01831400	-1.19558000
H	1.70204900	0.50913800	-1.30772600
C	3.53608000	-2.34399200	-0.77711600
H	3.54681700	-3.16900100	-0.07099700
H	3.15341300	-2.65617900	-1.74323100
H	4.52073700	-1.89520400	-0.86488300

293

294

(MSA)₃·(MA)₂:

Atoms	X	Y	Z
N	0.81161200	-0.82222900	-1.85056500
H	0.89265000	0.10493900	-1.42122000
H	0.17907000	-1.38783200	-1.25578400
C	0.22868100	-0.74546000	-3.20471200
H	-0.75870800	-0.30208700	-3.11948900
H	0.86519900	-0.13581600	-3.83847800
H	0.14529300	-1.74819600	-3.61138400

Atoms	X	Y	Z
N	0.62135600	0.67595500	1.80677100
H	0.07530400	1.54369300	1.78829400
H	1.37504800	0.76400900	1.09367400
C	1.15621200	0.36468800	3.15127900
H	0.32542200	0.25388300	3.84149900
H	1.73468800	-0.54943500	3.08482700
H	1.80447100	1.17489000	3.46993700
S	-2.11390700	-1.82449300	0.25407300
O	-1.18528900	-2.35854400	-0.73860200
O	-3.17953700	-0.99078600	-0.37609200
O	-1.47501000	-1.13375500	1.37200300
H	-0.03552100	-0.05882100	1.49728800
C	-2.98071500	-3.21256400	0.92483500
H	-3.68243600	-2.83952600	1.66422000
H	-3.49614100	-3.70794400	0.10784700
H	-2.24396800	-3.86977100	1.37657100
S	3.46928900	-0.18155000	-0.03773500
O	3.37111300	-0.69378500	1.32120700
O	2.45123600	0.87727600	-0.28606700
O	3.43693200	-1.20446900	-1.09043300
H	1.77152200	-1.20681800	-1.81147100
C	5.04475100	0.62016600	-0.18709000
H	5.10148900	1.39466000	0.57147900
H	5.80980900	-0.13414000	-0.02928500
H	5.11693300	1.04270400	-1.18431700
S	-1.80110300	2.03746600	-0.13193700
O	-0.88459700	1.09400100	-0.75073600
O	-1.33163000	2.67891100	1.07826300
O	-3.15780300	1.37960400	0.09970400
H	-3.14963000	0.29832800	-0.10451500
C	-2.17597200	3.31269500	-1.29561200
H	-2.56549200	2.84544100	-2.19447600
H	-2.91356100	3.96705400	-0.84103700
H	-1.25172700	3.84714300	-1.49422000

295

296 (MSA)₃·(MA)₃:

Atoms	X	Y	Z
N	2.91376300	1.57069900	-0.43565700
H	2.73386200	1.04460100	0.43311400
H	2.26991500	2.39969800	-0.46019100
C	4.34508000	1.89122500	-0.58031200
H	4.91677900	0.96834900	-0.54542900
H	4.50888400	2.39121200	-1.52985200
H	4.64787500	2.54438800	0.23193000

Atoms	X	Y	Z
N	-0.31584900	-1.15465800	-1.94710900
H	-0.46152900	-0.16188700	-1.71295200
H	-0.80866700	-1.64680200	-1.17894400
C	-0.86681600	-1.51002900	-3.26881600
H	-0.34524100	-0.95113600	-4.04019000
H	-0.73340800	-2.57452700	-3.43652900
H	-1.92097200	-1.25321700	-3.26703200
N	-0.32538100	-0.34130800	2.03027200
H	-0.51607100	0.66646200	1.88837900
H	0.68957100	-0.47551700	1.99821500
C	-0.94517800	-0.84807900	3.26943600
H	-2.01326400	-0.66824800	3.19779700
H	-0.74872300	-1.91275800	3.35226100
H	-0.53153100	-0.32195000	4.12451700
S	-0.12606000	2.44552000	0.07203700
O	-2.92603800	0.41901100	1.00460900
O	0.91460100	3.38946700	-0.38149900
O	-0.29222200	2.42487700	1.52529700
H	-0.72325000	-0.84764700	1.22422500
C	-1.65511000	2.98882900	-0.62588300
H	-1.82543000	3.99935800	-0.26582900
H	-1.55947400	2.96788900	-1.70710300
H	-2.42358400	2.30118000	-0.28319000
S	2.31911600	-1.66583600	0.20218400
O	1.02448100	-2.31675300	0.35346400
O	2.57357300	-0.64585600	1.24252400
O	2.53231900	-1.13338100	-1.16140000
H	0.68939900	-1.33605400	-1.85115800
C	3.56219500	-2.90920100	0.43557500
H	3.41071100	-3.67609700	-0.31791500
H	4.53587400	-2.44191600	0.32388800
H	3.43937300	-3.31760200	1.43398000
S	-2.99056500	-0.57104200	-0.06554500
O	-2.03132400	-1.68628300	0.16580800
O	-2.85944200	-0.02242700	-1.41577900
O	0.15214200	1.08758000	-0.45724200
H	2.59949700	0.89803600	-1.14152600
C	-4.60105600	-1.31651600	0.02429800
H	-4.66968400	-2.07377500	-0.75063400
H	-4.71216400	-1.75816100	1.00993800
H	-5.33573700	-0.53253200	-0.13317100

297

298 (SFA)₃:

Atoms	X	Y	Z
S	0.06337000	2.08953700	-0.09723500
O	-0.15395600	1.45280300	1.33737800
O	-0.04441300	1.01749200	-1.06067600
O	-0.81700200	3.20299700	-0.12865700
N	1.59933900	2.57815300	-0.19645700
H	0.39982700	0.63825100	1.40691700
H	1.86851800	3.20779600	0.54628200
H	2.23784000	1.80331000	-0.36495200
S	2.23090000	-1.00044900	0.01908600
O	1.11422100	-1.78949600	-0.72159200
O	2.86575800	-0.08826400	-0.88124400
O	1.68491500	-0.49916200	1.25831800
N	3.35485300	-2.11457900	0.41833100
H	0.22532000	-1.63839400	-0.27562800
H	3.84214100	-2.43939200	-0.40783300
H	2.94941400	-2.87981100	0.94332900
S	-2.40389800	-1.05929100	0.01333000
O	-2.20023900	-0.50155300	-1.43875400
O	-3.41774400	-2.04479500	-0.08299400
O	-1.09327700	-1.37974600	0.55139400
N	-2.93394500	0.15891600	0.94891700
H	-1.42544600	0.10894000	-1.44170500
H	-2.20495100	0.82869000	1.17127700
H	-3.78644000	0.57424500	0.59848700

299

300

(SFA)₃·(MA)₁:

Atoms	X	Y	Z
H	0.89701500	-2.30972500	-0.37448600
N	0.05884800	-2.06671500	0.16302500
C	0.11349700	-2.55308400	1.56121000
H	-0.78284400	-2.37739300	-0.32657800
H	1.00508300	-2.13948400	2.02071300
H	0.15653800	-3.63781300	1.56557000
H	-0.78239900	-2.20970900	2.06751900
S	-0.05397900	1.69157400	0.23185300
O	-0.05146100	0.49691200	-0.63684900
O	1.19074300	2.44540500	0.03653400
O	-1.27917100	2.46284500	0.07174700
N	-0.02992100	1.25612600	1.81895100
H	0.01720200	-1.02386100	0.10807800
H	-0.86838600	0.72276100	2.02785900
H	0.81579900	0.72621900	2.00451100
S	2.96834600	-0.40183700	-0.30260100
O	2.94821200	0.99594400	-0.93590700

Atoms	X	Y	Z
O	2.36751100	-0.35609100	1.00986600
O	2.48061100	-1.39950000	-1.21912800
N	4.56245300	-0.73753000	-0.09345900
H	2.18695000	1.61757600	-0.53712300
H	5.01462600	0.00579900	0.42589800
H	5.00606500	-0.86813000	-0.99515200
S	-3.13934300	-0.46354400	-0.20105600
O	-3.34527300	1.04690200	-0.47482100
O	-2.27320600	-0.62405900	0.94409900
O	-4.41097100	-1.10011300	-0.23400400
N	-2.27925400	-1.05307000	-1.49711400
H	-2.52230700	1.60270600	-0.24614200
H	-2.90929700	-1.13907000	-2.28640100
H	-1.51623900	-0.40810600	-1.70476300

301

302

(SFA)₃·(MA)₂:

Atoms	X	Y	Z
H	-0.44769100	-0.36772000	1.30094700
S	2.75847200	-0.51575700	0.34769200
O	2.54547700	-1.00614000	1.70533400
O	2.96802300	-1.52013000	-0.67365100
O	1.68905000	0.42694800	-0.06523100
N	-0.00768900	0.01115800	2.15184700
H	0.94569500	-0.40055100	2.18716400
C	-0.83538700	-0.29280900	3.33939700
H	-1.81279300	0.16143500	3.20550900
H	-0.35311900	0.10932000	4.22489300
H	-0.94350900	-1.36912000	3.41028100
H	0.85374700	-0.36365400	-1.34206700
S	-1.91838200	-1.94656600	-0.08122600
O	-1.48387000	-0.52926900	-0.26011600
O	-1.43727300	-2.72258300	-1.21430700
O	-1.59625500	-2.43800700	1.23806100
N	0.36827200	-0.68681300	-2.20597100
H	-0.11036300	-1.57280000	-1.98853500
C	1.32921600	-0.78864300	-3.32255700
H	1.76129200	0.19299200	-3.49317400
H	0.81828800	-1.13058900	-4.21737400
H	2.10894000	-1.48412400	-3.03039500
N	4.11888200	0.44849200	0.49051500
H	4.78452700	-0.05630000	1.06536100
H	4.52085300	0.57811600	-0.43117600
N	-3.58204500	-1.86733500	-0.11709300
H	-3.89734700	-1.83681600	-1.07967400

Atoms	X	Y	Z
H	-3.93938400	-2.70603100	0.32569900
H	0.08976800	1.01844700	1.98144400
H	-0.35448100	0.01980400	-2.35260800
S	-1.01002500	2.70621300	-0.35987600
O	-2.07518500	1.84176800	0.38342000
O	-0.59697600	1.99830000	-1.54316400
O	-1.51255300	4.03729100	-0.42888400
N	0.26766300	2.71493100	0.70381600
H	-1.98340800	0.87507500	0.10720200
H	0.50340600	3.67464500	0.91963500
H	1.05249500	2.19589300	0.30685600

303

304 (SFA)₃·(MA)₃:

Atoms	X	Y	Z
H	-1.44232900	-1.95662000	0.76326700
N	-0.54015900	-1.89680100	0.27057800
C	-0.65530700	-2.55646300	-1.05218600
H	0.24638300	-2.30817500	0.79577400
H	-1.46201600	-2.08102400	-1.60140800
H	-0.88185200	-3.60689600	-0.89678200
H	0.29727700	-2.45152000	-1.56056000
S	0.42241300	1.71245900	-0.48167600
O	0.12938600	0.85771400	0.68874600
O	-0.51308800	2.83804800	-0.53817200
O	1.82900800	2.09657600	-0.54169200
N	0.14487100	0.86746500	-1.87867500
H	-0.33226000	-0.88882500	0.17650700
H	0.74970200	0.05026600	-1.86488700
H	-0.83172100	0.58089700	-1.88031200
S	-3.61105500	-0.61224100	-0.12070400
O	-4.57458000	0.38575600	0.34855700
O	-2.44609300	0.03287700	-0.72859100
O	-3.26940000	-1.61880400	0.87851500
N	-4.28983100	-1.50279900	-1.36521500
H	-3.47454900	1.86272400	0.41423900
H	-4.66710500	-0.85765600	-2.05089500
H	-5.05190700	-2.04944200	-0.97867200
H	3.19203900	1.03454700	-0.77876600
N	4.22066900	0.87040200	-0.85423400
C	4.90338500	1.84524500	0.02658900
H	4.48391000	0.98231000	-1.82872200
H	4.57443600	1.63415000	1.03830200
H	4.59529400	2.84556400	-0.26011700
H	5.97946600	1.73043800	-0.06012300

Atoms	X	Y	Z
S	2.75946100	-1.55089300	0.43324900
O	4.18126400	-1.77119100	0.18827800
O	2.06044700	-1.03378800	-0.74860700
O	2.06472800	-2.66849200	1.06268400
N	2.74388800	-0.23346800	1.47718500
H	4.40544200	-0.11006800	-0.56124600
H	2.94943300	-0.56214200	2.41355000
H	1.81870700	0.19876600	1.44317300
H	-3.08804500	3.35440600	1.06353200
N	-2.74044600	2.41717300	0.88520000
C	-2.39105300	1.72091900	2.14854700
H	-1.88985600	2.50068300	0.26131200
H	-3.26422600	1.69658300	2.79291200
H	-1.56008900	2.23675000	2.61830500
H	-2.08768900	0.71351500	1.88839900