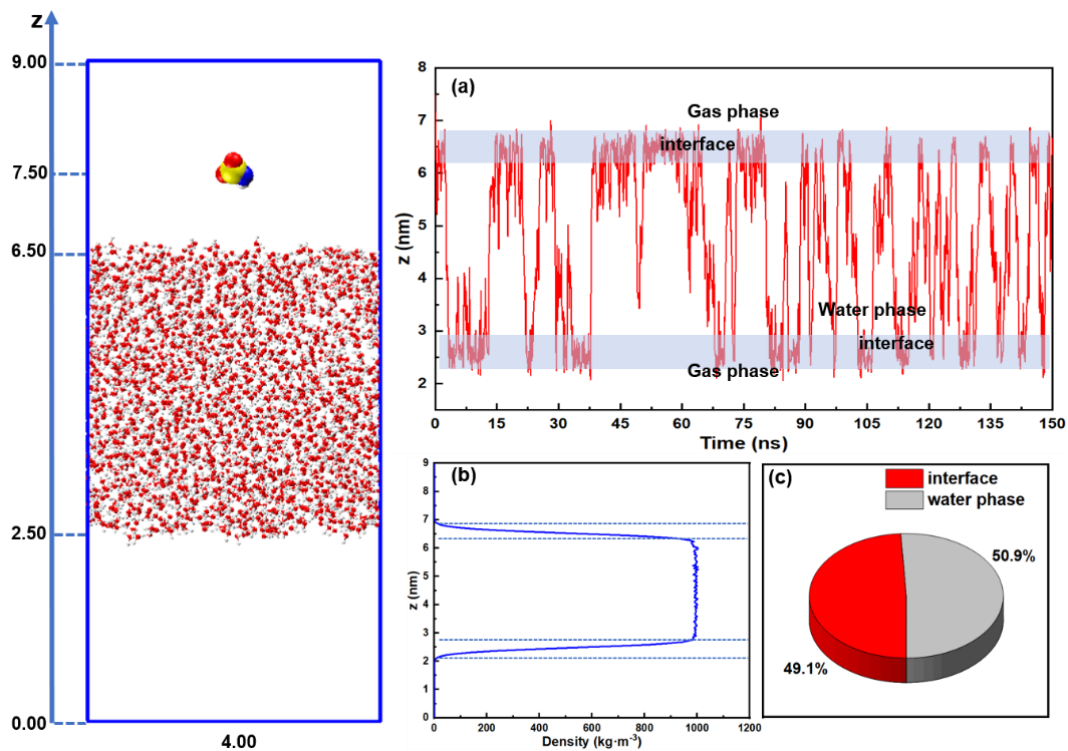


S. NO	Caption
S4	<b>Fig. S1</b> (a) The $z$ coordinates of HNSO <sub>2</sub> molecule as the function of simulation time; (b) the density profile of water; (c) the pie chart with the occurrence percentages of HNSO <sub>2</sub> molecule at the air-water interface and in water phase
S5	<b>Fig. S2</b> The optimized geometrical structures for the species involved in the HNSO <sub>2</sub> hydrolysis at several different levels of theory.
S6	<b>Table S1</b> The Energy barriers ( $\Delta E$ ) and unsigned error (UE) (kcal·mol <sup>-1</sup> ) for the HNSO <sub>2</sub> hydrolysis at different theoretical the potential energy profile ( $\Delta G$ ) correction
S7-S8	<b>Fig. S3</b> Optimized geometries of HNSO <sub>2</sub> , H <sub>2</sub> O, MSA, (H <sub>2</sub> O) <sub>2</sub> , HNSO <sub>2</sub> ···H <sub>2</sub> O and MSA···H <sub>2</sub> O at the M06-2X/6-311++G(2df,2pd) level (bond distances in Angstroms and angles in degrees) along with the stabilization energies of (H <sub>2</sub> O) <sub>2</sub> , HNSO <sub>2</sub> ···H <sub>2</sub> O and MSA···H <sub>2</sub> O at the CCSD(T)-F12/cc-pVDZ-F12//M06-2X/6-311++G(2df,2pd) level of theory
S9-S10	<b>Fig. S4</b> The optimized geometries and electric energies (in Hartree-Fock) for the complexes of HNSO <sub>2</sub> ···H <sub>2</sub> O···MSA at the M06-2X/6-311++G(2df,2pd) level of theory
S11	<b>Fig. S5</b> The potential energy profile ( $\Delta G$ ) for the hydrolysis reaction of HNSO <sub>2</sub> without (a) and with (b) H <sub>2</sub> O at the CCSD(T)-F12/cc-pVDZ-F12//M06-2X/6-311++G(2df,2pd) level of theory
S12	<b>Table S2</b> Zero point energy (ZPE/(kcal·mol <sup>-1</sup> )), entropies (S/(cal·mol <sup>-1</sup> ·K <sup>-1</sup> )), relative energies ( $\Delta E$ and $\Delta(E + \text{ZPE})$ /(kcal·mol <sup>-1</sup> )), enthalpies ( $\Delta H(298)$ /(kcal·mol <sup>-1</sup> )), and free energies ( $\Delta G(298)$ /(kcal·mol <sup>-1</sup> )) for the hydrolysis reaction of HNSO <sub>2</sub> without and with H <sub>2</sub> O and MSA
S13	<b>Table S3</b> Equilibrium constants (cm <sup>3</sup> ·molecule <sup>-1</sup> ) for the HNSO <sub>2</sub> ···H <sub>2</sub> O, H <sub>2</sub> O···H <sub>2</sub> O, and MSA···H <sub>2</sub> O complexes within the temperature range of 212.6-320.0 K
S14	<b>Table S4</b> The high-pressure limiting rate constant (cm <sup>3</sup> ·molecule <sup>-1</sup> ·s <sup>-1</sup> ) for the hydrolysis reaction of HNSO <sub>2</sub> with H <sub>2</sub> O and MSA within the temperature range of 212.6-320.0 K
S15-S17	<b>Part S1. Calculations of reaction rate coefficients</b>
S18	<b>Table S5</b> Rate coefficients ( $k$ , cm <sup>3</sup> ·molecule <sup>-1</sup> ·s <sup>-1</sup> ) for the hydrolysis of HNSO <sub>2</sub> by master equation within the temperature range of 212.6-320.0 K
S19	<b>Table S6</b> Concentrations (molecules·cm <sup>-3</sup> ) of H <sub>2</sub> O and MSA within the temperature range of 213-320 K and altitude range of 0-15 km
S20	<b>Fig. S7</b> The dynamic trajectories of MSA-assisted gaseous hydrolysis of HNSO <sub>2</sub>
S21	<b>Fig. S8</b> (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
S22	<b>Fig. S9</b> (a) The $z$ coordinates of complex HNSO <sub>2</sub> ···MSA as the function of simulation time; (b) the density profile of water; (c) the pie chart with the occurrence percentages of complex HNSO <sub>2</sub> ···MSA at the air-water interface and in water phase
S23	<b>Fig. S10</b> Snapshot structures taken from the BOMD simulations of HNSO <sub>2</sub> reaction at the air-water interface
S24	<b>Fig. S11</b> Snapshot structures taken from the BOMD simulations of MSA reaction at the air-water interface
S25-S28	<b>Fig. S12</b> BOMD simulation trajectories and snapshots of MSA <sup>-</sup> and H <sub>3</sub> O <sup>+</sup> ions forming mechanism via the chain structure routes in MSA-mediated hydration HNSO <sub>2</sub> at the air-water interface

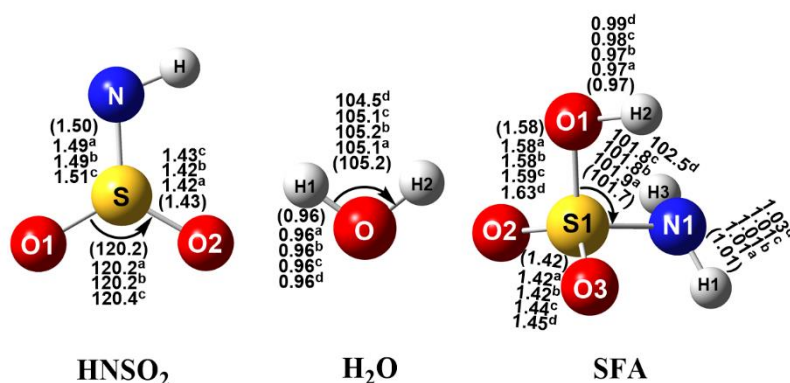
S29-S31	<b>Fig. S13</b> BOMD simulation trajectories and snapshots of $\text{MSA}^-$ and $\text{H}_3\text{O}^+$ ions forming mechanism via loop structure routes in MSA-mediated hydration $\text{HNSO}_2$ at the air-water interface
S32-S33	<b>Fig. S14</b> BOMD simulation trajectories and snapshots of proton exchange mechanism in MSA-mediated hydration $\text{HNSO}_2$ with a water molecule at the air-water interface
S34-S40	<b>Fig. S15</b> BOMD simulation trajectories and snapshots of proton exchange mechanism in MSA-mediated hydration $\text{HNSO}_2$ with two water molecules at the air-water interface
S40-S42	<b>Fig. S16</b> BOMD simulation trajectories and snapshots of proton exchange mechanism in MSA-mediated hydration $\text{HNSO}_2$ with three water molecules at the air-water interface
S43	<b>Part S2. Configurational sampling</b>
S44	<b>Fig. S17</b> 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. <sup>a</sup> The values obtained at the M06-2X/6-311++G(2df,2pd) level of theory. <sup>b</sup> 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.
S45	<b>Table S7</b> Comparison of calculated formation free energies ( $\Delta G$ ) at the M06-2X/6-311++G(2df,2pd) and the M06-2X/6-311++G(3df,3pd) levels
S46	<b>Fig. S18</b> The most stable configurations of the SFA-MSA-MA-based clusters identified at the M06-2X/6-311++G(2df,2pd) level of theory. The lengths of hydrogen bonds are given in Å (Color code: blue = nitrogen, yellow = sulfur, red = oxygen, gray = carbon, and white = hydrogen)
S47	<b>Fig. S19</b> (a) The $J(\text{cm}^{-3}\text{s}^{-1})$ and (b) $R$ as a function of [MSA] with [SFA] = $10^8$ molecules $\text{cm}^{-3}$ and three different [MA] (black line: [MA] = $2.5 \times 10^7$ molecules $\text{cm}^{-3}$ , red line: [MA] = $2.5 \times 10^8$ molecules $\text{cm}^{-3}$ , blue line: [MA] = $2.5 \times 10^9$ molecules $\text{cm}^{-3}$ ) at 238.15 K
S48	<b>Fig. S20</b> (a) The $J(\text{cm}^{-3}\text{s}^{-1})$ and (b) $R$ as a function of [MSA] with [SFA] = $10^8$ molecules $\text{cm}^{-3}$ and three different [MA] (black line: [MA] = $2.5 \times 10^7$ molecules $\text{cm}^{-3}$ , red line: [MA] = $2.5 \times 10^8$ molecules $\text{cm}^{-3}$ , blue line: [MA] = $2.5 \times 10^9$ molecules $\text{cm}^{-3}$ ) at 258.15 K
S49	<b>Fig. S21</b> (a) The $J(\text{cm}^{-3}\text{s}^{-1})$ and (b) $R$ as a function of [MSA] with [SFA] = $10^8$ molecules $\text{cm}^{-3}$ and three different [MA] (black line: [MA] = $2.5 \times 10^7$ molecules $\text{cm}^{-3}$ , red line: [MA] = $2.5 \times 10^8$ molecules $\text{cm}^{-3}$ , blue line: [MA] = $2.5 \times 10^9$ molecules $\text{cm}^{-3}$ ) at 298.15 K
S50	<b>Fig. S22.</b> 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 $\cdot\text{cm}^{-3}$ and [SFA] = $10^4$ , $10^6$ and $10^8$ molecules $\cdot\text{cm}^{-3}$ .
S51	<b>Fig. S23</b> Main cluster formation mechanism of MSA-MA-SFA-based system at 238.15 K, [MSA] = $10^7$ molecules $\cdot\text{cm}^{-3}$ , [MA] = $2.5 \times 10^8$ molecules $\cdot\text{cm}^{-3}$ , and [SFA] = $10^6$ molecules $\cdot\text{cm}^{-3}$ . The black arrows indicate the pure MSA-MA-based growth pathways. Blue arrows represent the pathways containing SFA
S52	<b>Fig. S24</b> Main cluster formation mechanism of MSA-MA-SFA-based system at 258.15 K, [MSA] = $10^7$ molecules $\cdot\text{cm}^{-3}$ , [MA] = $2.5 \times 10^8$ molecules $\cdot\text{cm}^{-3}$ , and [SFA] = $10^6$ molecules $\cdot\text{cm}^{-3}$ . The black arrows indicate the pure MSA-MA-based growth pathways. Blue arrows represent the pathways containing SFA
S53	<b>Fig. S25</b> Main cluster formation mechanism of MSA-MA-SFA-based system at 298.15 K, [MSA] = $10^7$ molecules $\cdot\text{cm}^{-3}$ , [MA] = $2.5 \times 10^8$ molecules $\cdot\text{cm}^{-3}$ , and [SFA] = $10^6$ molecules $\cdot\text{cm}^{-3}$ . The black arrows indicate the pure MSA-MA-based growth pathways. Blue arrows represent the pathways containing SFA
S54	<b>Table S8</b> The Gibbs free energy for the formation of $(\text{SFA})_x(\text{MSA})_y(\text{MA})_z$ ( $z \leq x + y \leq 3$ ) clusters $\Delta G$ (kcal $\cdot\text{mol}^{-1}$ ) at pressure of 1 atm and temperatures of 298.15, 278.15, 258.15 and 238.15 K

S55-S56	<b>Table S9</b> Evaporation rates $\gamma$ ( $\text{s}^{-1}$ ) for the studied clusters at different temperatures of 298.15, 278.15, 258.15 and 238.15 K
S57-S58	<b>Table S10</b> Collision coefficients ( $\beta$ , $\text{cm}^3\cdot\text{s}^{-1}$ ) for each cluster in the present study
S59	<b>Table S11</b> Total evaporation coefficients ( $\sum\gamma$ , $\text{s}^{-1}$ ) for each cluster in the present study
S60-S61	<b>Table S12</b> Ratios ( $\beta\cdot C/\sum\gamma$ ) between monomer molecule collisions and evaporation coefficients for each cluster involving SFA in the present study ([MSA] = $1.0 \times 10^7$ molecules $\cdot\text{cm}^{-3}$ , [MA] = $2.5 \times 10^7$ molecules $\cdot\text{cm}^{-3}$ , [SFA] = $1.0 \times 10^7$ molecules $\cdot\text{cm}^{-3}$ )
S62	<b>Table S13</b> The formation rate $J$ of MSA at the conditions of $T = 238.15$ K, [MSA] = $10^6$ - $10^8$ molecules $\cdot\text{cm}^{-3}$ , [MA] = $10^7$ - $10^{11}$ molecules $\cdot\text{cm}^{-3}$ , and [SFA] = 0, $10^8$ - $10^{12}$ molecules $\cdot\text{cm}^{-3}$ . MSA, MA and SFA represent methanesulfonic acid, methylamine and sulfamic acid, respectively
S63	<b>Table S14</b> The formation rate $J$ of MSA at the conditions of $T = 258.15$ K, [MSA] = $10^6$ - $10^8$ molecules $\cdot\text{cm}^{-3}$ , [MA] = $10^7$ - $10^{11}$ molecules $\cdot\text{cm}^{-3}$ , and [SFA] = 0, $10^8$ - $10^{12}$ molecules $\cdot\text{cm}^{-3}$ . MSA, MA and SFA represent methanesulfonic acid, methylamine and sulfamic acid, respectively
S64	<b>Table S15</b> The formation rate $J$ of MSA at the conditions of $T = 278.15$ K, [MSA] = $10^6$ - $10^8$ molecules $\cdot\text{cm}^{-3}$ , [MA] = $10^7$ - $10^{11}$ molecules $\cdot\text{cm}^{-3}$ , and [SFA] = 0, $10^8$ - $10^{12}$ molecules $\cdot\text{cm}^{-3}$ . MSA, MA and SFA represent methanesulfonic acid, methylamine and sulfamic acid, respectively
S65	<b>Table S16</b> The formation rate $J$ of MSA at the conditions of $T = 298.15$ K, [MSA] = $10^6$ - $10^8$ molecules $\cdot\text{cm}^{-3}$ , [MA] = $10^7$ - $10^{11}$ molecules $\cdot\text{cm}^{-3}$ , and [SFA] = 0, $10^8$ - $10^{12}$ molecules $\cdot\text{cm}^{-3}$ . MSA, MA and SFA represent methanesulfonic acid, methylamine and sulfamic acid, respectively
S66-S87	<b>Table S17</b> Cartesian coordinates of all molecules and clusters in the studied system



**Fig. S1** (a) The  $z$  coordinates of HNSO<sub>2</sub> molecule as the function of simulation time; (b) the density profile of water; (c) the pie chart with the occurrence percentages of HNSO<sub>2</sub> molecule at the air-water interface and in water phase





**Fig. S2** The optimized geometrical structures for the species involved in the HNSO<sub>2</sub> 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, <sup>d</sup> 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.).

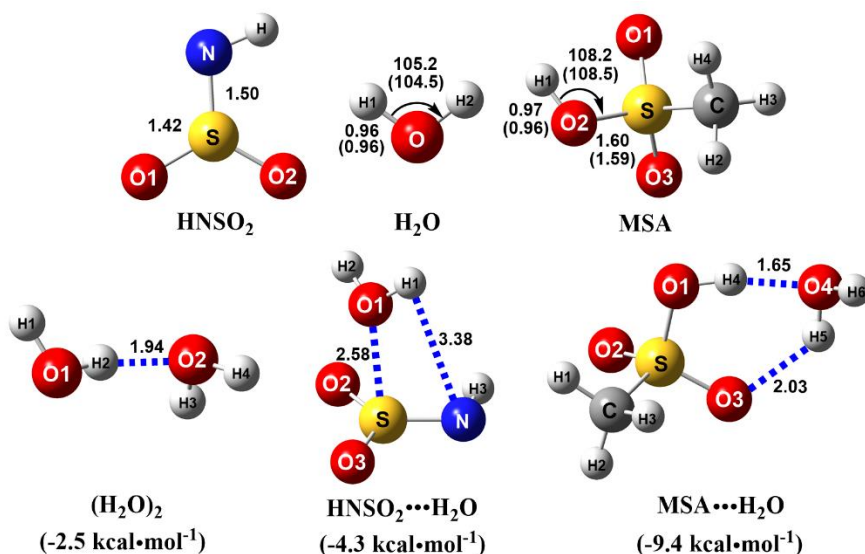
The geometric parameters of the reactants of HNSO<sub>2</sub>, H<sub>2</sub>O and NH<sub>2</sub>SO<sub>3</sub>H (SFA) have been displayed in Fig. S2. As seen in Fig. S2, the mean absolute deviation of calculated bond distances and bond angles between the M06-2X/6-311++G(2df,2pd) level and the experimental 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<sub>2</sub>, H<sub>2</sub>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<sub>2</sub> hydrolysis.

**Table S1** The Energy barriers ( $\Delta E$ ) and unsigned error (UE) ( $\text{kcal}\cdot\text{mol}^{-1}$ ) for the  $\text{HNSO}_2$  hydrolysis at different theoretical the potential energy profile ( $\Delta G$ ) correction

Methods	$\Delta E^a$	$\Delta E^b$	$\Delta E^c$	UE
CCSD(T)/CBS//M06-2X/ 6-311++G(2df,2pd)	3.4	29.7	-23.0	0.00
CCSD(T)-F12/cc-pVDZ-F12//M06-2X/ 6-311++G(2df,2pd)	3.6	30.6	-22.0	0.71

<sup>a</sup>, <sup>b</sup> and <sup>c</sup> respectively denote the species of pre-reactive complexes, transition states and products involved in the  $\text{HNSO}_2$  hydrolysis.

To further confirm the reliability of the CCSD(T)-F12/cc-pVDZ-F12//M06-2X/6-311++G(2df,2pd) level of theory, single-point energy calculations for the  $\text{HNSO}_2$  hydrolysis in the gas phase have been performed at two different levels of CCSD(T)/CBS and CCSD(T)-F12/cc-pVDZ-F12 based on the optimized geometries at the M06-2X/6-311++G(2df,2pd) level. Notably, the complete basis set (CBS) obtained by basis set extrapolation is used as the reference basis set. As presented in Table S1, compared with unsigned error calculated at the CCSD(T)/CBS//M06-2X/6-311++G(2df,2pd) level, unsigned errors calculated at CCSD(T)-F12/cc-pVDZ-F12//M06-2X/6-311++G(2df,2pd) was  $0.71 \text{ kcal}\cdot\text{mol}^{-1}$ . This suggests that the relative energies obtained at the CCSD(T)/aug-cc-pVDZ//M06-2X/6-311+G(2df,2pd) level was reasonable. Considering the computational accuracy and cost, the CCSD(T)/aug-cc-pVDZ//M06-2X/6-311+G(2df,2pd) method was chosen to calculate the single point energies of all the species involved in the  $\text{HNSO}_2$  hydrolysis.

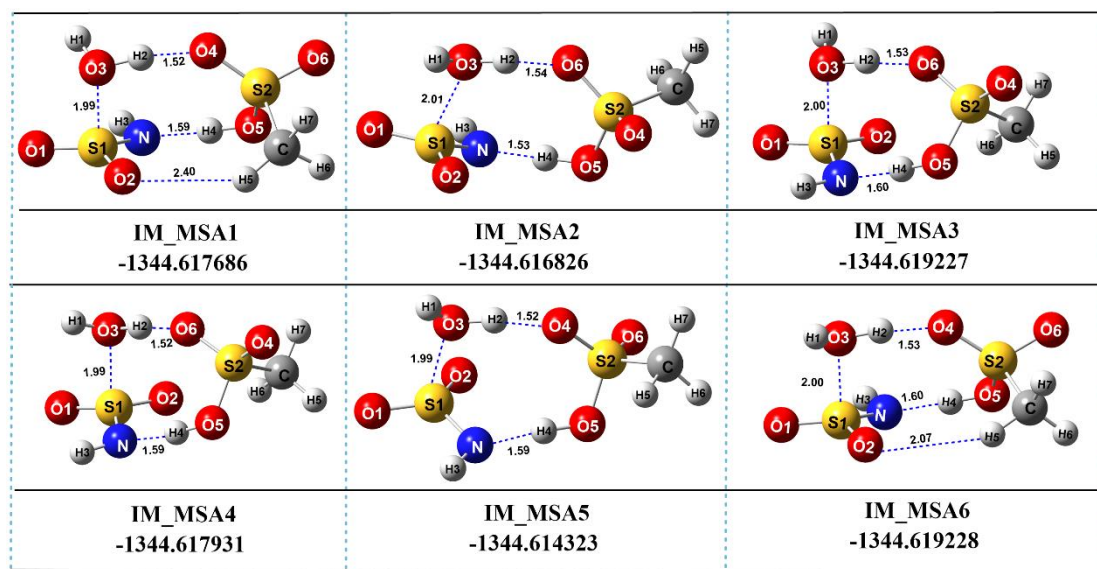


**Fig. S3** Optimized geometries of HNSO<sub>2</sub>, H<sub>2</sub>O, MSA, (H<sub>2</sub>O)<sub>2</sub>, HNSO<sub>2</sub>...H<sub>2</sub>O and MSA...H<sub>2</sub>O at the M06-2X/6-311++G(2df,2pd) level (bond distances in Angstroms and angles in degrees) along with the stabilization energies of (H<sub>2</sub>O)<sub>2</sub>, HNSO<sub>2</sub>...H<sub>2</sub>O and MSA...H<sub>2</sub>O at the CCSD(T)-F12/cc-pVDZ-F12//M06-2X/6-311++G(2df,2pd) level of theory

Fig. S2 illustrated the optimized geometries of monomer reactants of HNSO<sub>2</sub>, H<sub>2</sub>O 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(2df,2pd) level and the experimental values<sup>1, 2, 3</sup> were less than 0.01 Å and 0.5°, respectively. As for the dimer reactant of (H<sub>2</sub>O)<sub>2</sub>, single hydrogen bond geometry has been obtained, which was in good agreement with the previous reports<sup>4,5</sup> HNSO<sub>2</sub>...H<sub>2</sub>O and MSA...H<sub>2</sub>O displayed cage-like structures, and these geometrical structures were in good agreement with earlier findings<sup>6</sup>. The stabilization energies of (H<sub>2</sub>O)<sub>2</sub>, MSA...H<sub>2</sub>O with respect to the isolated reactants were in the range of -2.5 to -9.4 kcal·mol<sup>-1</sup>, and these energy values matched well with the earlier findings<sup>7</sup>.

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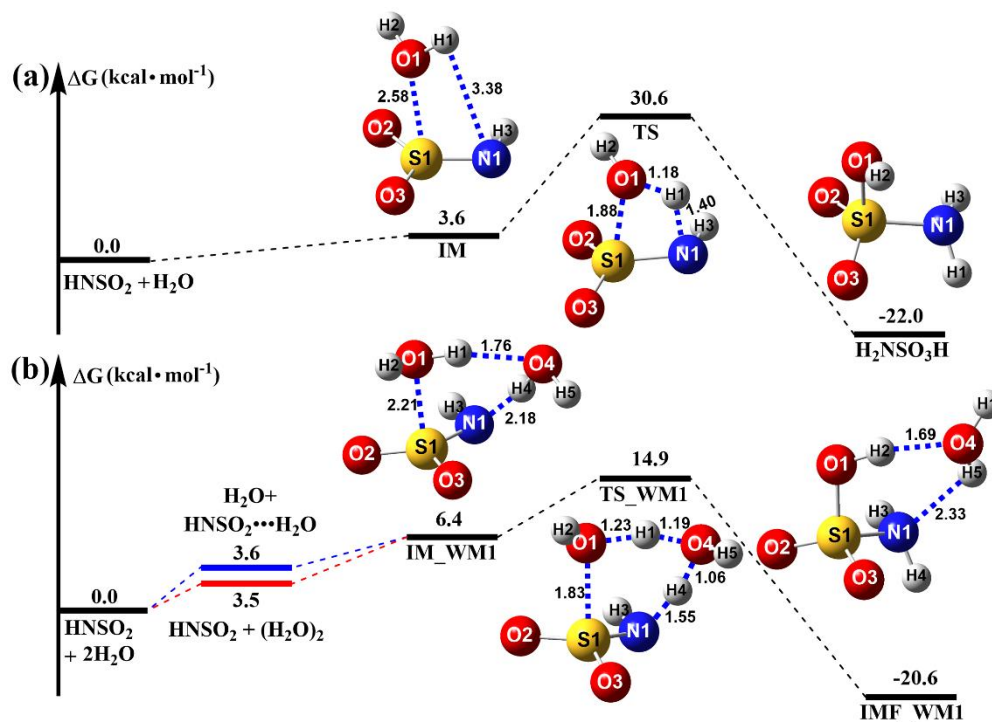


**Fig. S4** The optimized geometries and electric energies (in Hartree-Fock) for the complexes of  $\text{HNSO}_2 \cdots \text{H}_2\text{O} \cdots \text{MSA}$  at the M06-2X/6-311++G(2df,2pd) level of theory

To obtain the most stable configurations of  $\text{HNSO}_2 \cdots \text{H}_2\text{O} \cdots \text{MSA}$ , 500 auto-generated structures were produced by ABCcluster<sup>1,2</sup> software with TIP4P model<sup>3,4</sup> for  $\text{H}_2\text{O}$  and CHARMM force field<sup>5</sup> for  $\text{HNSO}_2$  and MSA. The generated structures were firstly optimized at the semi-empirical PM7 level by using MOPAC 2016<sup>6,7</sup>. Then, only structures with the following characteristics were selected and were optimized at the M06-2X/6-311++G(*d,p*) level: (i) the structures contains the  $\text{S}(\text{HNSO}_2) \cdots \text{O}(\text{H}_2\text{O})$  interaction of electron donor-acceptor (EDA); (ii) the structures facilitate the transfer of hydrogen atom from  $\text{H}_2\text{O}$  to  $\text{HNSO}_2$ . 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<sup>-1</sup> were re-optimized by the M06-2X/6-311++G(2df,2pd) level. As for the reactant complex  $\text{HNSO}_2 \cdots \text{H}_2\text{O} \cdots \text{MSA}$  its optimized geometries and stabilization energies have been illustrated in Fig. S2. As seen in Fig. S2, seven geometric isomers of  $\text{HNSO}_2 \cdots \text{H}_2\text{O} \cdots \text{MSA}$  (labeled as IM\_MSA $n$ ,  $n = 1-6$ ) have been optimized at the M06-2X/6-311++G(2df,2pd) level, where complex IM\_MSA1 is the most favorable complex with its binding energy larger by 0.8-3.1 kcal·mol<sup>-1</sup> than the other isomers. Based on the stable complex IM\_MSA1, Fig. 1 shows the favorable PES profile for the the hydrolysis reaction of  $\text{HNSO}_2$  with MSA.

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**Fig. S5** The potential energy profile ( $\Delta G$ ) for the hydrolysis reaction of  $\text{HNSO}_2$  without (a) and with (b)  $\text{H}_2\text{O}$  at the CCSD(T)-F12/cc-pVDZ-F12//M06-2X/6-311++G(2df,2pd) level of theory

115 **Table S2** Zero point energy (ZPE/(kcal·mol<sup>-1</sup>)), entropies (S/(cal·mol<sup>-1</sup>·K<sup>-1</sup>)), relative energies ( $\Delta E$   
 116 and  $\Delta(E + \text{ZPE})$ /(kcal·mol<sup>-1</sup>)), enthalpies ( $\Delta H(298)$ /(kcal·mol<sup>-1</sup>)), and free energies  
 117 ( $\Delta G(298)$ /(kcal·mol<sup>-1</sup>)) for the hydrolysis reaction of HNSO<sub>2</sub> without and with H<sub>2</sub>O and MSA

<i>Species</i>	ZPE	$\Delta E$	S	$\Delta G$	$\Delta(E + \text{ZPE})$	$\Delta H$
HNSO <sub>2</sub> + H <sub>2</sub> O	28.7	0.0	110.6	0.0	0.0	0.0
IM	30.3	-6.0	83.2	3.6	-4.4	-4.5
TS	29.2	20.2	71.9	30.6	20.6	19.1
IMF	32.8	-35.9	73.2	-22.0	-31.8	-33.2
HNSO <sub>2</sub> + 2H <sub>2</sub> O	42.3	0.0	155.7	0.0	0.0	0.0
HNSO <sub>2</sub> + (H <sub>2</sub> O) <sub>2</sub>	44.8	-5.0	133.2	3.5	-2.5	-3.2
HNSO <sub>2</sub> ···H <sub>2</sub> O + H <sub>2</sub> O	43.9	-6.0	128.3	3.6	-4.4	-4.5
IM_WM1	47.5	-17.1 (-20.3) <sup>a</sup>	89.1	6.4	-11.9	-13.5
TS_WM1	45.8	-8.2 (-12.1) <sup>a</sup>	79.8	14.9	-4.7	-7.7
IMF_WM1	48.7	-45.4 (-42.9) <sup>a</sup>	87.1	-20.6	-39.0	-41.0
HNSO <sub>2</sub> + H <sub>2</sub> O + MSA	68.2	0.0	185.4	0.0	0.0	0.0
HNSO <sub>2</sub> + MSA···H <sub>2</sub> O	70.5	-11.7	154.1	-0.9	-9.4	-10.2
HNSO <sub>2</sub> ···H <sub>2</sub> O + 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

118 <sup>a</sup> The value was taken from reference (Manonmani, G., Sandhiya, L., and Senthilkumar, K.: Hydrolysis of HNSO<sub>2</sub>:  
 119 A potential route for atmospheric production of H<sub>2</sub>SO<sub>4</sub> and NH<sub>3</sub>, Int J Quantum Chem, 120, e26182, 2020.)



**Table S3** Equilibrium constants ( $\text{cm}^3 \cdot \text{molecule}^{-1}$ ) for the  $\text{HNSO}_2 \cdots \text{H}_2\text{O}$ ,  $\text{H}_2\text{O} \cdots \text{H}_2\text{O}$ , and  $\text{MSA} \cdots \text{H}_2\text{O}$  complexes within the temperature range of 212.6-320.0 K

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

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

**Table S4** The high-pressure limiting rate constant ( $\text{cm}^3 \cdot \text{molecule}^{-1} \cdot \text{s}^{-1}$ ) for the hydrolysis reaction of  $\text{HNSO}_2$  with  $\text{H}_2\text{O}$  and MSA within the temperature range of 212.6-320.0 K

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

## Part S1. Calculations of reaction rate coefficients

The rate coefficients for the hydrolysis of HNSO<sub>2</sub> 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 Polyrates package<sup>1</sup>. Subsequently, on the basis of the HPL rate coefficients, the rate coefficients for the hydrolysis of HNSO<sub>2</sub> 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<sup>2</sup>. 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<sup>3</sup>, while the step transitioning between pre-reactive complexes and post-reactive complexes via transition states were evaluated using the RRKM theory<sup>4</sup> in combination with the asymmetric Eckart model.

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

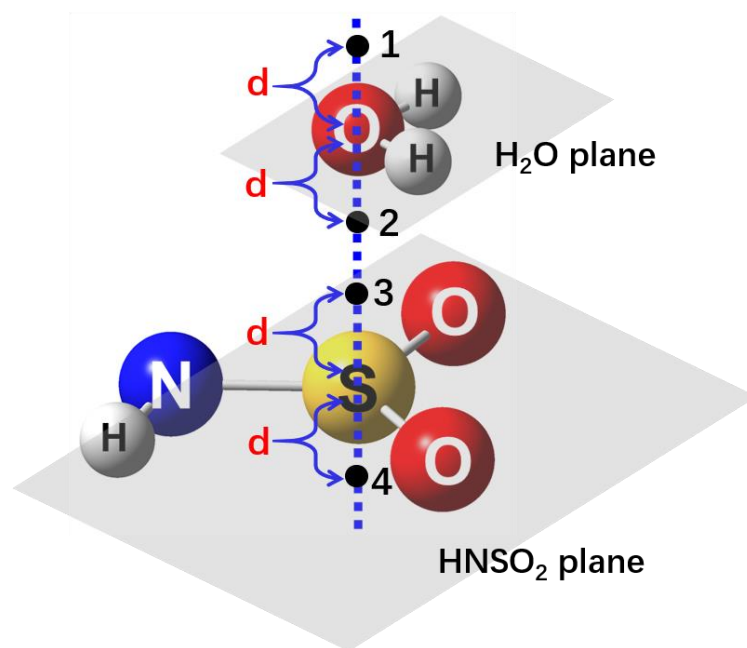
$$k(E) = \frac{W(E-E_0)}{h\rho(E)} \quad (\text{S1})$$

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

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

Herein, we describe the implementation details of the VRC-TST calculation<sup>5-8</sup>. 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<sub>2</sub> hydrolysis reaction, the pivot points of HNSO<sub>2</sub> (points 1 and 2) are located at a distance  $\pm d$  along its S axis, and the pivots of H<sub>2</sub>O (points 3 and 4) are located at a distance  $\pm d$  perpendicular to H<sub>2</sub>O molecule lane. As shown in Fig. S6, the Multiwfn package combined with the VMD software is adopted to visualize the reaction system and

help determine the location of pivot points. The reaction coordinate value ( $s$ ) is defined as the minimum of the distance ( $r_{ij}$ ) between the pivot point  $i$  ( $=1$  or  $2$ ) and pivot point  $j$  ( $=3$  or  $4$ ), where  $i$  and  $j$  represent the pivot points of  $\text{HNSO}_2$  and  $\text{H}_2\text{O}$  molecules, respectively. Hence, each of the four dividing surfaces is obtained by symmetrically placing two pivot points of each radical 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 four dividing surfaces (2-3), is determined by the locations of pivot points 2, 3 and the reaction coordinate  $s$ . There are total four pair of pivot points, the other three dividing surfaces (1-3, 1-4, 2-4) are defined by their corresponding pivot points and reaction coordinates  $s$ . Note that the locations of pivot points are critical to the rate constant calculation. Considering the difference between  $\text{HNSO}_2$  and  $\text{H}_2\text{O}$  molecules, the distance  $s$  between pivot points is varied from 2.5 to 6 Å for  $\text{HNSO}_2$  and  $\text{H}_2\text{O}$  in each case with a 0.5 Å grid increment.



**Fig. S6** The placements of the pivot points for the  $\text{HNSO}_2$  hydrolysis

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187

**Table S5** Rate coefficients ( $k$ ,  $\text{cm}^3 \cdot \text{molecule}^{-1} \cdot \text{s}^{-1}$ ) for the hydrolysis of  $\text{HNSO}_2$  by master equation within the temperature range of 212.6-320.0 K

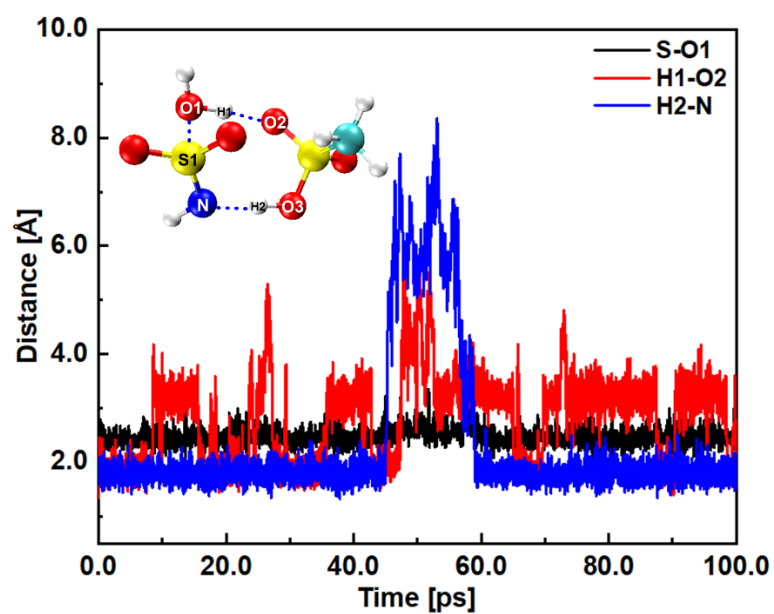
$T/\text{K}$	$k_{\text{R}}$
212.6	$2.55 \times 10^{-28}$
229.7	$3.78 \times 10^{-28}$
259.3	$1.04 \times 10^{-27}$
280.0	$2.70 \times 10^{-27}$
290.0	$4.53 \times 10^{-27}$
298.0	$7.02 \times 10^{-27}$
300.0	$7.86 \times 10^{-27}$
310.0	$1.39 \times 10^{-26}$
320.0	$2.50 \times 10^{-26}$

$k_{\text{R}}$  is the bimolecular rate constant for the hydrolysis of  $\text{HNSO}_2$ .

191 **Table S6** Concentrations (molecules·cm<sup>-3</sup>) of H<sub>2</sub>O and MSA within the temperature range of 213-320 K and altitude range of 0-15 km

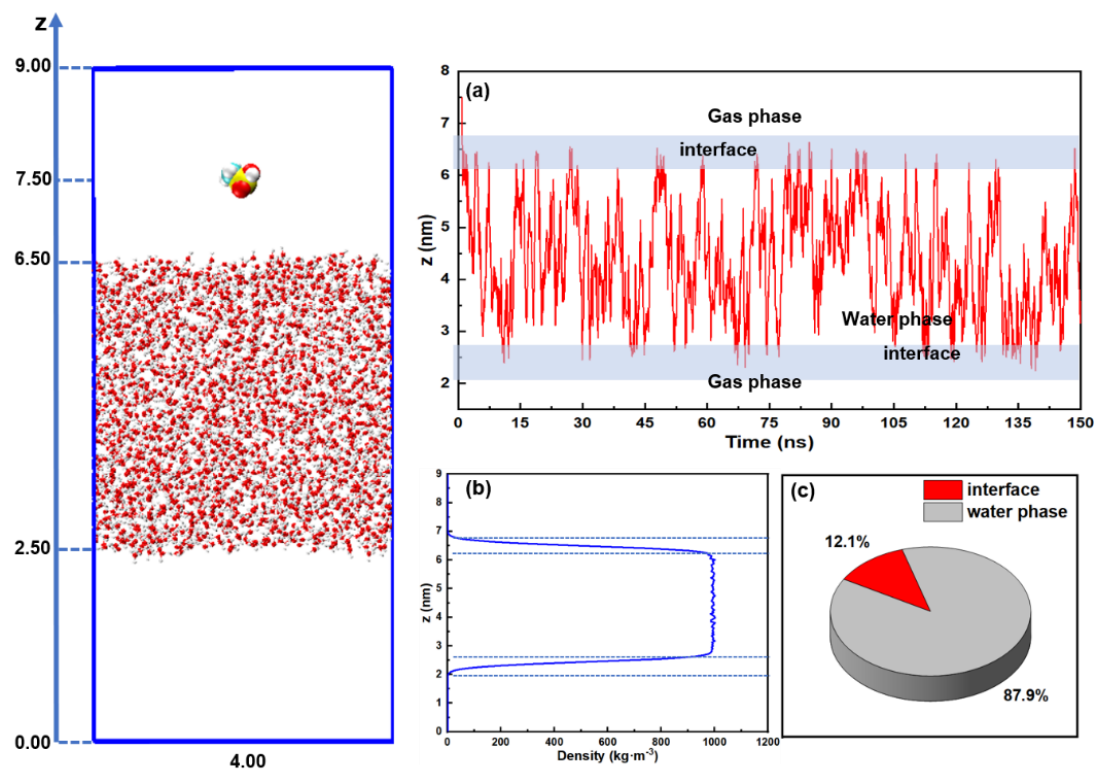
Altitude		0 km						5 km	10 km	15 km
T/K	RH	280.0	290.0	298.0	300.0	310.0	320.0	259.3	229.7	212.6
[H <sub>2</sub> O]	20%RH <sup>a</sup>	$5.16 \times 10^{16}$	$9.60 \times 10^{16}$	$1.50 \times 10^{17}$	$1.72 \times 10^{17}$	$2.92 \times 10^{17}$	$4.70 \times 10^{17}$			
	40%RH <sup>a</sup>	$1.03 \times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

192 <sup>a</sup> 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-  
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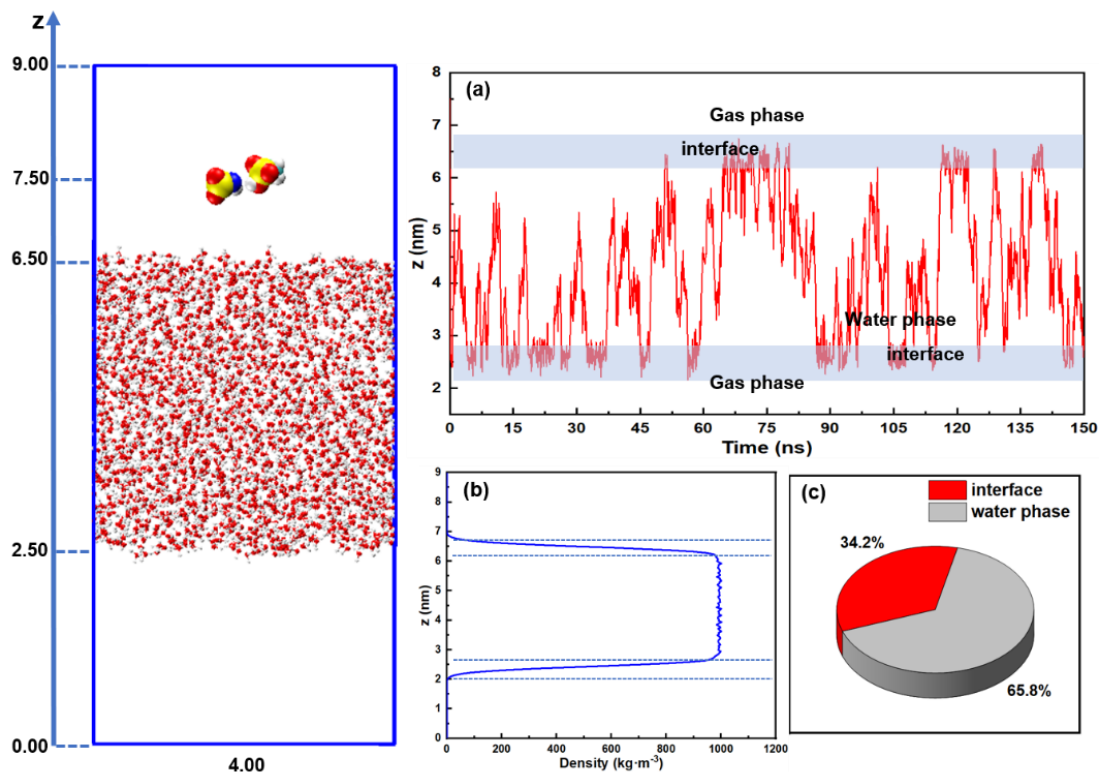


**Fig. S7** The dynamic trajectories of MSA-assisted gaseous hydrolysis of HNSO<sub>2</sub>

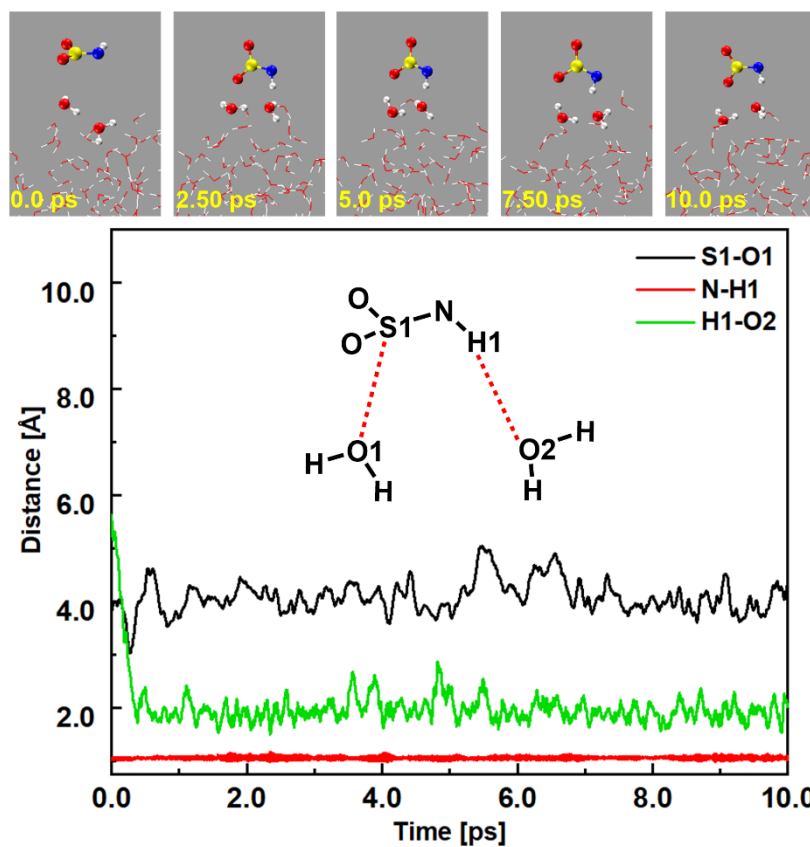




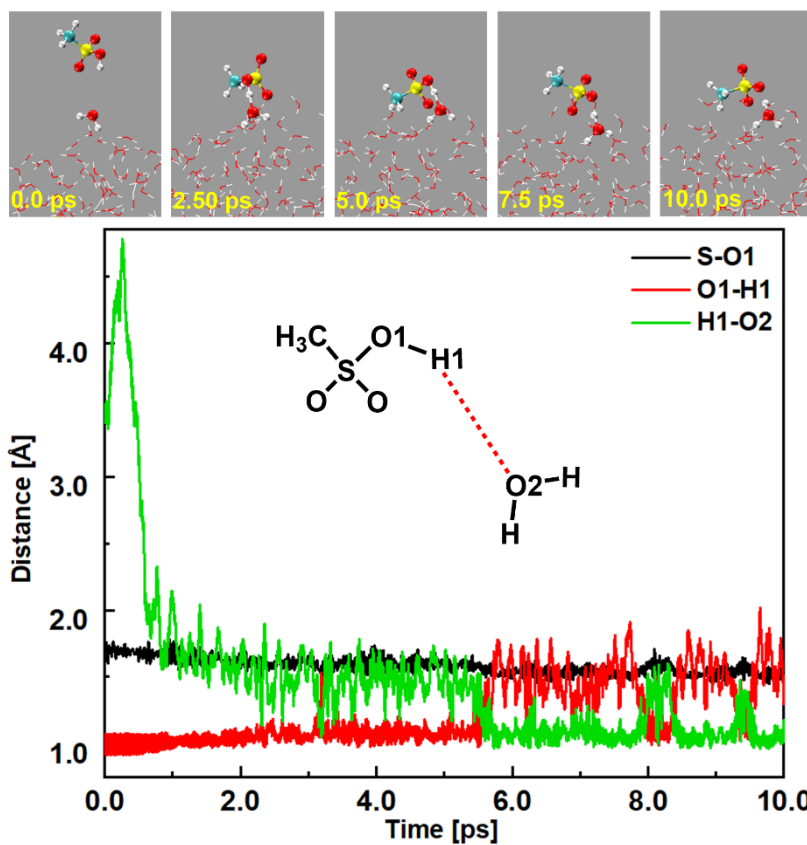
**Fig. S8** (a) The  $z$  coordinates of MSA molecule as the function of simulation time; (b) the density profile of water; (c) the pie chart with the occurrence percentages of MSA molecule at the air-water interface and in water phase



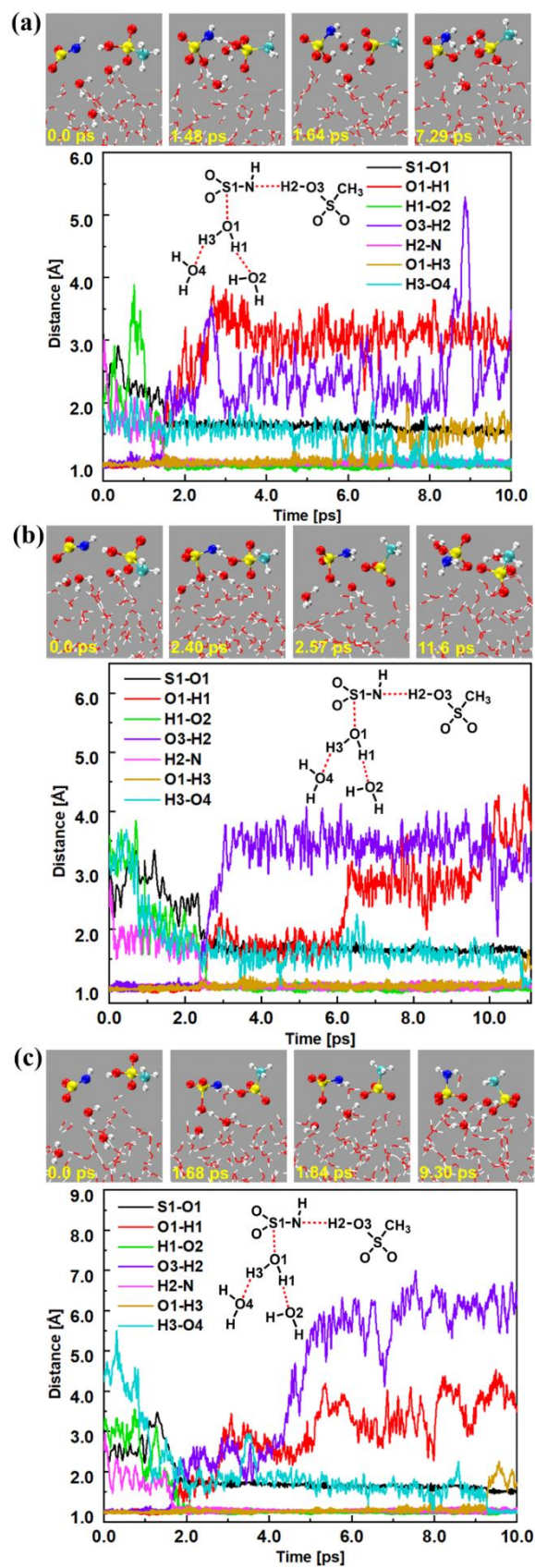
**Fig. S9** (a) The  $z$  coordinates of complex HNSO<sub>2</sub>...MSA as the function of simulation time; (b) the density profile of water; (c) the pie chart with the occurrence percentages of complex HNSO<sub>2</sub>...MSA at the air-water interface and in water phase

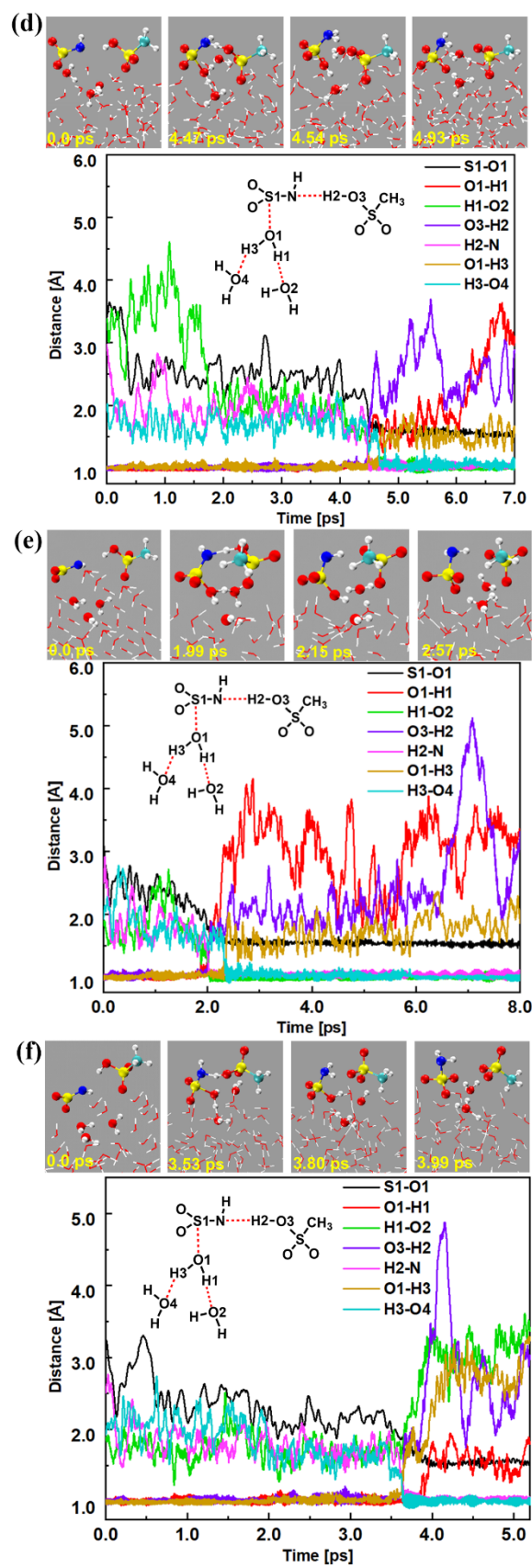


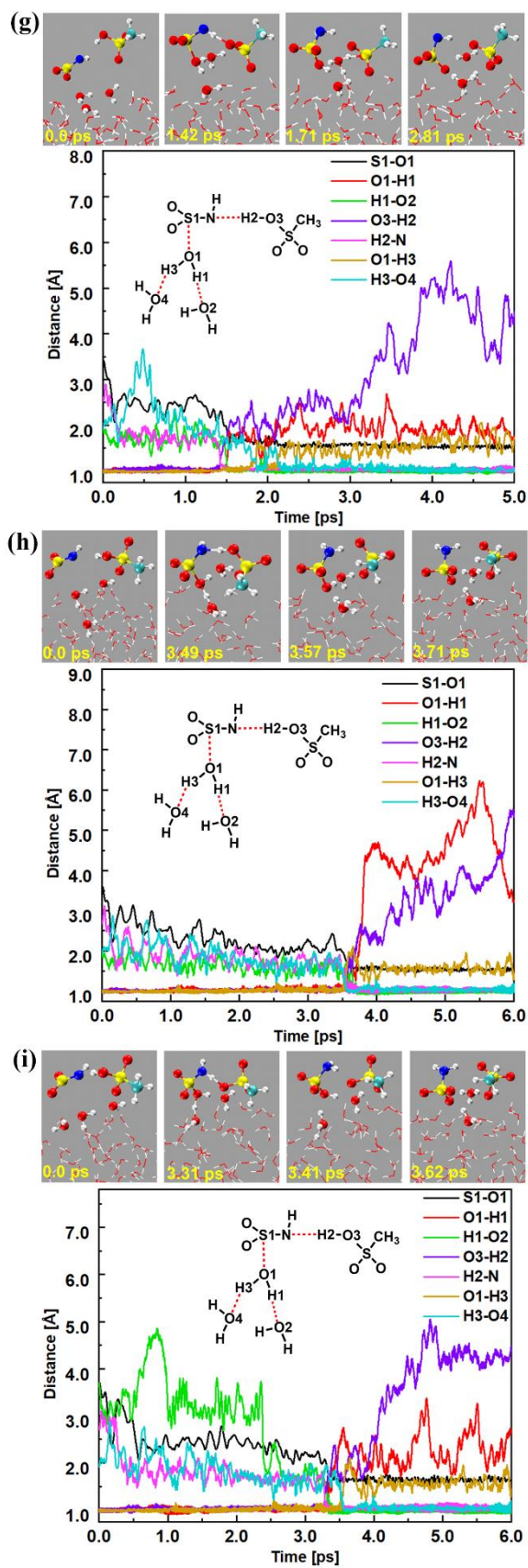
**Fig. S10** Snapshot structures taken from the BOMD simulations of HNSO<sub>2</sub> reaction at the air-water interface



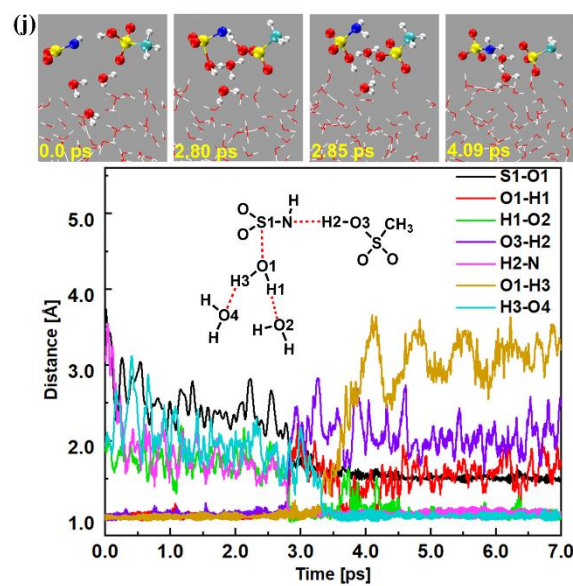
**Fig. S11** Snapshot structures taken from the BOMD simulations of MSA reaction at the air-water interface





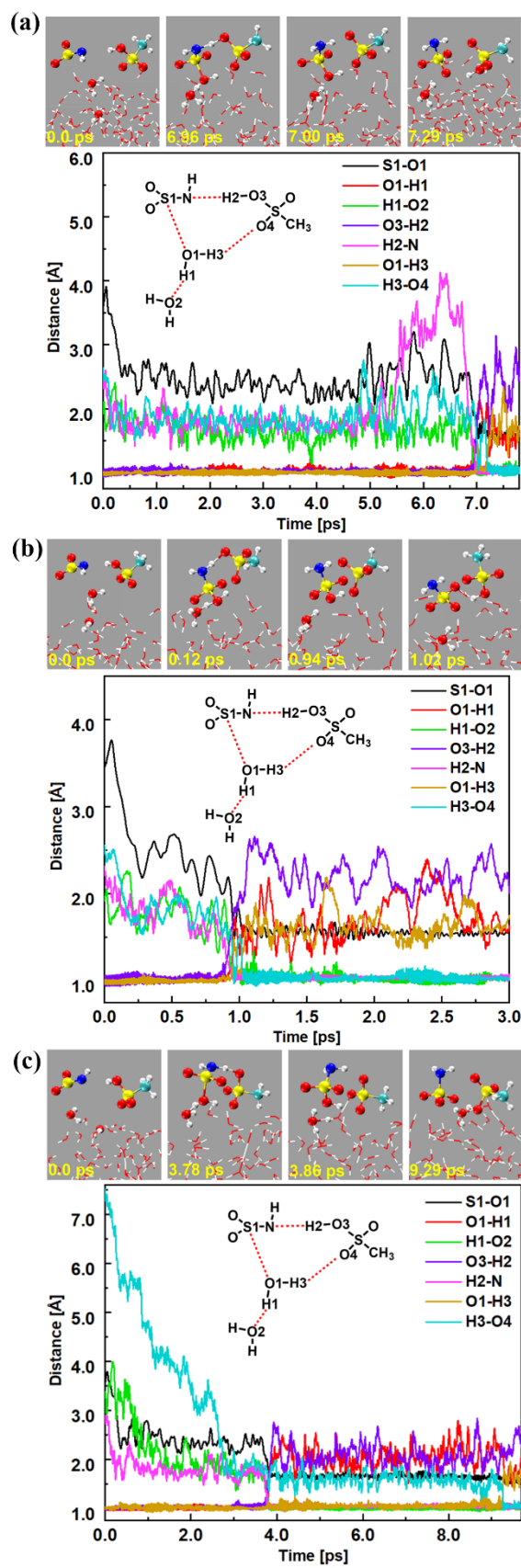


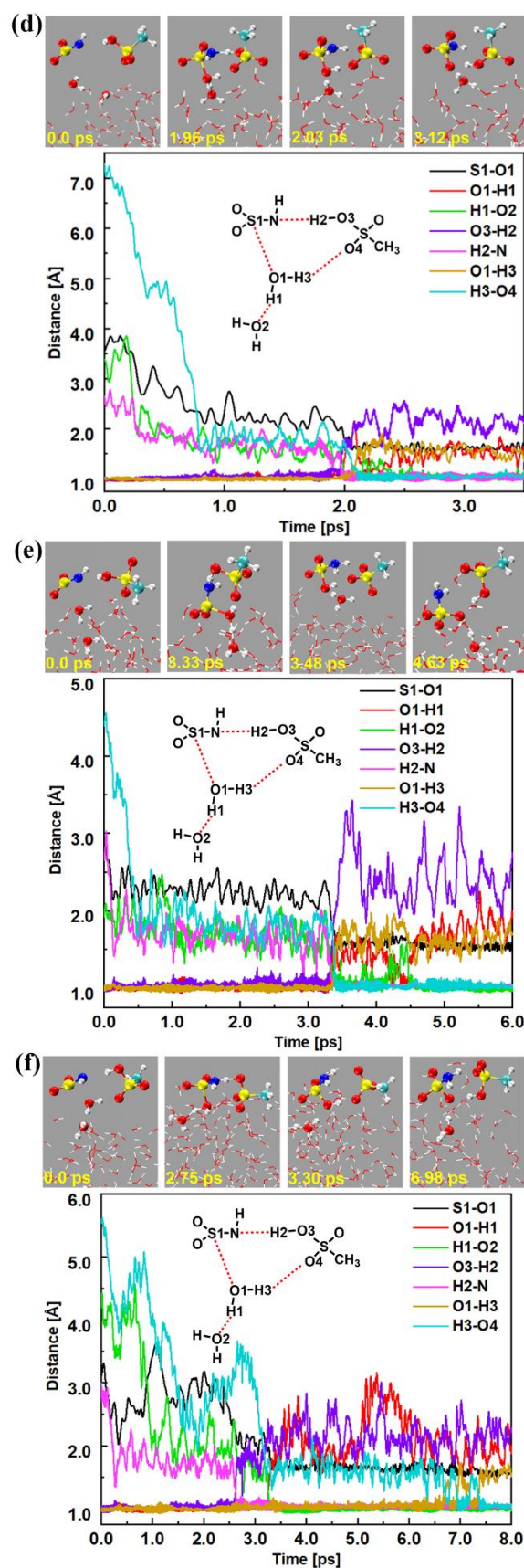


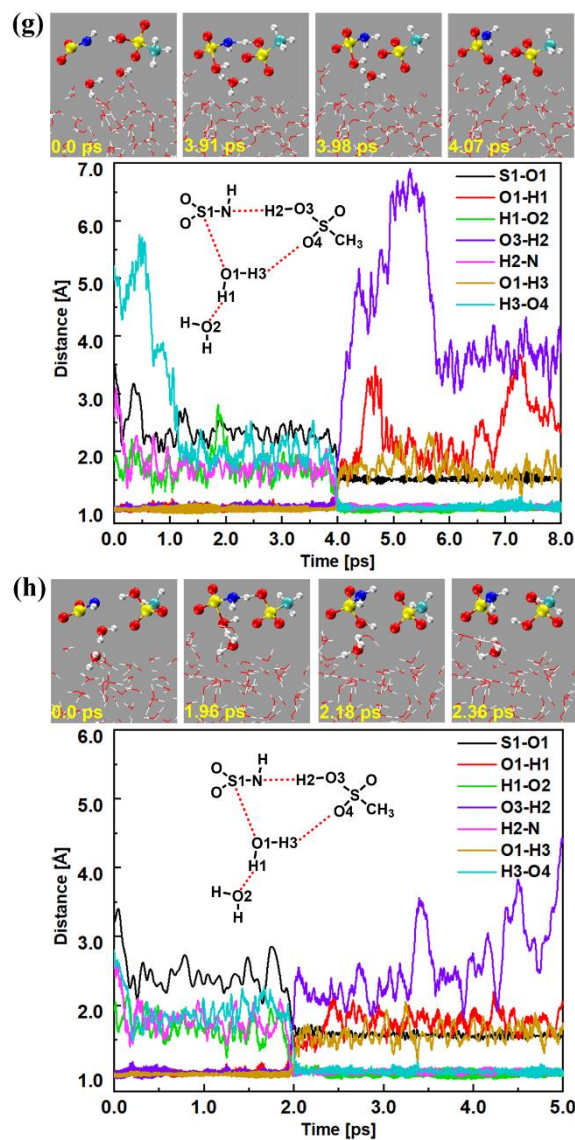


**Fig. S12** BOMD simulation trajectories and snapshots of  $\text{MSA}^-$  and  $\text{H}_3\text{O}^+$  ions forming mechanism via the chain structure routes in MSA-mediated hydration  $\text{HNSO}_2$  at the air-water interface

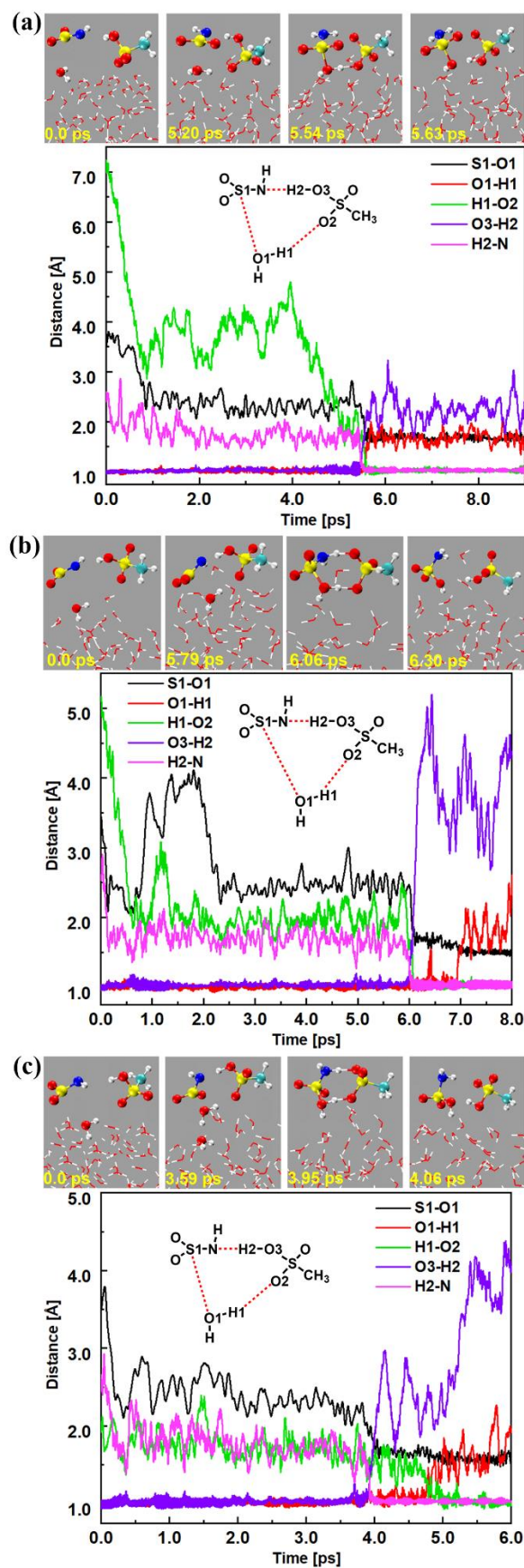


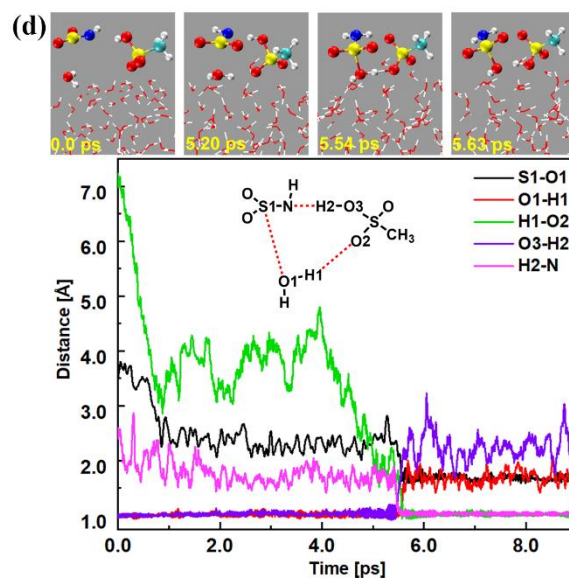






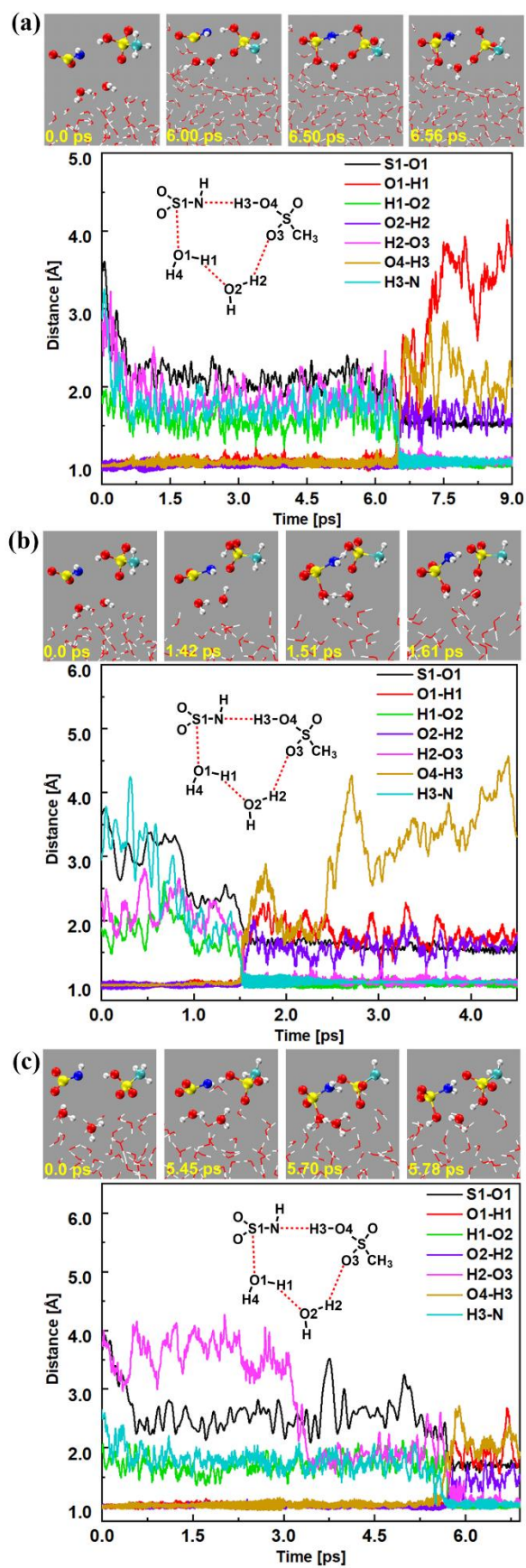
**Fig. S13** BOMD simulation trajectories and snapshots of  $\text{MSA}^-$  and  $\text{H}_3\text{O}^+$  ions forming mechanism via loop structure routes in  $\text{MSA}$ -mediated hydration  $\text{HNSO}_2$  at the air-water interface

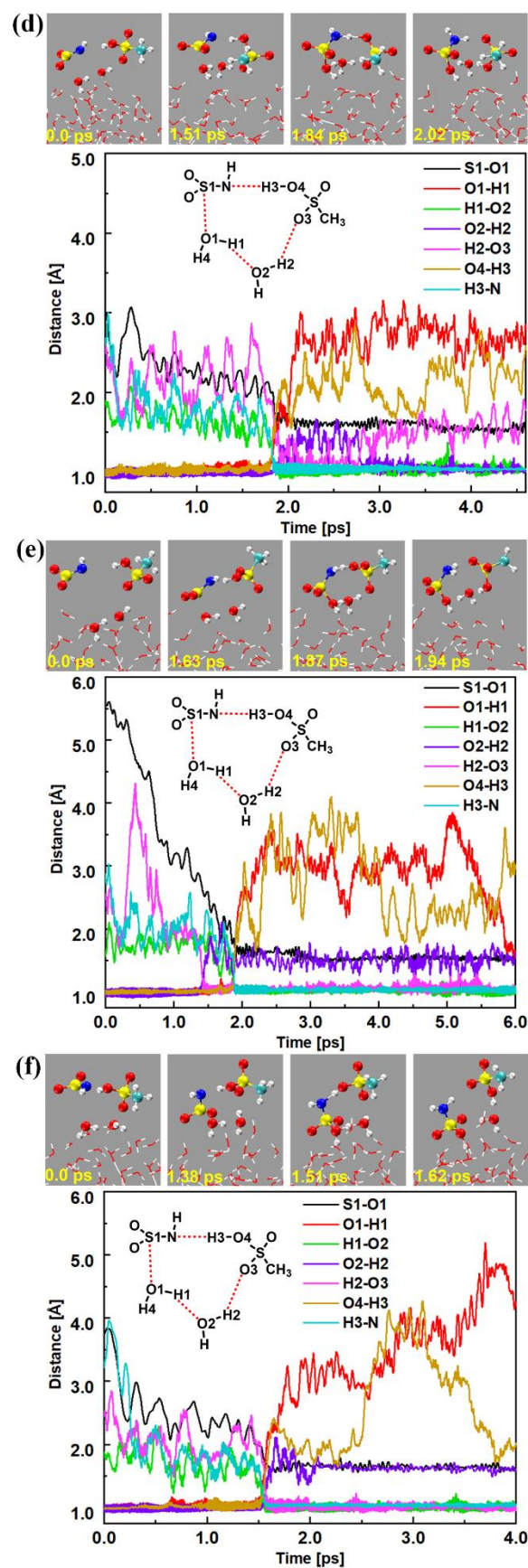


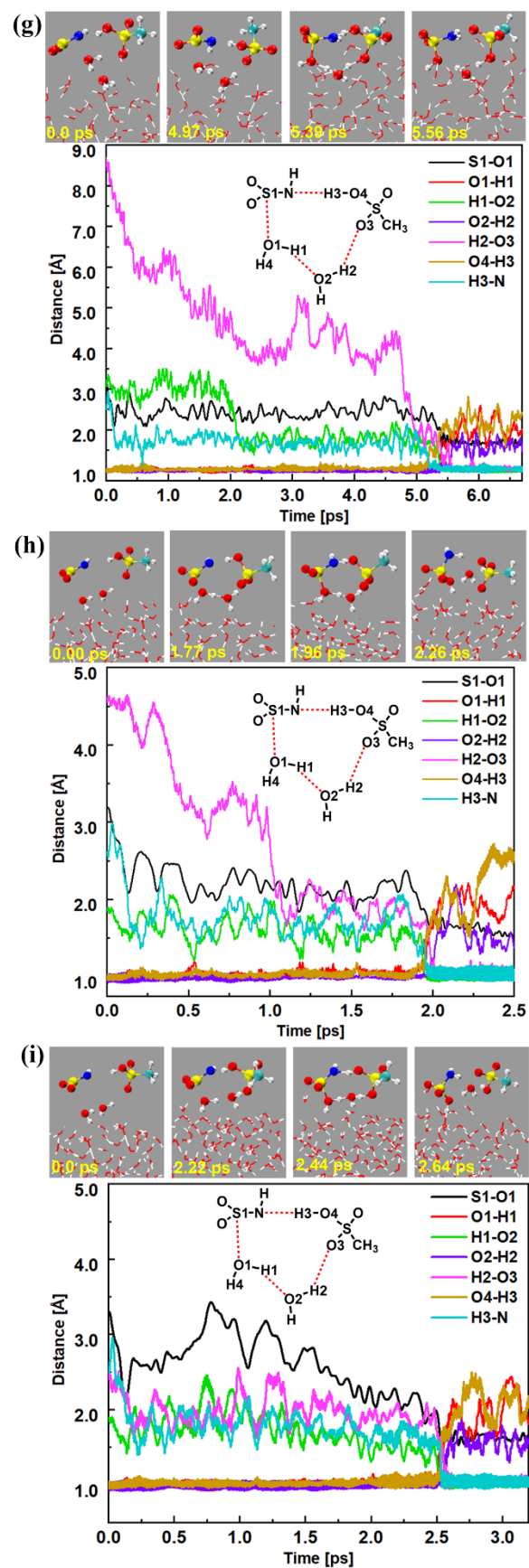


**Fig. S14** BOMD simulation trajectories and snapshots of proton exchange mechanism in MSA - mediated hydration  $\text{HNSO}_2$  with a water molecule at the air-water interface

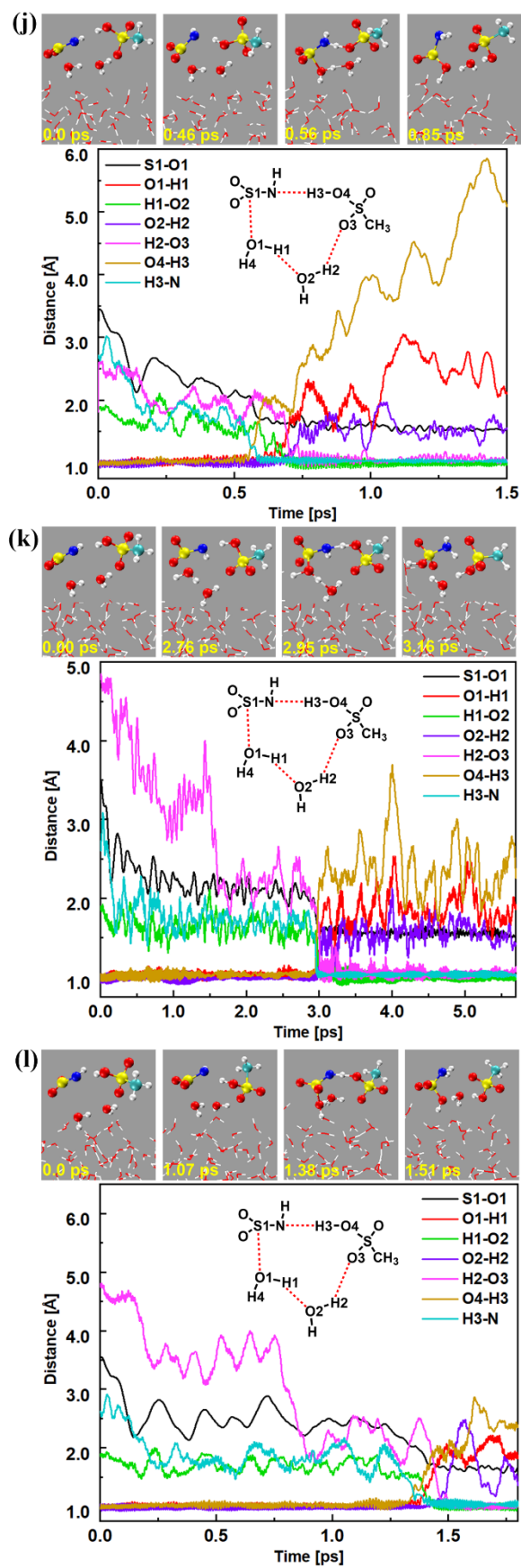


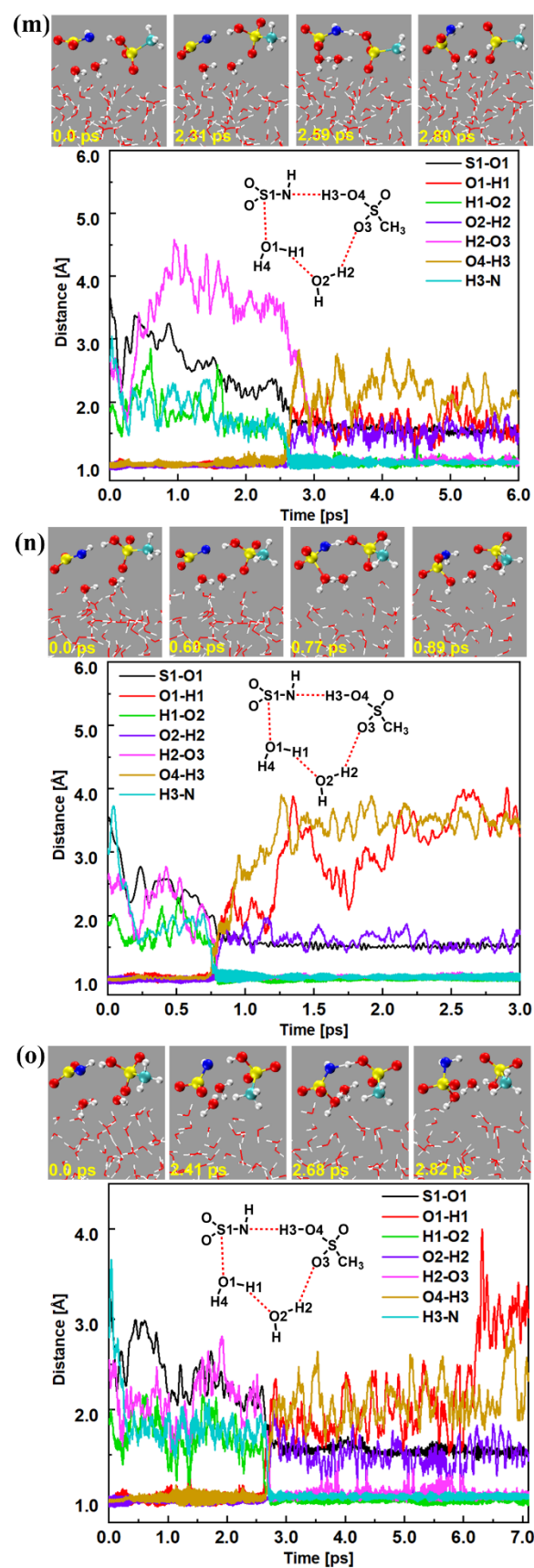


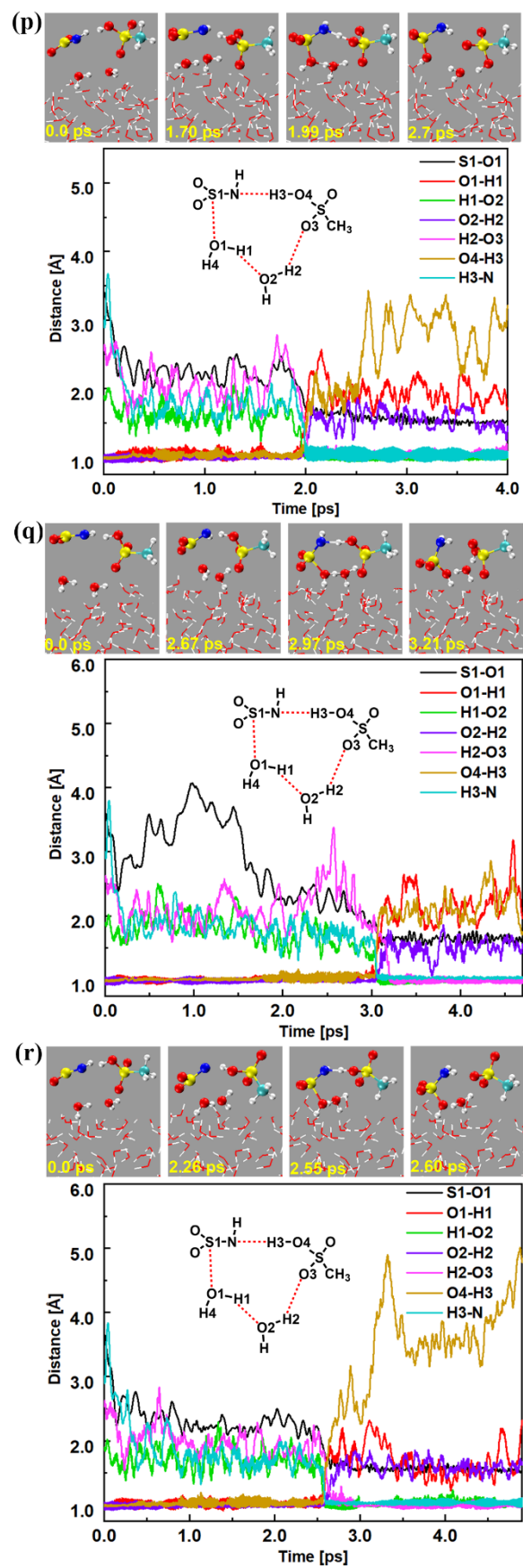


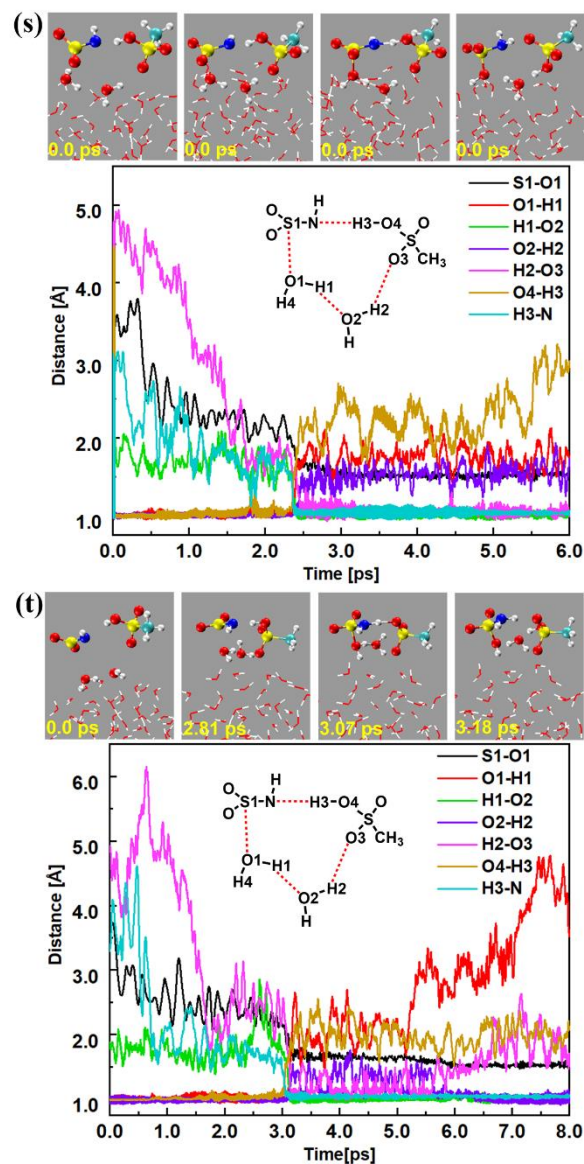




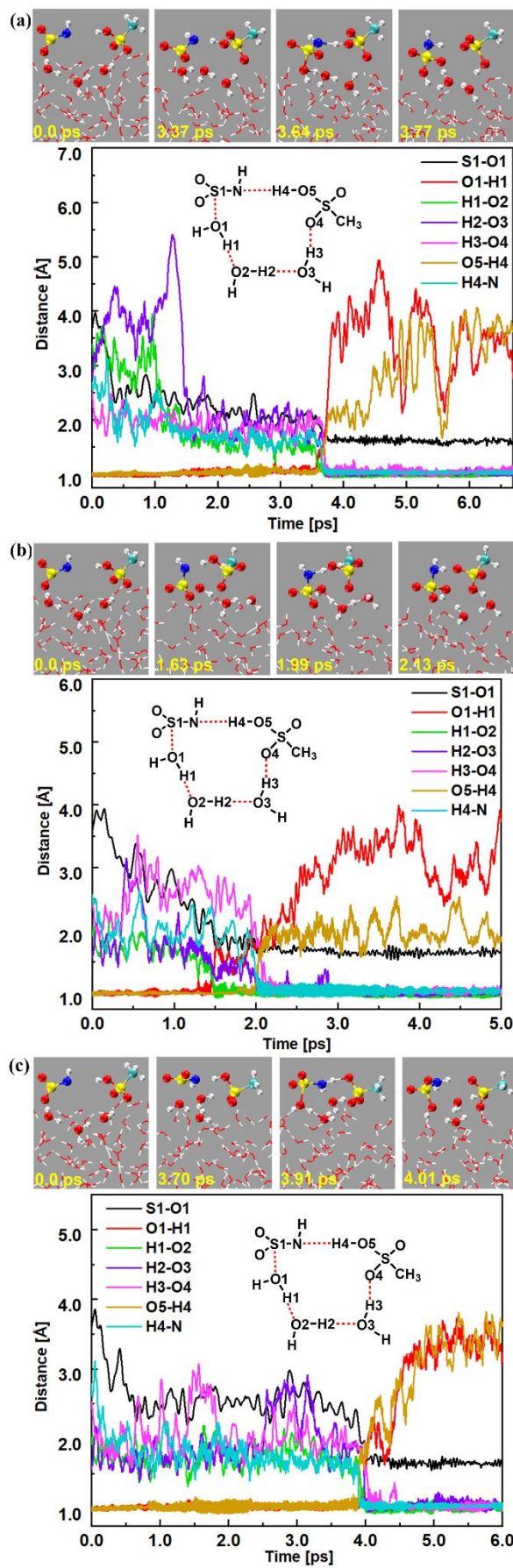


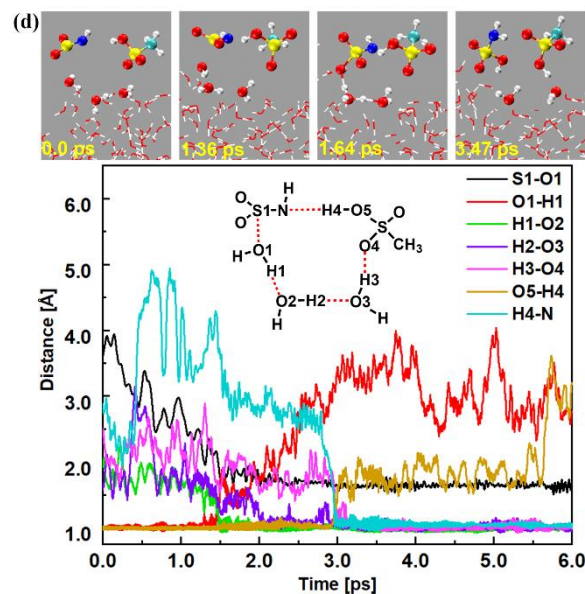






**Fig.S15** BOMD simulation trajectories and snapshots of proton exchange mechanism in MSA - mediated hydration HNSO<sub>2</sub> with two water molecules at the air-water interface





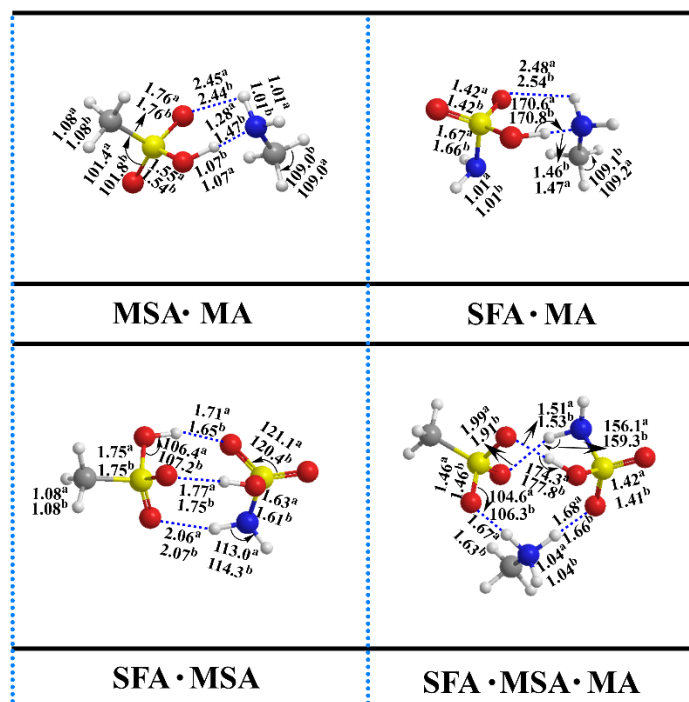
**Fig. S16** BOMD simulation trajectories and snapshots of proton exchange mechanism in MSA-mediated hydration of  $\text{HNSO}_2$  with three water molecules at the air-water interface



## 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  $(\text{SFA})_x(\text{MSA})_y(\text{MA})_z$  ( $0 \leq z \leq x + y \leq 3$ ) clusters. To locate the global minimum energy structure, the artificial bee colony algorithm was systematically employed by the ABCcluster program<sup>1, 2</sup> to generate  $n \times 1000$  ( $1 < n \leq 4$ ) initial random configurations for each cluster, and then, PM6 semi-empirical method<sup>3-5</sup> was used to further pre-optimize the produced configurations above. Second, up to 100 structures with relatively lower energies were selected from the  $n \times 1000$  structures (where  $1 < n \leq 4$ ), and a M06-2X/6-31+G(*d,p*)<sup>6</sup> level of theory was applied for subsequent optimization. Finally, further geometry optimization and frequency calculations at the M06-2X/6-311++G(2*df*,2*pd*)<sup>7</sup> 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(2*df*,2*pd*) 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<sup>8</sup>.

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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. <sup>a</sup> The values obtained at the M06-2X/6-311++G(2df,2pd) level of theory. <sup>b</sup> 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.



284 **Table S7** Comparison of calculated formation free energies ( $\Delta G$ ) at the M06-2X/6-311++G(2*df*,2*pd*) and the M06-  
 285 2X/6-311++G(3*df*,3*pd*) levels

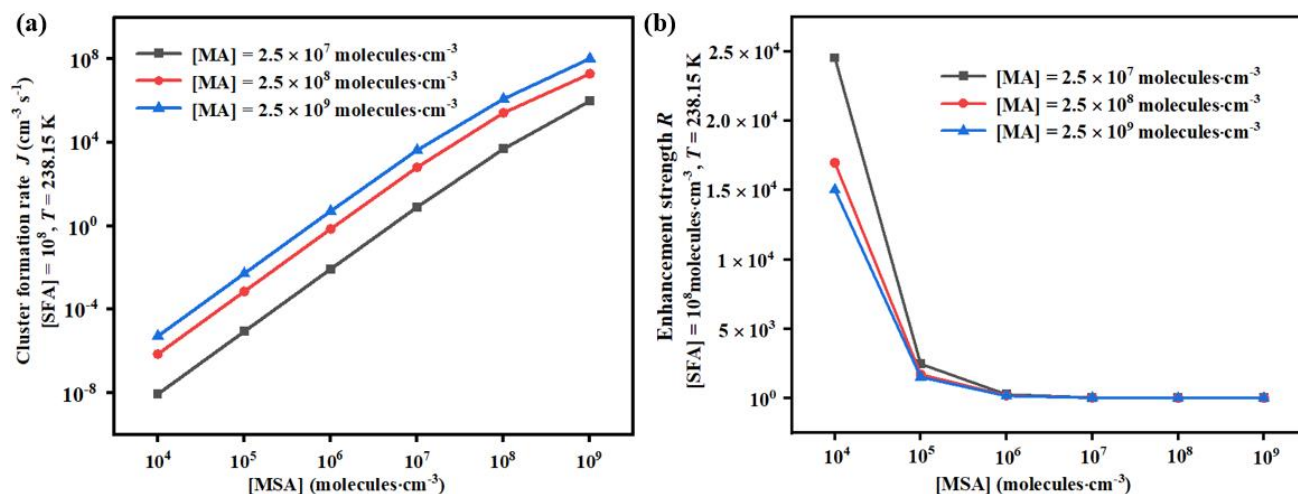
Cluster	M06-2X/6-311++G(2 <i>df</i> ,2 <i>pd</i> )	M06-2X/6-311++G(3 <i>df</i> ,3 <i>pd</i> )
	kcal·mol <sup>-1</sup>	
MSA·MA	-6.19	-6.55
MSA·SFA	-9.33	-9.54
MA·SFA	-6.01	-6.98
MSA·MA·SFA	-21.96	-23.71

286 We calculated the Gibbs free energy (in Table S7) for the MSA·MA, SFA·MA, MSA·SFA and  
 287 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  
 288 theory. The analysis of Gibbs free energy indicated that the predicted relative  $\Delta G$  of MSA·MA,  
 289 SFA·MA, MSA·SFA and MSA·SFA·MA clusters at the M06-2X/6-311++G(2*df*,2*pd*) level is nearly  
 290 close to the values at the M06-2X/6-311++G(3*df*,3*pd*) level, with differences of less than 1.75  
 291 kcal·mol<sup>-1</sup>. So, we chose the M06-2X/6-311++G(2*df*,2*pd*) method for further frequency calculations.  
 292 Relevant details are presented in Table S7.

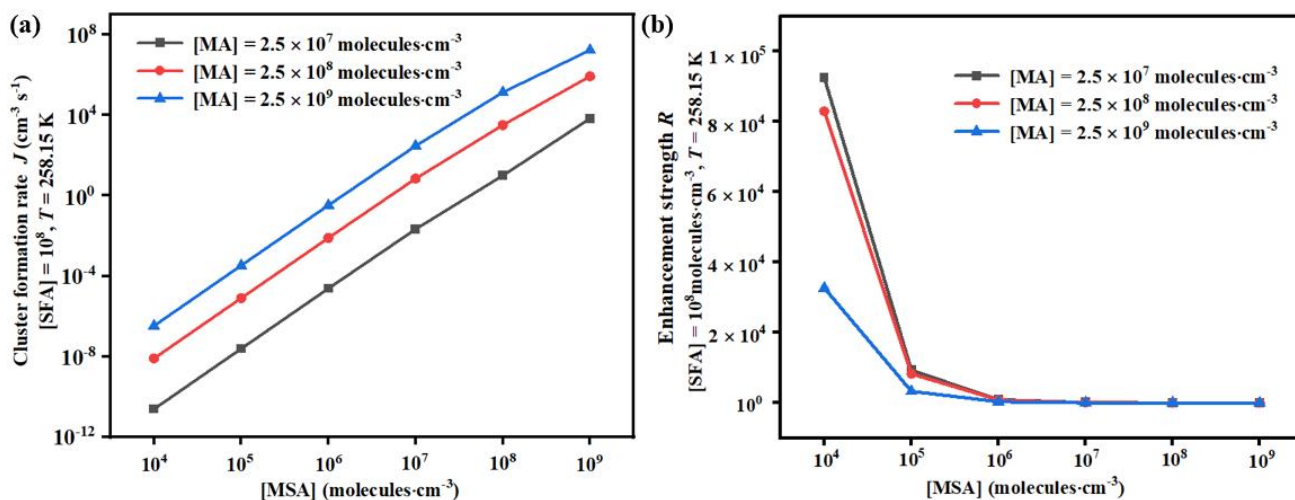
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 294

SFA · MSA	SFA · MA	SFA · MSA · MA	(SFA) <sub>2</sub> · MSA
SFA · (MSA) <sub>2</sub>	(SFA) <sub>2</sub> · MA	(SFA) <sub>2</sub> · MSA · MA	SFA · (MSA) <sub>2</sub> · MA
(SFA) <sub>3</sub> · MA	SFA · MSA · (MA) <sub>2</sub>	(SFA) <sub>2</sub> · (MA) <sub>2</sub>	(SFA) <sub>2</sub> · MSA · (MA) <sub>2</sub>
SFA · (MSA) <sub>2</sub> · (MA) <sub>2</sub>	(SFA) <sub>3</sub> · (MA) <sub>2</sub>	(SFA) <sub>2</sub> · MSA · (MA) <sub>3</sub>	(SFA) <sub>3</sub> · (MA) <sub>3</sub>

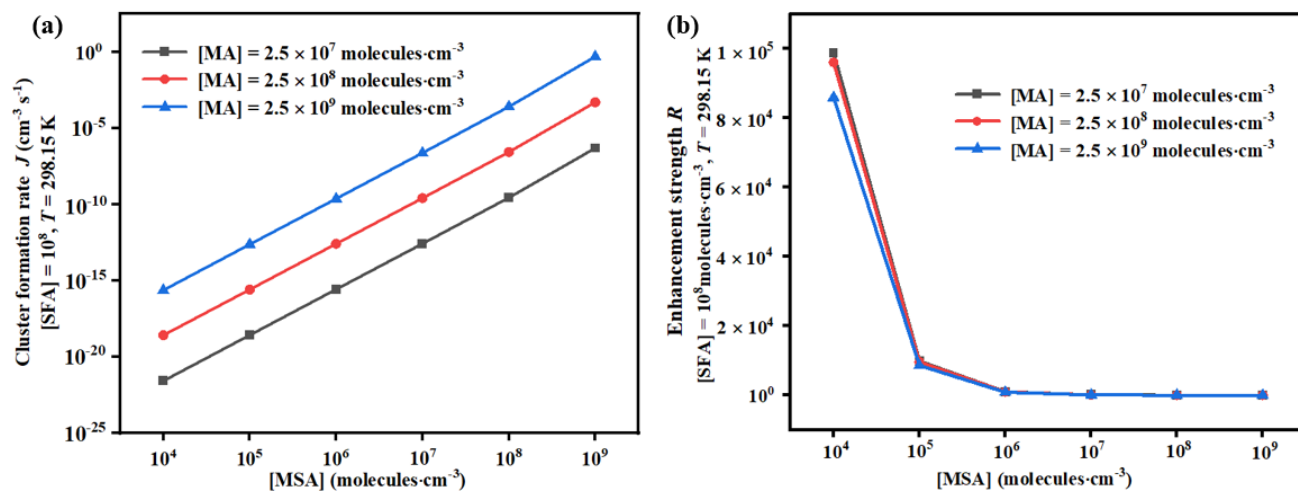
**Fig. S18** The most stable configurations of the SFA-MSA-MA-based clusters identified at the M06-2X/6-311++G(2df,2pd) level of theory. The lengths of hydrogen bonds are given in Å (Color code: blue = nitrogen, yellow = sulfur, red = oxygen, gray = carbon, and white = hydrogen)



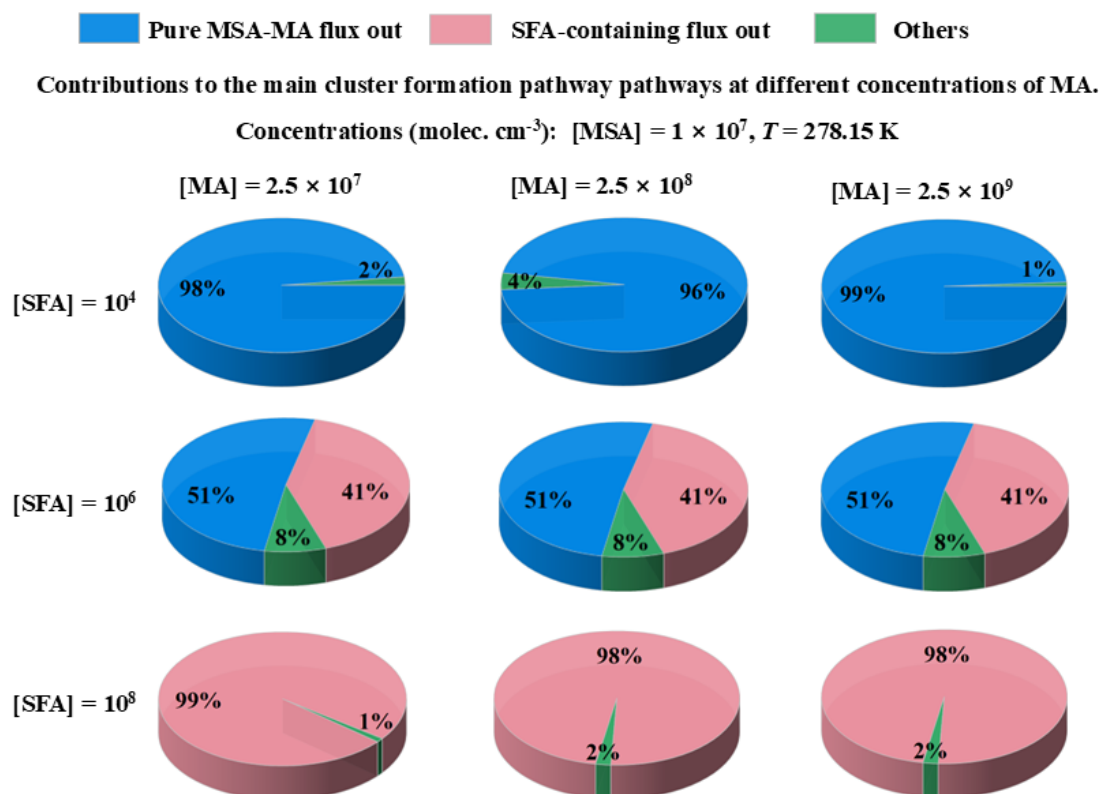
**Fig. S19** (a) The  $J$  ( $\text{cm}^{-3} \text{ s}^{-1}$ ) and (b)  $R$  as a function of  $[MSA]$  with  $[SFA] = 10^8 \text{ molecules cm}^{-3}$  and three different  $[MA]$  (black line:  $[MA] = 2.5 \times 10^7 \text{ molecules cm}^{-3}$ , red line:  $[MA] = 2.5 \times 10^8 \text{ molecules cm}^{-3}$ , blue line:  $[MA] = 2.5 \times 10^9 \text{ molecules cm}^{-3}$ ) at  $238.15 \text{ K}$



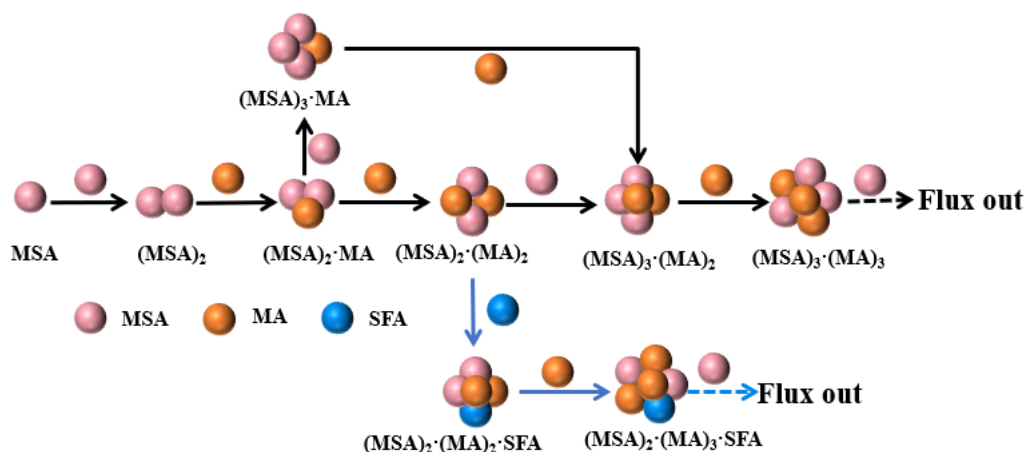
**Fig. S20** (a) The  $J$  ( $\text{cm}^{-3} \text{s}^{-1}$ ) and (b)  $R$  as a function of  $[\text{MSA}]$  with  $[\text{SFA}] = 10^8$  molecules  $\text{cm}^{-3}$  and three different  $[\text{MA}]$  (black line:  $[\text{MA}] = 2.5 \times 10^7$  molecules  $\text{cm}^{-3}$ , red line:  $[\text{MA}]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



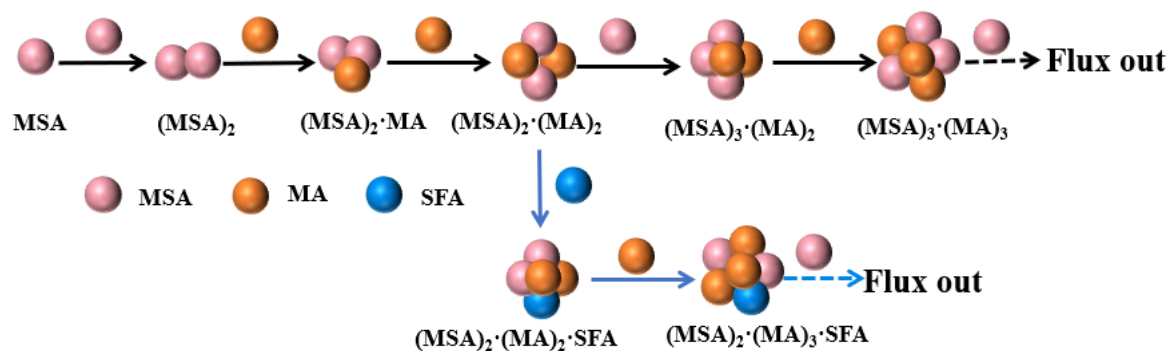
**Fig. S21** (a) The  $J$  (cm<sup>3</sup> s<sup>-1</sup>) and (b)  $R$  as a function of  $[MSA]$  with  $[SFA] = 10^8$  molecules cm<sup>-3</sup> and three different  $[MA]$  (black line:  $[MA] = 2.5 \times 10^7$  molecules cm<sup>-3</sup>, red line:  $[MA] = 2.5 \times 10^8$  molecules cm<sup>-3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



**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<sup>7</sup> molecules·cm<sup>-3</sup> and [SFA] = 10<sup>4</sup>, 10<sup>6</sup> and 10<sup>8</sup> molecules·cm<sup>-3</sup>.

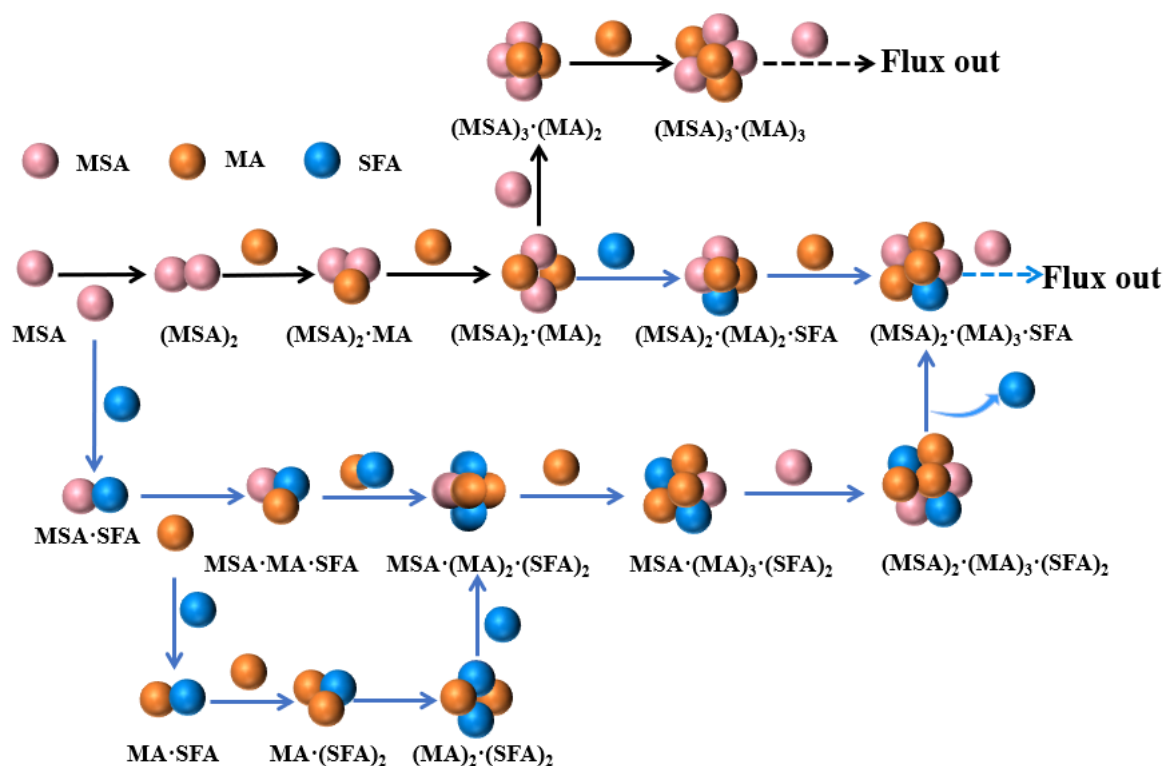


**Fig. S23** Main cluster formation mechanism of MSA-MA-SFA-based system at 238.15 K,  $[\text{MSA}] = 10^7$  molecules $\cdot\text{cm}^{-3}$ ,  $[\text{MA}] = 2.5 \times 10^8$  molecules $\cdot\text{cm}^{-3}$ , and  $[\text{SFA}] = 10^6$  molecules $\cdot\text{cm}^{-3}$ . The black arrows indicate the pure MSA-MA-based growth pathways. Blue arrows represent the pathways containing SFA



**Fig. S24** Main cluster formation mechanism of MSA-MA-SFA-based system at 258.15 K,  $[\text{MSA}] = 10^7$  molecules $\cdot\text{cm}^{-3}$ ,  $[\text{MA}] = 2.5 \times 10^8$  molecules $\cdot\text{cm}^{-3}$ , and  $[\text{SFA}] = 10^6$  molecules $\cdot\text{cm}^{-3}$ . The black arrows indicate the pure MSA-MA-based growth pathways. Blue arrows represent the pathways containing SFA





**Fig. S25** Main cluster formation mechanism of MSA-MA-SFA-based system at 298.15 K,  $[MSA] = 10^7$  molecules·cm<sup>-3</sup>,  $[MA] = 2.5 \times 10^8$  molecules·cm<sup>-3</sup>, and  $[SFA] = 10^6$  molecules·cm<sup>-3</sup>. The black arrows indicate the pure MSA-MA-based growth pathways. Blue arrows represent the pathways containing SFA

327 **Table S8** The Gibbs free energy for the formation of (SFA)<sub>x</sub>(MSA)<sub>y</sub>(MA)<sub>z</sub> ( $z \leq x + y \leq 3$ ) clusters  $\Delta G$  (kcal·mol<sup>-1</sup>)  
 328 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) <sup>a</sup>	-6.87	-7.56	-8.25
(MSA) <sub>2</sub>	-8.51 (-6.76) <sup>a</sup>	-9.27	-10.03	-10.79
(MSA) <sub>2</sub> ·MA	-21.17 (-20.36) <sup>a</sup>	-22.74	-24.31	-25.89
(MSA) <sub>2</sub> ·(MA) <sub>2</sub>	-34.05 (-34.97) <sup>a</sup>	-36.31	-38.59	-40.86
(MSA) <sub>3</sub>	-11.44 (-11.31) <sup>a</sup>	-13.06	-14.69	-16.32
(MSA) <sub>3</sub> ·MA	-30.29 (-31.68) <sup>a</sup>	-32.67	-35.06	-37.46
(MSA) <sub>3</sub> ·(MA) <sub>2</sub>	-46.76 (-46.45) <sup>a</sup>	-49.82	-52.90	-55.98
(MSA) <sub>3</sub> ·(MA) <sub>3</sub>	-59.17 (-59.33) <sup>a</sup>	-63.17	-67.19	-71.22
(SFA) <sub>2</sub>	-5.74(-5.76) <sup>b</sup>	-6.53	-7.32	-8.11
MA·SFA	-6.01	-6.73	-7.45	-8.17
(MA) <sub>2</sub> ·(SFA) <sub>2</sub>	-31.26	-33.53	-35.81	-38.09
MA·(SFA) <sub>2</sub>	-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) <sub>2</sub> ·SFA	-26.08	-28.48	-30.89	-33.31
(SFA) <sub>3</sub>	-11.87	-13.56	-15.27	-16.97
MSA <sub>2</sub> ·MA·SFA	-24.29	-26.66	-29.05	-31.44
(MSA) <sub>2</sub> ·(MA) <sub>2</sub> ·SFA	-44.62	-47.82	-51.03	-54.25
(MSA) <sub>2</sub> ·(MA) <sub>3</sub> ·SFA	-57.46	-61.43	-65.42	-69.41
MSA·(SFA) <sub>2</sub>	-12.26	-13.89	-15.52	-17.15
MA·(SFA) <sub>3</sub>	-29.46	-32.01	-34.57	-37.13
MSA·(MA) <sub>2</sub> ·(SFA) <sub>2</sub>	-45.12	-48.25	-51.39	-54.53
(MSA) <sub>2</sub> ·SFA	-9.11	-10.75	-12.40	-14.06
MSA·MA·(SFA) <sub>2</sub>	-31.11	-33.56	-36.01	-38.47
(MA) <sub>2</sub> ·(SFA) <sub>3</sub>	-44.04	-47.11	-50.19	-53.28
MSA·(MA) <sub>3</sub> ·(SFA) <sub>2</sub>	-62.91	-66.77	-70.63	-74.52
(MA) <sub>3</sub> ·(SFA) <sub>3</sub>	-53.82	-57.87	-61.94	-66.01

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

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

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

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

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

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

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

340 **Table S11** Total evaporation coefficients ( $\sum \gamma$ , s<sup>-1</sup>) for each cluster in the present study

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

**Table S12** Ratios ( $\beta \cdot C / \Sigma \gamma$ ) between monomer molecule collisions and evaporation coefficients for each cluster involving SFA in the present study ([MSA] =  $1.0 \times 10^7$  molecules·cm<sup>-3</sup>, [MA] =  $2.5 \times 10^7$  molecules·cm<sup>-3</sup>, [SFA] =  $1.0 \times 10^7$  molecules·cm<sup>-3</sup>)

		$(\beta \cdot C / \Sigma \gamma)$			
Clusters		298.15 K	278.15 K	258.15 K	238.15 K
Collision with MSA monomer: $C =$					
[MSA]					
MSA·MA		$1.05 \times 10^{-14}$	$7.21 \times 10^{-14}$	$6.72 \times 10^{-13}$	$9.19 \times 10^{-12}$
MSA·SFA		$1.32 \times 10^{-14}$	$9.71 \times 10^{-14}$	$9.81 \times 10^{-13}$	$1.48 \times 10^{-11}$
MA·SFA		$1.11 \times 10^{-15}$	$6.17 \times 10^{-15}$	$4.54 \times 10^{-14}$	$4.73 \times 10^{-13}$
(MSA) <sub>2</sub>		$8.82 \times 10^{-13}$	$9.11 \times 10^{-12}$	$1.36 \times 10^{-10}$	$3.25 \times 10^{-9}$
(SFA) <sub>2</sub>		$7.38 \times 10^{-15}$	$5.30 \times 10^{-14}$	$5.22 \times 10^{-13}$	$7.65 \times 10^{-12}$
(MSA) <sub>2</sub> ·MA		$3.58 \times 10^{-10}$	$6.77 \times 10^{-9}$	$2.04 \times 10^{-7}$	$1.09 \times 10^{-5}$
(MSA) <sub>2</sub> ·(MA) <sub>2</sub>		$6.48 \times 10^{-10}$	$1.01 \times 10^{-8}$	$2.46 \times 10^{-7}$	$1.03 \times 10^{-5}$
MA·(SFA) <sub>2</sub>		$2.10 \times 10^{-6}$	$6.92 \times 10^{-5}$	$3.94 \times 10^{-3}$	$4.43 \times 10^{-1}$
(MA) <sub>2</sub> ·(SFA) <sub>2</sub>		$6.52 \times 10^{-18}$	$2.45 \times 10^{-17}$	$1.15 \times 10^{-16}$	$7.09 \times 10^{-16}$
MSA·MA·SFA		$3.46 \times 10^{-10}$	$6.44 \times 10^{-9}$	$1.90 \times 10^{-7}$	$9.96 \times 10^{-6}$
MSA·(MA) <sub>2</sub> ·SFA		$3.45 \times 10^{-13}$	$3.86 \times 10^{-12}$	$6.36 \times 10^{-11}$	$1.69 \times 10^{-9}$
Collision with MA monomer: $C =$					
[MA]					
MSA·SFA		$6.85 \times 10^{-13}$	$5.04 \times 10^{-12}$	$5.09 \times 10^{-11}$	$7.69 \times 10^{-10}$
(MSA) <sub>2</sub>		$4.58 \times 10^{-11}$	$4.73 \times 10^{-10}$	$7.08 \times 10^{-9}$	$1.69 \times 10^{-7}$
(SFA) <sub>2</sub>		$3.83 \times 10^{-13}$	$2.75 \times 10^{-12}$	$2.71 \times 10^{-11}$	$3.97 \times 10^{-10}$
(MSA) <sub>2</sub> ·MA		$1.91 \times 10^{-8}$	$3.62 \times 10^{-7}$	$1.09 \times 10^{-5}$	$5.84 \times 10^{-4}$
MA·(SFA) <sub>2</sub>		$1.12 \times 10^{-4}$	$3.69 \times 10^{-3}$	$2.10 \times 10^{-1}$	$2.37 \times 10^1$
(MSA) <sub>2</sub> ·SFA		$1.16 \times 10^{-17}$	$5.02 \times 10^{-17}$	$2.75 \times 10^{-16}$	$2.01 \times 10^{-15}$
MSA·(SFA) <sub>2</sub>		$3.41 \times 10^{-15}$	$2.03 \times 10^{-14}$	$1.61 \times 10^{-13}$	$1.82 \times 10^{-12}$
(MSA) <sub>3</sub>		$2.76 \times 10^{-15}$	$1.76 \times 10^{-14}$	$1.50 \times 10^{-13}$	$1.87 \times 10^{-12}$
(SFA) <sub>3</sub>		$2.38 \times 10^{-19}$	$6.23 \times 10^{-19}$	$1.92 \times 10^{-18}$	$7.28 \times 10^{-18}$
(MSA) <sub>3</sub> ·MA		$1.10 \times 10^{-10}$	$1.35 \times 10^{-9}$	$2.49 \times 10^{-8}$	$7.59 \times 10^{-7}$
(MSA) <sub>3</sub> ·(MA) <sub>2</sub>		$4.69 \times 10^{-8}$	$8.68 \times 10^{-7}$	$2.55 \times 10^{-5}$	$1.34 \times 10^{-3}$
MA·(SFA) <sub>3</sub>		$3.88 \times 10^{-13}$	$4.63 \times 10^{-12}$	$8.16 \times 10^{-11}$	$2.36 \times 10^{-9}$
(MA) <sub>2</sub> ·(SFA) <sub>3</sub>		$5.06 \times 10^{-8}$	$9.16 \times 10^{-7}$	$2.60 \times 10^{-5}$	$1.28 \times 10^{-3}$
MSA·MA·SFA		$1.85 \times 10^{-8}$	$3.44 \times 10^{-7}$	$1.01 \times 10^{-5}$	$5.32 \times 10^{-4}$
(MSA) <sub>2</sub> ·MA·SFA		$1.12 \times 10^{-15}$	$5.80 \times 10^{-15}$	$3.91 \times 10^{-14}$	$3.67 \times 10^{-13}$
(MSA) <sub>2</sub> ·(MA) <sub>2</sub> ·SFA		$1.38 \times 10^{-9}$	$2.52 \times 10^{-8}$	$7.34 \times 10^{-7}$	$3.81 \times 10^{-5}$
MSA·MA·(SFA) <sub>2</sub>		$4.49 \times 10^{-12}$	$5.40 \times 10^{-11}$	$9.67 \times 10^{-10}$	$2.85 \times 10^{-8}$
MSA·(MA) <sub>2</sub> ·(SFA) <sub>2</sub>		$7.17 \times 10^{-8}$	$1.33 \times 10^{-6}$	$3.85 \times 10^{-5}$	$1.95 \times 10^{-3}$
Collision with SFA monomer: $C =$					
[SFA]					
MSA·MA		$9.60 \times 10^{-15}$	$6.58 \times 10^{-14}$	$6.13 \times 10^{-13}$	$8.38 \times 10^{-12}$
MSA·SFA		$1.21 \times 10^{-14}$	$8.89 \times 10^{-14}$	$8.98 \times 10^{-13}$	$1.36 \times 10^{-11}$



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

345

346 **Table S13** The formation rate  $J$  of MSA at the conditions of  $T = 238.15$  K,  $[\text{MSA}] = 10^6$ - $10^8$  molecules $\cdot\text{cm}^{-3}$ ,  $[\text{MA}] = 10^7$ - $10^{11}$  molecules $\cdot\text{cm}^{-3}$ , and  $[\text{SFA}] = 0, 10^8$ - $10^{12}$   
 347 molecules $\cdot\text{cm}^{-3}$ . 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] = $2.5 \times 10^7$	$3.54 \times 10^{-9}$	$4.80 \times 10^{-9}$	$1.62 \times 10^{-8}$	$1.30 \times 10^{-7}$	$1.22 \times 10^{-6}$	$8.69 \times 10^{-6}$
[MSA] = $10^5$	[MA] = $2.5 \times 10^8$	$4.27 \times 10^{-7}$	$5.34 \times 10^{-7}$	$1.49 \times 10^{-6}$	$1.10 \times 10^{-5}$	$1.02 \times 10^{-4}$	$7.26 \times 10^{-4}$
[MSA] = $10^5$	[MA] = $2.5 \times 10^9$	$3.47 \times 10^{-6}$	$4.21 \times 10^{-6}$	$1.08 \times 10^{-5}$	$7.60 \times 10^{-5}$	$6.78 \times 10^{-4}$	$5.23 \times 10^{-3}$
[MSA] = $10^6$	[MA] = $2.5 \times 10^7$	$3.48 \times 10^{-5}$	$3.61 \times 10^{-5}$	$4.71 \times 10^{-5}$	$1.58 \times 10^{-4}$	$1.22 \times 10^{-3}$	$8.64 \times 10^{-3}$
[MSA] = $10^6$	[MA] = $2.5 \times 10^8$	$4.19 \times 10^{-3}$	$4.29 \times 10^{-3}$	$5.22 \times 10^{-3}$	$1.45 \times 10^{-2}$	$1.04 \times 10^{-1}$	$7.20 \times 10^{-1}$
[MSA] = $10^6$	[MA] = $2.5 \times 10^9$	$3.40 \times 10^{-2}$	$3.47 \times 10^{-2}$	$4.11 \times 10^{-2}$	$1.04 \times 10^{-1}$	$6.90 \times 10^{-1}$	$5.14 \times 10^0$
[MSA] = $10^7$	[MA] = $2.5 \times 10^7$	$3.01 \times 10^{-1}$	$3.02 \times 10^{-1}$	$3.11 \times 10^{-1}$	$3.97 \times 10^{-1}$	$1.24 \times 10^0$	$8.08 \times 10^0$
[MSA] = $10^7$	[MA] = $2.5 \times 10^8$	$3.47 \times 10^1$	$3.48 \times 10^1$	$3.55 \times 10^1$	$4.28 \times 10^1$	$1.14 \times 10^2$	$6.53 \times 10^2$
[MSA] = $10^7$	[MA] = $2.5 \times 10^9$	$2.72 \times 10^2$	$2.73 \times 10^2$	$2.78 \times 10^2$	$3.26 \times 10^2$	$7.74 \times 10^2$	$4.31 \times 10^3$
[MSA] = $10^8$	[MA] = $2.5 \times 10^7$	$1.14 \times 10^3$	$1.14 \times 10^3$	$1.14 \times 10^3$	$1.17 \times 10^3$	$1.44 \times 10^3$	$4.98 \times 10^3$
[MSA] = $10^8$	[MA] = $2.5 \times 10^8$	$9.01 \times 10^4$	$9.01 \times 10^4$	$9.02 \times 10^4$	$9.19 \times 10^4$	$1.08 \times 10^5$	$2.64 \times 10^5$
[MSA] = $10^8$	[MA] = $2.5 \times 10^9$	$5.34 \times 10^5$	$5.34 \times 10^5$	$5.35 \times 10^5$	$5.42 \times 10^5$	$6.12 \times 10^5$	$1.23 \times 10^6$
[MSA] = $10^9$	[MA] = $2.5 \times 10^7$	$6.99 \times 10^5$	$6.99 \times 10^5$	$7.00 \times 10^5$	$7.02 \times 10^5$	$7.30 \times 10^5$	$9.89 \times 10^5$
[MSA] = $10^9$	[MA] = $2.5 \times 10^8$	$1.66 \times 10^7$	$1.66 \times 10^7$	$1.66 \times 10^7$	$1.67 \times 10^7$	$1.69 \times 10^7$	$1.97 \times 10^7$
[MSA] = $10^9$	[MA] = $2.5 \times 10^9$	$9.54 \times 10^7$	$9.54 \times 10^7$	$9.54 \times 10^7$	$9.55 \times 10^7$	$9.65 \times 10^7$	$1.06 \times 10^8$

348

349 **Table S14** The formation rate  $J$  of MSA at the conditions of  $T = 258.15$  K,  $[\text{MSA}] = 10^6$ - $10^8$  molecules $\cdot\text{cm}^{-3}$ ,  $[\text{MA}] = 10^7$ - $10^{11}$  molecules $\cdot\text{cm}^{-3}$ , and  $[\text{SFA}] = 0, 10^8$ - $10^{12}$   
350 molecules $\cdot\text{cm}^{-3}$ . 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] = $2.5 \times 10^7$	$2.63 \times 10^{-12}$	$5.59 \times 10^{-12}$	$3.22 \times 10^{-11}$	$2.98 \times 10^{-10}$	$2.96 \times 10^{-9}$	$2.43 \times 10^{-8}$
[MSA] = $10^5$	[MA] = $2.5 \times 10^8$	$9.62 \times 10^{-10}$	$1.87 \times 10^{-9}$	$1.00 \times 10^{-8}$	$9.19 \times 10^{-8}$	$9.18 \times 10^{-7}$	$7.97 \times 10^{-6}$
[MSA] = $10^5$	[MA] = $2.5 \times 10^9$	$1.02 \times 10^{-7}$	$1.47 \times 10^{-7}$	$5.60 \times 10^{-7}$	$4.68 \times 10^{-6}$	$4.48 \times 10^{-5}$	$3.31 \times 10^{-4}$
[MSA] = $10^6$	[MA] = $2.5 \times 10^7$	$2.61 \times 10^{-8}$	$2.90 \times 10^{-8}$	$5.52 \times 10^{-8}$	$3.17 \times 10^{-7}$	$2.93 \times 10^{-6}$	$2.40 \times 10^{-5}$
[MSA] = $10^6$	[MA] = $2.5 \times 10^8$	$9.54 \times 10^{-6}$	$1.04 \times 10^{-5}$	$1.84 \times 10^{-5}$	$9.88 \times 10^{-5}$	$9.10 \times 10^{-4}$	$7.86 \times 10^{-3}$
[MSA] = $10^6$	[MA] = $2.5 \times 10^9$	$1.00 \times 10^{-3}$	$1.05 \times 10^{-3}$	$1.45 \times 10^{-3}$	$5.49 \times 10^{-3}$	$4.48 \times 10^{-2}$	$3.28 \times 10^{-1}$
[MSA] = $10^7$	[MA] = $2.5 \times 10^7$	$2.44 \times 10^{-4}$	$2.47 \times 10^{-4}$	$2.69 \times 10^{-4}$	$4.93 \times 10^{-4}$	$2.73 \times 10^{-3}$	$2.12 \times 10^{-2}$
[MSA] = $10^7$	[MA] = $2.5 \times 10^8$	$8.75 \times 10^{-2}$	$8.83 \times 10^{-2}$	$9.50 \times 10^{-2}$	$1.63 \times 10^{-1}$	$8.47 \times 10^{-1}$	$6.90 \times 10^0$
[MSA] = $10^7$	[MA] = $2.5 \times 10^9$	$8.89 \times 10^0$	$8.92 \times 10^0$	$9.26 \times 10^0$	$1.26 \times 10^1$	$4.53 \times 10^1$	$2.94 \times 10^2$
[MSA] = $10^8$	[MA] = $2.5 \times 10^7$	$1.52 \times 10^0$	$1.52 \times 10^0$	$1.53 \times 10^0$	$1.61 \times 10^0$	$2.41 \times 10^0$	$9.90 \times 10^0$
[MSA] = $10^8$	[MA] = $2.5 \times 10^8$	$4.80 \times 10^2$	$4.80 \times 10^2$	$4.83 \times 10^2$	$5.06 \times 10^2$	$7.41 \times 10^2$	$3.17 \times 10^3$
[MSA] = $10^8$	[MA] = $2.5 \times 10^9$	$3.46 \times 10^4$	$3.46 \times 10^4$	$3.47 \times 10^4$	$3.57 \times 10^4$	$4.52 \times 10^4$	$1.35 \times 10^5$
[MSA] = $10^9$	[MA] = $2.5 \times 10^7$	$4.61 \times 10^3$	$4.61 \times 10^3$	$4.61 \times 10^3$	$4.63 \times 10^3$	$4.83 \times 10^3$	$6.79 \times 10^3$
[MSA] = $10^9$	[MA] = $2.5 \times 10^8$	$6.06 \times 10^5$	$6.06 \times 10^5$	$6.06 \times 10^5$	$6.09 \times 10^5$	$6.32 \times 10^5$	$8.51 \times 10^5$
[MSA] = $10^9$	[MA] = $2.5 \times 10^9$	$1.32 \times 10^7$	$1.32 \times 10^7$	$1.32 \times 10^7$	$1.33 \times 10^7$	$1.36 \times 10^7$	$1.69 \times 10^7$

351

352 **Table S15** The formation rate  $J$  of MSA at the conditions of  $T = 278.15$  K,  $[\text{MSA}] = 10^6$ - $10^8$  molecules $\cdot\text{cm}^{-3}$ ,  $[\text{MA}] = 10^7$ - $10^{11}$  molecules $\cdot\text{cm}^{-3}$ , and  $[\text{SFA}] = 0, 10^8$ - $10^{12}$   
 353 molecules $\cdot\text{cm}^{-3}$ . 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] = $2.5 \times 10^7$	$1.68 \times 10^{-17}$	$3.26 \times 10^{-17}$	$1.75 \times 10^{-16}$	$1.60 \times 10^{-15}$	$1.59 \times 10^{-14}$	$1.65 \times 10^{-13}$
[MSA] = $10^5$	[MA] = $2.5 \times 10^8$	$1.67 \times 10^{-14}$	$3.21 \times 10^{-14}$	$1.71 \times 10^{-13}$	$1.56 \times 10^{-12}$	$1.54 \times 10^{-11}$	$1.56 \times 10^{-10}$
[MSA] = $10^5$	[MA] = $2.5 \times 10^9$	$1.53 \times 10^{-11}$	$2.74 \times 10^{-11}$	$1.36 \times 10^{-10}$	$1.22 \times 10^{-9}$	$1.21 \times 10^{-8}$	$1.22 \times 10^{-7}$
[MSA] = $10^6$	[MA] = $2.5 \times 10^7$	$1.68 \times 10^{-13}$	$1.84 \times 10^{-13}$	$3.26 \times 10^{-13}$	$1.75 \times 10^{-12}$	$1.60 \times 10^{-11}$	$1.65 \times 10^{-10}$
[MSA] = $10^6$	[MA] = $2.5 \times 10^8$	$1.67 \times 10^{-10}$	$1.82 \times 10^{-10}$	$3.21 \times 10^{-10}$	$1.71 \times 10^{-9}$	$1.56 \times 10^{-8}$	$1.57 \times 10^{-7}$
[MSA] = $10^6$	[MA] = $2.5 \times 10^9$	$1.53 \times 10^{-7}$	$1.65 \times 10^{-7}$	$2.74 \times 10^{-7}$	$1.36 \times 10^{-6}$	$1.22 \times 10^{-5}$	$1.22 \times 10^{-4}$
[MSA] = $10^7$	[MA] = $2.5 \times 10^7$	$1.68 \times 10^{-9}$	$1.70 \times 10^{-9}$	$1.84 \times 10^{-9}$	$3.25 \times 10^{-9}$	$1.74 \times 10^{-8}$	$1.67 \times 10^{-7}$
[MSA] = $10^7$	[MA] = $2.5 \times 10^8$	$1.67 \times 10^{-6}$	$1.69 \times 10^{-6}$	$1.82 \times 10^{-6}$	$3.19 \times 10^{-6}$	$1.69 \times 10^{-5}$	$1.57 \times 10^{-4}$
[MSA] = $10^7$	[MA] = $2.5 \times 10^9$	$1.53 \times 10^{-3}$	$1.54 \times 10^{-3}$	$1.65 \times 10^{-3}$	$2.72 \times 10^{-3}$	$1.34 \times 10^{-2}$	$1.22 \times 10^{-1}$
[MSA] = $10^8$	[MA] = $2.5 \times 10^7$	$1.69 \times 10^{-5}$	$1.69 \times 10^{-5}$	$1.70 \times 10^{-5}$	$1.83 \times 10^{-5}$	$3.12 \times 10^{-5}$	$1.72 \times 10^{-4}$
[MSA] = $10^8$	[MA] = $2.5 \times 10^8$	$1.68 \times 10^{-2}$	$1.68 \times 10^{-2}$	$1.69 \times 10^{-2}$	$1.82 \times 10^{-2}$	$3.07 \times 10^{-2}$	$1.62 \times 10^{-1}$
[MSA] = $10^8$	[MA] = $2.5 \times 10^9$	$1.54 \times 10^1$	$1.54 \times 10^1$	$1.55 \times 10^1$	$1.64 \times 10^1$	$2.59 \times 10^1$	$1.22 \times 10^2$
[MSA] = $10^9$	[MA] = $2.5 \times 10^7$	$1.75 \times 10^{-1}$	$1.75 \times 10^{-1}$	$1.75 \times 10^{-1}$	$1.76 \times 10^{-1}$	$1.84 \times 10^{-1}$	$2.72 \times 10^{-1}$
[MSA] = $10^9$	[MA] = $2.5 \times 10^8$	$1.78 \times 10^2$	$1.78 \times 10^2$	$1.78 \times 10^2$	$1.79 \times 10^2$	$1.86 \times 10^2$	$2.68 \times 10^2$
[MSA] = $10^9$	[MA] = $2.5 \times 10^9$	$1.30 \times 10^5$	$1.30 \times 10^5$	$1.30 \times 10^5$	$1.31 \times 10^5$	$1.34 \times 10^5$	$1.73 \times 10^5$

354

355 **Table S16** The formation rate  $J$  of MSA at the conditions of  $T = 298.15$  K,  $[\text{MSA}] = 10^6$ - $10^8$  molecules $\cdot\text{cm}^{-3}$ ,  $[\text{MA}] = 10^7$ - $10^{11}$  molecules $\cdot\text{cm}^{-3}$ , and  $[\text{SFA}] = 0, 10^8$ - $10^{12}$   
 356 molecules $\cdot\text{cm}^{-3}$ . 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] = $2.5 \times 10^7$	$2.62 \times 10^{-23}$	$4.79 \times 10^{-23}$	$2.43 \times 10^{-22}$	$2.20 \times 10^{-21}$	$2.21 \times 10^{-20}$	$2.58 \times 10^{-19}$
[MSA] = $10^5$	[MA] = $2.5 \times 10^8$	$2.62 \times 10^{-20}$	$4.79 \times 10^{-20}$	$2.43 \times 10^{-19}$	$2.20 \times 10^{-18}$	$2.20 \times 10^{-17}$	$2.52 \times 10^{-16}$
[MSA] = $10^5$	[MA] = $2.5 \times 10^9$	$2.68 \times 10^{-17}$	$4.85 \times 10^{-17}$	$2.44 \times 10^{-16}$	$2.20 \times 10^{-15}$	$2.18 \times 10^{-14}$	$2.31 \times 10^{-13}$
[MSA] = $10^6$	[MA] = $2.5 \times 10^7$	$2.62 \times 10^{-19}$	$2.83 \times 10^{-19}$	$4.79 \times 10^{-19}$	$2.44 \times 10^{-18}$	$2.23 \times 10^{-17}$	$2.58 \times 10^{-16}$
[MSA] = $10^6$	[MA] = $2.5 \times 10^8$	$2.62 \times 10^{-16}$	$2.84 \times 10^{-16}$	$4.79 \times 10^{-16}$	$2.44 \times 10^{-15}$	$2.23 \times 10^{-14}$	$2.52 \times 10^{-13}$
[MSA] = $10^6$	[MA] = $2.5 \times 10^9$	$2.68 \times 10^{-13}$	$2.90 \times 10^{-13}$	$4.85 \times 10^{-13}$	$2.44 \times 10^{-12}$	$2.21 \times 10^{-11}$	$2.31 \times 10^{-10}$
[MSA] = $10^7$	[MA] = $2.5 \times 10^7$	$2.62 \times 10^{-15}$	$2.64 \times 10^{-15}$	$2.83 \times 10^{-15}$	$4.79 \times 10^{-15}$	$2.46 \times 10^{-14}$	$2.58 \times 10^{-13}$
[MSA] = $10^7$	[MA] = $2.5 \times 10^8$	$2.62 \times 10^{-12}$	$2.64 \times 10^{-12}$	$2.84 \times 10^{-12}$	$4.79 \times 10^{-12}$	$2.46 \times 10^{-11}$	$2.52 \times 10^{-10}$
[MSA] = $10^7$	[MA] = $2.5 \times 10^9$	$2.68 \times 10^{-9}$	$2.71 \times 10^{-9}$	$2.90 \times 10^{-9}$	$4.85 \times 10^{-9}$	$2.45 \times 10^{-8}$	$2.32 \times 10^{-7}$
[MSA] = $10^8$	[MA] = $2.5 \times 10^7$	$2.62 \times 10^{-11}$	$2.62 \times 10^{-11}$	$2.64 \times 10^{-11}$	$2.84 \times 10^{-11}$	$4.80 \times 10^{-11}$	$2.71 \times 10^{-10}$
[MSA] = $10^8$	[MA] = $2.5 \times 10^8$	$2.63 \times 10^{-8}$	$2.63 \times 10^{-8}$	$2.65 \times 10^{-8}$	$2.84 \times 10^{-8}$	$4.81 \times 10^{-8}$	$2.66 \times 10^{-7}$
[MSA] = $10^8$	[MA] = $2.5 \times 10^9$	$2.69 \times 10^{-5}$	$2.69 \times 10^{-5}$	$2.71 \times 10^{-5}$	$2.90 \times 10^{-5}$	$4.85 \times 10^{-5}$	$2.52 \times 10^{-4}$
[MSA] = $10^9$	[MA] = $2.5 \times 10^7$	$2.65 \times 10^{-7}$	$2.65 \times 10^{-7}$	$2.65 \times 10^{-7}$	$2.67 \times 10^{-7}$	$2.86 \times 10^{-7}$	$4.84 \times 10^{-7}$
[MSA] = $10^9$	[MA] = $2.5 \times 10^8$	$2.66 \times 10^{-4}$	$2.66 \times 10^{-4}$	$2.66 \times 10^{-4}$	$2.68 \times 10^{-4}$	$2.87 \times 10^{-4}$	$4.83 \times 10^{-4}$
[MSA] = $10^9$	[MA] = $2.5 \times 10^9$	$2.73 \times 10^{-1}$	$2.73 \times 10^{-1}$	$2.73 \times 10^{-1}$	$2.75 \times 10^{-1}$	$2.94 \times 10^{-1}$	$4.85 \times 10^{-1}$

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**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

**MA:**

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

**SFA:**

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

**(MSA)<sub>1</sub>·(MA)<sub>1</sub>:**

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

366

367 (MSA)<sub>1</sub>·(SFA)<sub>1</sub>:

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

368

369 (MSA)<sub>1</sub>·(SFA)<sub>1</sub>·(MA)<sub>1</sub>:

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

370

371 (MSA)<sub>1</sub>·(SFA)<sub>1</sub>·(MA)<sub>2</sub>:

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

372

373 (MSA)<sub>1</sub>·(SFA)<sub>2</sub>:

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

374

375 (MSA)<sub>1</sub>·(SFA)<sub>2</sub>·(MA)<sub>1</sub>:

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

376

377

(MSA)<sub>1</sub>·(SFA)<sub>2</sub>·(MA)<sub>2</sub>:

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

378

379 (MSA)<sub>1</sub>·(SFA)<sub>2</sub>·(MA)<sub>3</sub>:

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

380

381 (SFA)<sub>1</sub>·(MA)<sub>1</sub>:

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

382

383 (MSA)<sub>2</sub>:

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

384

385 (MSA)<sub>2</sub>·(MA)<sub>1</sub>:

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

386

387 **(MSA)<sub>2</sub>·(SFA)<sub>1</sub>:**

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

388

389 **(MSA)<sub>2</sub>·(SFA)<sub>1</sub>·(MA)<sub>1</sub>:**

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

390

391 (MSA)<sub>2</sub>·(SFA)<sub>1</sub>·(MA)<sub>2</sub>:

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

392

393 (MSA)<sub>2</sub>·(SFA)<sub>1</sub>·(MA)<sub>3</sub>:

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

394

395 (MSA)<sub>2</sub>·(MA)<sub>2</sub>:

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

396

397 (SFA)<sub>2</sub>:

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

398 (SFA)<sub>2</sub>·(MA)<sub>1</sub>:

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

399

400

**(SFA)<sub>2</sub>·(MA)<sub>2</sub>:**

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

401

402 (MSA)<sub>3</sub>:

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

403

(MSA)<sub>3</sub>·(MA)<sub>1</sub>:

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

404

405

(MSA)<sub>3</sub>·(MA)<sub>2</sub>:

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

406

407 (MSA)<sub>3</sub>·(MA)<sub>3</sub>:

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

408

409 (SFA)<sub>3</sub>:

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

410

411 (SFA)<sub>3</sub>·(MA)<sub>1</sub>:

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

412

413

**(SFA)<sub>3</sub>·(MA)<sub>2</sub>:**

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

414

415 (SFA)<sub>3</sub>·(MA)<sub>3</sub>:

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