Supporting information

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A novel formation mechanism of sulfamic acid and its enhancing effect on methanesulfonic acid-methylamine aerosol particle formation in agriculture-developed and coastal industrial areas

Hui Wang [a,‡], Shuqin Wei [a,‡], Jihuan Yang [a], Yanlong Yang [a], Rongrong Li [a], Rui Wang [a],

Chongqin Zhu [b,*], Tianlei Zhang [a,*] Changming Zhang [c],

[a] Shaanxi Key Laboratory of Catalysis, School of Chemical & Environment Science, Shaanxi University of Technology, Hanzhong, Shaanxi 723001, P. R. China

[b] College of Chemistry, Key Laboratory of Theoretical & Computational Photochemistry of Ministry of Education, Beijing Normal University, Beijing 100190, China.

[c] School of Mechanical Engineering, Shaanxi University of Technology, Hanzhong, Shaanxi 723001, P. R. China

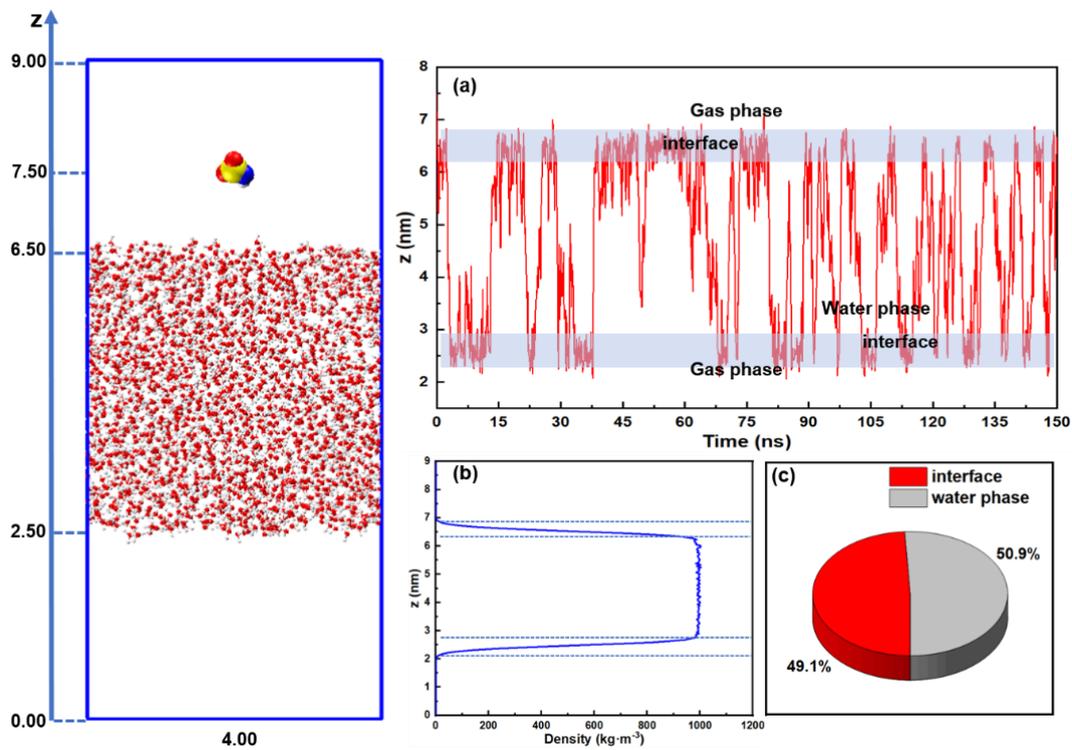| S. NO	Caption
S4	**Fig. S1** (a) The z coordinates of $HNSO_2$ molecule as the function of simulation time; (b) the density profile of water; (c) the pie chart with the occurrence percentages of $HNSO_2$ molecule at the air-water interface and in water phase
S5	**Fig. S2** The optimized geometrical structures for the species involved in the $HNSO_2$ hydrolysis at several different levels of theory.
S6	**Table S1** The Energy barriers (ΔE) and unsigned error (UE) (kcal·mol^{-1}) for the $HNSO_2$ hydrolysis at different theoretical the potential energy profile (ΔG) correction
S7-S8	**Fig. S3** Optimized geometries of $HNSO_2$, H_2O, MSA, $(H_2O)_2$, $HNSO_2\cdots H_2O$ and $MSA\cdots H_2O$ at the M06-2X/6-311++G(2df,2pd) level (bond distances in Angstroms and angles in degrees) along with the stabilization energies of $(H_2O)_2$, $HNSO_2\cdots H_2O$ and $MSA\cdots H_2O$ at the CCSD(T)-F12/cc-pVDZ-F12//M06-2X/6-311++G(2df,2pd) level of theory
S9-S10	**Fig. S4** The optimized geometries and electric energies (in Hartree-Fock) for the complexes of $HNSO_2\cdots H_2O\cdots$MSA at the M06-2X/6-311++G(2df,2pd) level of theory
S11	**Fig. S5** 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
S12	**Table S2** Zero point energy (ZPE/(kcal·mol^{-1})), entropies (S/(cal·mol^{-1}·K^{-1})), relative energies (ΔE and $\Delta(E + ZPE)$/(kcal·mol^{-1})), enthalpies (ΔH(298)/(kcal·mol^{-1})), and free energies (ΔG(298)/(kcal·mol^{-1})) for the hydrolysis reaction of $HNSO_2$ without and with H_2O and MSA
S13	**Table S3** Equilibrium constants (cm^3·molecule^{-1}) for the $HNSO_2\cdots H_2O$, $H_2O\cdots H_2O$, and $MSA\cdots H_2O$ complexes within the temperature range of 212.6-320.0 K

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* Corresponding authors, Tel: +86-0916-2641083, Fax: +86-0916-2641083.

E-mail: cqzhu@bnu.edu.cn (C. Q. Zhu), ztianlei88@l63.com (T. L. Zhang).

‡ These authors contributed equally to this work.

S48	**Fig. S20** (a) The J (cm^{-3} 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 × 10^7 molecules cm^{-3}, red line: [MA] = 2.5 × 10^8 molecules cm^{-3}, blue line: [MA] = 2.5 × 10^9 molecules cm^{-3}) at 258.15 K
S49	**Fig. S21**(a) The J (cm^{-3} 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 × 10^7 molecules cm^{-3}, red line: [MA] = 2.5 × 10^8 molecules cm^{-3}, blue line: [MA] = 2.5 × 10^9 molecules cm^{-3}) at 298.15 K
S50	**Fig. S22**. The influence of [MA] on the relative contribution of the pure MSA-MA-based clustering pathway and the SFA participation pathway to the system flux is analyzed at 278.15 K, [MSA] = 10^7 molecules·cm^{-3} and [SFA] = 10^4, 10^6 and 10^8 molecules·cm^{-3}.
S51	**Fig. S23** Main cluster formation mechanism of MSA-MA-SFA-based system at 238.15 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
S52	**Fig. S24** Main cluster formation mechanism of MSA-MA-SFA-based system at 258.15 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
S53	**Fig. S25** 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
S54	**Table S8** 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 and 238.15 K
S55-S56	**Table S9** Evaporation rates γ (s^{-1}) for the studied clusters at different temperatures of 298.15, 278.15, 258.15 and 238.15 K
S57-S58	**Table S10** Collision coefficients (β, cm^3·s^{-1}) for each cluster in the present study
S59	**Table S11** Total evaporation coefficients ($\sum\gamma$, s^{-1}) for each cluster in the present study
S60-S61	**Table S12** 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})
S62	**Table S13** 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 methanesulfonic acid, methylamine and sulfamic acid, respectively
S63	**Table S14** 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 methanesulfonic acid, methylamine and sulfamic acid, respectively
S64	**Table S15** 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 methanesulfonic acid, methylamine and sulfamic acid, respectively
S65	**Table S16** 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 methanesulfonic acid, methylamine and sulfamic acid, respectively
S66-S87	**Table S17** Cartesian coordinates of all molecules and clusters in the studied system

14

15 **Fig. S1** (a) The z coordinates of $HNSO_2$ molecule as the function of simulation time; (b) the density

16 profile of water; (c) the pie chart with the occurrence percentages of $HNSO_2$ molecule at the air-

17 water interface and in water phase

Fig. S2 The optimized geometrical structures for the species involved in the HNSO$_2$ hydrolysis at several different levels of theory.

[a, b and, c] respectively represents the values obtained at the M06-2X/6-311++G(3df,2pd), M062X/6-311++G(3df,3pd) and M06-2X/aug-cc-pVTZ level of theory, [d] represents the experimental values (The values in parentheses were obtained at the M06-2X/6-311++G(2df,2pd) level of theory; bond length is in angstrom and angle is in degree.).

The geometric parameters of the reactants of HNSO$_2$, H$_2$O and NH$_2$SO$_3$H (SFA) have been displayed in Fig. S2. As seen in Fig. S2, the mean absolute deviation of calculated bond distances and bond angles between the M06-2X/6-311++G(2df,2pd) level and the experimental reports were 0.02 Å and 0.57°, respectively. This reveals that the calculated bond distances and bond angles at the M06-2X/6-311++G(2df,2pd) level agree well with the available experimental values (From the pubchem database, https://pubchem.ncbi.nlm.nih.gov/#opennewwindow.). In addition, we have re-optimized all equilibrium structures of HNSO$_2$, H$_2$O and SFA at three different theoretical levels of M06-2X/6-311++G(3df,2pd), M062X/6-311++G(3df,3pd) and M06-2X/aug-cc-pVTZ levels. For the calculated geometrical parameters of these species, the mean absolute deviation of calculated bond distances and bond angles between the M06-2X/6-311+G(2df,2pd) level and the other levels were within 0.02 Å and 0.2°, respectively. Therefore, due to its efficiency, the M06-2X/6-311++G(2df,2pd) was adopted to optimize the geometries of all stationary points involved in the HNSO$_2$ hydrolysis.

37   **Table S1** The Energy barriers (ΔE) and unsigned error (UE) (kcal·mol^{-1}) for the HNSO$_2$ hydrolysis

38   at different theoretical the potential energy profile (ΔG) correction

Methods	ΔE [a]	ΔE [b]	ΔE [c]	UE
CCSD(T)/CBS//M06-2X/ 6-311++G(2*df*,2*pd*)	3.4	29.7	-23.0	0.00
CCSD(T)-F12/cc-pVDZ-F12//M06-2X/ 6-311++G(2*df*,2*pd*)	3.6	30.6	-22.0	0.71

39   [a, b and c] respectively denote the species of pre-reactive complexes, transition states and products involved in the
40   HNSO$_2$ hydrolysis.

41   To further confirm the reliability of the CCSD(T)-F12/cc-pVDZ-F12//M06-2X/6-

42   311++G(2*df*,2*pd*) level of theory, single-point energy calculations for the HNSO$_2$ hydrolysis in the

43   gas phase have been performed at two different levels of CCSD(T)/CBS and CCSD(T)-F12/cc-

44   pVDZ-F12 based on the optimized geometries at the M06-2X/6-311++G(2*df*,2*pd*) level. Notably,

45   the complete basis set (CBS) obtained by basis set extrapolation is used as the reference basis set.

46   As presented in Table S1, compared with unsigned error calculated at the CCSD(T)/CBS//M06-

47   2X/6-311++G(2*df*,2*pd*) level, unsigned errors calculated at CCSD(T)-F12/cc-pVDZ-F12//M06-

48   2X/6-311++G(2*df*,2*pd*) was 0.71 kcal·mol^{-1}. This suggests that the relative energies obtained at the

49   CCSD(T)/aug-cc-pVDZ//M06-2X/6-311+G(2*df*,2*pd*) level was reasonable. Considering the

50   computational accuracy and cost, the CCSD(T)/aug-cc-pVDZ//M06-2X/6-311+G(2*df*,2*pd*) method

51   was chosen to calculate the single point energies of all the species involved in the HNSO$_2$ hydrolysis.

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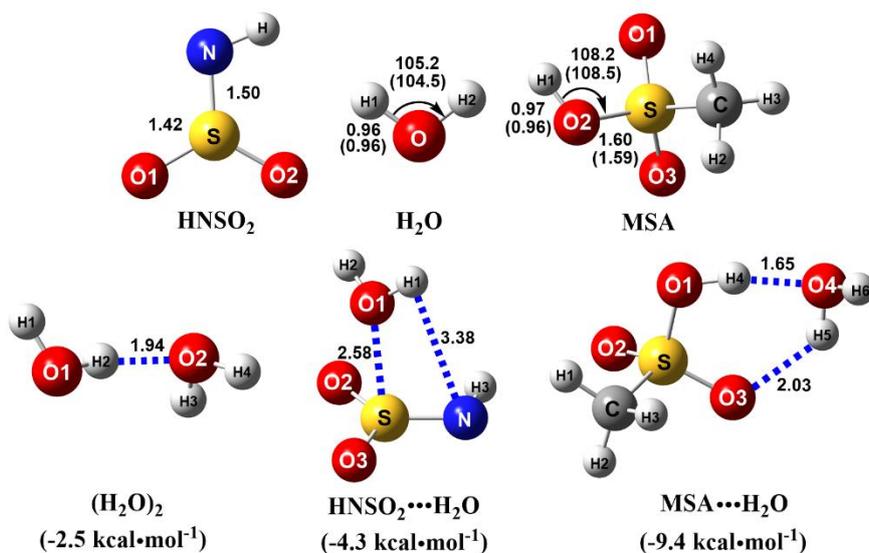
Fig. S3 Optimized geometries of $HNSO_2$, H_2O, MSA, $(H_2O)_2$, $HNSO_2\cdots H_2O$ and MSA$\cdots H_2O$ at the M06-2X/6-311++G(2*df*,2*pd*) level (bond distances in Angstroms and angles in degrees) along with the stabilization energies of $(H_2O)_2$, $HNSO_2\cdots H_2O$ and MSA$\cdots H_2O$ at the CCSD(T)-F12/cc-pVDZ-F12//M06-2X/6-311++G(2*df*,2*pd*) level of theory

Fig. S2 illustrated the optimized geometries of monomer reactants of $HNSO_2$, H_2O and MSA, which were consistent with the available experimental bond lengths (Å) and bond angles. The mean absolute deviation of bond lengths (Å) and bond angles (°) between the calculations at the M06-2X/6-311++G(2*df*,2*pd*) level and the experimental values [1, 2, 3] were less than 0.01 Å and 0.5°, respectively. As for the dimer reactant of $(H_2O)_2$, single hydrogen bond geometry has been obtained, which was in good agreement with the previous reports [4][5] $HNSO_2\cdots H_2O$ and MSA$\cdots H_2O$ displayed cage-like structures, and these geometrical structures were in good agreement with earlier findings [6]. The stabilization energies of $(H_2O)_2$, MSA$\cdots H_2O$ 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 findings [7].

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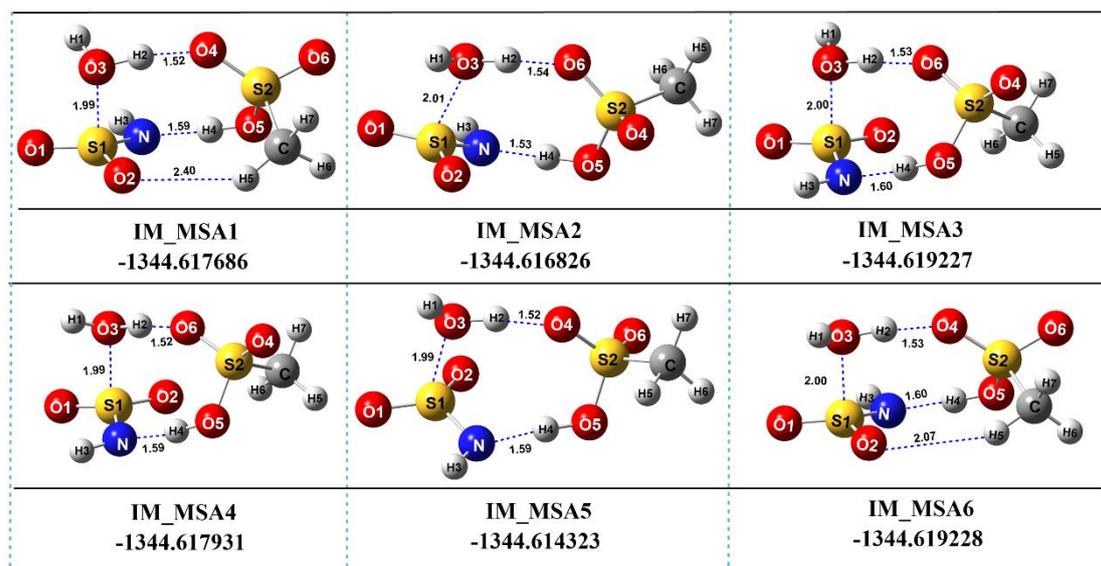
Fig. S4 The optimized geometries and electric energies (in Hartree-Fock) for the complexes of $HNSO_2\cdots H_2O\cdots MSA$ at the M06-2X/6-311++G(2*df*,2*pd*) level of theory

To obtain the most stable configurations of $HNSO_2\cdots H_2O\cdots MSA$, 500 auto-generated structures were produced by ABCluster [1, 2] software with TIP4P model [3, 4] for H_2O and CHARMM force field [5] for $HNSO_2$ and MSA. 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 $S(HNSO_2)\cdots O(H_2O)$ 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 $HNSO_2\cdots H_2O\cdots MSA$ its optimized geometries and stabilization energies have been illustrated in Fig. S2. As seen in Fig. S2, seven geometric isomers of $HNSO_2\cdots H_2O\cdots MSA$ (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 MSA.

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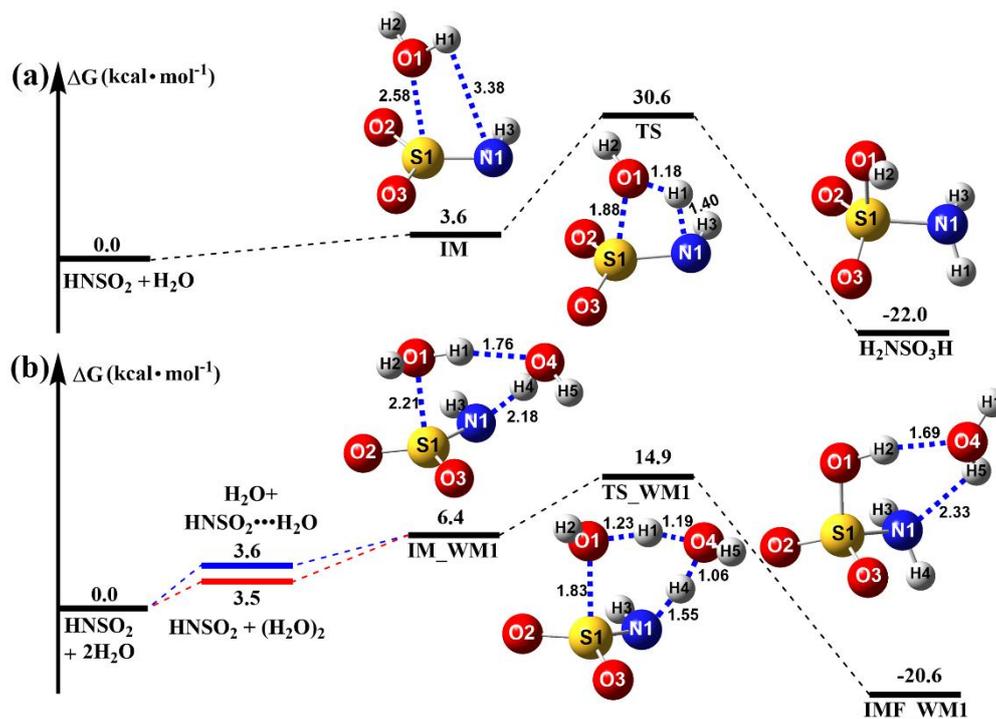
Fig. S5 The potential energy profile (ΔG) for the hydrolysis reaction of $HNSO_2$ without (a) and with (b) H_2O at the CCSD(T)-F12/cc-pVDZ-F12//M06-2X/6-311++G($2df,2pd$) level of theory

127 **Table S2** Zero point energy (ZPE/(kcal·mol^{-1})), entropies (S/(cal·mol^{-1}·K^{-1})), relative energies (ΔE
128 and $\Delta(E + \text{ZPE})$/(kcal·mol^{-1})), enthalpies ($\Delta H(298)$/(kcal·mol^{-1})), and free energies
129 ($\Delta G(298)$/(kcal·mol^{-1})) for the hydrolysis reaction of $HNSO_2$ without and with H_2O and MSA

Species	ZPE	ΔE	S	ΔG	$\Delta(E + \text{ZPE})$	ΔH
$HNSO_2$ + H_2O	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
$HNSO_2$ + $2H_2O$	42.3	0.0	155.7	0.0	0.0	0.0
$HNSO_2$ + $(H_2O)_2$	44.8	-5.0	133.2	3.5	-2.5	-3.2
$HNSO_2$···H_2O + H_2O	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_2O + MSA	68.2	0.0	185.4	0.0	0.0	0.0
$HNSO_2$ + MSA···H_2O	70.5	-11.7	154.1	-0.9	-9.4	-10.2
$HNSO_2$···H_2O + MSA	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

130 [a] The value was taken from reference (Manonmani, G., Sandhiya, L., and Senthilkumar, K.: Hydrolysis of $HNSO_2$:
131 A potential route for atmospheric production of H_2SO_4 and NH_3, Int J Quantum Chem, 120, e26182, 2020.)

132 **Table S3** Equilibrium constants ($cm^3 \cdot molecule^{-1}$) for the $HNSO_2 \cdots H_2O$, $H_2O \cdots H_2O$, and
133 MSA$\cdots H_2O$ complexes within the temperature range of 212.6-320.0 K

T/K	$HNSO_2 \cdots H_2O$	$H_2O \cdots H_2O$	MSA$\cdots H_2O$
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}

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

136 **Table S4** The high-pressure limiting rate constant ($cm^3 \cdot molecule^{-1} \cdot s^{-1}$) for the hydrolysis reaction
137 of $HNSO_2$ with H_2O and MSA within the temperature range of 212.6-320.0 K

T(K)	$HNSO_2 + H_2O$ $\rightarrow HNSO_2 \cdots H_2O$	$HNSO_2 +$ $H_2O \cdots H_2O$ $\rightarrow HNSO_2 \cdots$ $H_2O \cdots H_2O$	$HNSO_2 +$ MSA$\cdots H_2O$ $\rightarrow HNSO_2 \cdots$ MSA$\cdots H_2O$
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}

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Part S1. Calculations of reaction rate coefficients

The rate coefficients for the hydrolysis of $HNSO_2$ with MSA were calculated through a two-step process. Initially, the high-pressure-limit (HPL) rate coefficients were computed applying VRC-VTST methods within the Polyrate package [1]. Subsequently, on the basis of the HPL rate coefficients, the rate coefficients for the hydrolysis of $HNSO_2$ with MSA 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) program [2]. 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 calculations [3], while the step transitioning between pre-reactive complexes and post-reactive complexes via transition states were evaluated using the RRKM theory [4] in combination with the asymmetric Eckart model.

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

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

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

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.

Herein, we describe the implementation details of the VRC-TST calculation[5-8]. There are two assumptions in VRC-VTST calculation: (1) the contribution of the vibrational modes of reactants to the partition function is canceled by the corresponding contribution of transition states to the partition function; (2) the internal geometries of reactants are fixed along the reaction coordinate. The reaction coordinate in VRC-VTST is different from that in RP-VTST and determined by the pivot points of each reactant fragment. For the $HNSO_2$ hydrolysis reaction, the pivot points of $HNSO_2$ (points 1 and 2) are located at a distance ±d along its S axis, and the pivots of H_2O (points 3 and 4) are located at a distance ±d perpendicular to H_2O molecule lane. As shown in Fig. S6, the Multiwfn package combined with the VMD software is adopted to visualize the reaction system and

168 help determine the location of pivot points. The reaction coordinate value (s) is defined as the

169 minimum of the distance (r_{ij}) between the pivot point i (=1 or 2) and pivot point j (=3 or 4), where

170 i and j represent the pivot points of $HNSO_2$ and H_2O molecules, respectively. Hence, each of the

171 four dividing surfaces is obtained by symmetrically placing two pivot points of each radical

172 fragment (1-3, 1-4, 2-3, and 2-4). For example, if the reaction coordinate s is equal to r_{23}, one of the

173 four dividing surfaces (2-3), is determined by the locations of pivot points 2, 3 and the reaction

174 coordinate s. There are total four pair of pivot points, the other three dividing surfaces (1-3, 1-4, 2-

175 4) are defined by their corresponding pivot points and reaction coordinates s. Note that the locations

176 of pivot points are critical to the rate constant calculation. Considering the difference between

177 $HNSO_2$ and H_2O molecules, the distance s between pivot points is varied from 2.5 to 6 Å for $HNSO_2$

178 and H_2O in each case with a 0.5 Å grid increment.
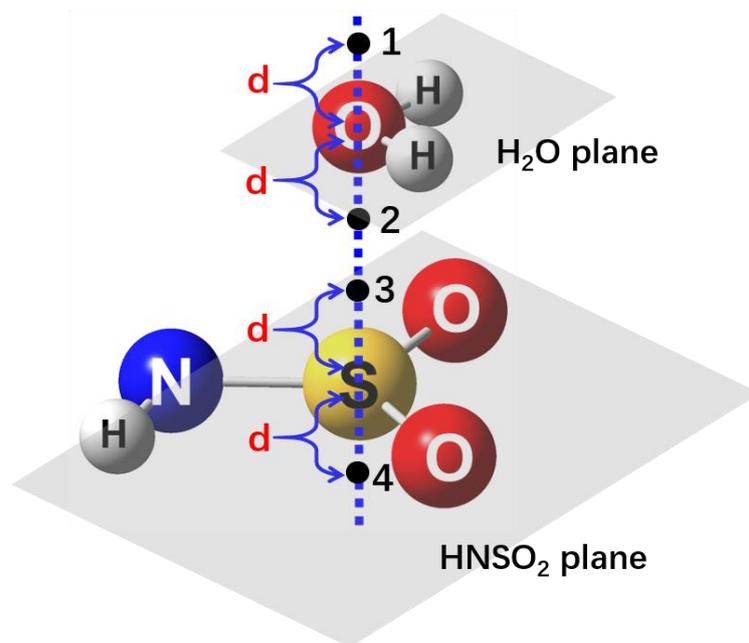
179

180 **Fig. S6** The placements of the pivot points for the $HNSO_2$ hydrolysis

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195   application to the $C_2H_3 + H \rightarrow C_2H_4$ reaction, JCP, 118, 5442-5455, 2003.

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198   polyatomics. New version announcement, Comput Phys Commun, 294, 108933, 2024.

199

200 **Table S5** Rate coefficients (k, $cm^3 \cdot molecule^{-1} \cdot s^{-1}$) for the hydrolysis of $HNSO_2$ by master equation
201 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}

202 k_R, is the bimolecular rate constant for the hydrolysis of $HNSO_2$.

203 **Table S6** Concentrations (molecules·cm^{-3}) of H_2O and MSA 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					

204 [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-
205 water complexes. J. Phys. Chem. A 117, 10381-10396, 2013.)

206 [b] The value was taken from reference (Shen, J., Elm, J., Xie, H.-B., Chen, J., Niu, J., and Vehkamaki, H.: Structural effects of amines in enhancing methanesulfonic acid-driven new particle
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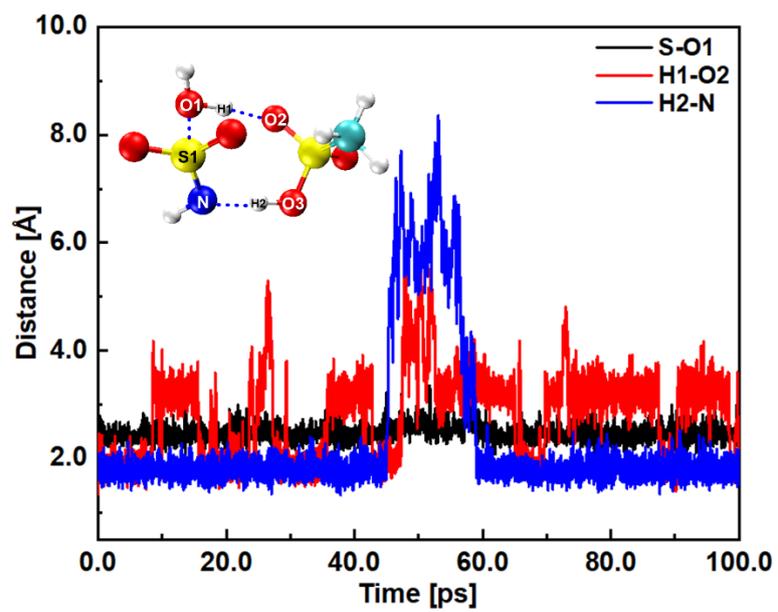
208

209 **Fig. S7** The dynamic trajectories of MSA-assisted gaseous hydrolysis of HNSO$_2$
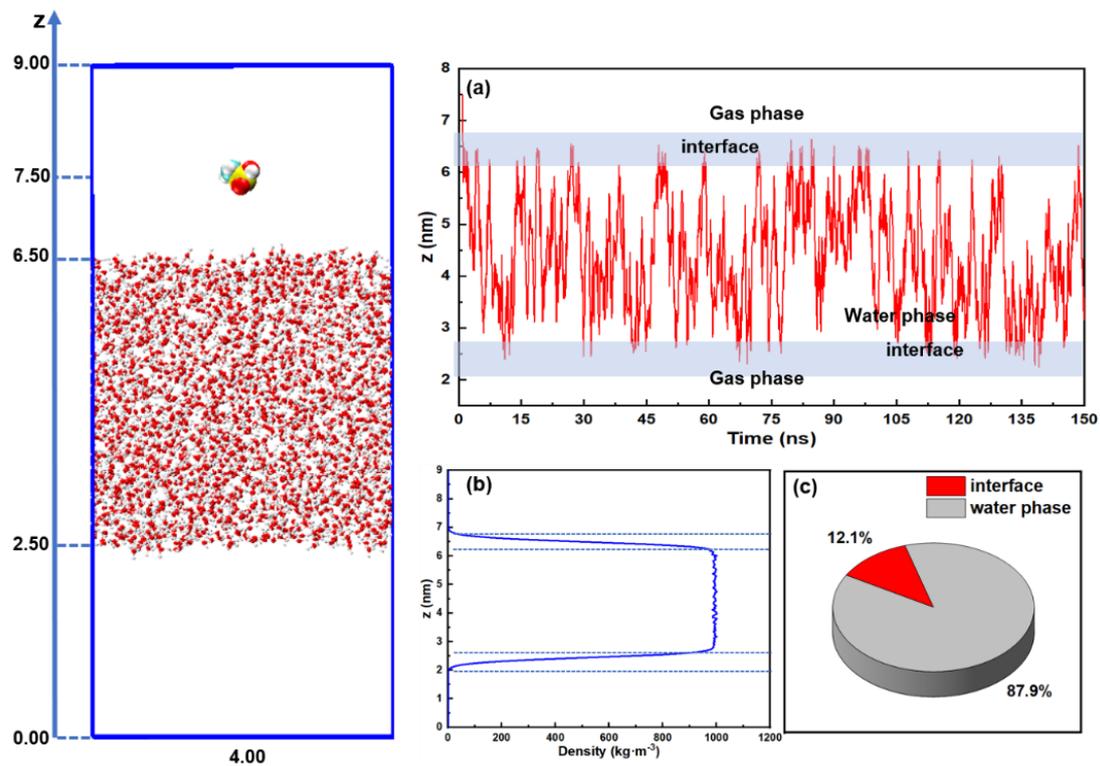
Fig. S8 (a) The *z* coordinates of MSA molecule as the function of simulation time; (b) the density profile of water; (c) the pie chart with the occurrence percentages of MSA molecule at the air-water interface and in water phase
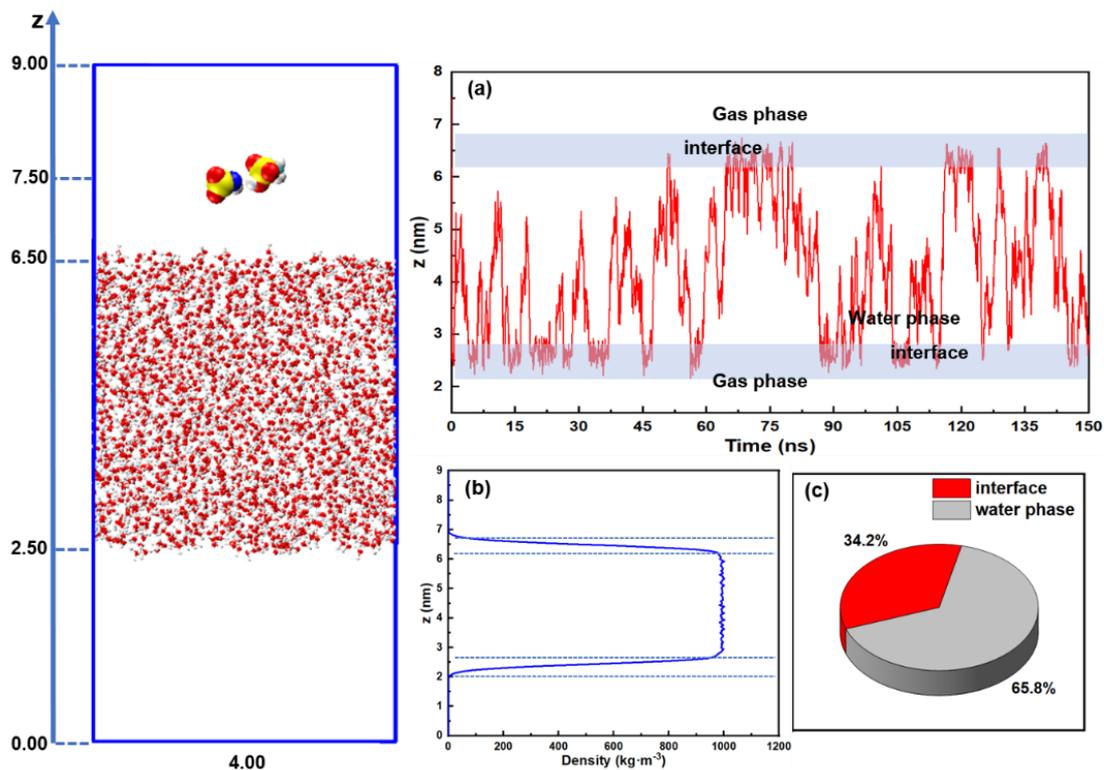
Fig. S9 (a) The z coordinates of complex $HNSO_2 \cdots MSA$ as the function of simulation time; (b) the density profile of water; (c) the pie chart with the occurrence percentages of complex $HNSO_2 \cdots MSA$ at the air-water interface and in water phase

218
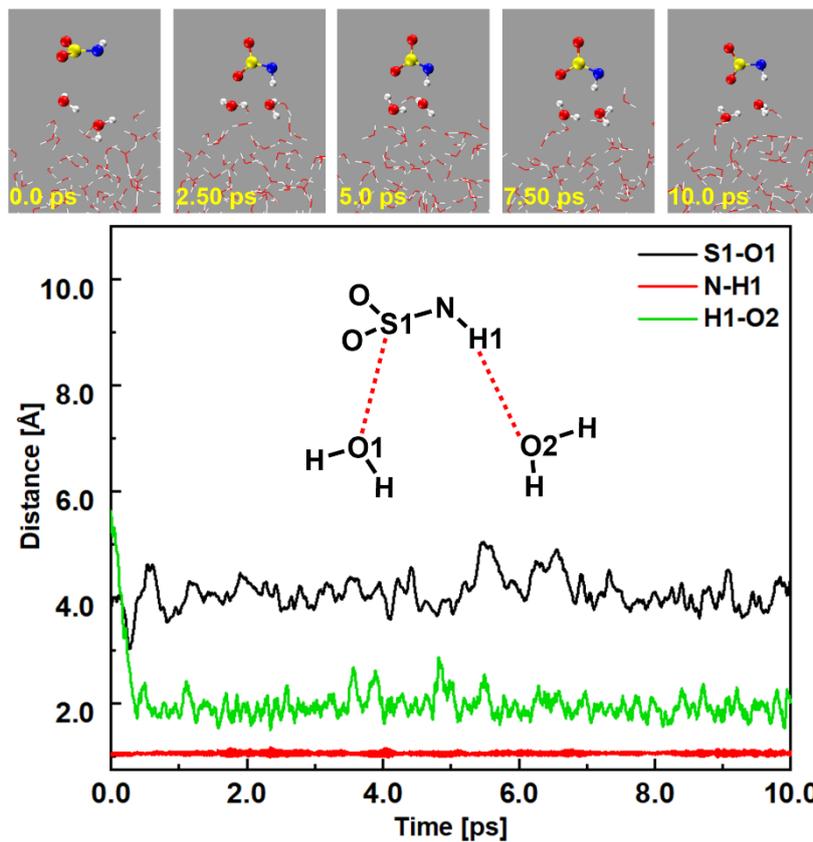
Fig. S10 Snapshot structures taken from the BOMD simulations of $HNSO_2$ reaction at the air-water interface

221
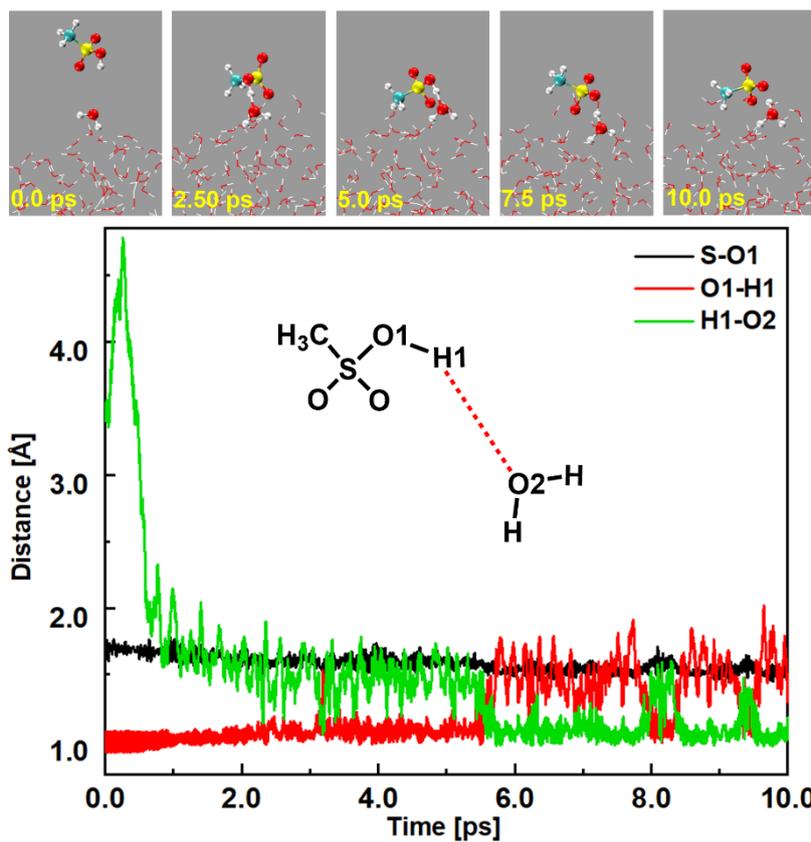
Fig. S11 Snapshot structures taken from the BOMD simulations of MSA reaction at the air-water interface

(g)

(h)

(i)
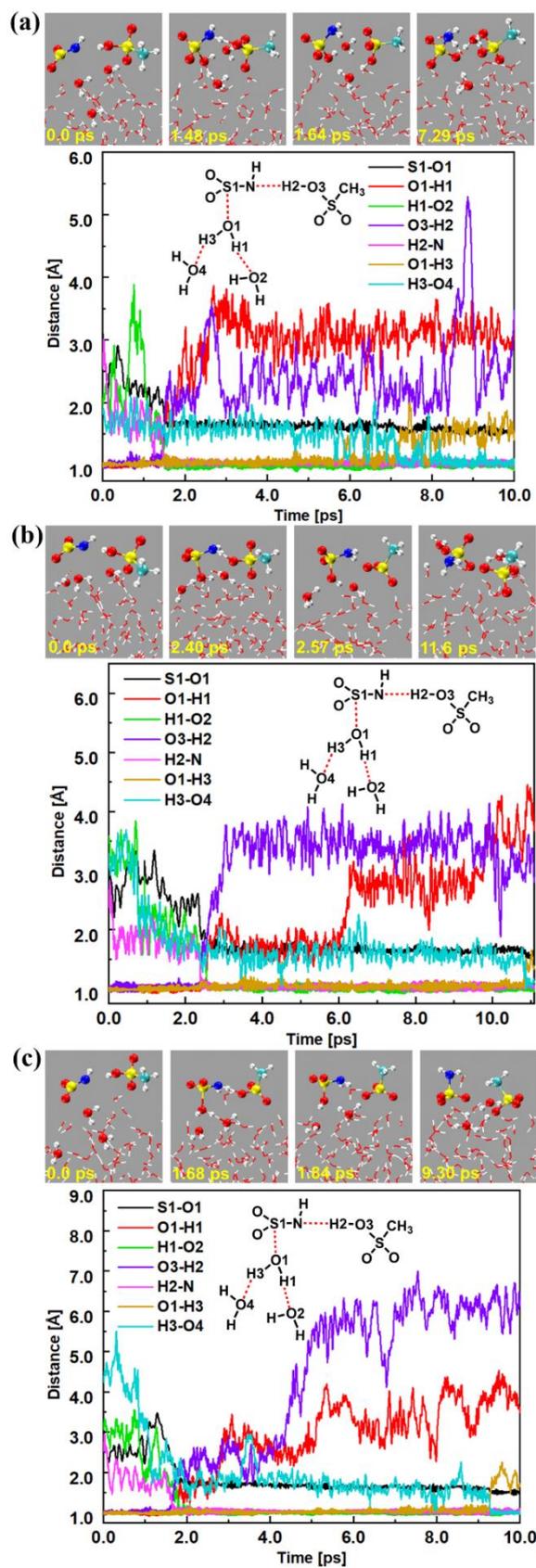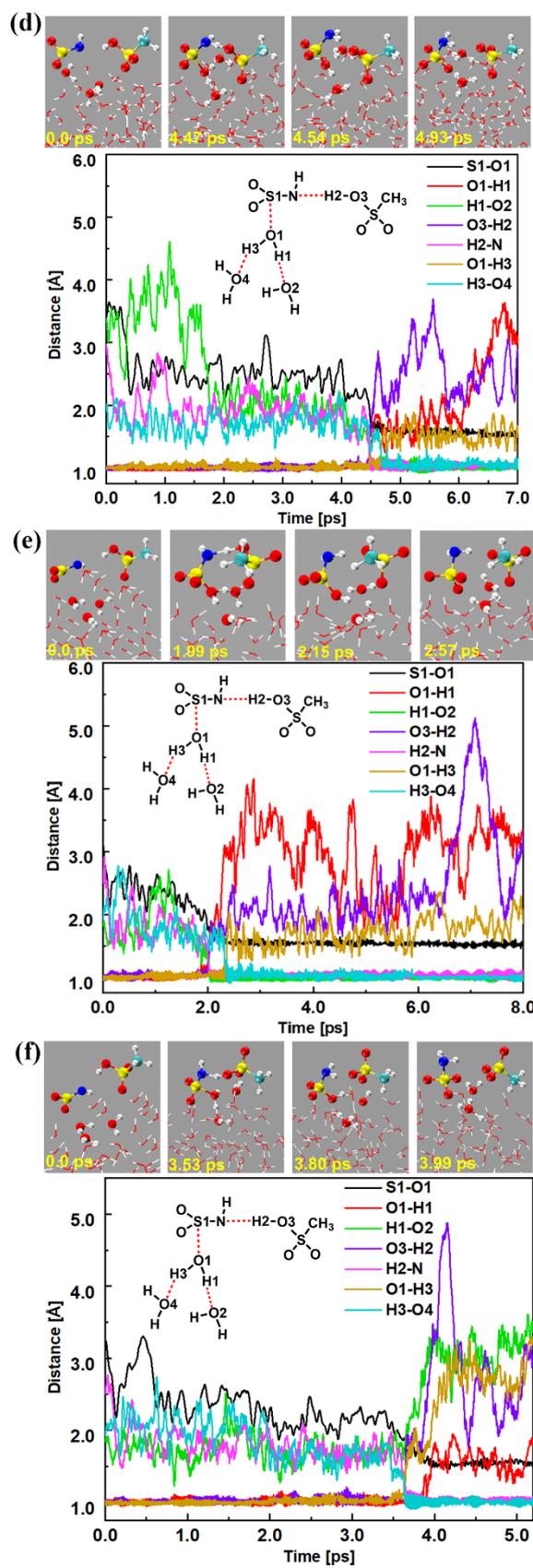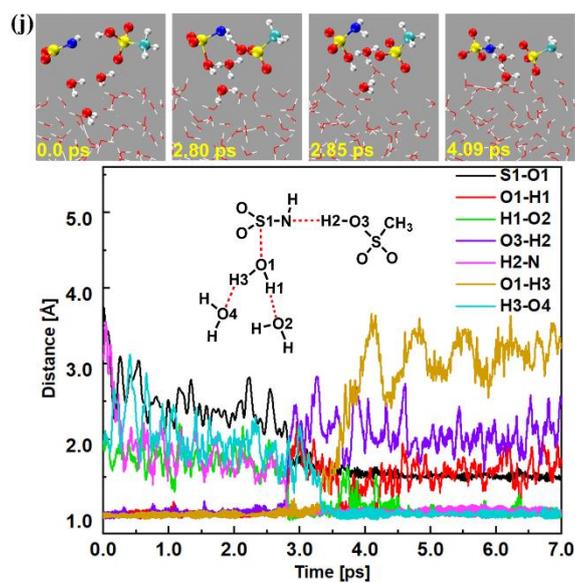
Fig. S12 BOMD simulation trajectories and snapshots of MSA⁻ and H_3O^+ ions forming mechanism via the chain structure routes in MSA-mediated hydration $HNSO_2$ at the air-water interface

(g)

(h)
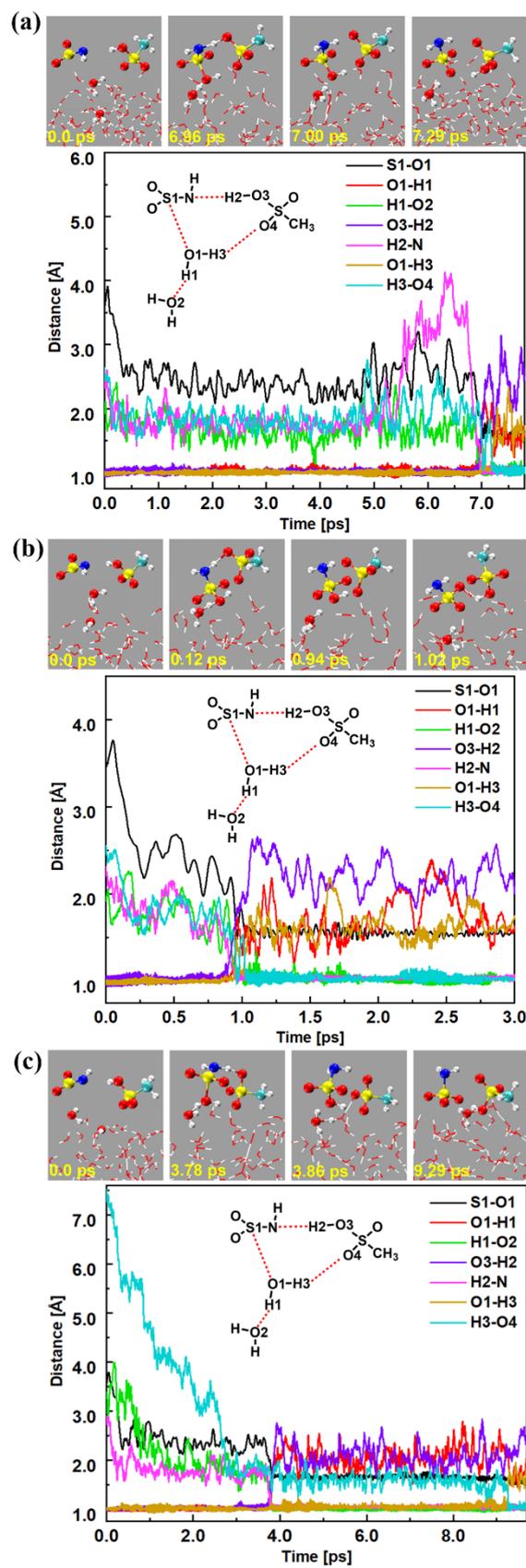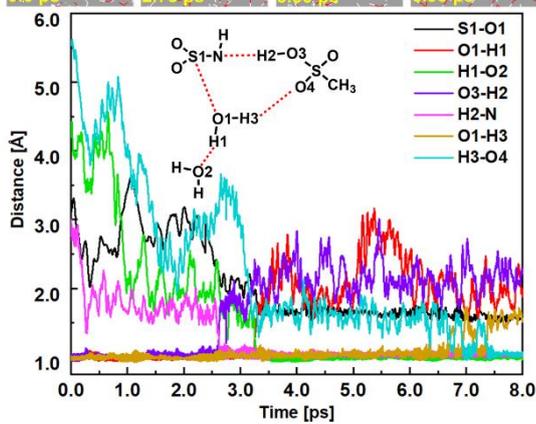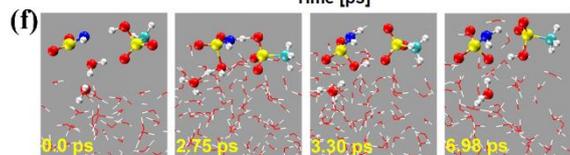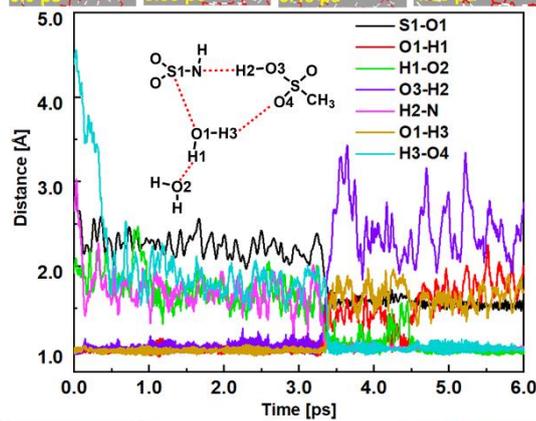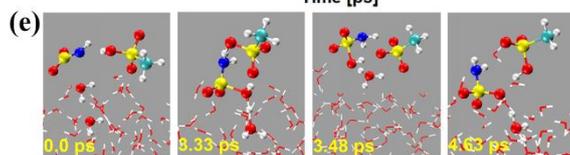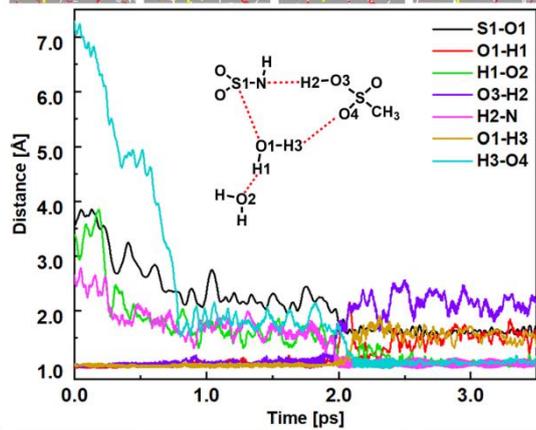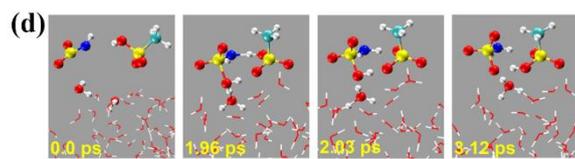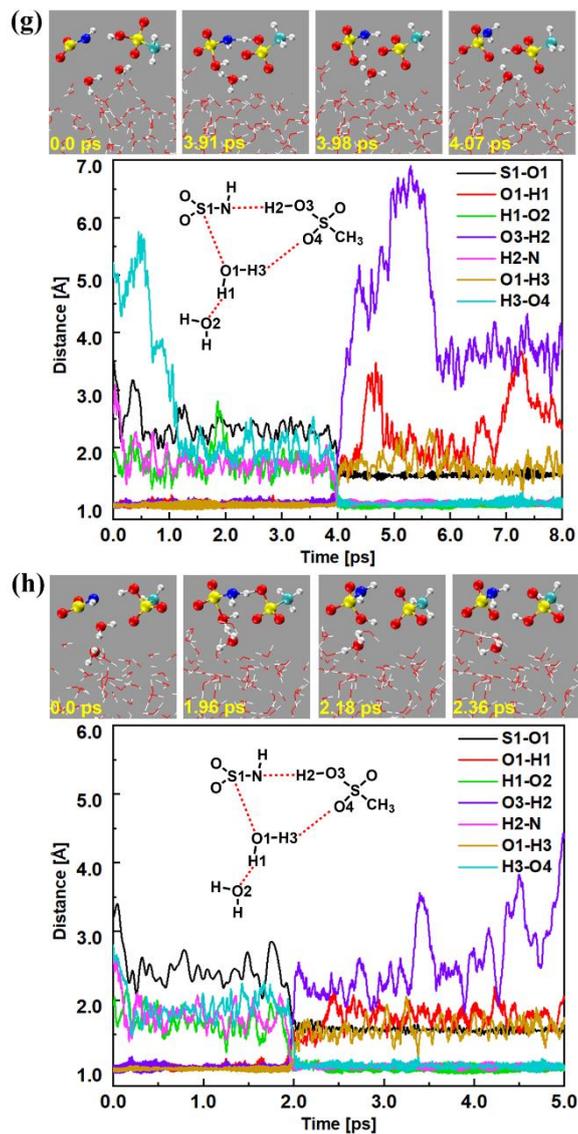
Fig. S13 BOMD simulation trajectories and snapshots of MSA⁻ and H_3O^+ ions forming mechanism via loop structure routes in MSA-mediated hydration $HNSO_2$ at the air-water interface
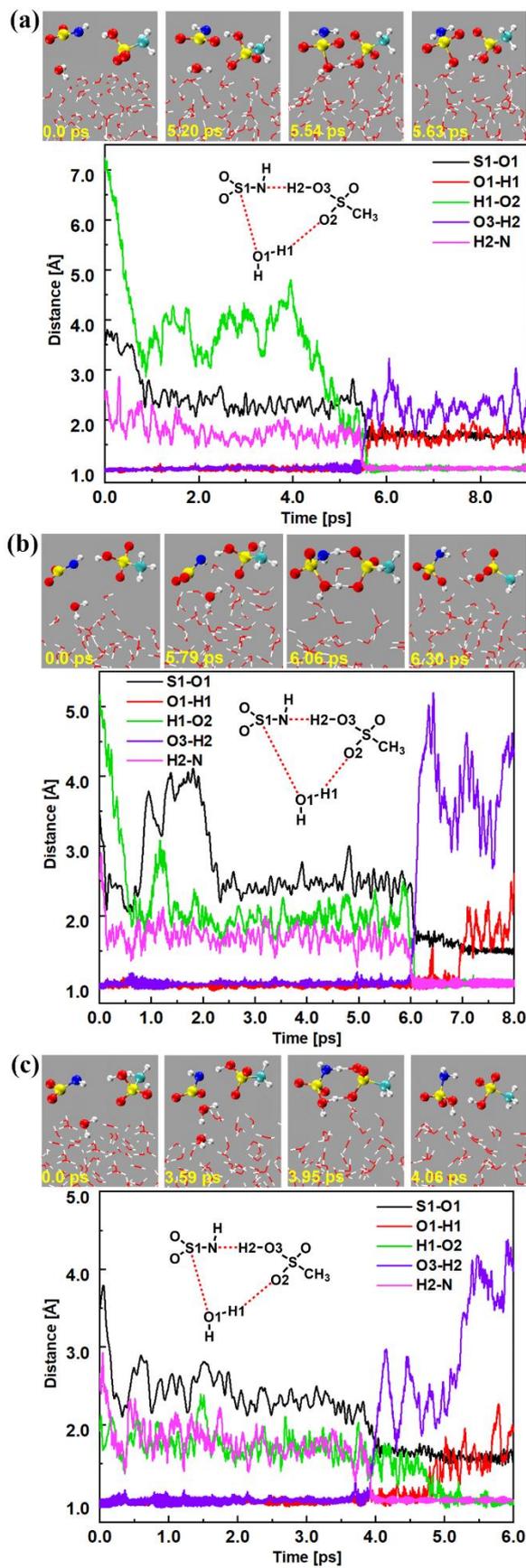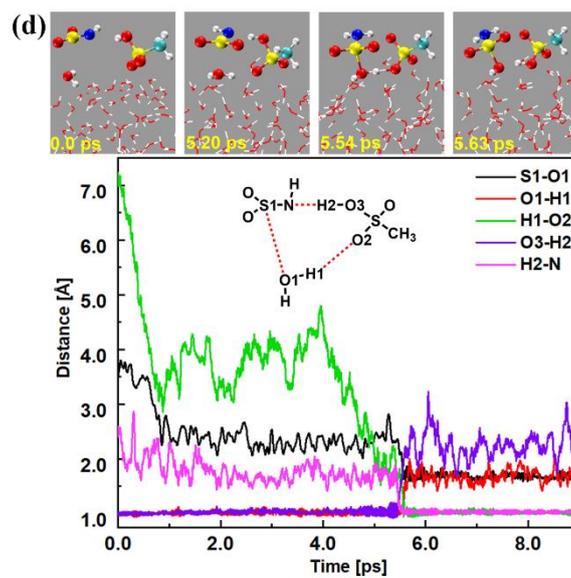
Fig. S14 BOMD simulation trajectories and snapshots of proton exchange mechanism in MSA - mediated hydration HNSO$_2$ with a water molecule at the air-water interface

(d)

(e)

(f)

(g)

(h)

(i)
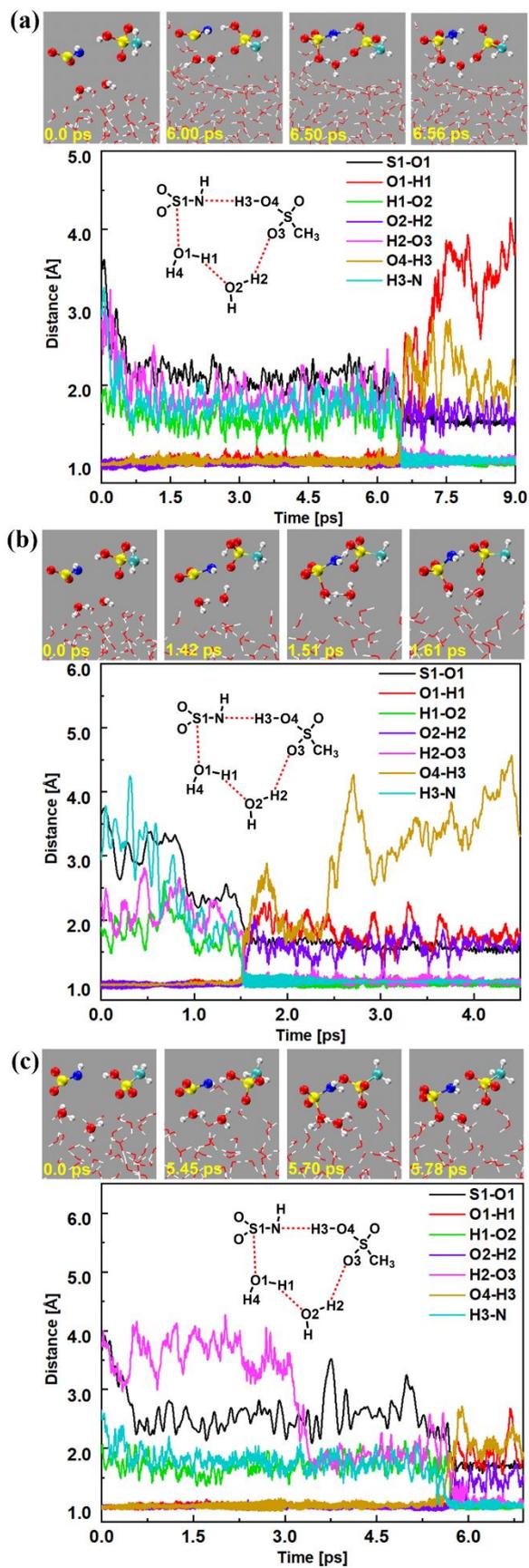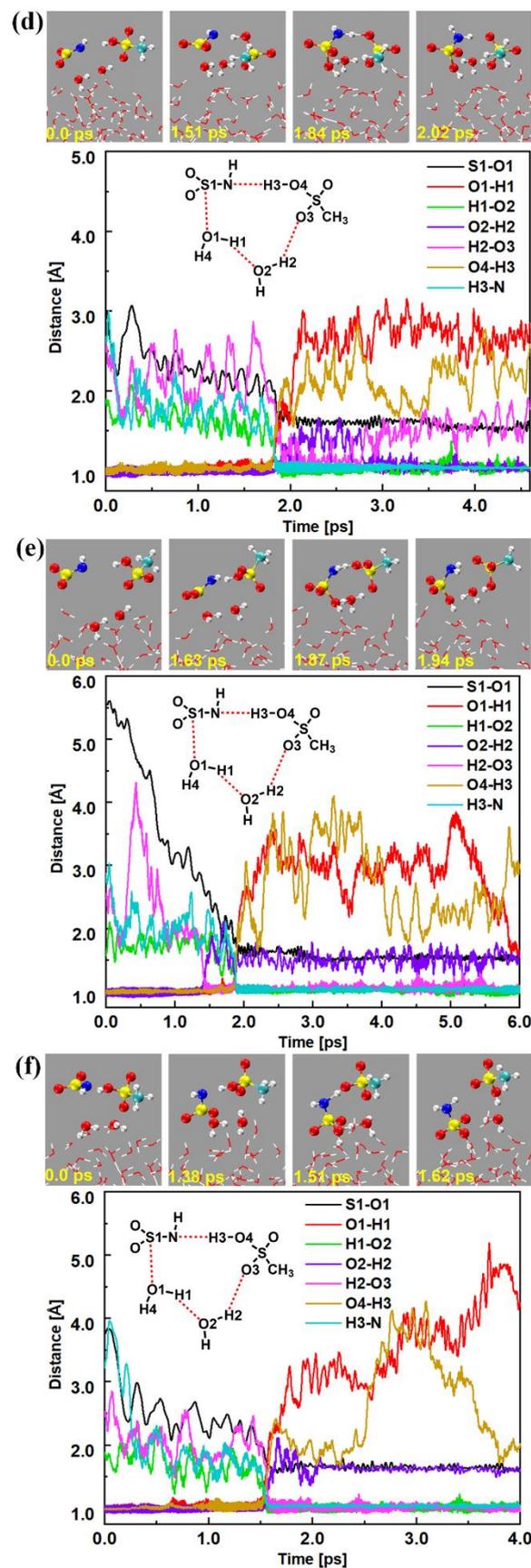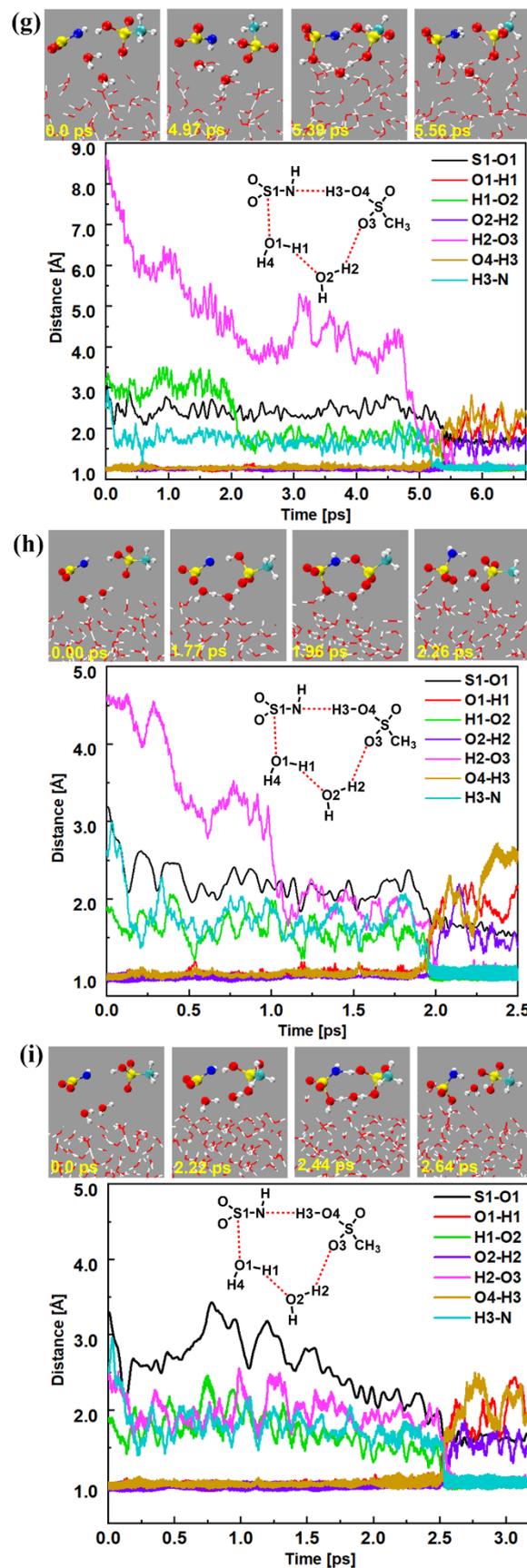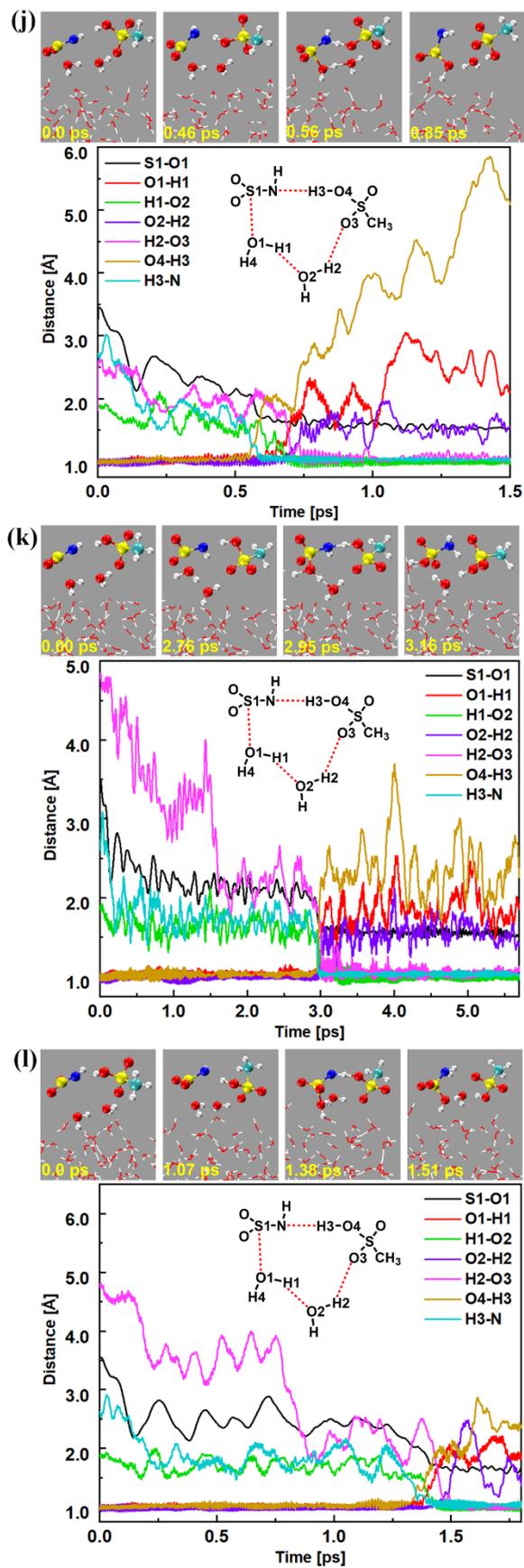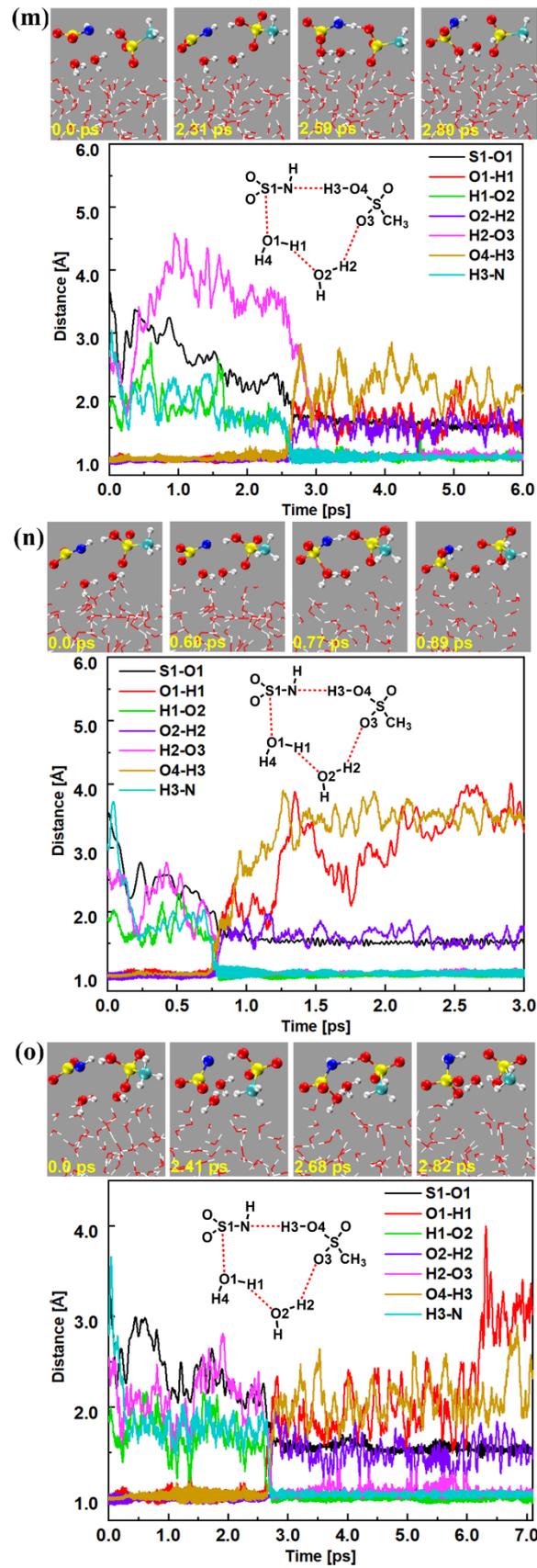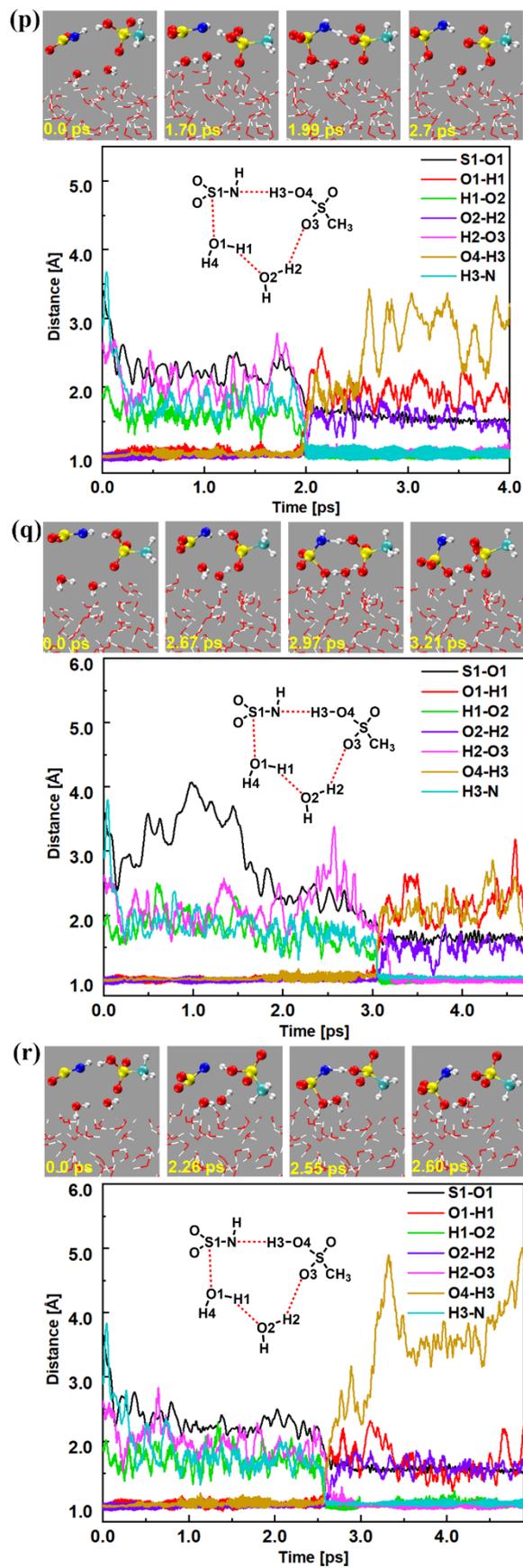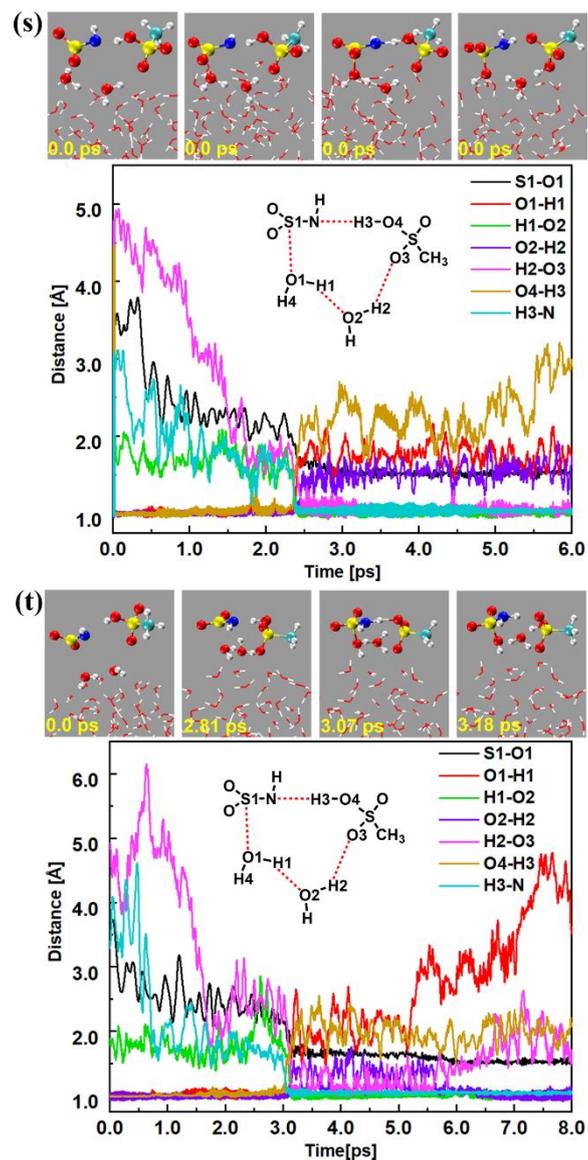
Fig.S15 BOMD simulation trajectories and snapshots of proton exchange mechanism in MSA -mediated hydration HNSO$_2$ with two water molecules at the air-water interface
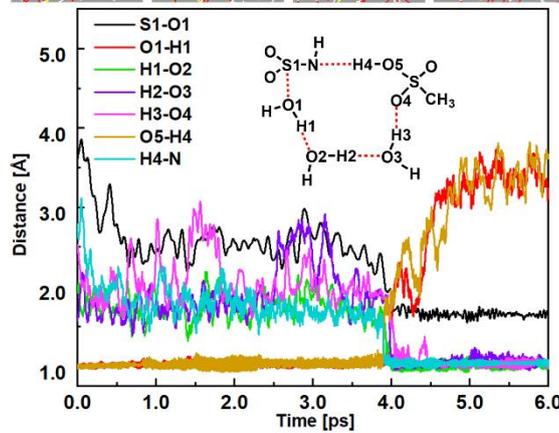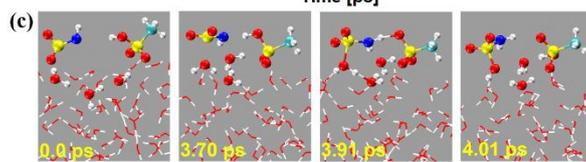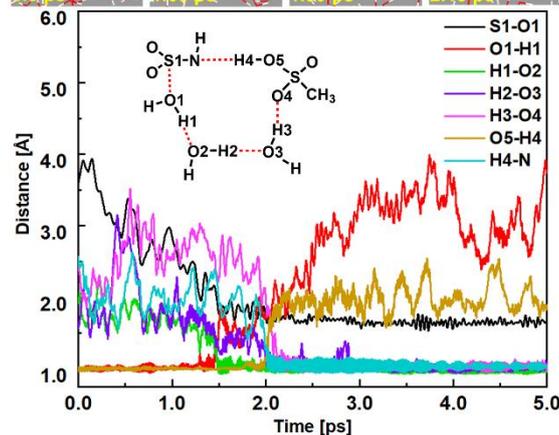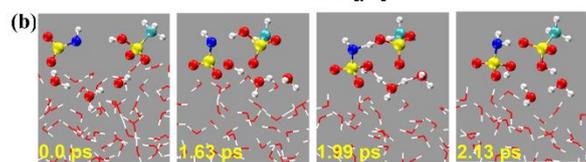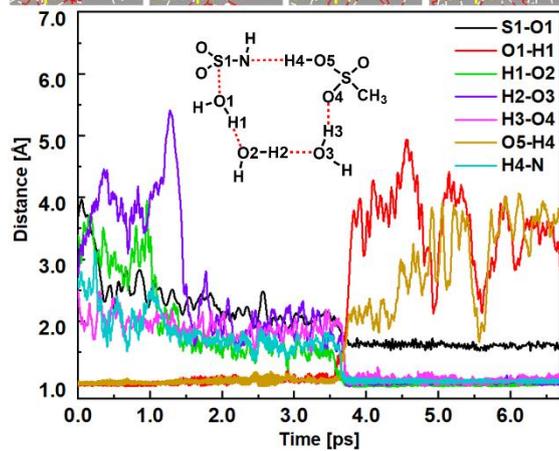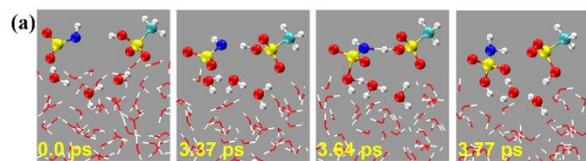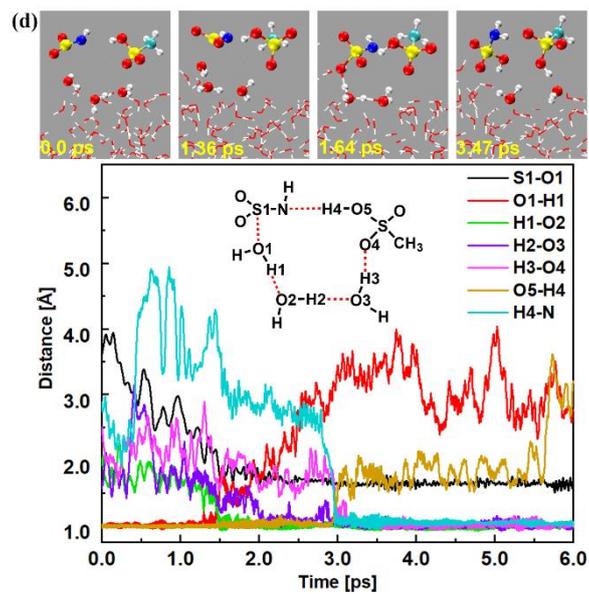
Fig. S16 BOMD simulation trajectories and snapshots of proton exchange mechanism in MSA-mediated hydration HNSO$_2$ with three water molecules at the air-water interface

Part S2. Configurational sampling

A multistep global minimum sampling scheme, which has previously been applied to study the atmospheric cluster formation, was employed to search for the global minima of the $(SFA)_x(MSA)_y(MA)_z$ $(0 \leqslant z \leqslant x + y \leqslant 3)$ clusters. To locate the global minimum energy structure, the artificial bee colony algorithm was systematically employed by the ABCluster program [1, 2] to generate n × 1000($1 < n \leq 4$) initial random configurations for each cluster, and then, PM6 semi-empirical method [3-5] was used to further pre-optimize the produced configurations above. Second, up to 100 structures with relatively lower energies were selected from the n × 1000 structures (where $1 < n \leq 4$), and a M06-2X/6-31+G(d,p) [6] level of theory was applied for subsequent optimization. Finally, further geometry optimization and frequency calculations at the M06-2X/6-311++G($2df,2pd$) [7] level of theory were performed to optimize the 10 best of 100 optimized configurations, and then the global minimum structure with the lowest energy was obtained. Subsequently, the M06-2X function combined with the 6-311++G($2df,2pd$) basis set was chosen as it has been proven to be accurate in estimating the thermodynamic properties of atmospheric clusters, such as organic acid-SA-amine clusters, amide-SA clusters or amino acid-SA clusters. In this study, all the density functional theory (DFT) calculations were implemented in the Gaussian 09 program [8].

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Fig. S17 The optimized geometries of the important precursors of atmospheric aerosol nucleation (MSA, MA and SFA), especially the main bond lengths and bond angles at two different theoretical levels. SFA, MSA and MA are the shorthand for formic acid, sulfuric acid and ammonia, respectively. [a] The values obtained at the M06-2X/6-311++G($2df$,$2pd$) level of theory. [b] The values obtained at the M06-2X/6-311++G($3df$,$3pd$) level of theory. Bond length is in angstrom and angle is in degree.

For the MSA·A, SFA·A, MSA·SFA and MSA·SFA·MA clusters, the geometric parameters (Fig. S17) at the M06-2X/6-311++G($3df$,$3pd$) and M06-2X/6-311++G($2df$,$2pd$) levels of theory were calculated. The geometrical structure analysis indicated that the bond lengths and angles obtained from both theoretical levels are close to each other. So, all optimizations and vibrational frequency were calculated at M06-2X/6-311++G($2df$,$2pd$) level.

Table S7 Comparison of calculated formation free energies (ΔG) at the M06-2X/6-311++G(2*df*,2*pd*) and the M06-2X/6-311++G(3*df*,3*pd*) levels

Cluster	M06-2X/6-311++G(2*df*,2*pd*)	M06-2X/6-311++G(3*df*,3*pd*)
	kcal·mol^{-1}	
MSA·MA	-6.19	-6.55
MSA·SFA	-9.33	-9.54
MA·SFA	-6.01	-6.98
MSA·MA·SFA	-21.96	-23.71

We calculated the Gibbs free energy (in Table S7) for the MSA·MA, SFA·MA, MSA·SFA and MSA·SFA·MA clusters at the M06-2X/6-311++G(3*df*,3*pd*) and M06-2X/6-311++G(2*df*,2*pd*) levels of theory. The analysis of Gibbs free energy indicated that the predicted relative ΔG of MSA·MA, SFA·MA, MSA·SFA and MSA·SFA·MA clusters at the M06-2X/6-311++G(2*df*,2*pd*) level is nearly close to the values at the M06-2X/6-311++G(3*df*,3*pd*) level, with differences of less than 1.75 kcal·mol^{-1}. So, we chose the M06-2X/6-311++G(2*df*,2*pd*) method for further frequency calculations. Relevant details are presented in Table S7.
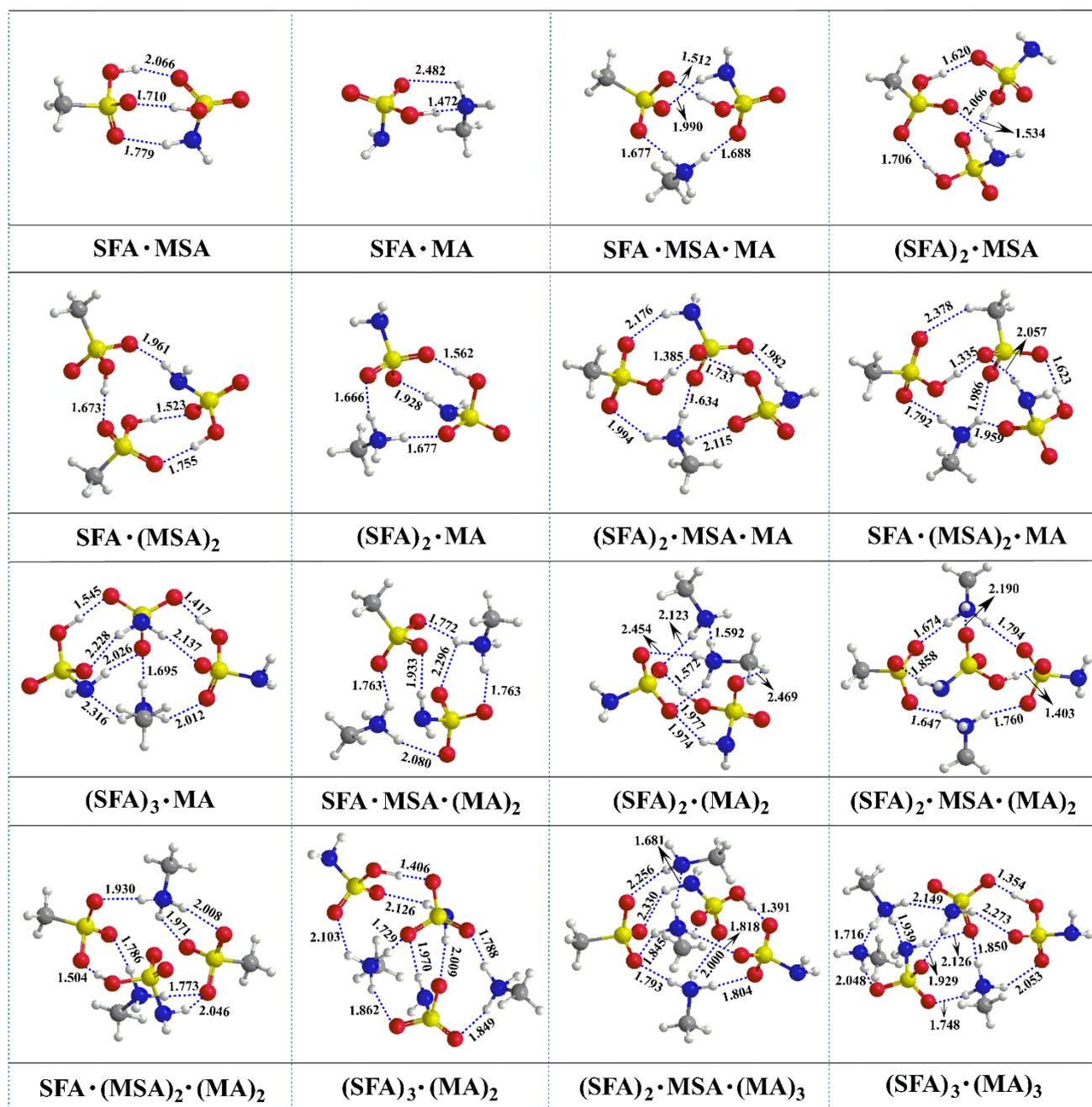
Fig. S18 The most stable configurations of the SFA-MSA-MA-based clusters identified at the M06-2X/6-311++G(2*df*,2*pd*) level of theory. The lengths of hydrogen bonds are given in Å (Color code: blue = nitrogen, yellow = sulfur, red = oxygen, gray = carbon, and white = hydrogen)
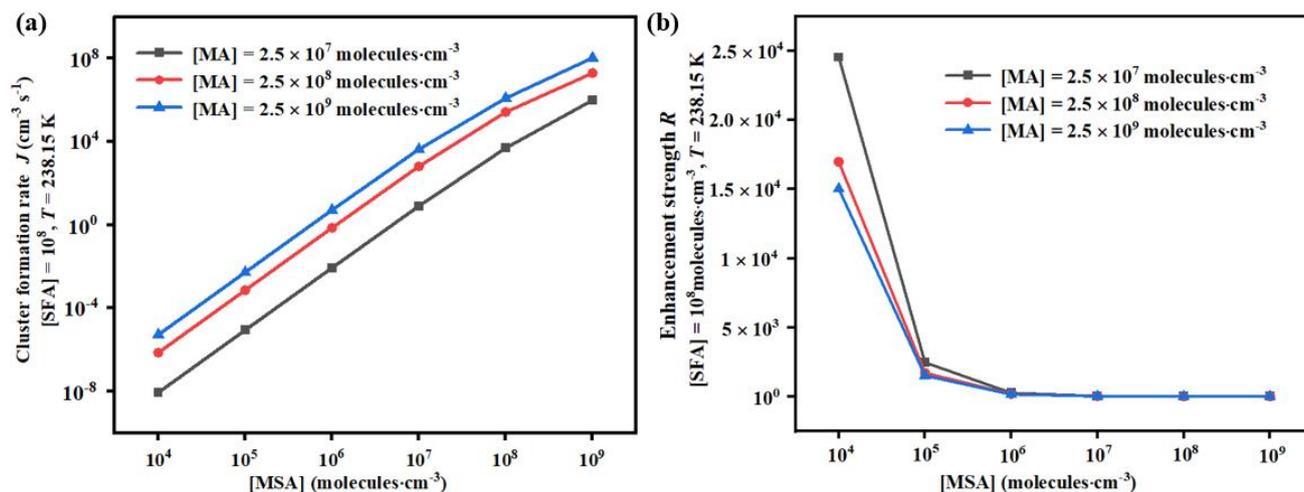
Fig. S19 (a) The J (cm^{-3} s^{-1}) and (b) R as a function of [MSA] with [SFA] = 10^8 molecules cm^{-3} and three different [MA] (black line: [MA] = 2.5×10^7 molecules cm^{-3}, red line: [MA] = 2.5×10^8 molecules cm^{-3}, blue line: [MA] = 2.5×10^9 molecules cm^{-3}) at 238.15 K

Fig. S20 (a) The J (cm^{-3} s^{-1}) and (b) R as a function of [MSA] with [SFA] = 10^8 molecules cm^{-3} and three different [MA] (black line: [MA] = 2.5×10^7 molecules cm^{-3}, red line: [MA] = 2.5×10^8 molecules cm^{-3}, blue line: [MA] = 2.5×10^9 molecules cm^{-3}) at 258.15 K

Fig. S21 (a) The J (cm^{-3} s^{-1}) and (b) R as a function of [MSA] with [SFA] = 10^8 molecules cm^{-3} and three different [MA] (black line: [MA] = 2.5×10^7 molecules cm^{-3}, red line: [MA] = 2.5×10^8 molecules cm^{-3}, blue line: [MA] = 2.5×10^9 molecules cm^{-3}) at 298.15 K

Pure MSA-MA flux out **SFA-containing flux out** **Others**

Contributions to the main cluster formation pathway pathways at different concentrations of MA.

Concentrations (molec. cm^{-3}): [MSA] = 1 × 10^7, T = 278.15 K

323

324   **Fig. S22**. The influence of [MA] on the relative contribution of the pure MSA-MA-based clustering pathway and the
325   SFA participation pathway to the system flux is analyzed at 278.15 K, [MSA] = 10^7 molecules·cm^{-3} and [SFA] = 10^4,
326   10^6 and 10^8 molecules·cm^{-3}.

Fig. S23 Main cluster formation mechanism of MSA-MA-SFA-based system at 238.15 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

Fig. S24 Main cluster formation mechanism of MSA-MA-SFA-based system at 258.15 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

Fig. S25 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

Table S8 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 and 238.15 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.)

347 **Table S9** Evaporation rates γ (s^{-1}) for the studied clusters at different temperatures of 298.15, 278.15, 258.15 and
348 238.15 K

Evaporation pathways	298.15 K	278.15 K	258.15 K	238.15 K
MSA·MA → MSA + MA	1.05×10^5	1.44×10^4	1.43×10^3	9.62×10^1
MSA·SFA → MSA + SFA	2.75×10^2	2.09×10^1	1.06×10^0	3.25×10^{-2}
MA·SFA → MA + SFA	1.26×10^5	1.66×10^4	1.59×10^3	1.03×10^2
$(MSA)_2$ → MSA + MSA	1.23×10^3	1.11×10^2	6.85×10^0	2.65×10^{-1}
$(SFA)_2$ → SFA + SFA	1.05×10^5	1.26×10^4	1.08×10^3	6.08×10^1
$(MSA)_2$·MA → $(MSA)_2$ + MA	2.90×10^0	1.43×10^{-1}	4.43×10^{-3}	7.64×10^{-5}
$(MSA)_2$·MA → MSA·MA + MSA	2.84×10^{-2}	9.29×10^{-4}	1.79×10^{-5}	1.77×10^{-7}
$(MSA)_2$·$(MA)_2$ → $(MSA)_2$·MA + MA	1.96×10^0	1.17×10^{-1}	4.48×10^{-3}	9.83×10^{-5}
MA·$(SFA)_2$ → $(SFA)_2$ + MA	2.82×10^{-4}	8.28×10^{-6}	1.41×10^{-7}	1.21×10^{-9}
MA·$(SFA)_2$ → MA·SFA + SFA	1.95×10^{-4}	5.22×10^{-6}	7.93×10^{-8}	5.96×10^{-10}
$(MA)_2$·$(SFA)_2$ → MA·$(SFA)_2$ + MA	1.93×10^4	2.04×10^3	1.50×10^2	7.06×10^0
$(MSA)_2$·SFA → $(MSA)_2$ + SFA	8.88×10^8	1.66×10^8	2.37×10^7	2.43×10^6
$(MSA)_2$·SFA → MSA·SFA + MSA	3.81×10^9	8.44×10^8	1.48×10^8	1.91×10^7
MSA·$(SFA)_2$ → $(SFA)_2$ + MSA	4.27×10^4	4.24×10^3	2.94×10^2	1.30×10^1
MSA·$(SFA)_2$ → MSA·SFA + SFA	1.69×10^7	2.66×10^6	3.11×10^5	2.53×10^4
$(MSA)_3$ → $(MSA)_2$ + MSA	1.89×10^7	2.78×10^6	3.01×10^5	2.23×10^4
$(SFA)_3$ → $(SFA)_2$ + SFA	7.60×10^4	6.96×10^3	4.38×10^2	1.74×10^1
$(MSA)_3$·MA → $(MSA)_2$·MA + MSA	5.28×10^2	4.00×10^1	2.01×10^0	6.10×10^{-2}
$(MSA)_3$·MA → $(MSA)_3$ + MA	7.77×10^{-5}	1.98×10^{-6}	2.85×10^{-8}	2.01×10^{-10}
$(MSA)_3$·$(MA)_2$ → $(MSA)_2$·$(MA)_2$ + MSA	1.44×10^0	7.28×10^{-2}	2.30×10^{-3}	4.04×10^{-5}
$(MSA)_3$·$(MA)_2$ → $(MSA)_3$·MA + MA	4.74×10^{-3}	1.88×10^{-4}	4.50×10^{-6}	5.73×10^{-8}
$(MSA)_3$·$(MA)_3$ → $(MSA)_3$·$(MA)_2$ + MA	8.39×10^2	4.86×10^1	1.81×10^0	3.82×10^{-2}
MA·$(SFA)_3$ → MA·$(SFA)_2$ + SFA	1.74×10^5	1.36×10^4	7.16×10^2	2.28×10^1
MA·$(SFA)_3$ → $(SFA)_3$ + MA	7.03×10^{-4}	1.76×10^{-5}	2.50×10^{-7}	1.73×10^{-9}
$(MA)_2$·$(SFA)_3$ → $(MA)_2$·$(SFA)_2$ + SFA	1.09×10^0	5.40×10^{-2}	1.67×10^{-3}	2.87×10^{-5}
$(MA)_2$·$(SFA)_3$ → MA·$(SFA)_3$ + MA	1.35×10^{-1}	9.04×10^{-3}	3.92×10^{-4}	9.95×10^{-6}
$(MA)_3$·$(SFA)_3$ → $(MA)_2$·$(SFA)_3$ + MA	3.03×10^6	3.94×10^5	3.71×10^4	2.33×10^3
MSA·SFA·MA → MA·SFA + 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
$MSA \cdot MA \cdot SFA \rightarrow MSA \cdot MA + SFA$	6.71×10^{-3}	1.88×10^{-4}	3.01×10^{-6}	2.41×10^{-8}
$MSA \cdot MA \cdot SFA \rightarrow MSA \cdot SFA + MA$	2.95×10^{0}	1.48×10^{-1}	4.67×10^{-3}	8.22×10^{-5}
$MSA \cdot (MA)_2 \cdot SFA \rightarrow MSA \cdot MA \cdot SFA + MA$	5.20×10^{6}	7.41×10^{5}	7.78×10^{4}	5.55×10^{3}
$(MSA)_2 \cdot MA \cdot SFA \rightarrow MSA \cdot MA \cdot SFA + MSA$	5.01×10^{7}	9.32×10^{6}	1.32×10^{6}	1.33×10^{5}
$(MSA)_2 \cdot MA \cdot SFA \rightarrow (MSA)_2 \cdot MA + SFA$	1.22×10^{7}	1.93×10^{6}	2.28×10^{5}	1.86×10^{4}
$(MSA)_2 \cdot MA \cdot SFA \rightarrow (MSA)_2 \cdot SFA + MA$	3.96×10^{-2}	1.67×10^{-3}	4.26×10^{-5}	5.85×10^{-7}
$(MSA)_2 \cdot (MA)_2 \cdot SFA \rightarrow MSA \cdot (MA)_2 \cdot SFA + MSA$	7.15×10^{-5}	1.78×10^{-6}	2.48×10^{-8}	1.68×10^{-10}
$(MSA)_2 \cdot (MA)_2 \cdot SFA \rightarrow (MSA)_2 \cdot (MA)_2 + SFA$	4.97×10^{1}	2.53×10^{0}	8.06×10^{-2}	1.43×10^{-3}
$(MSA)_2 \cdot (MA)_2 \cdot SFA \rightarrow (MSA)_2 \cdot MA \cdot SFA + MA$	8.46×10^{-6}	1.62×10^{-7}	1.67×10^{-9}	7.97×10^{-12}
$(MSA)_2 \cdot (MA)_3 \cdot SFA \rightarrow (MSA)_2 \cdot (MA)_2 \cdot SFA + MA$	2.58×10^{0}	1.35×10^{-1}	4.42×10^{-3}	8.09×10^{-5}
$MSA \cdot MA \cdot (SFA)_2 \rightarrow MA \cdot (SFA)_2 + MSA$	1.17×10^{4}	9.09×10^{2}	4.72×10^{1}	1.48×10^{0}
$MSA \cdot MA \cdot (SFA)_2 \rightarrow MSA \cdot MA \cdot SFA + SFA$	4.54×10^{2}	3.26×10^{1}	1.54×10^{0}	4.35×10^{-2}
$MSA \cdot MA \cdot (SFA)_2 \rightarrow MSA \cdot (SFA)_2 + MA$	8.61×10^{-5}	1.98×10^{-6}	2.52×10^{-8}	1.54×10^{-10}
$MSA \cdot (MA)_2 \cdot (SFA)_2 \rightarrow (MA)_2 \cdot (SFA)_2 + MSA$	1.90×10^{-1}	7.44×10^{-3}	1.76×10^{-4}	2.21×10^{-6}
$MSA \cdot (MA)_2 \cdot (SFA)_2 \rightarrow MSA \cdot (MA)_2 \cdot SFA + SFA$	2.81×10^{-5}	7.52×10^{-7}	1.14×10^{-8}	8.49×10^{-11}
$MSA \cdot (MA)_2 \cdot (SFA)_2 \rightarrow MSA \cdot MA \cdot (SFA)_2 + MA$	2.85×10^{-1}	1.51×10^{-2}	5.07×10^{-4}	9.58×10^{-6}
$MSA \cdot (MA)_3 \cdot (SFA)_2 \rightarrow MSA \cdot (MA)_2 \cdot (SFA)_2 + MA$	2.24×10^{5}	2.99×10^{4}	2.91×10^{3}	1.91×10^{2}

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350   **Table S10** Collision coefficients (β, cm^3·s^{-1}) for each cluster in the present study

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$^3 \cdot$s^{-1})			
	298.15 K	278.15 K	258.15 K	238.15 K
(MSA)$_2 \cdot$MA + SFA	9.59×10^{-11}	8.95×10^{-11}	8.31×10^{-11}	7.66×10^{-11}
(MSA)$_2 \cdot$SFA + MA	2.17×10^{-10}	2.03×10^{-10}	1.88×10^{-10}	1.73×10^{-10}
MSA$\cdot$(MA)$_2 \cdot$SFA + MSA	1.14×10^{-10}	1.07×10^{-10}	9.91×10^{-11}	9.14×10^{-11}
(MSA)$_2 \cdot$(MA)$_2$ + SFA	1.14×10^{-10}	1.06×10^{-10}	9.83×10^{-11}	9.07×10^{-11}
(MSA)$_2 \cdot$MA$\cdot$SFA + MA	2.80×10^{-10}	2.61×10^{-10}	2.42×10^{-10}	2.23×10^{-10}
(MSA)$_2 \cdot$(MA)$_2 \cdot$SFA + MA	2.73×10^{-10}	2.55×10^{-10}	2.37×10^{-10}	2.18×10^{-10}
MA$\cdot$(SFA)$_2$ + MSA	1.00×10^{-10}	9.34×10^{-11}	8.67×10^{-11}	7.99×10^{-11}
MSA$\cdot$MA$\cdot$SFA + SFA	9.39×10^{-11}	8.76×10^{-11}	8.13×10^{-11}	7.50×10^{-11}
MSA$\cdot$(SFA)$_2$ + MA	2.32×10^{-10}	2.16×10^{-10}	2.01×10^{-10}	1.85×10^{-10}
(MA)$_2 \cdot$(SFA)$_2$ + MSA	1.12×10^{-10}	1.05×10^{-10}	9.72×10^{-11}	8.97×10^{-11}
MSA$\cdot$(MA)$_2 \cdot$SFA + SFA	1.05×10^{-10}	9.83×10^{-11}	9.12×10^{-11}	8.42×10^{-11}
MSA$\cdot$MA$\cdot$(SFA)$_2$ + MA	6.02×10^{-10}	5.61×10^{-10}	5.21×10^{-10}	4.81×10^{-10}
MSA$\cdot$(MA)$_2 \cdot$(SFA)$_2$ + MA	2.80×10^{-10}	2.61×10^{-10}	2.43×10^{-10}	2.24×10^{-10}

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352   **Table S11** 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}

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	$(\beta \cdot C/\sum \gamma)$			
Clusters	298.15 K	278.15 K	258.15 K	238.15 K
Collision with MSA monomer: $C =$ [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}
(MSA)₂	8.82×10^{-13}	9.11×10^{-12}	1.36×10^{-10}	3.25×10^{-9}
(SFA)₂	7.38×10^{-15}	5.30×10^{-14}	5.22×10^{-13}	7.65×10^{-12}
(MSA)₂·MA	3.58×10^{-10}	6.77×10^{-9}	2.04×10^{-7}	1.09×10^{-5}
(MSA)₂·(MA)₂	6.48×10^{-10}	1.01×10^{-8}	2.46×10^{-7}	1.03×10^{-5}
MA·(SFA)₂	2.10×10^{-6}	6.92×10^{-5}	3.94×10^{-3}	4.43×10^{-1}
(MA)₂·(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·(MA)₂·SFA	3.45×10^{-13}	3.86×10^{-12}	6.36×10^{-11}	1.69×10^{-9}
Collision with MA monomer: $C =$ [MA]				
MSA·SFA	6.85×10^{-13}	5.04×10^{-12}	5.09×10^{-11}	7.69×10^{-10}
(MSA)₂	4.58×10^{-11}	4.73×10^{-10}	7.08×10^{-9}	1.69×10^{-7}
(SFA)₂	3.83×10^{-13}	2.75×10^{-12}	2.71×10^{-11}	3.97×10^{-10}
(MSA)₂·MA	1.91×10^{-8}	3.62×10^{-7}	1.09×10^{-5}	5.84×10^{-4}
MA·(SFA)₂	1.12×10^{-4}	3.69×10^{-3}	2.10×10^{-1}	2.37×10^{1}
(MSA)₂·SFA	1.16×10^{-17}	5.02×10^{-17}	2.75×10^{-16}	2.01×10^{-15}
MSA·(SFA)₂	3.41×10^{-15}	2.03×10^{-14}	1.61×10^{-13}	1.82×10^{-12}
(MSA)₃	2.76×10^{-15}	1.76×10^{-14}	1.50×10^{-13}	1.87×10^{-12}
(SFA)₃	2.38×10^{-19}	6.23×10^{-19}	1.92×10^{-18}	7.28×10^{-18}
(MSA)₃·MA	1.10×10^{-10}	1.35×10^{-9}	2.49×10^{-8}	7.59×10^{-7}
(MSA)₃·(MA)₂	4.69×10^{-8}	8.68×10^{-7}	2.55×10^{-5}	1.34×10^{-3}
MA·(SFA)₃	3.88×10^{-13}	4.63×10^{-12}	8.16×10^{-11}	2.36×10^{-9}
(MA)₂·(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}
(MSA)₂·MA·SFA	1.12×10^{-15}	5.80×10^{-15}	3.91×10^{-14}	3.67×10^{-13}
(MSA)₂·(MA)₂·SFA	1.38×10^{-9}	2.52×10^{-8}	7.34×10^{-7}	3.81×10^{-5}
MSA·MA·(SFA)₂	4.49×10^{-12}	5.40×10^{-11}	9.67×10^{-10}	2.85×10^{-8}
MSA·(MA)₂·(SFA)₂	7.17×10^{-8}	1.33×10^{-6}	3.85×10^{-5}	1.95×10^{-3}
Collision with SFA monomer: $C =$ [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	$(\beta \cdot C / \sum \gamma$			
	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}

357

358 **Table S13** 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}
359 molecules·cm^{-3}. MSA, MA and SFA represent methanesulfonic acid, methylamine and sulfamic 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

360

361 **Table S14** 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}
362 molecules·cm^{-3}. MSA, MA and SFA represent methanesulfonic acid, methylamine and sulfamic 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

363

364 **Table S15** 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}
365 molecules·cm^{-3}. MSA, MA and SFA represent methanesulfonic acid, methylamine and sulfamic 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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367 **Table S16** 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}
368 molecules·cm^{-3}. MSA, MA and SFA represent methanesulfonic acid, methylamine and sulfamic 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}

369

Table S17 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

372

373 **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

374

375 **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

376

377 **(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

378

379 **(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

380

381 **(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

382

383 **(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

384

385 **(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

386

387 **(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

388

389 **(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

390

391 **(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

392

393 **(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

394

395 **(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

396

397 **(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

398

399 **(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

400

401 **(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

402

403 **(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

404

405 **(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

406

407 **(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

408

409 **(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

410 **(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

411

412   **(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

413

414 **(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

415 **(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

416

417 **(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

418

419 **(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

420

421 **(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

422

423 **(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

424

425 **(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

426

(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

428