

# Supporting information

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## Enhancing SO<sub>3</sub> Hydrolysis and Nucleation: The Role of Formic Sulfuric Anhydride

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S.NO	Caption
S1	<b>Fig. S1</b> The optimized geometries of SO <sub>3</sub> and HCOOH, especially the main bond lengths and bond angles at two different theoretical levels. <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. <sup>c</sup> The values in parentheses are the experimental values. Bond length is in angstrom and angle is in degree.
S2	<b>Fig. S2.</b> BOMD simulation trajectories and snapshots of the FSA-assisted SO <sub>3</sub> hydrolysis reaction
S3	<b>Fig. S3.</b> Energy diagrams for H <sub>2</sub> SO <sub>4</sub> formation from the SO <sub>3</sub> + H <sub>2</sub> O reaction with and without H <sub>2</sub> O at the CCSD(T)-F12/cc-pVDZ-F12/M06-2X/6-311++G(2df,2pd) level of theory
S4	<b>Fig. S4.</b> Energy diagrams for SO <sub>3</sub> hydrolysis with HNO <sub>3</sub> (a), HCOOH (b) and H <sub>2</sub> SO <sub>4</sub> (c) at the CCSD(T)-F12/cc-pVDZ-F12/M06-2X/6-311+G(2df,2pd) level of theory
S4-S5	<b>Table S1.</b> Relative energies ( $\Delta E$ and $\Delta(E + ZPE)$ ), enthalpies ( $\Delta H$ ), entropy (S) and free energies ( $\Delta G$ ) for reactants, intermediates, transition states, and products in the SO <sub>3</sub> + H <sub>2</sub> SO <sub>4</sub> reaction, with and without H <sub>2</sub> O, and the SO <sub>3</sub> hydrolysis reaction, with and without H <sub>2</sub> O and H <sub>2</sub> SO <sub>4</sub> (units: kcal·mol <sup>-1</sup> for $\Delta E$ , $\Delta(E + ZPE)$ , $\Delta H$ , and $\Delta G$ ; kcal·mol <sup>-1</sup> ·K <sup>-1</sup> for S)
S6	<b>Fig. S5.</b> ESP-mapped van der Waals surface of HNO <sub>3</sub> (NA), H <sub>2</sub> SO <sub>4</sub> (SA), HCOOH (FA), (COOH) <sub>2</sub> (OA) and HCOOSO <sub>3</sub> H (FSA)
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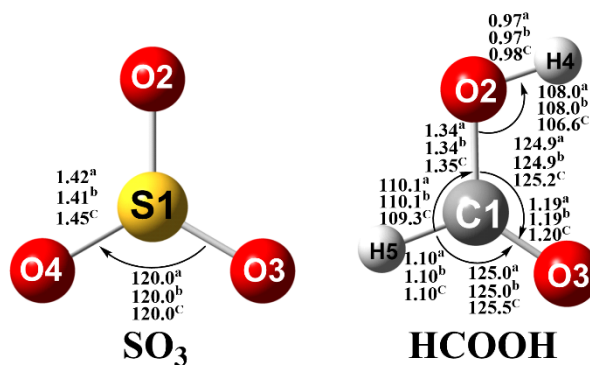
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	H <sub>2</sub> SO <sub>4</sub> , H <sub>2</sub> SO <sub>4</sub> ···H <sub>2</sub> O and (H <sub>2</sub> SO <sub>4</sub> ) <sub>2</sub> ), calculated using the master equation within the temperature range of 280-320 K
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S16	<b>Fig. S8.</b> Snapshot structures from BOMD simulations of the FSA reaction at the air-water interface. White, red, yellow and blue spheres represent H, O, S, and C atoms, respectively
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S32	<b>Table S12.</b> Formation rate ( <i>J</i> , s <sup>-1</sup> ) of FSA at <i>T</i> = 298.15 K with [SA] = 10 <sup>4</sup> - 10 <sup>8</sup> molecules·cm <sup>-3</sup> , [A] = 10 <sup>7</sup> - 10 <sup>11</sup> molecules·cm <sup>-3</sup> , and [FSA] = 10 <sup>3</sup> - 10 <sup>7</sup> molecules·cm <sup>-3</sup> .
S33	<b>Table S13.</b> Formation rate <i>J</i> (s <sup>-1</sup> ) of FSA at <i>T</i> = 278.15 K with [SA] = 10 <sup>4</sup> - 10 <sup>8</sup> molecules·cm <sup>-3</sup> , [A] = 10 <sup>7</sup> - 10 <sup>11</sup> molecules·cm <sup>-3</sup> , and [FSA] = 10 <sup>3</sup> - 10 <sup>7</sup> molecules·cm <sup>-3</sup>
S34	<b>Table S14.</b> Formation rate <i>J</i> (s <sup>-1</sup> ) of FSA at <i>T</i> = 258.15 K with [SA] = 10 <sup>4</sup> - 10 <sup>8</sup> molecules·cm <sup>-3</sup> , [A] = 10 <sup>7</sup> - 10 <sup>11</sup> molecules·cm <sup>-3</sup> , and [FSA] = 10 <sup>3</sup> - 10 <sup>7</sup> molecules·cm <sup>-3</sup>

S35	<b>Fig. S14.</b> (a) Cluster formation rate ( $J$ , $\text{cm}^{-3} \text{s}^{-1}$ ) with $[\text{SA}] = 10^4 \text{ molecules}\cdot\text{cm}^{-3}$ , $[\text{A}] = 10^7 \text{ molecules}\cdot\text{cm}^{-3}$ at three temperatures, (b) Cluster formation rate ( $J$ , $\text{cm}^{-3} \text{s}^{-1}$ ) with $[\text{SA}] = 10^8 \text{ molecules}\cdot\text{cm}^{-3}$ , $[\text{A}] = 10^{11} \text{ molecules}\cdot\text{cm}^{-3}$ at three temperatures (black: 258.15 K, red: 278.15 K, blue: 298.15 K)
S36	<b>Fig. S15.</b> (a) Cluster formation rate ( $J$ , $\text{cm}^{-3} \text{s}^{-1}$ ) and (b) enhancement factor ( $R$ ) as a function of $[\text{A}]$ with $[\text{FSA}] = 10^6 \text{ molecules}\cdot\text{cm}^{-3}$ and five different $[\text{SA}]$ concentrations (black: $[\text{SA}] = 10^4 \text{ molecules}\cdot\text{cm}^{-3}$ , red: $[\text{SA}] = 10^5 \text{ molecules}\cdot\text{cm}^{-3}$ , blue: $[\text{SA}] = 10^6 \text{ molecules}\cdot\text{cm}^{-3}$ , green: $[\text{SA}] = 10^7 \text{ molecules}\cdot\text{cm}^{-3}$ , purple: $[\text{SA}] = 10^8 \text{ molecules}\cdot\text{cm}^{-3}$ ) at 258.15 K
S37	<b>Fig. S16.</b> (a) Cluster formation rate ( $J$ , $\text{cm}^{-3} \text{s}^{-1}$ ) and (b) enhancement factor ( $R$ ) as a function of $[\text{A}]$ with $[\text{FSA}] = 10^6 \text{ molecules}\cdot\text{cm}^{-3}$ and five different $[\text{SA}]$ concentrations (black: $[\text{SA}] = 10^4 \text{ molecules}\cdot\text{cm}^{-3}$ , red: $[\text{SA}] = 10^5 \text{ molecules}\cdot\text{cm}^{-3}$ , blue: $[\text{SA}] = 10^6 \text{ molecules}\cdot\text{cm}^{-3}$ , green: $[\text{SA}] = 10^7 \text{ molecules}\cdot\text{cm}^{-3}$ , purple: $[\text{SA}] = 10^8 \text{ molecules}\cdot\text{cm}^{-3}$ ) at 298.15 K
S38	<b>Fig. S17.</b> Main pathways of clusters growth under conditions of $T = 258.15 \text{ K}$ , $[\text{SA}] = 10^6 \text{ molecules}\cdot\text{cm}^{-3}$ , $[\text{A}] = 10^9 \text{ molecules}\cdot\text{cm}^{-3}$ , and $[\text{FSA}] = 10^3\text{-}10^7 \text{ molecules}\cdot\text{cm}^{-3}$ . Blue and orange fluxes represent the pathways of the SA-A-based and SA-A-FSA-based cluster, respectively
S39	<b>Fig. S18.</b> Main pathways of clusters growth under conditions of $T = 298.15 \text{ K}$ , $[\text{SA}] = 10^6 \text{ molecules}\cdot\text{cm}^{-3}$ , $[\text{A}] = 10^9 \text{ molecules}\cdot\text{cm}^{-3}$ , and $[\text{FSA}] = 10^3\text{-}10^7 \text{ molecules}\cdot\text{cm}^{-3}$ . The blue and orange fluxes represent the pathways of the SA-A-based and SA-A-FSA-based cluster, respectively
S40-S58	<b>Table S15.</b> Cartesian coordinates of all molecules and clusters in this study

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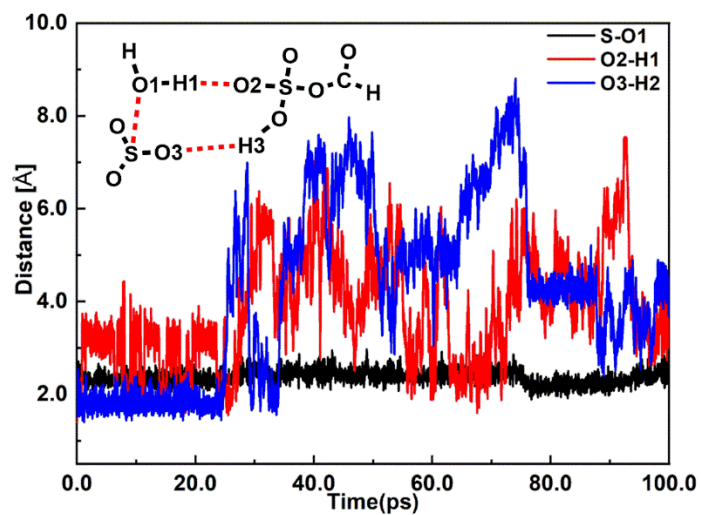


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18 **Fig. S1** The optimized geometries of SO<sub>3</sub> and HCOOH, especially the main bond lengths and bond angles at two  
 19 different theoretical levels. <sup>a</sup> The values obtained at the M06-2X/6-311++G(2df,2pd) level of theory. <sup>b</sup> The values  
 20 obtained at the M06-2X/6-311++G(3df,3pd) level of theory. <sup>c</sup> The values in parentheses are the experimental values.  
 21 Bond length is in angstrom and angle is in degree.

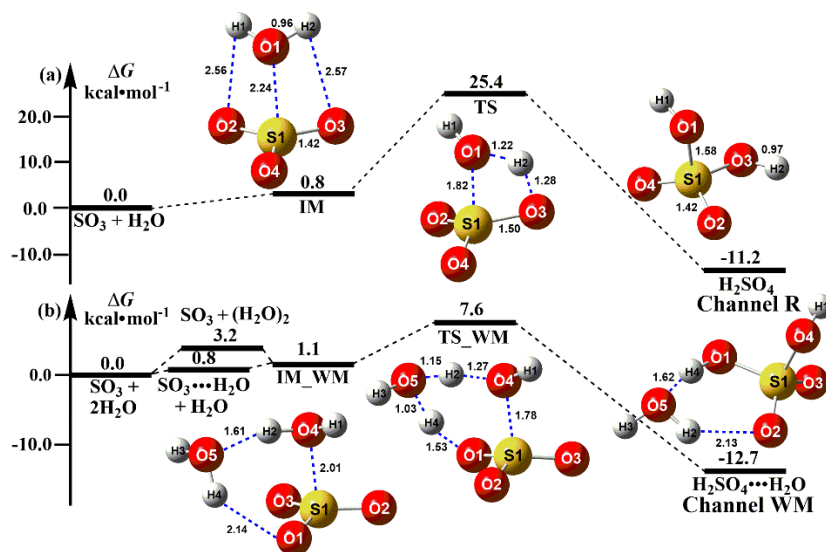
22 The geometric parameters of the SO<sub>3</sub> and HCOOH reactants, calculated at the M06-2X/6-311++G(2df,2pd)  
 23 level, are presented in Fig. S1. As seen in Fig. S1, the mean absolute deviations between the calculated bond  
 24 distances and bond angles at the M06-2X/6-311++G(2df,2pd) level and the experimental data are 0.01 Å and 0.60°,  
 25 respectively. This reveals that the calculated bond distances and bond angles at the M06-2X/6-311++G(2df,2pd)  
 26 level are consistent with the available experimental data (From the NIST chemistry webbook,  
 27 <http://webbook.nist.gov/chemistry>). Besides, the bond lengths and angles obtained from the M06-2X/6-  
 28 311++G(2df,2pd) level are close to the values calculated at the M06-2X/6-311++G(3df,3pd) level (Fig. S1). Thus,  
 29 the 6-311++G(2df,2pd) basis set was selected for all M06-2X calculations, as it provides an optimal balance between  
 30 accuracy and computational efficiency when compared to the 6-311++G(3df,3pd).

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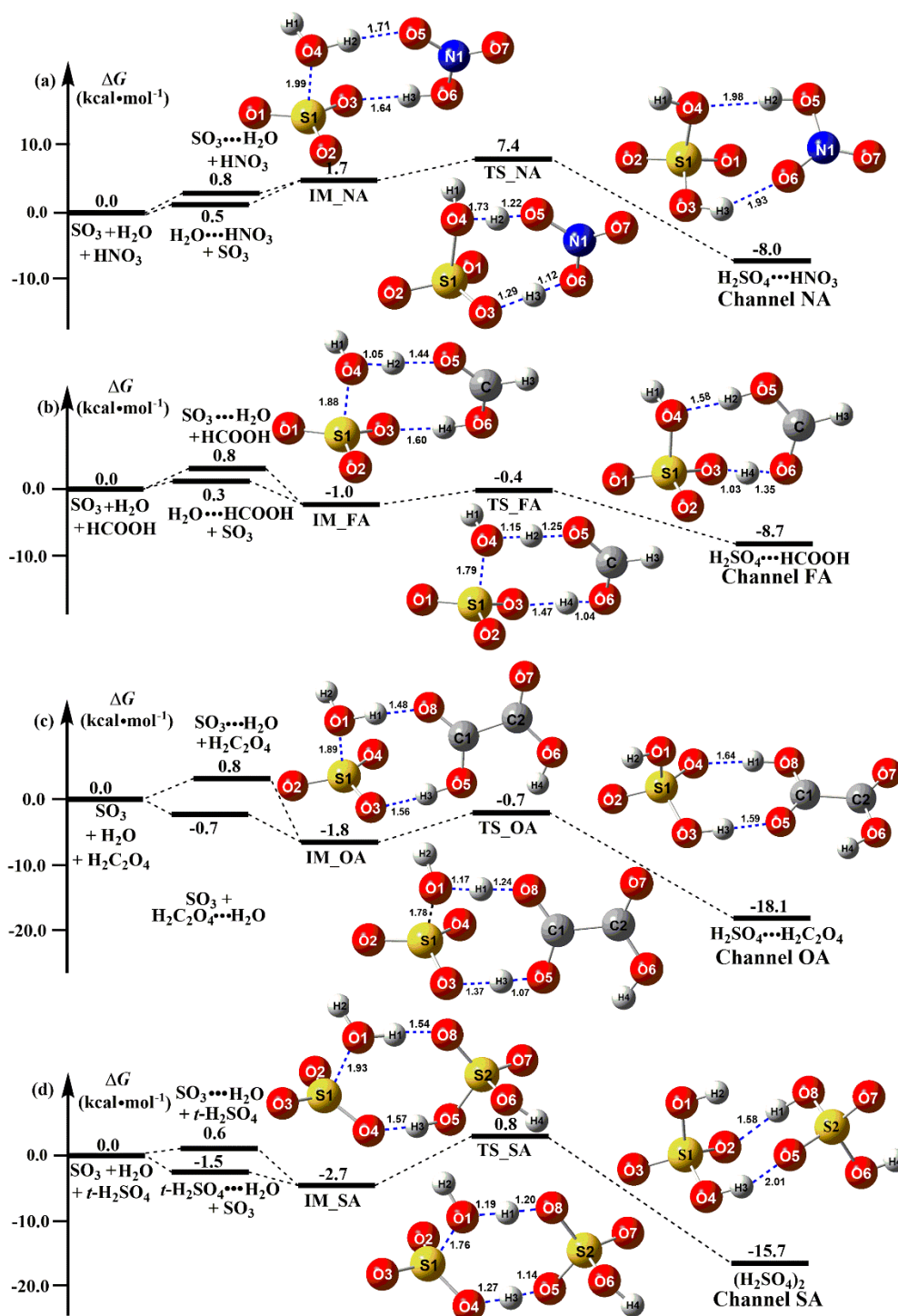


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33 **Fig. S2.** BOMD simulation trajectories and snapshots of the FSA-assisted  $\text{SO}_3$  hydrolysis reaction



**Fig. S3.** Energy diagrams for H<sub>2</sub>SO<sub>4</sub> formation from the SO<sub>3</sub> + H<sub>2</sub>O reaction with and without H<sub>2</sub>O at the CCSD(T)-F12/cc-pVDZ-F12//M06-2X/6-311++G(2df,2pd) level of theory



**Fig. S4.** Energy diagrams for SO<sub>3</sub> hydrolysis with HNO<sub>3</sub> (a), HCOOH (b) and H<sub>2</sub>SO<sub>4</sub> (c) at the CCSD(T)-F12/cc-pVDZ-F12//M06-2X/6-311+G(2df,2pd) level of theory

40 **Table S1.** Relative energies ( $\Delta E$  and  $\Delta(E + \text{ZPE})$ ), enthalpies ( $\Delta H$ ), entropy (S) and free energies ( $\Delta G$ ) for reactants,  
 41 intermediates, transition states, and products in the  $\text{SO}_3 + \text{H}_2\text{SO}_4$  reaction, with and without  $\text{H}_2\text{O}$ , and the  $\text{SO}_3$   
 42 hydrolysis reaction, with and without  $\text{H}_2\text{O}$  and  $\text{H}_2\text{SO}_4$  (units:  $\text{kcal}\cdot\text{mol}^{-1}$  for  $\Delta E$ ,  $\Delta(E + \text{ZPE})$ ,  $\Delta H$ , and  $\Delta G$ ;  $\text{kcal}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$  for S)  
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<i>Species</i>	ZPE	$\Delta E$	S	$\Delta G$	$\Delta(E+\text{ZPE})$	$\Delta H$
$\text{SO}_3 + \text{H}_2\text{O} + \text{FSA}$	52.9	0.0	188.3	0.0	0.0	0.0
$\text{SO}_3\cdots\text{H}_2\text{O} + \text{FSA}$	24.0	-9.4	77.9	0.8(0.33) <sup>a</sup>	-7.0	-7.6
$\text{SO}_3 + \text{FSA}\cdots\text{H}_2\text{O}$	47.1	-12.7	95.6	-1.8	-10.4	-11.2
IM	56.9	-26.4	115.3	-2.0	-22.4	-23.7
TS	53.7	-21.6	110.4	0.5	-20.7	-22.7
$\text{H}_2\text{SO}_4\cdots\text{FSA}$	57.4	-37.1	118.1	-12.9	-32.6	-33.8
$\text{SO}_3 + \text{H}_2\text{O}$	21.6	0.0	106.2	0.0	0.0	0.0
$\text{SO}_3\cdots\text{H}_2\text{O}$	24.0	-9.4	77.9	0.8(0.33) <sup>a</sup> (0.62) <sup>b</sup>	-7.0	-7.6
$\text{TS}_{\text{SA}}$	22.3	15.7	70.4	25.4 (25.7) <sup>a</sup>	16.4	14.7
$\text{H}_2\text{SO}_4$	25.2	-23.6	71.8	-11.2(-10.72) <sup>a</sup>	-20.0	-21.4
$\text{SO}_3 + \text{H}_2\text{O} + \text{H}_2\text{O}$	35.2	0.0	151.3	0.0	0.0	0.0
$\text{SO}_3\cdots\text{H}_2\text{O} + \text{H}_2\text{O}$	24.0	-9.4	77.9	0.8(0.33) <sup>a</sup> (0.62) <sup>b</sup>	-7.0	-7.6
$\text{SO}_3 + (\text{H}_2\text{O})_2$	29.5	-5.0	68.6	3.2(2.68) <sup>a</sup>	-2.7	-3.3
$\text{SO}_3\cdots(\text{H}_2\text{O})_2$	40.7	-21.6	87.4	1.1(0.8) <sup>c</sup>	-16.0	-17.9
$\text{TS}_{\text{SA\_WM}}$	39.1	-14.5	80.1	7.6(6.7) <sup>c</sup>	-10.6	-13.6
$\text{H}_2\text{SO}_4\cdots\text{H}_2\text{O}$	41.0	-36.0	85.5	-12.7(-11.9) <sup>c</sup>	-30.2	-32.3
$\text{SO}_3 + \text{H}_2\text{O} + \text{HNO}_3$	38.9	0.0	169.5	0.0	0.0	0.0
$\text{SO}_3 + \text{HNO}_3\cdots\text{H}_2\text{O}$	41.0	-8.4	139.4	0.5	-7.9 (-8.1) <sup>c</sup>	-8.4
$\text{SO}_3\cdots\text{H}_2\text{O} + \text{HNO}_3$	41.2	-7.8	141.4	0.8	-7.2 (-7.4) <sup>c</sup>	-7.8
IM_NA	42.8	-18.1	103.2	1.7	-17.1 (-17.2) <sup>c</sup>	-18.1
TS_NA	39.9	-15.2	93.6	7.4	-13.2 (-13.5) <sup>c</sup>	-15.2
$\text{H}_2\text{SO}_4\cdots\text{HNO}_3$	43.4	-28.6	100.6	-8.0	-27.4 (-27.8) <sup>c</sup>	-28.6
$\text{SO}_3 + \text{H}_2\text{O} + \text{HCOOH}$	43.2	0.0	165.5	0.0	0.0	0.0
$\text{SO}_3 + \text{HCOOH}\cdots\text{H}_2\text{O}$	45.6	-10.2	134.8	0.3	-7.7	-8.5
$\text{SO}_3\cdots\text{H}_2\text{O} + \text{HCOOH}$	45.5	-9.5	137.4	0.8	-7.2	-7.8
IM_FA	47.4	-25.7	94.1	-1.8(-2.0) <sup>b</sup>	-21.5	-23.1
TS_FA	45.9	-23.9	89.4	-0.8(-1.0) <sup>b</sup>	-21.2	-23.5
$\text{H}_2\text{SO}_4\cdots\text{HCOOH}$	48.0	-40.9	130.8	-8.7(-8.3) <sup>b</sup>	-36.1	-37.7
$\text{SO}_3 + \text{H}_2\text{O} + \text{H}_2\text{C}_2\text{O}_4$	52.9	0.0	181.7	0.0	0.0	0.0
$\text{SO}_3 + \text{H}_2\text{C}_2\text{O}_4\cdots\text{H}_2\text{O}$	55.3	-11.8	150.1	-0.7	-10.6 (-11.1) <sup>d</sup>	-10.1
$\text{SO}_3\cdots\text{H}_2\text{O} + \text{H}_2\text{C}_2\text{O}_4$	55.3	-9.5	153.6	0.8	-7.2 (-7.4) <sup>d</sup>	-7.8
IM_OA	57.1	-26.3	109.1	-1.8	-23.3 (-23.5) <sup>d</sup>	-23.5
TS_OA	54.7	-23.5	104.5	-0.7	-23.0 (-23.5) <sup>d</sup>	-23.8
$\text{H}_2\text{SO}_4\cdots\text{H}_2\text{C}_2\text{O}_4$	57.6	-42.7	110.0	-18.1	-39.3 (-39.1) <sup>d</sup>	-39.5



SO <sub>3</sub> + H <sub>2</sub> O + <i>t</i> -H <sub>2</sub> SO <sub>4</sub>	46.9	0.0	177.8	0.0	0.0	0.0
SO <sub>3</sub> + H <sub>2</sub> SO <sub>4</sub> ···H <sub>2</sub> O	49.1	-12.4	146.3	-1.5	-10.1 (-10.1) <sup>e</sup>	-10.9
SO <sub>3</sub> ···H <sub>2</sub> O + H <sub>2</sub> SO <sub>4</sub>	49.2	-9.5	149.7	0.6	-7.2 (-7.0) <sup>e</sup>	-7.8
IM_SA	50.8	-26.2	108.4	-1.5	-22.2 (-21.3) <sup>e</sup>	-23.4
TS_SA	47.5	-20.5	102.1	2.1	-19.9 (-19.9) <sup>e</sup>	-21.8
(H <sub>2</sub> SO <sub>4</sub> ) <sub>2</sub>	51.6	-40.6	105.2	-14.3	-35.9 (-35.4) <sup>e</sup>	-37.4

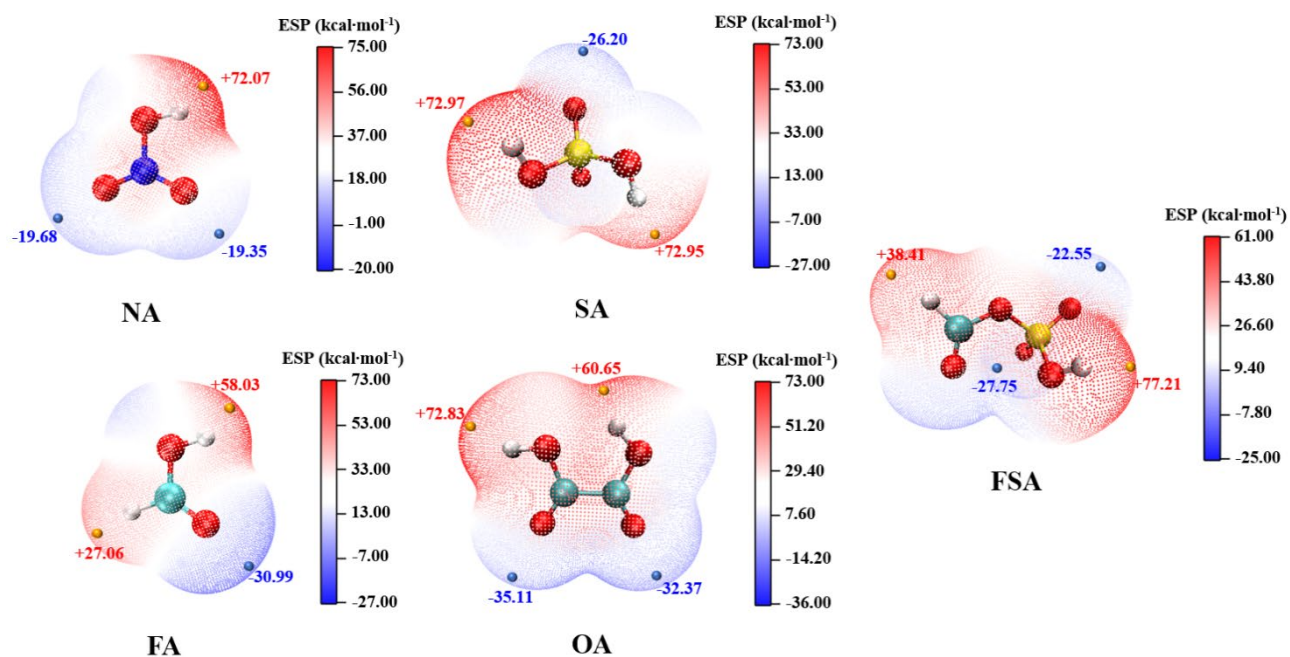
<sup>a</sup> The value was taken from reference (*Chem. Phys. Lett.*, **2013**, 581, 26-29.)

<sup>b</sup> The value was taken from reference (*Chem. Phys. Chem.*, **2012**, 13, 323-329.)

<sup>c</sup> The value was taken from reference (*J. Phys. Chem. A*, **2021**, 123, 3131-3141.)

<sup>d</sup> The value was taken from reference (*Atmos. Chem. Phys.*, **2019**, 19, 2833-2844.)

<sup>e</sup> The value was taken from reference (*J. Am. Chem. Soc.*, **2012**, 134, 20632-20644.)



**Fig. S5.** ESP-mapped van der Waals surface of  $\text{HNO}_3$  (NA),  $\text{H}_2\text{SO}_4$  (SA),  $\text{HCOOH}$  (FA),  $(\text{COOH})_2$  (OA) and  $\text{HCOOSO}_3\text{H}$  (FSA)

53 **Table S2.** Equilibrium constants (molecules·cm<sup>-3</sup>) for FSA···H<sub>2</sub>O, SO<sub>3</sub>···H<sub>2</sub>O, SO<sub>3</sub>···FSA and (H<sub>2</sub>O)<sub>2</sub> within the temperature range of 280-320 K

<i>T</i> /K	FSA···H <sub>2</sub> O	SO <sub>3</sub> ···H <sub>2</sub> O	(H <sub>2</sub> O) <sub>2</sub>	HCOOH···H <sub>2</sub> O	HNO <sub>3</sub> ···H <sub>2</sub> O	H <sub>2</sub> C <sub>2</sub> O <sub>4</sub> ···H <sub>2</sub> O	H <sub>2</sub> SO <sub>4</sub> ···H <sub>2</sub> O	SO <sub>3</sub> ···FSA
280	2.63 × 10 <sup>-18</sup>	2.45 × 10 <sup>-20</sup>	2.86 × 10 <sup>-22</sup>	3.11 × 10 <sup>-20</sup> (2.69 × 10 <sup>-20</sup> ) <sup>b</sup>	4.48 × 10 <sup>-20</sup>	3.07 × 10 <sup>-18</sup>	1.53 × 10 <sup>-18</sup>	1.80 × 10 <sup>-22</sup>
290	1.37 × 10 <sup>-18</sup>	1.59 × 10 <sup>-20</sup>	2.42 × 10 <sup>-22</sup>	1.91 × 10 <sup>-20</sup>	2.75 × 10 <sup>-20</sup>	1.58 × 10 <sup>-18</sup>	8.12 × 10 <sup>-19</sup>	1.50 × 10 <sup>-22</sup>
298	8.40 × 10 <sup>-19</sup>	1.14 × 10 <sup>-20</sup> (6.44 × 10 <sup>-20</sup> ) <sup>a</sup>	2.14 × 10 <sup>-22</sup> (2.34 × 10 <sup>-21</sup> ) <sup>a</sup>	1.33 × 10 <sup>-20</sup> (1.10 × 10 <sup>-20</sup> ) <sup>b</sup>	1.91 × 10 <sup>-20</sup> (4.07 × 10 <sup>-20</sup> ) <sup>c</sup>	9.65 × 10 <sup>-19</sup>	5.05 × 10 <sup>-19</sup> (3.88 × 10 <sup>-19</sup> ) <sup>d</sup>	1.31 × 10 <sup>-22</sup>
300	7.47 × 10 <sup>-19</sup>	1.06 × 10 <sup>-20</sup>	2.08 × 10 <sup>-22</sup>	1.22 × 10 <sup>-20</sup>	1.75 × 10 <sup>-20</sup>	8.56 × 10 <sup>-19</sup>	4.50 × 10 <sup>-19</sup>	1.27 × 10 <sup>-22</sup>
310	4.23 × 10 <sup>-19</sup>	7.25 × 10 <sup>-21</sup>	1.80 × 10 <sup>-22</sup>	7.99 × 10 <sup>-21</sup>	1.14 × 10 <sup>-20</sup>	4.83 × 10 <sup>-19</sup>	2.60 × 10 <sup>-19</sup>	1.09 × 10 <sup>-22</sup>
320	2.49 × 10 <sup>-19</sup>	5.10 × 10 <sup>-21</sup>	1.58 × 10 <sup>-22</sup>	5.40 × 10 <sup>-21</sup> (4.24 × 10 <sup>-21</sup> ) <sup>b</sup>	7.71 × 10 <sup>-21</sup>	2.82 × 10 <sup>-19</sup>	1.55 × 10 <sup>-19</sup>	9.49 × 10 <sup>-23</sup>

54 <sup>a</sup> The value was taken from reference (*J. Am. Chem. Soc.*, **2012**, *134*, 20632-20644)

55 <sup>b</sup> The value was taken from reference (*ChemPhysChem.*, **2012**, *13*, 323-329)

56 <sup>c</sup> The value was taken from reference (*RSC Adv.*, **2015**, *5*, 32941-32949)

57 <sup>d</sup> The value was taken from reference (*J. Phys. Chem. A*, **2021**, *125*, 2642-2652)

58 **Table S3.** Concentrations (molecules·cm<sup>-3</sup>) of H<sub>2</sub>O, FSA···H<sub>2</sub>O and SO<sub>3</sub>···H<sub>2</sub>O within the temperature range of 280-  
59 320 K<sup>a</sup>

Catalysts	RH	280 K	290 K	298 K	300 K	310 K	320 K
H <sub>2</sub> O	20%RH <sup>b</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>b</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>b</sup>	$1.55 \times 10^{17}$	$2.87 \times 10^{17}$	$4.50 \times 10^{17}$	$5.15 \times 10^{17}$	$8.77 \times 10^{17}$	$1.41 \times 10^{18}$
	80%RH <sup>b</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>b</sup>	$2.58 \times 10^{17}$	$4.78 \times 10^{17}$	$7.70 \times 10^{17}$	$8.58 \times 10^{17}$	$1.46 \times 10^{18}$	$2.35 \times 10^{18}$
FSA···H <sub>2</sub> O	20%RH <sup>b</sup>	$1.36 \times 10^6$	$1.32 \times 10^6$	$1.26 \times 10^6$	$1.28 \times 10^6$	$1.24 \times 10^6$	$1.17 \times 10^6$
	40%RH <sup>b</sup>	$2.71 \times 10^6$	$2.62 \times 10^6$	$2.60 \times 10^6$	$2.56 \times 10^6$	$2.47 \times 10^6$	$2.34 \times 10^6$
	60%RH <sup>b</sup>	$4.08 \times 10^6$	$3.94 \times 10^6$	$3.78 \times 10^6$	$3.85 \times 10^6$	$3.71 \times 10^6$	$3.51 \times 10^6$
	80%RH <sup>b</sup>	$5.45 \times 10^6$	$5.24 \times 10^6$	$5.21 \times 10^6$	$5.12 \times 10^6$	$4.95 \times 10^6$	$4.69 \times 10^6$
	100%RH <sup>b</sup>	$6.80 \times 10^6$	$6.55 \times 10^6$	$6.47 \times 10^6$	$6.41 \times 10^6$	$6.18 \times 10^6$	$5.86 \times 10^6$
SO <sub>3</sub> ···H <sub>2</sub> O	20%RH <sup>b</sup>	1.76	2.09	2.34	2.47	2.84	3.19
	40%RH <sup>b</sup>	3.52	4.17	4.83	4.93	5.69	6.38
	60%RH <sup>b</sup>	5.30	6.26	7.01	7.40	8.54	9.56
	80%RH <sup>b</sup>	7.08	8.33	9.66	9.86	11.4	12.8
	100%RH <sup>b</sup>	8.82	1.04	1.20	12.3	14.2	15.9

60 <sup>a</sup> All of the equilibrium constants were calculated by using energies computed at CCSD(T)-F12a/cc-pVDZ-F12//M06-2X/6-  
61 311++G(2df,2pd) level and partition functions obtained at the M06-2X/6-311++G(2df,2pd) level.

62 <sup>b</sup> The values are reported from reference (*J. Phys. Chem. A*, **2013**, *117*, 10381-10396)

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**Part 1. Calculations details of high-pressure-limit (HPL) rate constants**

The VRC-VTST calculations were carried out with the potential surface obtained by using CCSD(T)-F12/cc-pVDZ-F12//M06-2X/6-311+G(2df,2pd), and were performed by variationally minimizing the rate constant with respect to the distance  $s$  between pivot points and with respect to the location of the pivot points. Specifically, using two pivot points produces a single-faceted dividing surface for the hydrolysis of  $\text{SO}_3$  with  $X$  ( $X = \text{H}_2\text{O}$ ,  $\text{HCOOH}$ ,  $\text{HNO}_3$  and  $\text{H}_2\text{SO}_4$ ). Such as, using two pivot points produces a single-faceted dividing surface for the reaction of  $\text{FSA}\cdots\text{H}_2\text{O} + \text{SO}_3$ . One pivot point is located at a distance  $d$  from the center of mass (COM) of  $\text{FSA}\cdots\text{H}_2\text{O}$ , where the vector connecting the pivot point with  $\text{SO}_3\cdots\text{H}_2\text{O}$ 's COM is perpendicular to the  $\text{SO}_3$  plane, and the other pivot point is located at a distance  $d$  from the COM of catalyst  $\text{FSA}\cdots\text{H}_2\text{O}$ , where the vector connecting the pivot point with catalyst FSA's COM is perpendicular to catalyst  $\text{FSA}\cdots\text{H}_2\text{O}$  plane. The lengths of these vectors are fixed successively at 0.2 Å. The reaction coordinate  $s$  is the distance between a pivot point on one reactant and a pivot point on the other reactant. The distance  $s$  between pivot points is varied from 2.5 to 8.0 Å for  $\text{FSA}\cdots\text{H}_2\text{O} + \text{SO}_3$  in each case with a 0.2 Å grid increment. The details of the VRC-VTST calculations can be seen in the supporting information of reference.<sup>1</sup>

**References:**

- (1) Bao, J. L.; Zhang, X.; Truhlar, D. G. Barrierless association of  $\text{CF}_2$  and dissociation of  $\text{C}_2\text{F}_4$  by variational transition-state theory and system-specific quantum Rice-Ramsperger-Kassel theory. *Proc. Natl. Acad. Sci. U. S. A.* **2016**, *113*, 13606-13611.

82 **Table S4.** High-pressure limiting rate constants ( $\text{cm}^3 \cdot \text{molecules}^{-1} \cdot \text{s}^{-1}$ ) for the reactants to pre-reactive complex  
83 process in  $\text{SO}_3$  hydrolysis with and without  $X$  ( $X = \text{H}_2\text{O}$ ,  $\text{NH}_3$ ,  $\text{HCOOH}$ ,  $(\text{COOH})_2$ ,  $\text{HNO}_3$ ,  $\text{H}_2\text{SO}_4$ ,  $\text{H}_2\text{SO}_4 \cdots \text{H}_2\text{O}$   
84 and  $(\text{H}_2\text{SO}_4)_2$ ), calculated using the master equation within the temperature range of 280-320 K

$T(\text{K})$	$\text{SO}_3 + \text{H}_2\text{O} \rightarrow \text{IM}$	$\text{SO}_3 \cdots \text{H}_2\text{O} + \text{H}_2\text{O} \rightarrow \text{IM\_WM}$	$\text{SO}_3 + \text{NH}_3 \cdots \text{H}_2\text{O} \rightarrow \text{IM\_AM}$
280	$1.07 \times 10^{-10}$	$2.17 \times 10^{-10}$	$1.88 \times 10^{-10}$
290	$1.09 \times 10^{-10}$	$2.21 \times 10^{-10}$	$1.92 \times 10^{-10}$
298	$1.10 \times 10^{-10}$	$2.24 \times 10^{-10}$	$1.94 \times 10^{-10}$
300	$1.10 \times 10^{-10}$	$2.25 \times 10^{-10}$	$1.95 \times 10^{-10}$
310	$1.12 \times 10^{-10}$	$2.28 \times 10^{-10}$	$1.98 \times 10^{-10}$
320	$1.14 \times 10^{-10}$	$2.32 \times 10^{-10}$	$2.01 \times 10^{-10}$
$T(\text{K})$	$\text{SO}_3 + \text{HNO}_3 \cdots \text{H}_2\text{O} \rightarrow \text{IM\_NA}$	$\text{SO}_3 + \text{HCOOH} \cdots \text{H}_2\text{O} \rightarrow \text{IM\_FA}$	$\text{SO}_3 + \text{H}_2\text{C}_2\text{O}_4 \cdots \text{H}_2\text{O} \rightarrow \text{IM\_OA}$
280	$9.15 \times 10^{-11}$	$1.25 \times 10^{-10}$	$9.33 \times 10^{-11}$
290	$9.32 \times 10^{-11}$	$1.27 \times 10^{-10}$	$9.50 \times 10^{-11}$
298	$9.44 \times 10^{-11}$	$1.29 \times 10^{-10}$	$9.63 \times 10^{-11}$
300	$9.47 \times 10^{-11}$	$1.30 \times 10^{-10}$	$9.66 \times 10^{-11}$
310	$9.63 \times 10^{-11}$	$1.32 \times 10^{-10}$	$9.82 \times 10^{-11}$
320	$9.79 \times 10^{-11}$	$1.34 \times 10^{-10}$	$9.98 \times 10^{-11}$
$T(\text{K})$	$\text{SO}_3 + \text{H}_2\text{SO}_4 \cdots \text{H}_2\text{O} \rightarrow \text{IM\_SA}$	$\text{SO}_3 + \text{FSA} \cdots \text{H}_2\text{O} \rightarrow \text{IM\_FSA}$	
280	$1.06 \times 10^{-10}$	$3.09 \times 10^{-11}$	
290	$1.07 \times 10^{-10}$	$3.14 \times 10^{-11}$	
298	$1.09 \times 10^{-10}$	$3.18 \times 10^{-11}$	
300	$1.09 \times 10^{-10}$	$3.19 \times 10^{-11}$	
310	$1.11 \times 10^{-10}$	$3.25 \times 10^{-11}$	
320	$1.13 \times 10^{-10}$	$3.30 \times 10^{-11}$	

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## Part 2. Details of Master Equation Solver for Multi-Energy Well Reactions

The rate constants for  $\text{SO}_3 + \text{H}_2\text{O} \cdots X$  ( $X = \text{H}_2\text{O}$ ,  $\text{NH}_3$ ,  $\text{HCOOH}$ ,  $\text{HNO}_3$ ,  $\text{H}_2\text{C}_2\text{O}_4$ ,  $\text{H}_2\text{SO}_4$ ,  $\text{H}_2\text{SO}_4 \cdots \text{H}_2\text{O}$  and  $(\text{H}_2\text{SO}_4)_2$ ) and  $\text{SO}_3 \cdots \text{H}_2\text{O} + Y$  reactions within the temperature range of 280-320 K and the pressure range of 10-760 Torr were calculated by using the Master Equation Solver for Multi-Energy Well Reactions (MESMER).<sup>1</sup> Specifically, as for  $\text{SO}_3 + \text{H}_2\text{O} \cdots X$  and  $\text{SO}_3 \cdots \text{H}_2\text{O} + X$  reaction, the barrierless bimolecular reaction steps were evaluated by using Inverse Laplace Transform (ILT) method, whereas, the rate determining steps were obtained by employing the RRKM theory. The ILT methods<sup>2-3</sup> and RRKM theory<sup>4-5</sup> 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), where  $W(E-E_0)$  is the rovibrational sum of states (SOS) at the optimized transition state (TS) geometry,  $E_0$  is the reaction threshold energy,  $h$  is Planck's constant,  $\rho(E)$  is the density of rovibrational states of the reactant, and  $Q(\beta)$  is the corresponding canonical partition function. Moreover, the electronic geometries, vibrational frequencies, and rotational constants were calculated at the M06-2X/6-311+G(2df,2pd) level and single-point energy calculations were refined at the CCSD(T)-F12/cc-pVDZ-F12 level for the modeling. The one-dimensional asymmetric Eckart potential<sup>6</sup> was used to treat the tunneling effect in the RRKM calculation. In addition, The Lennard-Jones (L-J) parameters  $\epsilon/k_B = 82$  K and  $\sigma = 3.798$  Å were used for  $\text{N}_2$ <sup>7-8</sup> while  $\epsilon/k_B = 420.08$  K and  $\sigma = 2.89$  Å were estimated for  $\text{H}_2\text{SO}_4$  and its isomer. It was noted that the hindered internal rotation.<sup>9-18</sup>

## Reference:

- (1) Glowacki, D. R.; Liang, C. H.; Morley, C.; Pilling, M. J.; Robertson, S. H. MESMER: an open-source master equation solver for multi-energy well reactions. *J. Phys. Chem. A* **2012**, *116*, 9545-9560.
- (2) Horváth, G.; Horváth, I.; Almousa, S. A.-D.; Telek, M. Numerical inverse Laplace transformation using concentrated matrix exponential distributions. *Perform. Evaluation* **2020**, *137*, 102067.
- (3) Kumar, A.; Mallick, S.; Kumar, P. Oxidation of  $\text{HOSO}^\cdot$  by  $\text{Cl}^\cdot$ : a new source of  $\text{SO}_2$  in the atmosphere? *Phys. Chem. Chem. Phys.* **2021**, *23*, 18707-18711.
- (4) Mai, T. V.-T.; Duong, M. V.; Nguyen, H. T.; Huynh, L. K. J. P. C. C. P. Ab initio kinetics of the  $\text{HOSO}_2 + {}^3\text{O}_2 \rightarrow \text{SO}_3 + \text{HO}_2$  reaction. *Phys. Chem. Chem. Phys.* **2018**, *20*, 6677-6687.
- (5) Mallick, S.; Kumar, A.; Kumar, P. Oxidation of  $\text{HOSO}$  by  $\text{NH}_2$ : A new path for the formation of an acid rain precursor. *Chem. Phys. Lett.* **2021**, *773*, 138536.
- (6) Eckart, C. The penetration of a potential barrier by electrons. *Phys. Rev. B* **1930**, *35*, 1303.
- (7) Hippler, H.; Troe, J.; Wendelken, H. J. Collisional deactivation of vibrationally highly excited polyatomic molecules. II. Direct observations for excited toluene. *J. Chem. Phys.* **1983**, *78*, 6709-6717.
- (8) Reid, R. C.; Prausnitz, J. M.; Poling, B. E. The properties of gases and liquids. **1987**.

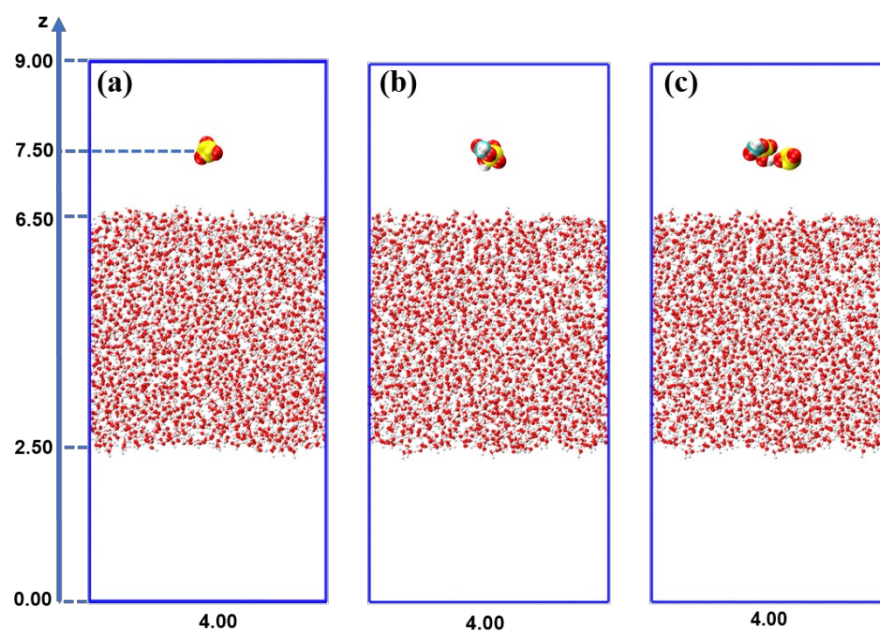
- 119 (9) Le, X. T.; Mai, T. V.-T.; Duong, M. v.; Huynh, L. K. Kinetics of hydrogen abstraction from desflurane by OH and Cl radicals-A  
120 theoretical study. *Chem. Phys. Lett.* **2019**, 728, 142-147.
- 121 (10) Le, X. T.; Mai, T. V.-T.; Lin, K. C.; Huynh, L. K. Low temperature oxidation kinetics of biodiesel molecules: Rate rules for  
122 concerted HO<sub>2</sub> elimination from alkyl ester peroxy radicals. *J. Phys. Chem. A* **2018**, 122, 8259-8273.
- 123 (11) Mai, T. V. T.; Duong, M. v.; Nguyen, H. T.; Lin, K. C.; Huynh, L. K. Kinetics of thermal unimolecular decomposition of acetic  
124 anhydride: An integrated deterministic and stochastic model. *J. Phys. Chem. A* **2017**, 121, 3028-3036.
- 125 (12) Mai, T. V. T.; Duong, M. V.; Nguyen, H. T.; Lin, K. C.; Huynh, L. K. Ab initio chemical kinetics of the CH<sub>2</sub>OO + C<sub>2</sub>F<sub>4</sub> reaction.  
126 *Chem. Phys. Lett.* **2018**, 706, 280-284.
- 127 (13) Mai, T. V. T.; Huynh, L. K. Ab initio kinetics of the C<sub>2</sub>H<sub>2</sub> + NH<sub>2</sub> reaction: a revisited study. *Phys. Chem. Chem. Phys.* **2019**, 21,  
128 17232-17239.
- 129 (14) Mai, T. V. T.; Raghunath, P.; Le, X. T.; Huynh, L. K.; Nam, P. C.; Lin, M. C. Ab initio chemical kinetics for the HCCO + OH  
130 reaction. *Chem. Phys. Lett.* **2014**, 592, 175-181.
- 131 (15) Mai, T. V. T.; Ratkiewicz, A.; Duong, M. V.; Huynh, L. K. Direct ab initio study of the C<sub>6</sub>H<sub>6</sub> + CH<sub>3</sub>/C<sub>2</sub>H<sub>5</sub> = C<sub>6</sub>H<sub>5</sub> + CH<sub>4</sub>/C<sub>2</sub>H<sub>6</sub>  
132 reactions. *Chem. Phys. Lett.* **2016**, 646, 102-109.
- 133 (16) Mai, T. V. T.; Nguyen, H. T.; Huynh, L. K. Ab initio dynamics of hydrogen abstraction from N<sub>2</sub>H<sub>4</sub> by OH radicals: an RRKM-  
134 based master equation study. *Phys. Chem. Chem. Phys.* **2019**, 21, 23733-23741.
- 135 (17) Mai, T. V. T.; Nguyen, H. T.; Huynh, L. K. Kinetics of hydrogen abstraction from CH<sub>3</sub>SH by OH radicals: An ab initio RRKM-  
136 based master equation study. *Atmos. Environ.* **2020**, 242, 117833.
- 137 (18) Reiner, T.; Arnold, F. Laboratory investigations of gaseous sulfuric acid formation via SO<sub>3</sub> + H<sub>2</sub>O + M → H<sub>2</sub>SO<sub>4</sub> + M:  
138 Measurement of the rate constant and product identification. *J. Chem. Phys.* **1994**, 101, 7399-7407.
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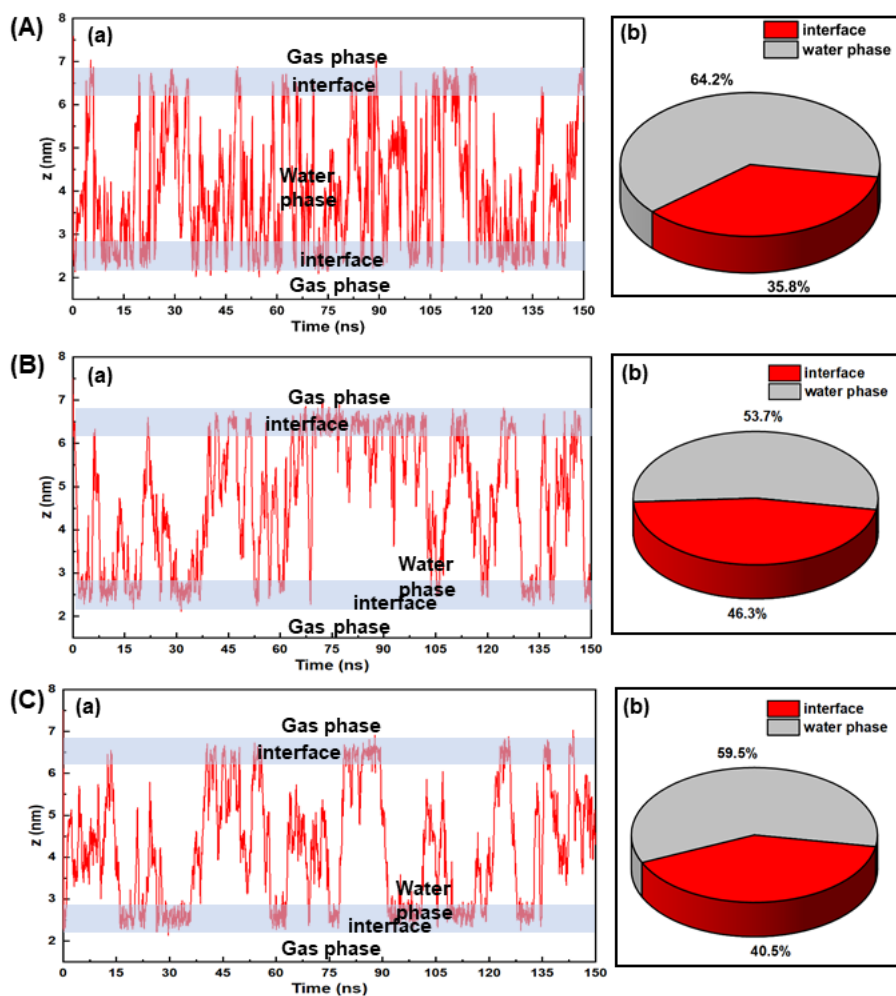
140 **Table S5.** Rate ratios for SO<sub>3</sub> hydrolysis with FSA compared to H<sub>2</sub>O and  $X$  ( $X = \text{HCOOH}$ ,  $(\text{COOH})_2$ ,  $\text{HNO}_3$  and  
141  $\text{H}_2\text{SO}_4$ ) within the temperature range of 280-320 K

$T/\text{K}$	$[Y]$	280	290	298	300	310	320
$\nu_{\text{SA\_FSA}}/\nu_{\text{SA\_WM}}$	20%RH	$7.04 \times 10^{-7}$	$3.55 \times 10^{-7}$	$2.16 \times 10^{-7}$	$1.87 \times 10^{-7}$	$1.04 \times 10^{-7}$	$6.11 \times 10^{-8}$
	40%RH	$3.53 \times 10^{-7}$	$1.78 \times 10^{-7}$	$1.05 \times 10^{-7}$	$9.36 \times 10^{-8}$	$5.19 \times 10^{-8}$	$3.06 \times 10^{-8}$
	60%RH	$2.34 \times 10^{-7}$	$1.19 \times 10^{-7}$	$7.22 \times 10^{-8}$	$6.23 \times 10^{-8}$	$3.46 \times 10^{-8}$	$2.04 \times 10^{-8}$
	80%RH	$1.75 \times 10^{-7}$	$8.92 \times 10^{-8}$	$5.24 \times 10^{-8}$	$4.68 \times 10^{-8}$	$2.59 \times 10^{-8}$	$1.53 \times 10^{-8}$
	100%RH	$1.41 \times 10^{-7}$	$7.13 \times 10^{-8}$	$4.22 \times 10^{-8}$	$3.74 \times 10^{-8}$	$2.08 \times 10^{-8}$	$1.22 \times 10^{-8}$
$\nu_{\text{SA\_FSA}}/\nu_{\text{SA\_VFA}}$	$10^8$	$2.89 \times 10^0$	$2.72 \times 10^0$	$2.61 \times 10^0$	$2.58 \times 10^0$	$2.47 \times 10^0$	$2.38 \times 10^0$
	$10^{11}$	$3.79 \times 10^{-2}$	$3.62 \times 10^{-2}$	$3.38 \times 10^{-2}$	$3.32 \times 10^{-2}$	$3.24 \times 10^{-2}$	$3.02 \times 10^{-2}$
	$10^{11}$	$2.89 \times 10^{-3}$	$2.72 \times 10^{-3}$	$2.61 \times 10^{-3}$	$2.58 \times 10^{-3}$	$2.47 \times 10^{-3}$	$2.38 \times 10^{-3}$
$\nu_{\text{SA\_OA}}/\nu_{\text{SA\_OA}}$	$10^7$	$1.27 \times 10^{-1}$	$1.31 \times 10^{-1}$	$1.34 \times 10^{-1}$	$1.35 \times 10^{-1}$	$1.38 \times 10^{-1}$	$1.27 \times 10^{-1}$
	$10^9$	$1.27 \times 10^{-3}$	$1.31 \times 10^{-3}$	$1.34 \times 10^{-3}$	$1.35 \times 10^{-3}$	$1.38 \times 10^{-3}$	$1.27 \times 10^{-3}$
$\nu_{\text{SA\_FSA}}/\nu_{\text{SA\_VNA}}$	$10^9$	$3.71 \times 10^1$	$3.72 \times 10^1$	$3.73 \times 10^1$	$3.73 \times 10^1$	$3.70 \times 10^1$	$3.61 \times 10^1$
	$10^{11}$	$3.71 \times 10^{-1}$	$3.72 \times 10^{-1}$	$3.73 \times 10^{-1}$	$3.73 \times 10^{-1}$	$3.70 \times 10^{-1}$	$3.61 \times 10^{-1}$
$\nu_{\text{SA\_FSA}}/\nu_{\text{SA\_SA}}$	$10^6$	$6.26 \times 10^0$	$6.85 \times 10^0$	$7.40 \times 10^0$	$7.70 \times 10^0$	$8.42 \times 10^0$	$9.20 \times 10^0$
	$10^7$	$4.88 \times 10^{-1}$	$5.21 \times 10^{-1}$	$5.48 \times 10^{-1}$	$5.54 \times 10^{-1}$	$5.89 \times 10^{-1}$	$6.26 \times 10^{-1}$
	$10^8$	$6.26 \times 10^{-2}$	$6.85 \times 10^{-2}$	$7.40 \times 10^{-2}$	$7.70 \times 10^{-2}$	$8.42 \times 10^{-2}$	$9.20 \times 10^{-2}$

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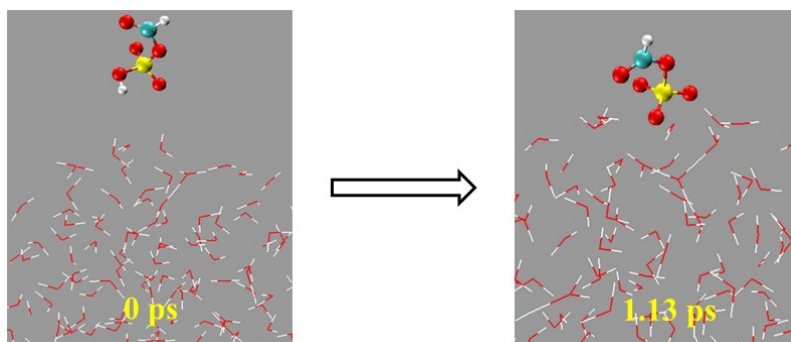


**Fig. S6** The initial configuration of the 150 ns NVT simulation of (a)  $\text{SO}_3$ , (b) FSA and (c)  $\text{SO}_3$ -FSA complex.



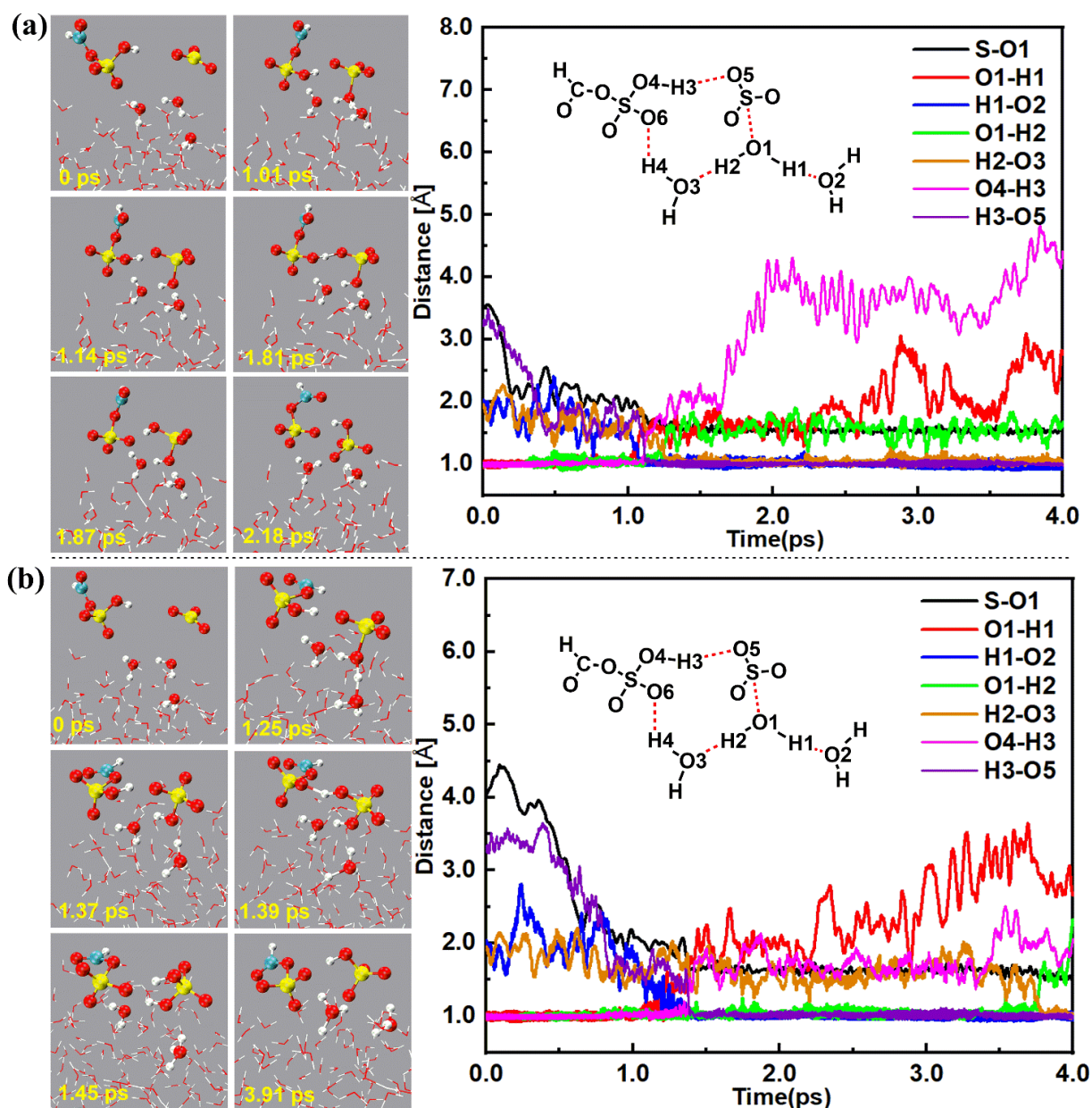
**Fig. S7.** Z coordinates of  $\text{SO}_3$  (A), FSA (B) and  $\text{SO}_3$ -FSA complex (C) as the function of simulation time, along with (a) the water density profile and (b) a pie chart showing occurrence percentages (c) at the air-water interface and in the water phase

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152 **Fig. S8.** Snapshot structures from BOMD simulations of the FSA reaction at the air-water interface. White, red,  
153 yellow and blue spheres represent H, O, S, and C atoms, respectively



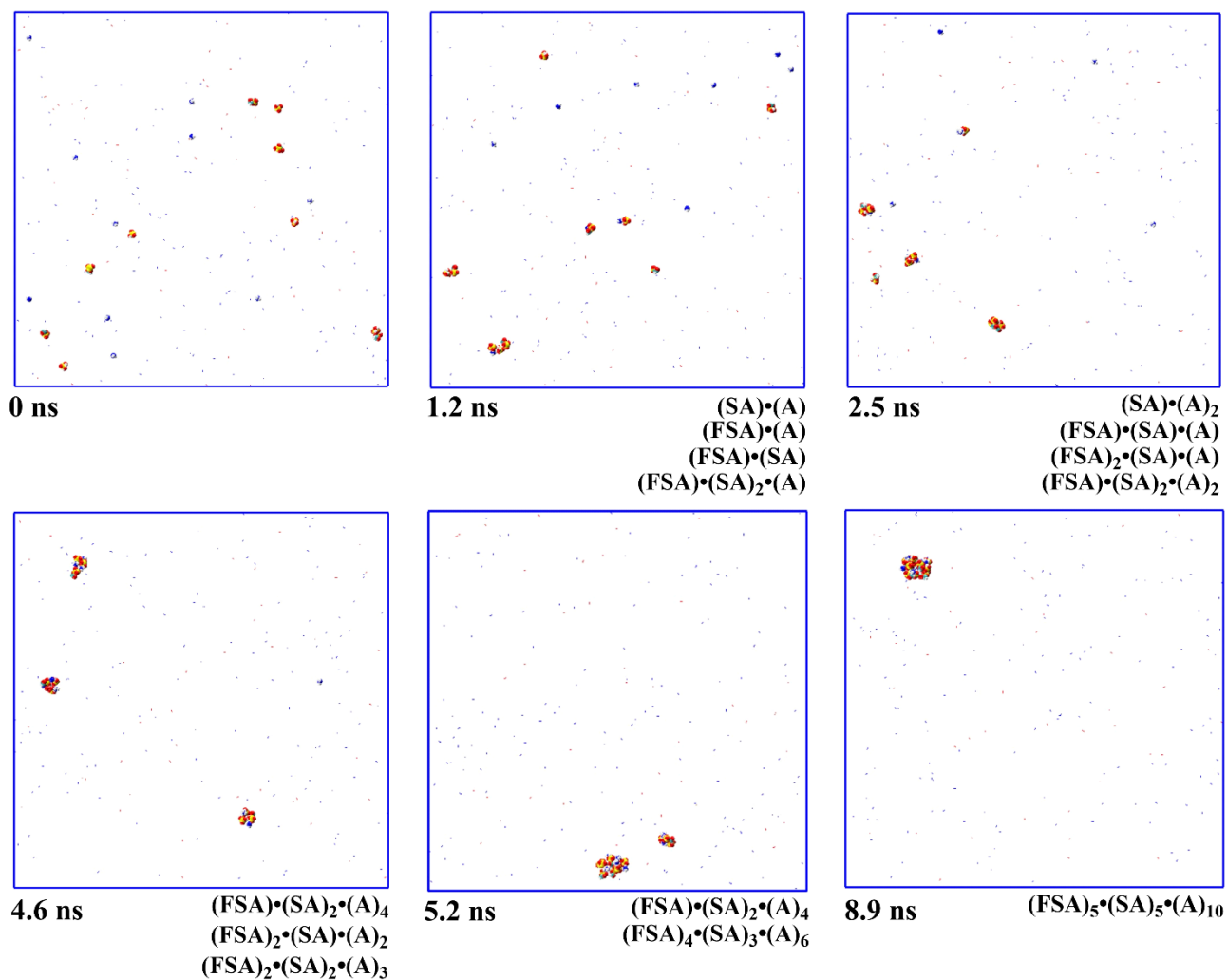
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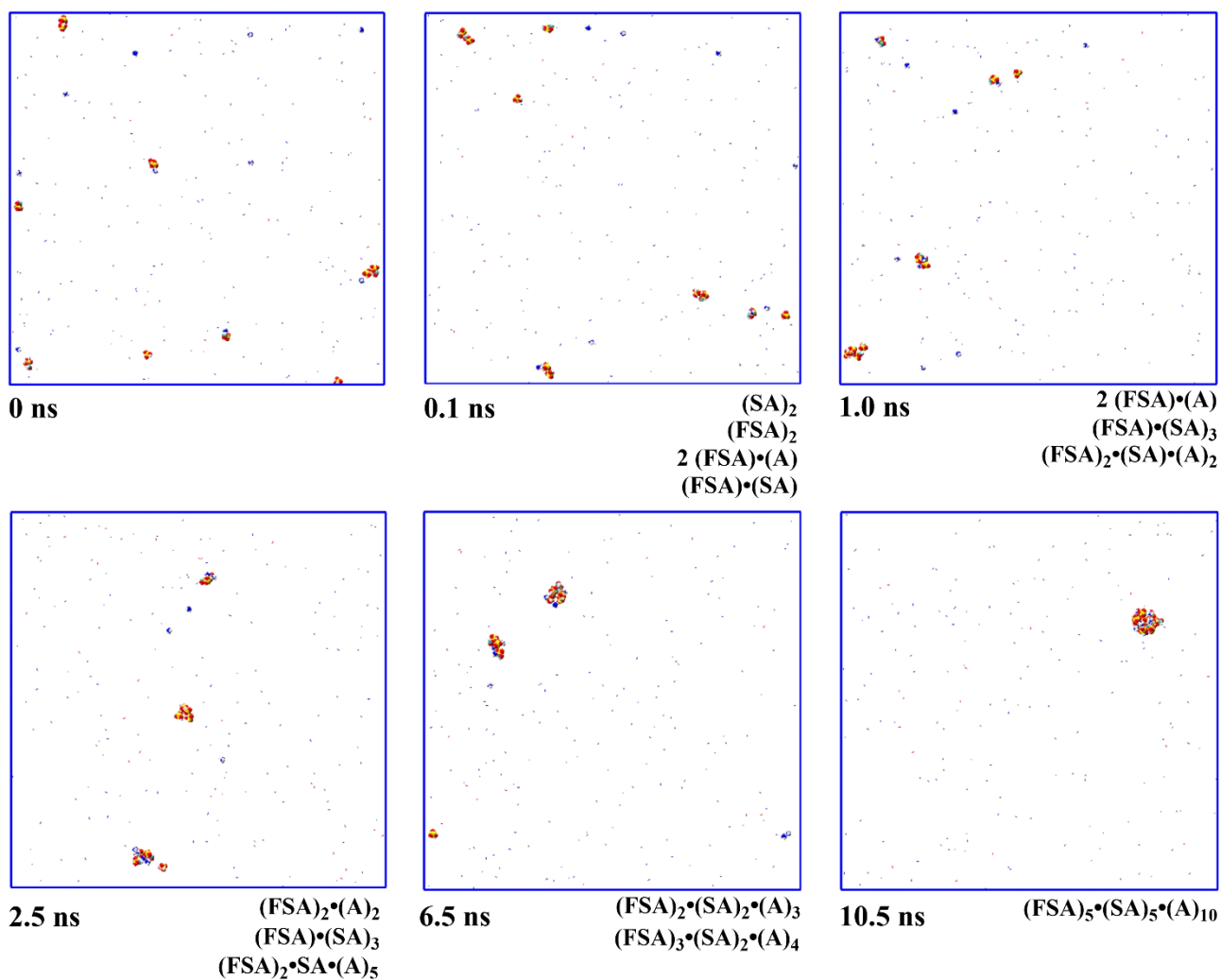
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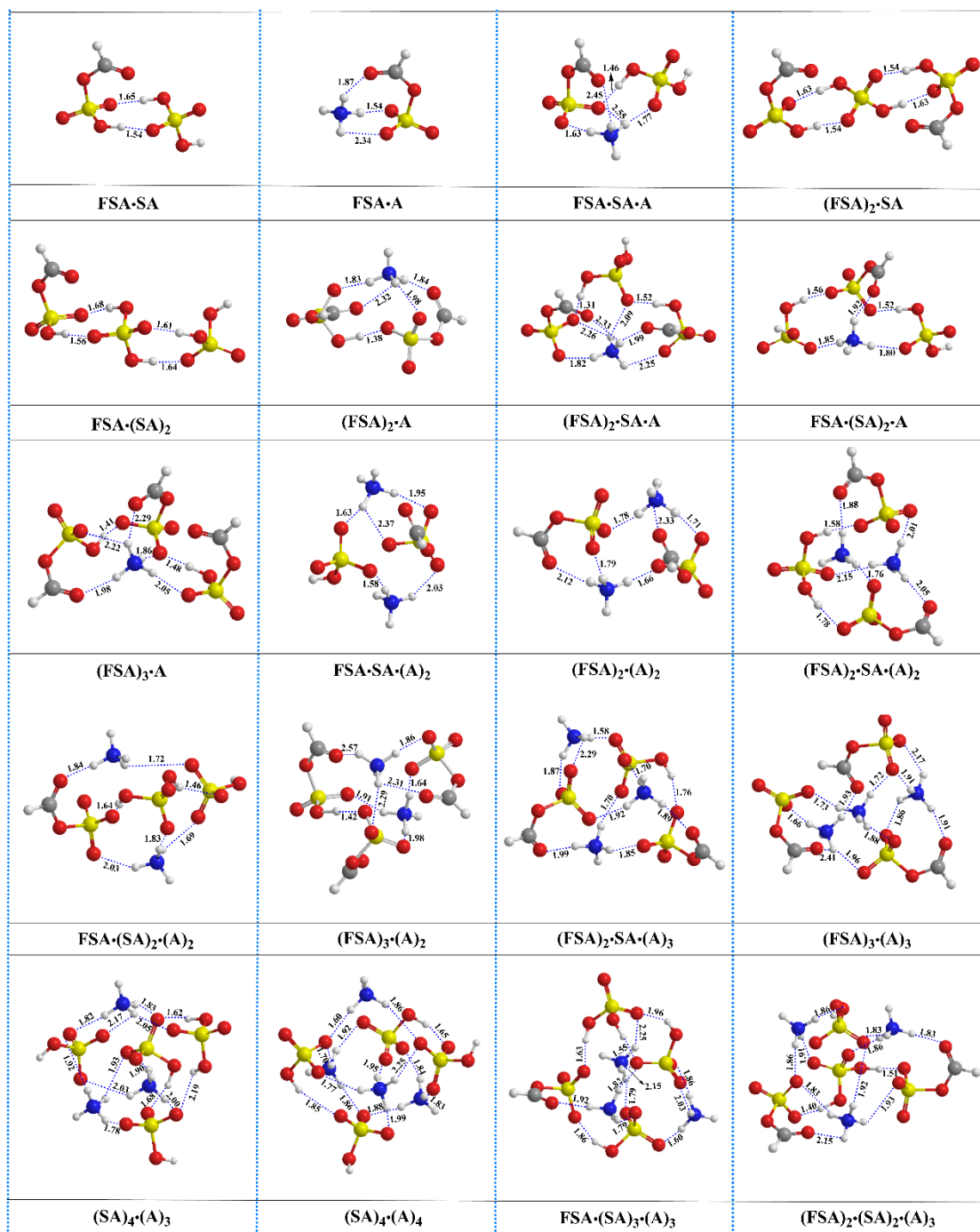
**Fig. S9.** BOMD simulations of  $\text{HSO}_4^- \cdots \text{FSA}^- \cdots \text{H}_3\text{O}^+$  ion pair formation from  $\text{SO}_3$  hydrolysis with FSA at the air-water interface (Top panel: Snapshot structures showing the formation of  $\text{HSO}_4^- \cdots \text{FSA}^- \cdots \text{H}_3\text{O}^+$  ion pair. Lower panel: Time evolution of key bond distances (S-O1, O5-H3, and O1-H2) involved in the mechanism.)



**Fig. S10.** Snapshots of nucleation simulation of FSA, SA and A using the VDW representation, with N<sub>2</sub> and O<sub>2</sub> shown using the line drawing method at 278.15 K

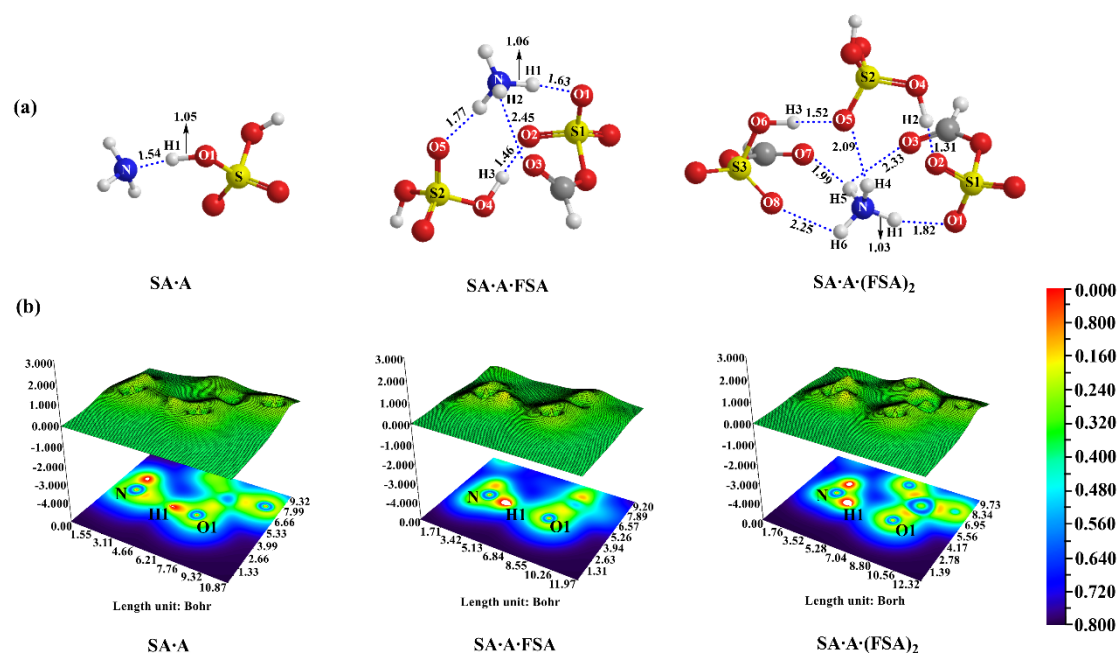


**Fig. S11.** Snapshots of nucleation simulation of FSA, SA and A using the VDW representation, with N<sub>2</sub> and O<sub>2</sub> shown using the line drawing method at 298.15 K



**Fig. S12.** Most stable configurations of FSA-SA-A-based clusters identified at the M06-2X/6-311++G(2df,2pd) level of theory. Hydrogen bond lengths are given in Å.





**Fig. S13** The most stable configurations of SA·A, SA·A·FSA and SA·A·(FSA)<sub>2</sub> clusters along with the corresponding relief Aps with the projection of localized orbital locator (LOL), hydrogen bonds are shown as dashed lines

As shown in Fig. S11, in contrast to the pure SA-A cluster, where proton transfer from SA to A has not occurred, the proton in the SA·A·FSA cluster is fully transferred from FSA to A. This is evidenced by the green region between H1 and O1 and the red region between H1 and N1 in Fig. 11(b), and the LBO of the newly formed H1···N1 bond in the SA·A·FSA cluster is 0.606 a.u. Similar to the SA·A·FSA cluster, the MA in the SA·A·(FSA)<sub>2</sub> cluster is protonated (Fig. 11(b)), but to a greater extent. This is reflected in the LBO values from Table S6, where the newly formed H1···N1 bond in the SA·A·(FSA)<sub>2</sub> cluster shows an LBO of 0.695, higher than the 0.606 observed in the SA·A·FSA cluster. Moreover, this is evidenced by the significant increase in electron density (ρ) at the bond critical points (BCPs) of the N···H1 bond, along with a more negative Laplacian (∇<sup>2</sup>ρ) (see Table S1). These analysis demonstrate that the FSA molecule not only strengthens the hydrogen bonding between SA and A but also facilitates proton transfer from SA to A, thereby increasing the stability of the SA-A cluster.

**Table S6** The bond length  $r$  (Å), electron density  $\rho$  (a.u.) and Laplacian electron density  $\nabla^2\rho$  (a.u.) at corresponding BCPs. Laplacian bond order (LBO) of the newly formed covalent bond among SA, FSA and A molecules

Cluster	Bonds	$r$ (Å)	$\rho$ (a.u.)	$\nabla^2\rho$ (a.u.)	LBO (a.u.)
SA·A	O1-H1···N-H2	1.54	0.0811	0.0262	-
	O1-H1	1.05	0.2688	-1.7786	-
SA·A·FSA	S-O1···H1-N	1.63	0.0559	0.0978	-
	H1-N	1.06	0.3004	-1.8041	0.606
SA·A·(FSA) <sub>2</sub>	S-O1···H1-N	1.82	0.0335	0.1064	-
	H1-N	1.03	0.3249	-1.9502	0.695

190 **Table S7.** Gibbs free energy change  $\Delta G$  (kcal·mol<sup>-1</sup>) for the formation of all clusters at 1 atm and  
 191 temperatures of 298.15, 278.15, and 258.15K

Clusters	$T = 298.15$ K	$T = 278.15$ K	$T = 258.15$ K
SA·A	-5.85 (-7.33) <sup>a</sup>	-6.49 (-7.94) <sup>a</sup>	-7.12 (-8.54) <sup>a</sup>
(SA) <sub>2</sub>	-8.33 (-8.42) <sup>a</sup>	-9.00 (-9.10) <sup>a</sup>	-9.68 (-9.77) <sup>a</sup>
(SA) <sub>2</sub> ·A	-21.34 (-20.84) <sup>a</sup>	-22.86 (-22.41) <sup>a</sup>	-24.38 (-23.96) <sup>a</sup>
(SA) <sub>2</sub> ·(A) <sub>2</sub>	-27.91 (-26.55) <sup>a</sup>	-30.13 (-28.81) <sup>a</sup>	-32.34 (-31.04) <sup>a</sup>
(SA) <sub>3</sub>	-13.19 (-13.91) <sup>a</sup>	-14.72 (-15.46) <sup>a</sup>	-16.25 (-17.00) <sup>a</sup>
(SA) <sub>3</sub> ·A	-30.23 (-30.19) <sup>a</sup>	-32.53 (-32.52) <sup>a</sup>	-34.82 (-34.85) <sup>a</sup>
(SA) <sub>3</sub> ·(A) <sub>2</sub>	-43.08 (-41.79) <sup>a</sup>	-46.09 (-44.87) <sup>a</sup>	-49.09 (-47.94) <sup>a</sup>
(SA) <sub>3</sub> ·(A) <sub>3</sub>	-53.69 (-52.79) <sup>a</sup>	-57.50 (-56.64) <sup>a</sup>	-61.32 (-60.47) <sup>a</sup>
(FSA) <sub>2</sub>	-1.81	-2.58	-3.34
FSA·A	-8.54	-9.28	-10.02
(FSA) <sub>2</sub> ·(A) <sub>2</sub>	-31.41	-33.61	-35.81
(FSA) <sub>2</sub> ·A	-18.73	-20.29	-21.86
SA·FSA	-4.93	-5.69	-6.45
SA·FSA·A	-17.78	-19.30	-20.82
SA·FSA·(A) <sub>2</sub>	-20.41	-22.72	-25.03
(FSA) <sub>3</sub>	2.44	0.86	-0.73
(SA) <sub>2</sub> ·FSA·A	-22.53	-25.02	-27.52
(SA) <sub>2</sub> ·FSA·(A) <sub>2</sub>	-43.76	-46.87	-49.98
(SA) <sub>2</sub> ·FSA·(A) <sub>3</sub>	-54.83	-58.66	-62.49
SA·(FSA) <sub>2</sub>	-8.48	-10.09	-11.71
(FSA) <sub>3</sub> ·A	-26.13	-28.47	-30.81
SA·(FSA) <sub>2</sub> ·(A) <sub>2</sub>	-38.33	-41.48	-44.64
(SA) <sub>2</sub> ·FSA	-12.00	-13.50	-15.01
SA·(FSA) <sub>2</sub> ·A	-22.84	-25.06	-27.30
(FSA) <sub>3</sub> ·(A) <sub>2</sub>	-37.55	-40.61	-43.68

192	Continued table			
	SA·(FSA) <sub>2</sub> ·(A) <sub>3</sub>	-57.73	-61.56	-65.39
	(FSA) <sub>3</sub> ·(A) <sub>3</sub>	-54.24	-58.02	-61.81
193	*Calculated at DLPNO-CCSD(T)/aug-cc-pVTZ//M06-2X/6-311++G(2df,2pd) level of theory.			
194	<sup>a</sup> The values in parentheses taken from reference ( <i>J. Chem. Phys.</i> , 2017, 146, 184308)			

**Table S8.** Evaporation rates ( $\gamma$ ,  $\text{s}^{-1}$ ) of the studied clusters at 298.15, 278.15, and 258.15K

Evaporation pathways	298.15 K	278.15 K	258.15 K
$\text{SA} \cdot \text{A} \rightarrow \text{SA} + \text{A}$	$1.86 \times 10^5$	$2.89 \times 10^4$	$3.37 \times 10^3$
$\text{SA} \cdot \text{FSA} \rightarrow \text{SA} + \text{FSA}$	$5.85 \times 10^5$	$8.15 \times 10^4$	$8.34 \times 10^3$
$\text{A} \cdot \text{FSA} \rightarrow \text{A} + \text{FSA}$	$2.01 \times 10^3$	$1.86 \times 10^2$	$1.19 \times 10^1$
$(\text{SA})_2 \rightarrow \text{SA} + \text{SA}$	$1.68 \times 10^3$	$1.79 \times 10^2$	$1.35 \times 10^1$
$(\text{FSA})_2 \rightarrow \text{FSA} + \text{FSA}$	$1.23 \times 10^8$	$2.48 \times 10^7$	$3.87 \times 10^6$
$(\text{SA})_2 \cdot \text{A} \rightarrow (\text{SA})_2 + \text{A}$	$1.58 \times 10^0$	$7.09 \times 10^{-2}$	$1.97 \times 10^{-3}$
$(\text{SA})_2 \cdot \text{A} \rightarrow \text{SA} \cdot \text{A} + \text{SA}$	$1.20 \times 10^{-2}$	$3.70 \times 10^{-4}$	$6.67 \times 10^{-6}$
$(\text{SA})_2 \cdot (\text{A})_2 \rightarrow (\text{SA})_2 \cdot \text{A} + \text{A}$	$8.35 \times 10^4$	$1.07 \times 10^4$	$9.93 \times 10^2$
$\text{A} \cdot (\text{FSA})_2 \rightarrow (\text{FSA})_2 + \text{A}$	$1.79 \times 10^{-3}$	$5.40 \times 10^{-5}$	$9.48 \times 10^{-7}$
$\text{A} \cdot (\text{FSA})_2 \rightarrow \text{A} \cdot \text{FSA} + \text{FSA}$	$1.06 \times 10^2$	$6.98 \times 10^0$	$2.98 \times 10^{-1}$
$(\text{A})_2 \cdot (\text{FSA})_2 \rightarrow \text{A} \cdot (\text{FSA})_2 + \text{A}$	$2.48 \times 10^0$	$1.68 \times 10^{-1}$	$7.46 \times 10^{-3}$
$(\text{SA})_2 \cdot \text{FSA} \rightarrow (\text{SA})_2 + \text{FSA}$	$6.63 \times 10^6$	$9.52 \times 10^5$	$1.01 \times 10^5$
$(\text{SA})_2 \cdot \text{FSA} \rightarrow \text{SA} \cdot \text{FSA} + \text{SA}$	$1.67 \times 10^4$	$1.84 \times 10^3$	$1.43 \times 10^2$
$\text{SA} \cdot (\text{FSA})_2 \rightarrow (\text{FSA})_2 + \text{SA}$	$3.17 \times 10^4$	$3.03 \times 10^3$	$2.01 \times 10^2$
$\text{SA} \cdot (\text{FSA})_2 \rightarrow \text{SA} \cdot \text{FSA} + \text{FSA}$	$7.77 \times 10^6$	$1.07 \times 10^6$	$1.09 \times 10^5$
$(\text{SA})_3 \rightarrow (\text{SA})_2 + \text{SA}$	$7.21 \times 10^5$	$8.57 \times 10^4$	$7.29 \times 10^3$
$(\text{FSA})_3 \rightarrow (\text{FSA})_2 + \text{FSA}$	$3.79 \times 10^{12}$	$1.45 \times 10^{12}$	$4.74 \times 10^{11}$
$(\text{SA})_3 \cdot \text{A} \rightarrow (\text{SA})_2 \cdot \text{A} + \text{SA}$	$7.77 \times 10^2$	$6.50 \times 10^1$	$3.67 \times 10^0$
$(\text{SA})_3 \cdot \text{A} \rightarrow (\text{SA})_3 + \text{A}$	$1.63 \times 10^{-3}$	$5.16 \times 10^{-5}$	$9.54 \times 10^{-7}$
$(\text{SA})_3 \cdot (\text{A})_2 \rightarrow (\text{SA})_2 \cdot (\text{A})_2 + \text{SA}$	$2.29 \times 10^{-2}$	$8.66 \times 10^{-4}$	$1.97 \times 10^{-5}$
$(\text{SA})_3 \cdot (\text{A})_2 \rightarrow (\text{SA})_3 \cdot \text{A} + \text{A}$	$2.17 \times 10^0$	$1.26 \times 10^{-1}$	$4.68 \times 10^{-3}$
$(\text{SA})_3 \cdot (\text{A})_3 \rightarrow (\text{SA})_3 \cdot (\text{A})_2 + \text{A}$	$1.11 \times 10^2$	$7.11 \times 10^0$	$2.97 \times 10^{-1}$
$\text{A} \cdot (\text{FSA})_3 \rightarrow \text{A} \cdot (\text{FSA})_2 + \text{FSA}$	$1.12 \times 10^4$	$1.13 \times 10^3$	$7.87 \times 10^1$
$\text{A} \cdot (\text{FSA})_3 \rightarrow (\text{FSA})_3 + \text{A}$	$5.07 \times 10^{-12}$	$4.03 \times 10^{-14}$	$1.51 \times 10^{-16}$
$(\text{A})_2 \cdot (\text{FSA})_3 \rightarrow (\text{A})_2 \cdot (\text{FSA})_2 + \text{FSA}$	$1.15 \times 10^5$	$1.15 \times 10^4$	$7.96 \times 10^2$
$(\text{A})_2 \cdot (\text{FSA})_3 \rightarrow \text{A} \cdot (\text{FSA})_3 + \text{A}$	$2.18 \times 10^1$	$1.46 \times 10^0$	$6.45 \times 10^{-2}$
$(\text{A})_3 \cdot (\text{FSA})_3 \rightarrow (\text{A})_2 \cdot (\text{FSA})_3 + \text{A}$	$3.33 \times 10^{-3}$	$1.20 \times 10^{-4}$	$2.59 \times 10^{-6}$
$\text{SA} \cdot \text{FSA} \cdot \text{A} \rightarrow \text{A} \cdot \text{FSA} + \text{SA}$	$4.60 \times 10^2$	$3.67 \times 10^1$	$1.98 \times 10^0$

Continued table

$SA \cdot A \cdot FSA \rightarrow SA \cdot A + FSA$	$5.79 \times 10^0$	$2.75 \times 10^{-1}$	$8.13 \times 10^{-3}$
$SA \cdot A \cdot FSA \rightarrow SA \cdot FSA + A$	$1.91 \times 10^0$	$1.01 \times 10^{-1}$	$3.41 \times 10^{-3}$
$SA \cdot (A)_2 \cdot FSA \rightarrow SA \cdot A \cdot FSA + A$	$6.00 \times 10^7$	$1.04 \times 10^7$	$1.36 \times 10^6$
$(SA)_2 \cdot A \cdot FSA \rightarrow SA \cdot A \cdot FSA + SA$	$8.11 \times 10^5$	$7.82 \times 10^4$	$5.22 \times 10^3$
$(SA)_2 \cdot A \cdot FSA \rightarrow (SA)_2 \cdot A + FSA$	$4.37 \times 10^8$	$6.49 \times 10^7$	$7.10 \times 10^6$
$(SA)_2 \cdot A \cdot FSA \rightarrow (SA)_2 \cdot FSA + A$	$9.95 \times 10^1$	$4.63 \times 10^0$	$1.33 \times 10^{-1}$
$(SA)_2 \cdot (A)_2 \cdot FSA \rightarrow SA \cdot (A)_2 \cdot FSA + SA$	$1.96 \times 10^{-8}$	$2.74 \times 10^{-10}$	$1.97 \times 10^{-12}$
$(SA)_2 \cdot (A)_2 \cdot FSA \rightarrow (SA)_2 \cdot (A)_2 + FSA$	$9.26 \times 10^{-3}$	$2.69 \times 10^{-4}$	$4.49 \times 10^{-6}$
$(SA)_2 \cdot (A)_2 \cdot FSA \rightarrow (SA)_2 \cdot A \cdot FSA + A$	$1.38 \times 10^{-6}$	$3.46 \times 10^{-8}$	$4.91 \times 10^{-10}$
$(SA)_2 \cdot (A)_3 \cdot FSA \rightarrow (SA)_2 \cdot (A)_2 \cdot FSA + A$	$5.28 \times 10^1$	$3.74 \times 10^0$	$1.75 \times 10^{-1}$
$SA \cdot A \cdot (FSA)_2 \rightarrow A \cdot (FSA)_2 + SA$	$2.40 \times 10^6$	$4.40 \times 10^5$	$6.13 \times 10^4$
$SA \cdot A \cdot (FSA)_2 \rightarrow SA \cdot A \cdot FSA + FSA$	$5.91 \times 10^5$	$8.88 \times 10^4$	$9.85 \times 10^3$
$SA \cdot A \cdot (FSA)_2 \rightarrow SA \cdot (FSA)_2 + A$	$1.45 \times 10^{-1}$	$8.37 \times 10^{-3}$	$3.09 \times 10^{-4}$
$SA \cdot (A)_2 \cdot (FSA)_2 \rightarrow (A)_2 \cdot (FSA)_2 + SA$	$2.51 \times 10^4$	$1.92 \times 10^3$	$9.86 \times 10^1$
$SA \cdot (A)_2 \cdot (FSA)_2 \rightarrow SA \cdot (A)_2 \cdot FSA + FSA$	$2.37 \times 10^{-4}$	$5.85 \times 10^{-6}$	$8.09 \times 10^{-8}$
$SA \cdot (A)_2 \cdot (FSA)_2 \rightarrow SA \cdot A \cdot (FSA)_2 + A$	$2.31 \times 10^{-2}$	$6.56 \times 10^{-4}$	$1.07 \times 10^{-5}$
$SA \cdot (A)_3 \cdot (FSA)_2 \rightarrow SA \cdot (A)_2 \cdot (FSA)_2 + A$	$3.38 \times 10^{-5}$	$9.53 \times 10^{-7}$	$1.54 \times 10^{-8}$

**Table S9.** Collision coefficients ( $\beta$ ,  $\text{cm}^3 \text{s}^{-1}$ ) for each cluster

Collisions	$\beta \text{ (cm}^3\text{s}^{-1}\text{)}$		
	298.15 K	278.15 K	258.15 K
SA + A	$1.48 \times 10^{-10}$	$1.38 \times 10^{-10}$	$1.28 \times 10^{-10}$
SA + FSA	$9.85 \times 10^{-11}$	$9.19 \times 10^{-11}$	$8.53 \times 10^{-11}$
FSA + A	$1.49 \times 10^{-10}$	$1.39 \times 10^{-10}$	$1.29 \times 10^{-10}$
SA + SA	$8.69 \times 10^{-11}$	$8.11 \times 10^{-11}$	$7.53 \times 10^{-11}$
FSA + FSA	$1.07 \times 10^{-10}$	$9.95 \times 10^{-11}$	$9.24 \times 10^{-11}$
(SA) <sub>2</sub> + A	$2.23 \times 10^{-10}$	$2.08 \times 10^{-10}$	$1.93 \times 10^{-10}$
SA·A + SA	$1.11 \times 10^{-10}$	$1.03 \times 10^{-10}$	$9.59 \times 10^{-11}$
(SA) <sub>2</sub> ·A + A	$2.24 \times 10^{-10}$	$2.09 \times 10^{-10}$	$1.94 \times 10^{-10}$
(FSA) <sub>2</sub> + A	$1.85 \times 10^{-10}$	$1.72 \times 10^{-10}$	$1.60 \times 10^{-10}$
FSA·A + FSA	$1.28 \times 10^{-10}$	$1.20 \times 10^{-10}$	$1.11 \times 10^{-10}$
(FSA) <sub>2</sub> ·A + A	$1.98 \times 10^{-10}$	$1.85 \times 10^{-10}$	$1.71 \times 10^{-10}$
(SA) <sub>2</sub> + FSA	$1.33 \times 10^{-10}$	$1.24 \times 10^{-10}$	$1.15 \times 10^{-10}$
SA·FSA + SA	$1.03 \times 10^{-10}$	$9.61 \times 10^{-11}$	$8.92 \times 10^{-11}$
(FSA) <sub>2</sub> + SA	$9.89 \times 10^{-11}$	$9.23 \times 10^{-11}$	$8.57 \times 10^{-11}$
SA·FSA + FSA	$1.25 \times 10^{-10}$	$1.16 \times 10^{-10}$	$1.08 \times 10^{-10}$
(SA) <sub>2</sub> + SA	$1.08 \times 10^{-10}$	$1.00 \times 10^{-10}$	$9.32 \times 10^{-11}$
(FSA) <sub>2</sub> + FSA	$1.17 \times 10^{-10}$	$1.09 \times 10^{-10}$	$1.01 \times 10^{-10}$
SA + (SA) <sub>2</sub> ·A	$1.05 \times 10^{-10}$	$9.78 \times 10^{-11}$	$9.08 \times 10^{-11}$
(SA) <sub>3</sub> + A	$2.09 \times 10^{-10}$	$1.95 \times 10^{-10}$	$1.81 \times 10^{-10}$
(SA) <sub>2</sub> ·(A) <sub>2</sub> + SA	$1.23 \times 10^{-10}$	$1.15 \times 10^{-10}$	$1.07 \times 10^{-10}$
(SA) <sub>3</sub> ·A + A	$2.32 \times 10^{-10}$	$2.17 \times 10^{-10}$	$2.01 \times 10^{-10}$
(SA) <sub>3</sub> ·(A) <sub>2</sub> + A	$2.72 \times 10^{-10}$	$2.54 \times 10^{-10}$	$2.35 \times 10^{-10}$
(FSA) <sub>2</sub> ·A + FSA	$1.21 \times 10^{-10}$	$1.13 \times 10^{-10}$	$1.05 \times 10^{-10}$
(FSA) <sub>3</sub> + A	$1.84 \times 10^{-10}$	$1.72 \times 10^{-10}$	$1.60 \times 10^{-10}$
(FSA) <sub>2</sub> ·(A) <sub>2</sub> + FSA	$1.50 \times 10^{-10}$	$1.40 \times 10^{-10}$	$1.30 \times 10^{-10}$
(FSA) <sub>3</sub> ·A + A	$2.10 \times 10^{-10}$	$1.96 \times 10^{-10}$	$1.82 \times 10^{-10}$
(FSA) <sub>3</sub> ·(A) <sub>2</sub> + A	$2.35 \times 10^{-10}$	$2.20 \times 10^{-10}$	$2.04 \times 10^{-10}$
FSA·A + SA	$1.12 \times 10^{-10}$	$1.04 \times 10^{-10}$	$9.69 \times 10^{-11}$
SA·A + FSA	$1.31 \times 10^{-10}$	$1.22 \times 10^{-10}$	$1.14 \times 10^{-10}$
SA·FSA + A	$2.04 \times 10^{-10}$	$1.91 \times 10^{-10}$	$1.77 \times 10^{-10}$
SA·FSA·A + A	$2.05 \times 10^{-10}$	$1.91 \times 10^{-10}$	$1.77 \times 10^{-10}$
SA·FSA·A + SA	$9.92 \times 10^{-11}$	$9.26 \times 10^{-11}$	$8.59 \times 10^{-11}$

$(SA)_2 \cdot A + FSA$	$1.31 \times 10^{-10}$	$1.22 \times 10^{-10}$	$1.14 \times 10^{-10}$
$(SA)_2 \cdot FSA + A$	$2.11 \times 10^{-10}$	$1.97 \times 10^{-10}$	$1.83 \times 10^{-10}$
$SA \cdot FSA \cdot (A)_2 + SA$	$1.06 \times 10^{-10}$	$9.93 \times 10^{-11}$	$9.22 \times 10^{-11}$
$(SA)_2 \cdot (A)_2 + FSA$	$1.57 \times 10^{-10}$	$1.46 \times 10^{-10}$	$1.36 \times 10^{-10}$
$(SA)_2 \cdot FSA \cdot A + A$	$2.09 \times 10^{-10}$	$1.95 \times 10^{-10}$	$1.81 \times 10^{-10}$
$(SA)_2 \cdot FSA \cdot (A)_2 + A$	$2.81 \times 10^{-10}$	$2.62 \times 10^{-10}$	$2.44 \times 10^{-10}$
$(FSA)_2 \cdot A + SA$	$1.00 \times 10^{-10}$	$9.35 \times 10^{-11}$	$8.68 \times 10^{-11}$
$SA \cdot FSA \cdot A + FSA$	$1.22 \times 10^{-10}$	$1.14 \times 10^{-10}$	$1.06 \times 10^{-10}$
$SA \cdot (FSA)_2 + A$	$2.00 \times 10^{-10}$	$1.86 \times 10^{-10}$	$1.73 \times 10^{-10}$
$(FSA)_2 \cdot (A)_2 + SA$	$1.21 \times 10^{-10}$	$1.13 \times 10^{-10}$	$1.05 \times 10^{-10}$
$SA \cdot FSA \cdot (A)_2 + FSA$	$1.33 \times 10^{-10}$	$1.24 \times 10^{-10}$	$1.15 \times 10^{-10}$
$SA \cdot (FSA)_2 \cdot A + A$	$2.14 \times 10^{-10}$	$2.00 \times 10^{-10}$	$1.85 \times 10^{-10}$
$SA \cdot (FSA)_2 \cdot (A)_2 + A$	$2.33 \times 10^{-10}$	$2.17 \times 10^{-10}$	$2.02 \times 10^{-10}$



201 **Table S10.** Total evaporation coefficients ( $\sum\gamma$ , s<sup>-1</sup>) for each cluster

Clusters	$\sum\gamma$ , (s <sup>-1</sup> )		
	298.15 K	278.15 K	258.15 K
SA·A	$1.86 \times 10^5$	$2.89 \times 10^4$	$3.37 \times 10^3$
SA·FSA	$5.85 \times 10^5$	$8.15 \times 10^4$	$8.34 \times 10^3$
A·FSA	$2.01 \times 10^3$	$1.86 \times 10^2$	$1.19 \times 10^1$
(SA) <sub>2</sub>	$1.68 \times 10^3$	$1.79 \times 10^2$	$1.35 \times 10^1$
(FSA) <sub>2</sub>	$1.23 \times 10^8$	$2.48 \times 10^7$	$3.87 \times 10^6$
(SA) <sub>2</sub> ·A	$1.59 \times 10^0$	$7.12 \times 10^{-2}$	$1.98 \times 10^{-3}$
(SA) <sub>2</sub> ·(A) <sub>2</sub>	$8.35 \times 10^4$	$1.07 \times 10^4$	$9.93 \times 10^2$
A·(FSA) <sub>2</sub>	$1.06 \times 10^2$	$6.98 \times 10^0$	$2.98 \times 10^{-1}$
(A) <sub>2</sub> ·(FSA) <sub>2</sub>	$2.48 \times 10^0$	$1.68 \times 10^{-1}$	$7.46 \times 10^{-3}$
(SA) <sub>2</sub> ·FSA	$6.65 \times 10^6$	$9.54 \times 10^5$	$1.01 \times 10^5$
SA·(FSA) <sub>2</sub>	$7.80 \times 10^6$	$1.08 \times 10^6$	$1.09 \times 10^5$
(SA) <sub>3</sub>	$7.21 \times 10^5$	$8.57 \times 10^4$	$7.29 \times 10^3$
(FSA) <sub>3</sub>	$3.79 \times 10^{12}$	$1.45 \times 10^{12}$	$4.74 \times 10^{11}$
(SA) <sub>3</sub> ·A	$7.77 \times 10^2$	$6.50 \times 10^1$	$3.67 \times 10^0$
(SA) <sub>3</sub> ·(A) <sub>2</sub>	$2.19 \times 10^0$	$1.26 \times 10^{-1}$	$4.70 \times 10^{-3}$
(SA) <sub>3</sub> ·(A) <sub>3</sub>	$1.11 \times 10^2$	$7.11 \times 10^0$	$2.97 \times 10^{-1}$
A·(FSA) <sub>3</sub>	$1.12 \times 10^4$	$1.13 \times 10^3$	$7.87 \times 10^1$
(A) <sub>2</sub> ·(FSA) <sub>3</sub>	$1.15 \times 10^5$	$1.15 \times 10^4$	$7.96 \times 10^2$
(A) <sub>3</sub> ·(FSA) <sub>3</sub>	$3.33 \times 10^{-3}$	$1.20 \times 10^{-4}$	$2.59 \times 10^{-6}$
SA·A·FSA	$4.68 \times 10^2$	$3.71 \times 10^1$	$1.99 \times 10^0$
SA·(A) <sub>2</sub> ·FSA	$6.00 \times 10^7$	$1.04 \times 10^7$	$1.36 \times 10^6$
SA <sub>2</sub> ·A·FSA	$4.37 \times 10^8$	$6.49 \times 10^7$	$7.10 \times 10^6$
(SA) <sub>2</sub> ·(A) <sub>2</sub> ·FSA	$9.26 \times 10^{-3}$	$2.69 \times 10^{-4}$	$4.49 \times 10^{-6}$
(SA) <sub>2</sub> ·(A) <sub>3</sub> ·FSA	$5.28 \times 10^1$	$3.74 \times 10^0$	$1.75 \times 10^{-1}$
SA·A·(FSA) <sub>2</sub>	$2.99 \times 10^6$	$5.28 \times 10^5$	$7.12 \times 10^4$
SA·(A) <sub>2</sub> ·(FSA) <sub>2</sub>	$2.51 \times 10^4$	$1.92 \times 10^3$	$9.86 \times 10^1$
SA·(A) <sub>3</sub> ·(FSA) <sub>2</sub>	$3.38 \times 10^{-5}$	$9.53 \times 10^{-7}$	$1.54 \times 10^{-8}$

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**Table S11.** Ratios ( $\beta C/\Sigma\gamma$ ) of monomer collisions to evaporation coefficients for each FSA-involved cluster in this study.  $[SA] = 1.0 \times 10^7$  molecules $\cdot$ cm $^{-3}$ ,  $[A] = 1.0 \times 10^{10}$  molecules $\cdot$ cm $^{-3}$ ,  $[FSA] = 1.0 \times 10^6$  molecules $\cdot$ cm $^{-3}$

Clusters	$\beta C/\Sigma\gamma$		
	298.15 K	278.15 K	258.15 K
Collision with SA monomer: $C = [SA]$			
SA $\cdot$ A	$5.97 \times 10^{-15}$	$3.58 \times 10^{-14}$	$2.85 \times 10^{-13}$
SA $\cdot$ FSA	$1.76 \times 10^{-15}$	$1.18 \times 10^{-14}$	$1.07 \times 10^{-13}$
A $\cdot$ FSA	$5.58 \times 10^{-13}$	$5.62 \times 10^{-12}$	$8.13 \times 10^{-11}$
(SA) $_2$	$6.42 \times 10^{-13}$	$5.61 \times 10^{-12}$	$6.90 \times 10^{-11}$
(FSA) $_2$	$8.03 \times 10^{-18}$	$3.72 \times 10^{-17}$	$2.21 \times 10^{-16}$
(SA) $_2\cdot$ A	$6.60 \times 10^{-10}$	$1.37 \times 10^{-8}$	$4.58 \times 10^{-7}$
(SA) $_2\cdot$ (A) $_2$	$1.48 \times 10^{-14}$	$1.07 \times 10^{-13}$	$1.07 \times 10^{-12}$
A $\cdot$ (FSA) $_2$	$9.44 \times 10^{-12}$	$1.34 \times 10^{-10}$	$2.91 \times 10^{-9}$
(A) $_2\cdot$ (FSA) $_2$	$4.88 \times 10^{-10}$	$6.73 \times 10^{-9}$	$1.40 \times 10^{-7}$
SA $\cdot$ A $\cdot$ FSA	$2.12 \times 10^{-12}$	$2.49 \times 10^{-11}$	$4.33 \times 10^{-10}$
SA $\cdot$ (A) $_2\cdot$ FSA	$1.77 \times 10^{-17}$	$9.57 \times 10^{-17}$	$6.77 \times 10^{-16}$
(SA) $_2\cdot$ (A) $_3\cdot$ FSA	$5.32 \times 10^{-11}$	$7.01 \times 10^{-10}$	$1.39 \times 10^{-8}$
Collision with A monomer: $C = [A]$			
SA $\cdot$ FSA	$3.49 \times 10^{-12}$	$2.34 \times 10^{-11}$	$2.12 \times 10^{-10}$
(SA) $_2$	$1.33 \times 10^{-9}$	$1.16 \times 10^{-8}$	$1.43 \times 10^{-7}$
(FSA) $_2$	$1.50 \times 10^{-14}$	$6.95 \times 10^{-14}$	$4.13 \times 10^{-13}$
(SA) $_2\cdot$ A	$1.41 \times 10^{-6}$	$2.94 \times 10^{-5}$	$9.80 \times 10^{-4}$
A $\cdot$ (FSA) $_2$	$1.87 \times 10^{-8}$	$2.65 \times 10^{-7}$	$5.75 \times 10^{-6}$
(SA) $_2\cdot$ FSA	$3.18 \times 10^{-13}$	$2.07 \times 10^{-12}$	$1.82 \times 10^{-11}$
SA $\cdot$ (FSA) $_2$	$2.56 \times 10^{-13}$	$1.73 \times 10^{-12}$	$1.59 \times 10^{-11}$
(SA) $_3$	$2.90 \times 10^{-12}$	$2.27 \times 10^{-11}$	$2.48 \times 10^{-10}$
(FSA) $_3$	$4.87 \times 10^{-19}$	$1.19 \times 10^{-18}$	$3.37 \times 10^{-18}$
(SA) $_3\cdot$ A	$2.99 \times 10^{-9}$	$3.33 \times 10^{-8}$	$5.47 \times 10^{-7}$
(SA) $_3\cdot$ (A) $_2$	$1.24 \times 10^{-6}$	$2.01 \times 10^{-5}$	$5.00 \times 10^{-4}$
A $\cdot$ (FSA) $_3$	$1.88 \times 10^{-10}$	$1.74 \times 10^{-9}$	$2.31 \times 10^{-8}$
(A) $_2\cdot$ (FSA) $_3$	$2.05 \times 10^{-11}$	$1.91 \times 10^{-10}$	$2.56 \times 10^{-9}$
SA $\cdot$ A $\cdot$ FSA	$4.37 \times 10^{-9}$	$5.14 \times 10^{-8}$	$8.91 \times 10^{-7}$
(SA) $_2\cdot$ A $\cdot$ FSA	$4.78 \times 10^{-15}$	$3.00 \times 10^{-14}$	$2.55 \times 10^{-13}$

Continued table

$(SA)_2 \cdot (A)_2 \cdot FSA$	$3.04 \times 10^{-4}$	$9.75 \times 10^{-3}$	$5.42 \times 10^{-1}$
$SA \cdot A \cdot (FSA)_2$	$7.15 \times 10^{-13}$	$3.78 \times 10^{-12}$	$2.60 \times 10^{-11}$
$SA \cdot (A)_2 \cdot (FSA)_2$	$9.29 \times 10^{-11}$	$1.13 \times 10^{-9}$	$2.04 \times 10^{-8}$
Collision with FSA monomer: $C=[FSA]$			
$SA \cdot A$	$7.07 \times 10^{-16}$	$4.24 \times 10^{-15}$	$3.37 \times 10^{-14}$
$SA \cdot FSA$	$2.13 \times 10^{-16}$	$1.43 \times 10^{-15}$	$1.30 \times 10^{-14}$
$A \cdot FSA$	$6.39 \times 10^{-14}$	$6.44 \times 10^{-13}$	$9.32 \times 10^{-12}$
$(SA)_2$	$7.94 \times 10^{-14}$	$6.93 \times 10^{-13}$	$8.52 \times 10^{-12}$
$(FSA)_2$	$9.48 \times 10^{-19}$	$4.39 \times 10^{-18}$	$2.61 \times 10^{-17}$
$(SA)_2 \cdot A$	$8.26 \times 10^{-11}$	$1.72 \times 10^{-9}$	$5.74 \times 10^{-8}$
$(SA)_2 \cdot (A)_2$	$1.88 \times 10^{-15}$	$1.37 \times 10^{-14}$	$1.37 \times 10^{-13}$
$A \cdot (FSA)_2$	$1.14 \times 10^{-12}$	$1.62 \times 10^{-11}$	$3.52 \times 10^{-10}$
$(A)_2 \cdot (FSA)_2$	$6.05 \times 10^{-11}$	$8.35 \times 10^{-10}$	$1.74 \times 10^{-8}$
$SA \cdot A \cdot FSA$	$2.61 \times 10^{-13}$	$3.07 \times 10^{-12}$	$5.33 \times 10^{-11}$
$SA \cdot (A)_2 \cdot FSA$	$2.22 \times 10^{-18}$	$1.20 \times 10^{-17}$	$8.48 \times 10^{-17}$

208 **Table S12.** Formation rate ( $J$ ,  $s^{-1}$ ) of FSA at  $T = 298.15$  K with  $[SA] = 10^4 - 10^8$  molecules $\cdot$ cm $^{-3}$ ,  $[A]$   
209  $= 10^7 - 10^{11}$  molecules $\cdot$ cm $^{-3}$ , and  $[FSA] = 10^3 - 10^7$  molecules $\cdot$ cm $^{-3}$ .

[SA]	[A]	[FSA] = $10^3$	[FSA] = $10^4$	[FSA] = $10^5$	[FSA] = $10^6$	[FSA] = $10^7$
[SA] = $10^4$	[A] = $10^7$	$2.90 \times 10^{-29}$	$7.30 \times 10^{-28}$	$1.11 \times 10^{-24}$	$9.56 \times 10^{-21}$	$7.88 \times 10^{-17}$
[SA] = $10^4$	[A] = $10^8$	$2.90 \times 10^{-26}$	$7.30 \times 10^{-25}$	$1.11 \times 10^{-21}$	$9.56 \times 10^{-28}$	$7.88 \times 10^{-14}$
[SA] = $10^4$	[A] = $10^9$	$2.90 \times 10^{-23}$	$7.30 \times 10^{-22}$	$1.11 \times 10^{-18}$	$9.56 \times 10^{-15}$	$7.88 \times 10^{-11}$
[SA] = $10^4$	[A] = $10^{10}$	$2.86 \times 10^{-20}$	$7.22 \times 10^{-18}$	$1.11 \times 10^{-15}$	$9.57 \times 10^{-12}$	$7.88 \times 10^{-8}$
[SA] = $10^4$	[A] = $10^{11}$	$2.50 \times 10^{-17}$	$6.59 \times 10^{-16}$	$1.11 \times 10^{-12}$	$9.67 \times 10^{-9}$	$7.95 \times 10^{-5}$
[SA] = $10^5$	[A] = $10^7$	$4.23 \times 10^{-26}$	$2.90 \times 10^{-25}$	$7.29 \times 10^{-24}$	$1.08 \times 10^{-20}$	$7.95 \times 10^{-17}$
[SA] = $10^5$	[A] = $10^8$	$4.23 \times 10^{-23}$	$2.90 \times 10^{-22}$	$7.29 \times 10^{-21}$	$1.08 \times 10^{-17}$	$7.95 \times 10^{-14}$
[SA] = $10^5$	[A] = $10^9$	$4.23 \times 10^{-20}$	$2.90 \times 10^{-19}$	$7.28 \times 10^{-18}$	$1.08 \times 10^{-14}$	$7.95 \times 10^{-11}$
[SA] = $10^5$	[A] = $10^{10}$	$4.19 \times 10^{-17}$	$2.86 \times 10^{-16}$	$7.21 \times 10^{-15}$	$1.08 \times 10^{-11}$	$7.95 \times 10^{-8}$
[SA] = $10^5$	[A] = $10^{11}$	$3.86 \times 10^{-14}$	$2.50 \times 10^{-13}$	$6.57 \times 10^{-12}$	$1.09 \times 10^{-8}$	$8.02 \times 10^{-5}$
[SA] = $10^6$	[A] = $10^7$	$2.01 \times 10^{-22}$	$4.23 \times 10^{-22}$	$2.90 \times 10^{-21}$	$7.14 \times 10^{-20}$	$8.88 \times 10^{-17}$
[SA] = $10^6$	[A] = $10^8$	$2.01 \times 10^{-19}$	$4.23 \times 10^{-19}$	$2.90 \times 10^{-18}$	$7.14 \times 10^{-17}$	$8.88 \times 10^{-14}$
[SA] = $10^6$	[A] = $10^9$	$2.01 \times 10^{-16}$	$4.23 \times 10^{-16}$	$2.89 \times 10^{-15}$	$7.13 \times 10^{-14}$	$8.88 \times 10^{-11}$
[SA] = $10^6$	[A] = $10^{10}$	$2.00 \times 10^{-13}$	$4.19 \times 10^{-13}$	$2.85 \times 10^{-12}$	$7.05 \times 10^{-11}$	$8.88 \times 10^{-8}$
[SA] = $10^6$	[A] = $10^{11}$	$1.97 \times 10^{-10}$	$3.85 \times 10^{-10}$	$2.49 \times 10^{-9}$	$6.39 \times 10^{-8}$	$8.91 \times 10^{-5}$
[SA] = $10^7$	[A] = $10^7$	$1.79 \times 10^{-18}$	$2.01 \times 10^{-18}$	$4.23 \times 10^{-18}$	$2.87 \times 10^{-17}$	$6.03 \times 10^{-16}$
[SA] = $10^7$	[A] = $10^8$	$1.79 \times 10^{-15}$	$2.01 \times 10^{-15}$	$4.23 \times 10^{-15}$	$2.87 \times 10^{-14}$	$6.03 \times 10^{-13}$
[SA] = $10^7$	[A] = $10^9$	$1.79 \times 10^{-12}$	$2.01 \times 10^{-12}$	$4.23 \times 10^{-12}$	$2.86 \times 10^{-11}$	$6.02 \times 10^{-10}$
[SA] = $10^7$	[A] = $10^{10}$	$1.79 \times 10^{-9}$	$2.00 \times 10^{-9}$	$4.17 \times 10^{-9}$	$2.81 \times 10^{-8}$	$5.91 \times 10^{-7}$
[SA] = $10^7$	[A] = $10^{11}$	$1.78 \times 10^{-6}$	$1.96 \times 10^{-6}$	$3.75 \times 10^{-6}$	$2.34 \times 10^{-5}$	$5.07 \times 10^{-4}$
[SA] = $10^8$	[A] = $10^7$	$1.77 \times 10^{-14}$	$1.79 \times 10^{-14}$	$2.02 \times 10^{-14}$	$4.26 \times 10^{-14}$	$2.65 \times 10^{-13}$
[SA] = $10^8$	[A] = $10^8$	$1.77 \times 10^{-11}$	$1.79 \times 10^{-11}$	$2.02 \times 10^{-11}$	$4.26 \times 10^{-11}$	$2.65 \times 10^{-10}$
[SA] = $10^8$	[A] = $10^9$	$1.77 \times 10^{-8}$	$1.79 \times 10^{-8}$	$2.01 \times 10^{-8}$	$4.24 \times 10^{-8}$	$2.63 \times 10^{-7}$
[SA] = $10^8$	[A] = $10^{10}$	$1.77 \times 10^{-5}$	$1.79 \times 10^{-5}$	$2.00 \times 10^{-5}$	$4.07 \times 10^{-5}$	$2.46 \times 10^{-4}$
[SA] = $10^8$	[A] = $10^{11}$	$1.76 \times 10^{-2}$	$1.78 \times 10^{-2}$	$1.90 \times 10^{-2}$	$3.12 \times 10^{-2}$	$1.55 \times 10^{-1}$

210 SA, A and FSA represent sulfuric acid, ammonia and formic sulfuric anhydride, respectively.

211 **Table S13.** Formation rate  $J$  ( $\text{s}^{-1}$ ) of FSA at  $T = 278.15$  K with  $[\text{SA}] = 10^4 - 10^8$  molecules $\cdot\text{cm}^{-3}$ ,  $[\text{A}]$   
 212  $= 10^7 - 10^{11}$  molecules $\cdot\text{cm}^{-3}$ , and  $[\text{FSA}] = 10^3 - 10^7$  molecules $\cdot\text{cm}^{-3}$

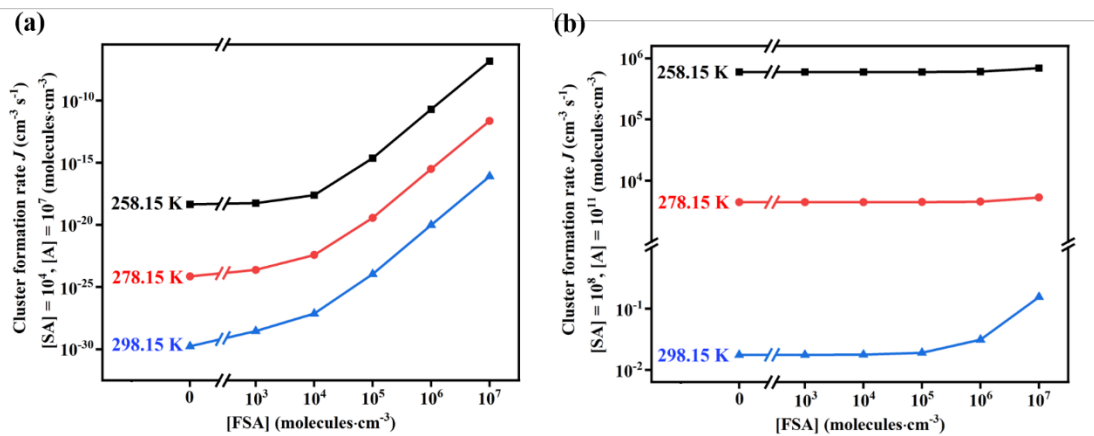
[SA]	[A]	[FSA] = $10^3$	[FSA] = $10^4$	[FSA] = $10^5$	[FSA] = $10^6$	[FSA] = $10^7$
[SA] = $10^4$	[A] = $10^7$	$2.38 \times 10^{-24}$	$3.78 \times 10^{-23}$	$3.70 \times 10^{-20}$	$3.10 \times 10^{-16}$	$2.27 \times 10^{-12}$
[SA] = $10^4$	[A] = $10^8$	$2.37 \times 10^{-21}$	$3.76 \times 10^{-20}$	$3.70 \times 10^{-17}$	$3.11 \times 10^{-13}$	$2.27 \times 10^{-9}$
[SA] = $10^4$	[A] = $10^9$	$2.28 \times 10^{-18}$	$3.60 \times 10^{-17}$	$3.69 \times 10^{-14}$	$3.11 \times 10^{-10}$	$2.27 \times 10^{-6}$
[SA] = $10^4$	[A] = $10^{10}$	$1.75 \times 10^{-15}$	$2.63 \times 10^{-14}$	$3.66 \times 10^{-11}$	$3.12 \times 10^{-7}$	$2.29 \times 10^{-3}$
[SA] = $10^4$	[A] = $10^{11}$	$9.07 \times 10^{-13}$	$1.26 \times 10^{-11}$	$3.77 \times 10^{-8}$	$3.31 \times 10^{-4}$	$2.40 \times 10^0$
[SA] = $10^5$	[A] = $10^7$	$8.77 \times 10^{-21}$	$2.38 \times 10^{-20}$	$3.76 \times 10^{-19}$	$3.56 \times 10^{-16}$	$2.29 \times 10^{-12}$
[SA] = $10^5$	[A] = $10^8$	$8.76 \times 10^{-18}$	$2.37 \times 10^{-17}$	$3.75 \times 10^{-16}$	$3.56 \times 10^{-13}$	$2.29 \times 10^{-9}$
[SA] = $10^5$	[A] = $10^9$	$8.68 \times 10^{-15}$	$2.28 \times 10^{-14}$	$3.59 \times 10^{-13}$	$3.55 \times 10^{-10}$	$2.29 \times 10^{-6}$
[SA] = $10^5$	[A] = $10^{10}$	$8.10 \times 10^{-12}$	$1.75 \times 10^{-11}$	$2.62 \times 10^{-10}$	$3.52 \times 10^{-7}$	$2.30 \times 10^{-3}$
[SA] = $10^5$	[A] = $10^{11}$	$6.46 \times 10^{-9}$	$9.06 \times 10^{-9}$	$1.25 \times 10^{-7}$	$3.61 \times 10^{-4}$	$2.41 \times 10^0$
[SA] = $10^6$	[A] = $10^7$	$7.42 \times 10^{-17}$	$8.78 \times 10^{-17}$	$2.38 \times 10^{-16}$	$3.65 \times 10^{-15}$	$2.58 \times 10^{-12}$
[SA] = $10^6$	[A] = $10^8$	$7.42 \times 10^{-14}$	$8.77 \times 10^{-14}$	$2.37 \times 10^{-13}$	$3.63 \times 10^{-12}$	$2.58 \times 10^{-9}$
[SA] = $10^6$	[A] = $10^9$	$7.40 \times 10^{-11}$	$8.68 \times 10^{-11}$	$2.28 \times 10^{-10}$	$3.47 \times 10^{-9}$	$2.57 \times 10^{-6}$
[SA] = $10^6$	[A] = $10^{10}$	$7.26 \times 10^{-8}$	$8.10 \times 10^{-8}$	$1.73 \times 10^{-7}$	$2.50 \times 10^{-6}$	$2.54 \times 10^{-3}$
[SA] = $10^6$	[A] = $10^{11}$	$6.21 \times 10^{-5}$	$6.43 \times 10^{-5}$	$8.97 \times 10^{-5}$	$1.18 \times 10^{-3}$	$2.58 \times 10^0$
[SA] = $10^7$	[A] = $10^7$	$7.30 \times 10^{-13}$	$7.44 \times 10^{-13}$	$8.85 \times 10^{-13}$	$2.39 \times 10^{-12}$	$2.84 \times 10^{-11}$
[SA] = $10^7$	[A] = $10^8$	$7.30 \times 10^{-10}$	$7.44 \times 10^{-10}$	$8.83 \times 10^{-10}$	$2.37 \times 10^{-9}$	$2.82 \times 10^{-8}$
[SA] = $10^7$	[A] = $10^9$	$7.29 \times 10^{-7}$	$7.42 \times 10^{-7}$	$8.71 \times 10^{-7}$	$2.26 \times 10^{-6}$	$2.66 \times 10^{-5}$
[SA] = $10^7$	[A] = $10^{10}$	$7.17 \times 10^{-4}$	$7.24 \times 10^{-4}$	$8.02 \times 10^{-4}$	$1.63 \times 10^{-3}$	$1.78 \times 10^{-2}$
[SA] = $10^7$	[A] = $10^{11}$	$5.97 \times 10^{-1}$	$5.99 \times 10^{-1}$	$6.18 \times 10^{-1}$	$8.25 \times 10^{-1}$	$7.67 \times 10^0$
[SA] = $10^8$	[A] = $10^7$	$7.49 \times 10^{-9}$	$7.51 \times 10^{-9}$	$7.70 \times 10^{-9}$	$9.50 \times 10^{-9}$	$2.47 \times 10^{-8}$
[SA] = $10^8$	[A] = $10^8$	$7.49 \times 10^{-6}$	$7.51 \times 10^{-6}$	$7.69 \times 10^{-6}$	$9.45 \times 10^{-6}$	$2.43 \times 10^{-5}$
[SA] = $10^8$	[A] = $10^9$	$7.46 \times 10^{-3}$	$7.47 \times 10^{-3}$	$7.61 \times 10^{-3}$	$9.02 \times 10^{-3}$	$2.14 \times 10^{-2}$
[SA] = $10^8$	[A] = $10^{10}$	$7.11 \times 10^0$	$7.12 \times 10^0$	$7.17 \times 10^0$	$7.66 \times 10^0$	$1.24 \times 10^1$
[SA] = $10^8$	[A] = $10^{11}$	$4.43 \times 10^3$	$4.43 \times 10^3$	$4.44 \times 10^3$	$4.52 \times 10^3$	$5.28 \times 10^3$

213 SA, A and FSA represent sulfuric acid, ammonia and formic sulfuric anhydride, respectively

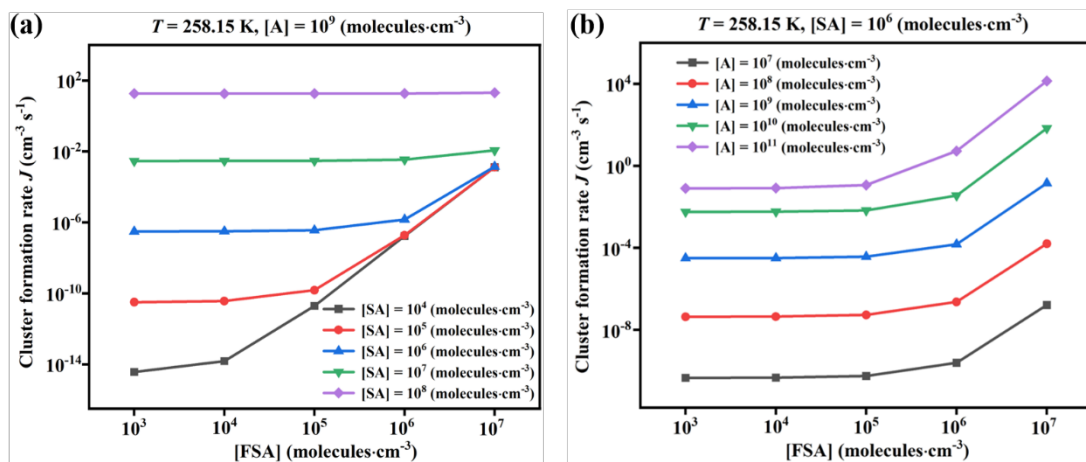
**Table S14.** Formation rate  $J$  ( $\text{s}^{-1}$ ) of FSA at  $T = 258.15$  K with  $[\text{SA}] = 10^4 - 10^8$  molecules $\cdot\text{cm}^{-3}$ ,  $[\text{A}] = 10^7 - 10^{11}$  molecules $\cdot\text{cm}^{-3}$ , and  $[\text{FSA}] = 10^3 - 10^7$  molecules $\cdot\text{cm}^{-3}$

[SA]	[A]	[FSA] = $10^3$	[FSA] = $10^4$	[FSA] = $10^5$	[FSA] = $10^6$	[FSA] = $10^7$
[SA] = $10^4$	[A] = $10^7$	$5.49 \times 10^{-19}$	$2.46 \times 10^{-18}$	$2.28 \times 10^{-15}$	$1.95 \times 10^{-11}$	$1.43 \times 10^{-7}$
[SA] = $10^4$	[A] = $10^8$	$5.25 \times 10^{-16}$	$2.31 \times 10^{-15}$	$2.25 \times 10^{-12}$	$1.92 \times 10^{-8}$	$1.42 \times 10^{-4}$
[SA] = $10^4$	[A] = $10^9$	$3.70 \times 10^{-13}$	$1.52 \times 10^{-12}$	$1.97 \times 10^{-9}$	$1.72 \times 10^{-5}$	$1.29 \times 10^{-1}$
[SA] = $10^4$	[A] = $10^{10}$	$6.90 \times 10^{-11}$	$3.80 \times 10^{-10}$	$9.50 \times 10^{-7}$	$8.49 \times 10^{-3}$	$6.33 \times 10^1$
[SA] = $10^4$	[A] = $10^{11}$	$1.22 \times 10^{-9}$	$6.01 \times 10^{-8}$	$3.52 \times 10^{-4}$	$3.09 \times 10^0$	$1.34 \times 10^4$
[SA] = $10^5$	[A] = $10^7$	$4.55 \times 10^{-15}$	$5.49 \times 10^{-15}$	$2.46 \times 10^{-14}$	$2.20 \times 10^{-11}$	$1.44 \times 10^{-7}$
[SA] = $10^5$	[A] = $10^8$	$4.38 \times 10^{-12}$	$5.25 \times 10^{-12}$	$2.31 \times 10^{-11}$	$2.17 \times 10^{-8}$	$1.43 \times 10^{-4}$
[SA] = $10^5$	[A] = $10^9$	$3.17 \times 10^{-9}$	$3.70 \times 10^{-9}$	$1.52 \times 10^{-8}$	$1.90 \times 10^{-5}$	$1.29 \times 10^{-1}$
[SA] = $10^5$	[A] = $10^{10}$	$5.93 \times 10^{-7}$	$6.88 \times 10^{-7}$	$3.78 \times 10^{-6}$	$9.15 \times 10^{-3}$	$6.36 \times 10^1$
[SA] = $10^5$	[A] = $10^{11}$	$8.51 \times 10^{-6}$	$1.21 \times 10^{-5}$	$5.93 \times 10^{-4}$	$3.22 \times 10^0$	$1.34 \times 10^4$
[SA] = $10^6$	[A] = $10^7$	$4.47 \times 10^{-11}$	$4.56 \times 10^{-11}$	$5.52 \times 10^{-11}$	$2.44 \times 10^{-10}$	$1.60 \times 10^{-7}$
[SA] = $10^6$	[A] = $10^8$	$4.31 \times 10^{-8}$	$4.39 \times 10^{-8}$	$5.27 \times 10^{-8}$	$2.28 \times 10^{-7}$	$1.58 \times 10^{-4}$
[SA] = $10^6$	[A] = $10^9$	$3.10 \times 10^{-5}$	$3.15 \times 10^{-5}$	$3.67 \times 10^{-5}$	$1.47 \times 10^{-4}$	$1.41 \times 10^{-1}$
[SA] = $10^6$	[A] = $10^{10}$	$5.69 \times 10^{-3}$	$5.78 \times 10^{-3}$	$6.69 \times 10^{-3}$	$3.56 \times 10^{-2}$	$6.72 \times 10^1$
[SA] = $10^6$	[A] = $10^{11}$	$7.92 \times 10^{-2}$	$8.19 \times 10^{-2}$	$1.16 \times 10^{-1}$	$5.25 \times 10^0$	$1.37 \times 10^4$
[SA] = $10^7$	[A] = $10^7$	$4.54 \times 10^{-7}$	$4.55 \times 10^{-7}$	$4.66 \times 10^{-7}$	$5.79 \times 10^{-7}$	$2.26 \times 10^{-6}$
[SA] = $10^7$	[A] = $10^8$	$4.34 \times 10^{-4}$	$4.34 \times 10^{-4}$	$4.44 \times 10^{-4}$	$5.43 \times 10^{-4}$	$2.05 \times 10^{-3}$
[SA] = $10^7$	[A] = $10^9$	$2.92 \times 10^{-1}$	$2.92 \times 10^{-1}$	$2.97 \times 10^{-1}$	$3.44 \times 10^{-1}$	$1.15 \times 10^0$
[SA] = $10^7$	[A] = $10^{10}$	$4.53 \times 10^1$	$4.53 \times 10^1$	$4.59 \times 10^1$	$5.18 \times 10^1$	$2.24 \times 10^2$
[SA] = $10^7$	[A] = $10^{11}$	$5.53 \times 10^2$	$5.54 \times 10^2$	$5.68 \times 10^2$	$7.49 \times 10^2$	$1.89 \times 10^2$
[SA] = $10^8$	[A] = $10^7$	$5.34 \times 10^{-3}$	$5.34 \times 10^{-3}$	$5.37 \times 10^{-3}$	$5.66 \times 10^{-3}$	$7.69 \times 10^{-3}$
[SA] = $10^8$	[A] = $10^8$	$4.65 \times 10^0$	$4.65 \times 10^0$	$4.67 \times 10^0$	$4.83 \times 10^0$	$6.12 \times 10^0$
[SA] = $10^8$	[A] = $10^9$	$1.84 \times 10^3$	$1.84 \times 10^3$	$1.84 \times 10^3$	$1.86 \times 10^3$	$2.03 \times 10^3$
[SA] = $10^8$	[A] = $10^{10}$	$1.03 \times 10^5$	$1.03 \times 10^5$	$1.03 \times 10^5$	$1.03 \times 10^5$	$1.09 \times 10^5$
[SA] = $10^8$	[A] = $10^{11}$	$5.97 \times 10^5$	$5.97 \times 10^5$	$5.97 \times 10^5$	$6.03 \times 10^5$	$6.87 \times 10^5$

SA, A and FSA represent sulfuric acid, ammonia and formic sulfuric anhydride, respectively

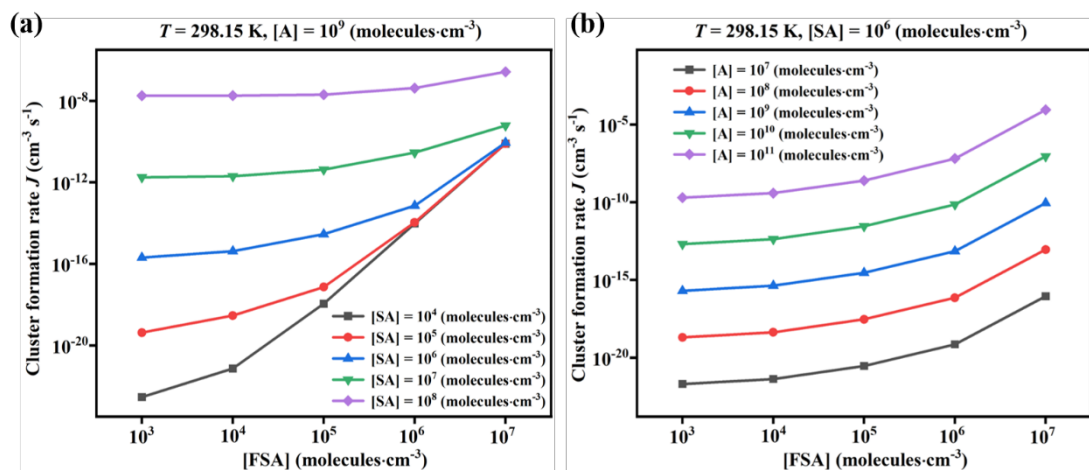


**Fig. S14.** (a) Cluster formation rate ( $J$ ,  $\text{cm}^3 \text{s}^{-1}$ ) with  $[SA] = 10^4$   $\text{molecules} \cdot \text{cm}^{-3}$ ,  $[A] = 10^7$   $\text{molecules} \cdot \text{cm}^{-3}$  at three temperatures, (b) Cluster formation rate ( $J$ ,  $\text{cm}^3 \text{s}^{-1}$ ) with  $[SA] = 10^8$   $\text{molecules} \cdot \text{cm}^{-3}$ ,  $[A] = 10^{11}$   $\text{molecules} \cdot \text{cm}^{-3}$  at three temperatures (black: 258.15 K, red: 278.15 K, blue: 298.15 K)

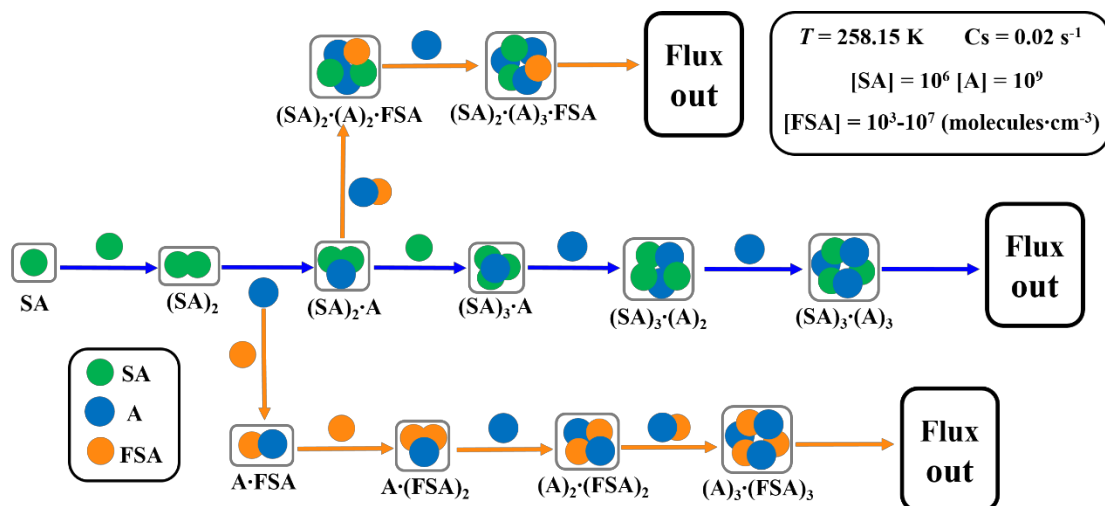


**Fig. S15.** The cluster formation rate ( $J$ ,  $\text{cm}^3 \text{s}^{-1}$ ) as a function of (a)  $[SA]$  and (b)  $[A]$ , with different concentrations of  $[FSA] = 10^3$ - $10^7 \text{ molecules} \cdot \text{cm}^{-3}$  at 258.15 K.

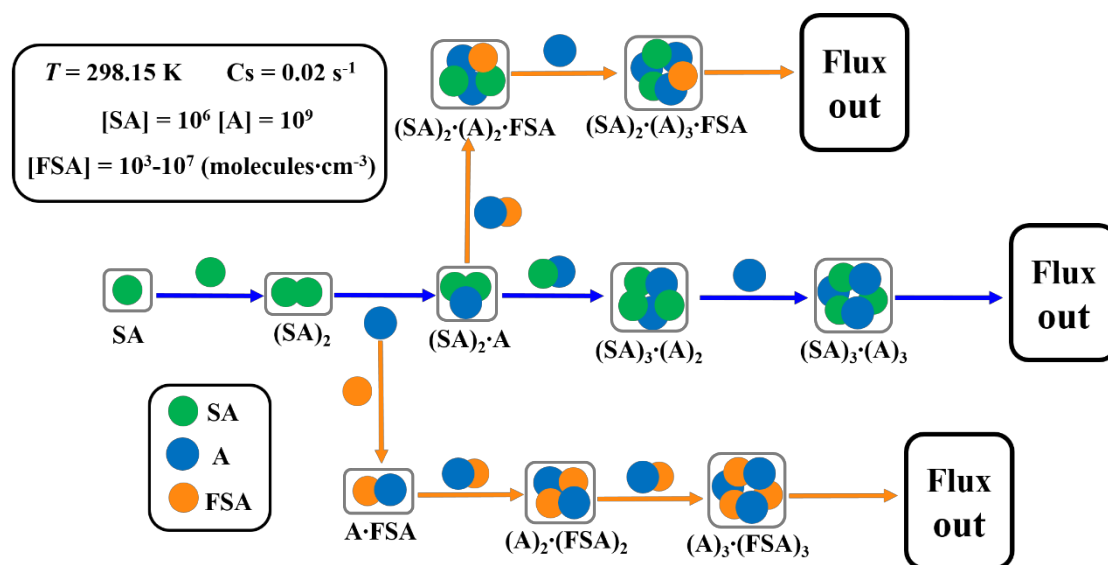




**Fig. S16.** The cluster formation rate ( $J$ ,  $\text{cm}^3 \text{ s}^{-1}$ ) as a function of (a)  $[SA]$  and (b)  $[A]$ , with different concentrations of  $[FSA] = 10^3$ - $10^7 \text{ molecules}\cdot\text{cm}^{-3}$  at 298.15 K



**Fig. S17.** Main pathways of clusters growth under conditions of  $T = 258.15 \text{ K}$ ,  $[\text{SA}] = 10^6$  molecules·cm<sup>-3</sup>,  $[\text{A}] = 10^9$  molecules·cm<sup>-3</sup>, and  $[\text{FSA}] = 10^3\text{-}10^7$  molecules·cm<sup>-3</sup>. Blue and orange fluxes represent the pathways of the SA-A-based and SA-A-FSA-based cluster, respectively



**Fig. S18.** Main pathways of clusters growth under conditions of  $T = 298.15 \text{ K}$ ,  $[SA] = 10^6$  molecules·cm<sup>-3</sup>,  $[A] = 10^9$  molecules·cm<sup>-3</sup>, and  $[FSA] = 10^3\text{-}10^7$  molecules·cm<sup>-3</sup>. The blue and orange fluxes represent the pathways of the SA-A-based and SA-A-FSA-based cluster, respectively

**Table S15.** Cartesian coordinates of all molecules and clusters in this study

SA

Atom	X	Y	Z
S	-0.00000100	0.00000200	-0.15545600
O	0.65765000	-1.06508500	-0.82224200
O	-0.65766000	1.06510800	-0.82220400
O	1.02424100	0.67764400	0.84020100
O	-1.02423000	-0.67766800	0.84019400
H	1.69311900	0.03016000	1.09984500
H	-1.69310700	-0.03019100	1.09986300

A

Atom	X	Y	Z
N	0.00000000	0.11213000	0.00000000
H	-0.94020500	-0.26169700	0.00000000
H	0.47010300	-0.26160800	0.81428100
H	0.47010300	-0.26160800	-0.81428100

FSA

Atom	X	Y	Z
S	-0.73245600	-0.00003100	0.084092000
O	-1.86438700	-0.67719800	-0.41027000
O	-0.37942100	1.13847800	-0.92486400
O	-0.61218900	0.46342500	1.41730000
O	1.78817900	-0.59587800	-0.05562900
H	0.51177600	-1.04252700	-0.16626600
C	2.47070900	-1.44826000	-0.09353000
H	2.10711400	0.54561400	0.04517600
O	0.41637300	1.60168100	-0.60677600

SA·A

Atom	X	Y	Z
S	-0.59827600	-0.11336800	0.08617500
O	0.10893200	-0.09214100	1.32834700
O	-1.74906500	-0.92894600	-0.10565200
O	0.39576600	-0.37422800	-1.06128100
O	-1.03681100	1.39710200	-0.16132600
H	1.37463300	-0.19089300	-0.73462700
H	-1.78503200	1.40349300	-0.77106700
N	2.73855300	0.04357600	-0.05140800
H	3.20053200	0.91724700	-0.27070200
H	3.40981800	-0.70549900	-0.16620600

247

248

H	2.45200800	0.07021600	0.92295000
FSA·A			
Atom	X	Y	Z
S	-2.06986300	-1.43720000	-0.02487300
O	-2.28947300	-0.45708400	0.19881300
O	-1.74977800	-1.89068700	0.82786100
O	-2.84681600	-1.92440600	-0.45419300
O	0.87085200	-0.31194100	0.02282000
H	2.28806200	-0.35459200	-0.03984100
H	0.16258200	-0.81847000	-1.16009200
N	0.21548900	-0.69441000	1.25156800
H	-0.61216000	1.88395400	-0.03391400
H	0.60096100	1.37010700	-0.07332800
C	-0.55396200	2.97630800	-0.08844400
H	-1.65868000	1.29398800	0.04496400
O	-1.19891900	-1.32936600	-0.65773400

249

250

(SA) <sub>2</sub>			
Atom	X	Y	Z
S	2.03944100	0.07517400	0.11329500
O	1.06831400	-0.09670000	1.16086600
O	3.31172000	0.62626400	0.39691600
O	2.20680700	-1.37335100	-0.48979500
H	2.98774000	-1.40489100	-1.05933100
O	1.41198000	0.87974800	-1.04535300
H	0.44673500	0.64256800	-1.15033500
O	-1.06831700	0.09668400	-1.16087000
S	-2.03944300	-0.07517400	-0.11329500
O	-1.41198700	-0.87975200	1.04535400
O	-3.31172900	-0.62625000	-0.39691000
O	-2.20678900	1.37335500	0.48979100
H	-0.44674000	-0.64257900	1.15033500
H	-2.98771900	1.40490700	1.05933100

251

252

(FSA) <sub>2</sub>			
Atom	X	Y	Z
S	-2.10673800	-0.64032400	-0.24218500
O	-3.16703900	-1.51334400	-0.55398700
O	-1.52529400	-0.99650900	1.13623900
O	-1.04397200	-0.39901200	-1.17532800
C	-2.13419400	1.83567000	0.56745300

O	-2.82560300	0.78565000	0.01405000
H	-2.78175100	2.71571600	0.54331000
O	-1.03853400	1.77228500	1.00367700
H	-0.58548000	-0.67711000	1.22411800
S	2.10673800	-0.64032400	0.24218400
O	3.16703900	-1.51334400	0.55398700
O	1.52529400	-0.99650900	-1.13623900
O	1.04397200	-0.39901200	1.17532900
C	2.13419400	1.83567000	-0.56745300
O	2.82560300	0.78565000	-0.01405100
H	2.78175100	2.71571600	-0.54331100
O	1.03853300	1.77228500	-1.00367600
H	0.58547900	-0.67711100	-1.22411600

253

254 SA·FSA

Atom	X	Y	Z
S	2.22843800	-0.00423900	0.07863900
O	3.23791900	0.97524400	0.24010300
O	1.27077300	-0.25369000	1.12244200
O	2.90768300	-1.40834000	-0.15214600
O	1.49401400	0.26141300	-1.25288200
H	3.74994700	-1.28862800	-0.61125600
H	0.56250200	-0.08538900	-1.23312600
S	-1.93817600	-0.60901300	-0.05970300
O	-3.06674300	-1.45127200	-0.05756800
O	-1.24859400	-0.62326500	1.30624500
O	-0.95965800	-0.70137600	-1.10956400
C	-1.73682200	1.97561700	-0.03610200
O	-2.56398900	0.88882400	-0.12069700
H	-2.34435400	2.88083400	-0.11348900
O	-0.56291500	1.92177700	0.10376500
H	-0.25926600	-0.42300400	1.23392100

255

256 (SA)<sub>2</sub>·A

Atom	X	Y	Z
S	-1.77231300	-0.34077900	-0.04909000
O	-1.07131700	0.16352900	1.14296700
O	-0.99847000	-1.34675900	-0.75741300
O	-3.07876600	-1.07528900	0.45986500
H	-2.85067000	-1.96938800	0.74413600
O	-2.28848200	0.74869000	-0.85700500
H	-1.40689900	2.09302200	-0.44210900
O	1.42804700	1.08270500	-0.53209900

S	2.06372500	-0.11895200	-0.01742600
O	1.43416000	-0.42809800	1.36683400
O	3.47167000	-0.14405700	0.10310200
O	1.62893900	-1.30669600	-0.91181400
H	0.44446700	-0.24695300	1.34915800
H	0.63395000	-1.35519900	-0.95819300
N	-0.64527900	2.68400200	-0.01766800
H	0.24045900	2.13587500	-0.15608200
H	-0.82981700	2.75595300	0.97931500
H	-0.58337400	3.60217400	-0.44379900

257

258 SA·A·FSA

Atom	X	Y	Z
S	0.55397800	2.48299400	-0.70439700
O	0.45073600	3.03570100	0.14224400
O	-0.24090200	1.81899900	-0.72850000
O	0.55144200	3.07525400	-1.52784700
O	2.13527700	-0.46863900	-0.40785800
H	3.00805500	-1.52978200	-0.75383900
H	2.68481300	0.87791700	-0.40902500
N	0.80219000	-0.48805700	-1.02270300
H	1.05345300	0.02665000	1.93691500
H	1.81162200	-0.79790800	1.20606800
S	0.96935400	-0.36474900	2.95539900
O	0.53492900	1.03427100	1.55561300
O	1.44609600	1.92109200	-0.62581400
O	-2.37916900	-0.14053600	-0.01737800
O	-1.84312000	1.07847500	-0.55578700
H	-3.21751400	-0.11977900	1.12909100
H	-1.25121700	-1.15558600	0.21694100
C	-3.19108800	-0.76047000	-1.22541400
H	-0.40838300	-0.93672100	-0.33532800
O	-3.77401000	-1.45628600	-0.89463100

259

260 (FSA)<sub>2</sub>·A

Atom	X	Y	Z
N	0.53599000	1.62901700	1.53538100
H	1.33593800	1.86879000	0.92730000
H	0.73156800	0.67470000	1.86455300
H	0.44707100	2.27841600	2.30898800
S	1.82396600	-0.88183100	-0.13231500
O	1.80719000	-2.19493100	-0.66933400
O	0.78405400	0.02834200	-0.65823700

O	2.03005200	-0.70863300	1.28211100
C	3.54095800	1.04184400	-0.61837800
O	3.20543000	-0.22448100	-0.83384200
H	4.47964800	1.26606200	-1.13446400
O	2.93793700	1.85135900	0.03095800
H	-0.33133500	1.59116000	0.97715900
S	-2.52000400	0.36564800	-0.62012600
O	-3.66487200	0.56839600	-1.41984700
O	-1.50362100	-0.51119700	-1.31541400
O	-1.89506900	1.47643000	0.04285400
C	-2.24247400	-1.05306800	1.54702500
O	-3.07199100	-0.63666600	0.56714800
H	-2.78840400	-1.72915800	2.21135200
O	-1.10228300	-0.73486600	1.67210600
H	-0.49533300	-0.33683700	-1.02340400

261

262 (SA)<sub>3</sub>

Atom	X	Y	Z
S	0.17750700	1.30695000	-0.05944900
O	-0.09390200	0.06719200	-0.78009000
O	1.37463700	1.98332600	-0.44312400
H	3.10843900	1.28610800	-0.37359300
O	0.17205700	0.99707200	1.45713200
O	-1.00451000	2.25666600	-0.18455500
O	3.82087700	0.61891100	-0.31555500
S	3.23113400	-0.76663900	0.09084400
O	4.31169100	-1.65664100	0.25254200
O	2.42122500	-1.20817600	-1.17323700
O	-2.41639300	-1.20536900	-1.04774400
H	1.51320800	-0.84728200	-1.14877900
H	-1.52390100	-0.77676800	-0.99149200
O	2.28428500	-0.56330900	1.16270100
O	-3.14100400	0.86502300	0.01296900
H	0.93006700	0.38422300	1.63170700
H	-1.88155500	1.76156800	-0.09917000
O	-4.69818200	-1.03136200	-0.32527500
S	-3.39889000	-0.55000200	-0.04775200
O	-2.91048600	-1.08369200	1.35077700
H	-3.26462400	-1.96992300	1.51070800

263

264 (FSA)<sub>3</sub>

Atom	X	Y	Z
S	-3.23194400	-0.59637700	-0.25851000



O	-4.51319100	-0.86236400	-0.79376300
O	-2.16008800	-1.00223500	-1.29416100
O	-2.89865700	0.66721800	0.37672000
C	-1.85890000	-1.89976900	1.47204800
O	-3.06403200	-1.70774200	0.87655800
H	-1.98901700	-2.60927700	2.25876100
O	-0.84291000	-1.38849500	1.16683800
H	-1.29933600	-0.54007000	-1.10837700
S	0.10009300	2.06276100	-0.68190000
O	0.68944600	2.80847500	-1.72092700
O	-1.24487000	2.69328800	-0.27988000
O	-0.06913400	0.63672600	-0.77376700
C	0.63470800	1.90232600	1.85577600
O	1.02955900	2.34576900	0.60712100
H	1.44694200	2.12286300	2.55616800
O	-0.41216400	1.38226800	2.09994300
H	-1.84632800	2.00376500	0.11677500
S	3.07446000	-0.57195000	0.10911000
O	4.22086400	-0.50151200	0.92477800
O	1.84116100	-0.60394300	1.05586400
O	2.81545200	0.29037500	-0.98445400
C	2.06960000	-2.60418700	-1.11004100
O	3.15002600	-2.10354300	-0.48818400
H	2.36905000	-3.56437900	-1.57315100
O	0.97890500	-2.08765900	-1.12358800
H	1.00155600	-0.64709400	0.55113200

265

266 (SA)<sub>2</sub>·FSA

Atom	X	Y	Z
S	0.31393300	0.27128100	0.80272400
O	1.41010300	1.14724900	1.09984700
O	-0.86402600	0.38006700	1.61620000
O	0.76621500	0.97877800	-0.09423400
O	-0.03223000	-1.06706500	-0.95553900
H	1.68969000	-1.50955800	-0.84556300
H	-0.90520200	-1.19916600	0.89051400
S	-3.54538300	0.50006100	-0.68317400
O	-4.49435400	-1.30305700	0.52329200
O	-3.27097300	0.08072500	-0.90098400
O	-2.31119600	-0.76729700	-0.24322500
C	-3.72422400	-1.80240900	-0.34368500
O	-4.34249300	-0.42685700	1.22451000
H	-4.41327900	-0.82986600	-0.97754600

O	-2.62724100	1.77061100	-0.73336400
H	-2.33757500	0.55060600	-0.76049900
S	4.17910500	2.51668200	-1.13704700
O	5.55665000	1.96342400	-0.33226800
O	3.19718500	-0.06954300	1.36773100
O	3.73034400	-0.24299300	-0.32449600
O	3.99097900	-0.56491400	-0.36294300
H	4.45057900	-1.25396600	-0.04119100
H	3.02693100	0.34216500	-1.71845100

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268

SA·(FSA)<sub>2</sub>

Atom	X	Y	Z
S	0.00000300	-0.00002800	0.64830500
O	-0.75790100	0.97127900	-0.09591600
O	0.75794500	-0.97141300	-0.09578700
O	-0.93532600	-0.74113000	1.61626600
O	0.93529600	0.74117800	1.61622700
H	-1.89125600	-0.51059200	1.45471200
H	1.89122100	0.51056900	1.45478500
S	4.12652700	-0.41133700	0.05570600
O	5.38190600	-1.04011800	0.15954000
O	3.18315600	-1.22394000	-0.83248000
O	3.43564500	0.04122300	1.23295100
C	3.38169200	1.71437500	-1.22313300
O	4.41750700	0.90281500	-0.85685100
H	3.78099100	2.54795700	-1.80636700
O	2.24469900	1.52681200	-0.94873200
H	2.21091700	-1.07916900	-0.58578700
S	-4.12653200	0.41133400	0.05572300
O	-5.38190500	1.04011300	0.15962200
O	-3.18316800	1.22400700	-0.83241000
O	-3.43564800	-0.04131800	1.23293200
C	-3.38168200	-1.71429500	-1.22323100
O	-4.41750600	-0.90274600	-0.85692800
H	-3.78097400	-2.54781300	-1.80656000
O	-2.24470000	-1.52677500	-0.94875300
H	-2.21093000	1.07916500	-0.58578600

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270

(SA)<sub>2</sub>·(A)<sub>2</sub>

Atom	X	Y	Z
S	-2.06184100	0.03024000	-0.13465200
O	-2.04117600	1.44224200	0.23783700
O	-3.44180400	-0.18999500	-0.89528300

O	-1.07447700	-0.35111100	-1.12711700
O	-2.07527000	-0.85956100	1.02215600
H	-0.62565200	2.17366500	0.71126100
H	-4.16339900	0.11236500	-0.33044200
S	2.14824600	-0.06917100	-0.20933500
O	1.98617900	-1.44915800	-0.67010100
O	1.31072900	0.84270300	-1.21025200
O	1.44496800	0.08726200	1.09667700
O	3.46837600	0.47040600	-0.23135200
H	0.82649800	-2.09927000	0.18550400
H	0.42274300	0.42956900	-1.33621000
N	0.16605000	-2.42220400	0.96179200
H	-0.03648600	-3.41297000	0.89015000
H	0.64646900	-2.21664600	1.83389300
H	-0.71778100	-1.86109400	0.94374900
N	0.35020200	2.43893700	0.98896700
H	0.35301500	3.05370700	1.79434900
H	0.86196200	1.50602200	1.17669400
H	0.81620300	2.87810800	0.19901900

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272 SA·(A)<sub>2</sub>·FSA

Atom	X	Y	Z
N	-0.56014400	-2.50162300	-1.18465600
H	-0.51312700	-3.31715500	-0.58087000
H	0.24189900	-1.86322200	-0.91499800
H	-0.49089300	-2.76590600	-2.16129700
S	-2.01210800	0.36785000	-0.31238200
O	-2.62217700	1.67359200	-0.33240400
O	-2.86486200	-0.78410300	-0.47660100
O	-0.76692500	0.28066100	-1.05249400
C	-0.91367900	-0.71721100	1.84228300
O	-1.51723600	0.35112600	1.30152900
H	-0.57047200	-0.46665600	2.84999400
O	-0.78402900	-1.78897100	1.33362300
H	-1.44645400	-2.00919800	-0.99711800
S	2.27254000	-0.09072400	0.06125900
O	1.71174100	-1.31696200	-0.48662400
O	3.65606800	-0.17762300	0.42225600
O	1.39806600	0.55074600	1.04932200
O	2.21153500	0.99868500	-1.15471900
H	0.58368300	1.79927500	0.53551600
H	3.04161700	0.92588300	-1.63930400
N	0.14155800	2.61144100	-0.00672300

H	0.55313300	3.49885700	0.25954500
H	-0.88044200	2.61495600	0.10152100
H	0.34885200	2.38648600	-0.98017800

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274 (A)<sub>2</sub>·(FSA)<sub>2</sub>

Atom	X	Y	Z
N	0.51148200	2.21605000	0.26359000
H	1.25940400	2.30709700	-0.42793300
H	0.90111700	1.54792200	0.95568500
H	0.28671200	3.11166600	0.68183300
S	2.00305500	-0.65065500	0.17540100
O	1.96884000	-2.07899400	0.23914100
O	1.28396600	-0.07317100	-0.95522100
O	1.80990200	0.07670500	1.41292700
C	4.01436400	0.89889400	-0.42278200
O	3.61354300	-0.35473100	-0.20718100
H	5.08904000	0.90567600	-0.63275600
O	3.33419100	1.88415700	-0.40110200
H	-0.32876000	1.77240300	-0.18012500
S	-2.85590100	0.42548300	-0.36412200
O	-3.93486700	1.34816000	-0.43110200
O	-3.12220300	-0.94470500	-0.76286000
O	-1.56411400	0.89502700	-0.85432000
C	-1.73688800	-0.53841800	1.81611900
O	-2.61719500	0.32824700	1.31127800
H	-1.77253100	-0.50324200	2.91060600
O	-1.00327200	-1.24862300	1.19472600
H	-1.64200600	-1.71722000	-1.14245700
N	-0.65735500	-1.99590300	-1.35904500
H	-0.07627600	-1.13464800	-1.37477700
H	-0.58601000	-2.49305000	-2.23965100
H	-0.27922600	-2.55431300	-0.59300400

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276 (SA)<sub>3</sub>·A

Atom	X	Y	Z
N	-0.08306900	0.43034300	2.52884500
H	-0.96686500	0.21892000	2.01889600
H	0.62338000	-0.24748900	2.20270400
H	-0.22034100	0.36070000	3.53139300
S	1.14064300	1.97416100	-0.15831000
O	0.06648000	0.98458200	-0.29616000
O	1.25367800	2.50665600	1.17335800
H	0.26824900	1.36202900	2.25930200

O	2.38467600	1.45066900	-0.74121700
S	-2.89899900	-0.31614900	-0.11437500
O	-2.20892100	-1.35592600	-1.04413200
O	-2.49532900	1.05527200	-0.72151700
O	-4.29806300	-0.45733500	-0.25192500
O	-2.29521200	-0.43001100	1.19720400
H	-1.28439900	-1.55011900	-0.76684000
H	-1.51456700	1.18329100	-0.61120100
S	1.62500000	-1.74705900	-0.06495200
O	2.49474900	-3.05585900	-0.03919200
O	2.25892200	-0.95907300	-1.19405200
O	0.28429300	-2.14902000	-0.39499600
O	1.85113600	-1.10561700	1.19884400
H	2.13547100	-3.69945900	-0.66426200
H	2.33436100	0.08623200	-0.99483800
O	0.75413400	3.22380900	-1.04837100
H	0.93553700	3.03305100	-1.97763000

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278 (SA)<sub>2</sub>·A·FSA

Atom	X	Y	Z
N	-0.37923500	-1.61848700	0.51393000
H	-0.72962600	-2.40970400	1.04954400
H	0.61354800	-1.73754800	0.24637300
H	-0.97316100	-1.47534100	-0.31706500
S	-0.23533500	1.63051300	-0.41786400
O	-0.59344800	2.73170700	-1.26140300
O	-1.27494000	1.13832600	0.51765900
O	0.48704200	0.49589900	-1.04079700
C	1.47787000	1.52350300	1.56386900
O	0.92242100	2.30063300	0.61194800
H	2.24428000	2.09621900	2.09896000
O	1.18910400	0.37975000	1.79207600
H	-0.43577500	-0.75476800	1.07033400
S	3.46041000	-0.86448500	-0.13695200
O	2.35495100	-1.80366900	-0.11698500
O	4.25092200	-0.61065900	1.03805700
O	2.97998300	0.49720400	-0.72930600
O	4.43249900	-1.41597100	-1.27920500
H	1.98448300	0.47621100	-0.98085100
H	5.32608200	-1.07672400	-1.11191400
S	-3.72981600	-0.75109400	-0.18716200
O	-2.66648800	-1.11059000	-1.10242900
O	-5.07856600	-1.19843800	-0.37289200

O	-3.75240800	0.78833300	0.05631900
O	-3.18410400	-1.31740600	1.23325100
H	-2.79817900	1.10930800	0.18164000
H	-3.90410900	-1.27914400	1.88357000

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280 SA·A·(FSA)<sub>2</sub>

Atom	X	Y	Z
N	-0.12726200	-1.84684600	-0.42365600
H	0.30849300	-1.60355300	0.47046200
H	-0.28726300	-0.95610800	-0.90261100
H	0.51118100	-2.42022500	-0.96687400
S	-3.40300200	-0.97176800	-0.54312600
O	-4.70177800	-0.85341600	-1.09550800
O	-2.88019700	-2.29154100	-0.28317200
O	-2.36887300	-0.11436700	-1.18227100
C	-2.55236400	-0.17279100	1.80472900
O	-3.58880700	-0.26086200	0.95576800
H	-2.88968400	0.28121100	2.74123200
O	-1.43280000	-0.52042400	1.58134300
H	-1.05776800	-2.27053000	-0.27560300
S	-0.25221100	2.13698400	0.04135500
O	0.43061200	0.96247800	-0.48801800
O	0.04848200	2.56374800	1.36310400
O	-1.73585800	1.98059400	-0.17501200
O	0.16874700	3.28151800	-0.96129200
H	-2.04361000	1.05180300	-0.67223200
H	0.08108400	4.14035300	-0.52685300
S	3.56124100	-0.57648400	-0.61780300
O	4.82862700	-0.50502300	-1.23130200
O	2.96657000	0.82490200	-0.47074200
O	2.56900100	-1.51049300	-1.04742500
C	2.94634400	-1.06786900	1.86862000
O	3.92467600	-0.93558800	0.94565400
H	3.40228000	-1.26938700	2.84190000
O	1.77876500	-0.97724300	1.66017700
H	1.94844500	0.84432700	-0.44116800

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282 A·(FSA)<sub>3</sub>

Atom	X	Y	Z
N	-0.31846600	-1.49948400	0.67567200
H	-1.00334800	-2.06692100	0.16388500
H	-0.77180200	-1.15287300	1.52238100
H	0.54405300	-2.00898400	0.86222200

S	-3.42516100	-0.19026100	0.29706900
O	-4.27466000	0.93609500	0.38980700
O	-2.28213200	0.00913100	0.69515100
O	-2.97552600	-0.87595500	1.46499600
C	-3.74718800	-2.48517100	0.88445500
O	-4.29436800	-1.29629000	0.56047200
H	-4.49879900	-3.09560300	1.39193400
O	-2.62659800	-2.82814200	0.66717500
H	-0.06789300	-0.67510200	0.10923100
S	0.26628700	2.09574900	0.91638700
O	1.03928000	2.96583600	1.72091300
O	-1.18402100	2.17778300	1.04326400
O	0.70654400	0.68857800	0.88803900
C	0.00065800	2.05210700	1.67455700
O	0.58458700	2.63920000	0.61320300
H	0.33227000	2.55245000	2.58850500
O	-0.75973100	1.13591700	1.63079200
H	-1.89658100	0.98841500	0.80336800
S	3.48657100	-1.27416200	0.43973400
O	4.62554500	-1.84089600	1.04710800
O	3.11859600	0.03917700	1.11501600
O	2.32543100	-2.06055300	0.15648600
C	3.25522000	-0.10370000	1.87784200
O	4.06376600	-0.74995200	1.01519600
H	3.83056200	0.17029600	2.76677800
O	2.10010100	0.13305200	1.70383000
H	2.13097500	0.32021800	-1.00381200

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284

(SA)<sub>3</sub>·(A)<sub>2</sub>

Atom	X	Y	Z
N	0.00518100	-2.07016200	0.13235300
H	-0.75853200	-2.16079900	-0.55462500
H	0.93474300	-1.88806300	-0.30515600
H	0.03719300	-2.89913000	0.71738900
N	-2.34720800	1.90536900	1.66490700
H	-3.28300000	2.15582800	1.35682500
H	-2.15626000	2.28748100	2.58494300
H	-2.28784300	0.86629500	1.66909200
S	-3.05154400	-0.82064200	-0.13076300
O	-2.54077100	-1.86675900	-0.99529000
O	-2.97918700	0.51386700	-0.72804800
O	-2.49768700	-0.83783600	1.22061400
H	-1.36657100	0.64835200	-1.39460500

S	0.28837400	1.51641400	-0.40036800
O	-0.38382400	0.61467600	-1.49818000
O	1.58674500	1.85904500	-0.92585500
O	-0.60465300	2.64712900	-0.17390700
O	0.36418400	0.67575900	0.81966400
H	-0.22309800	-1.24829000	0.70426700
H	-1.64624200	2.26948800	0.94588000
O	-4.59477800	-1.12522500	0.10609000
H	-5.01675300	-1.29530900	-0.74583900
S	3.45174800	-0.69237600	0.13959600
O	3.87133700	0.63659300	-0.53293900
O	2.71916700	-0.25160100	1.44404300
O	4.61983900	-1.39864900	0.50930300
O	2.47134100	-1.33631400	-0.71283100
H	3.05627700	1.14908100	-0.79026500
H	1.83331600	0.16880500	1.23453400

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286 (SA)<sub>2</sub>· (A)<sub>2</sub>·FSA

Atom	X	Y	Z
S	2.40391200	-1.07942500	-0.36129600
O	1.71053700	-1.25313700	-1.62432800
O	3.93485000	-1.39284600	-0.64312600
O	2.45422600	0.30895400	0.10438500
O	1.97479500	-1.98921100	0.68846800
H	0.16014500	-0.66201200	-2.06959300
H	4.02118800	-2.30963400	-0.93347400
S	0.13090500	2.77099300	0.23948700
O	0.52718100	2.22941500	1.51602800
O	0.95491200	2.04616800	-0.86784700
O	-1.32140800	2.28625400	-0.08580200
O	0.15960200	4.16954900	0.02567800
H	0.71912300	0.51593200	2.14015500
H	1.59722700	1.33912600	-0.47051200
N	0.82421100	-0.40948600	2.59019800
H	1.30829900	-0.31796500	3.47661200
H	-0.09695100	-0.84199200	2.70844700
H	1.35056700	-1.03668200	1.93661900
N	-0.54682000	0.00432200	-2.44844900
H	-1.48253800	-0.21180200	-2.07199100
H	-0.26303100	0.93496800	-2.12694200
H	-0.55070900	-0.03008600	-3.46270000
S	-1.51508900	-1.52449700	0.46380600
O	-1.31946500	-2.13805600	1.74464700



O	-0.84361300	-0.22355000	0.34583800
O	-1.43521900	-2.32475700	-0.71761100
C	-3.73537000	-0.45623000	-0.42866100
O	-3.15087300	-1.09347000	0.57740100
H	-4.80124800	-0.32047400	-0.22130800
O	-3.20123700	-0.05980200	-1.42839300
H	-1.36154100	1.31689700	0.11975700

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SA·(A)<sub>2</sub>·(FSA)<sub>2</sub>

Atom	X	Y	Z
N	0.88963900	0.53209400	2.15145900
H	1.84966900	0.41081100	1.79133900
H	0.83420700	0.13754200	3.08575900
H	0.62595400	1.51890800	2.14764400
S	2.05308100	-1.52499800	-0.28033400
O	1.86208800	-2.52535200	-1.29162100
O	1.56829600	-0.21036900	-0.69826200
O	1.74324300	-1.87586600	1.07550400
C	4.24923600	-0.40930500	0.52002400
O	3.72193000	-1.32633400	-0.28834800
H	5.33771900	-0.39884700	0.41336200
O	3.64710000	0.31648900	1.26178000
H	0.22502200	0.02316400	1.53083500
S	-2.47028500	-0.12945100	0.31801600
O	-2.80915800	1.05221100	1.08298300
O	-2.93186600	-0.17716900	-1.03705100
O	-1.09183800	-0.56319500	0.51862600
C	-3.25017700	-2.56141200	0.62325600
O	-3.35078200	-1.31108700	1.10186400
H	-3.89023600	-3.22717300	1.20973100
O	-2.57184200	-2.91559000	-0.29470100
H	-1.31172900	-1.82703100	-1.49415100
N	-0.68616600	-1.32213500	-2.13810800
H	-0.53976600	-0.38179800	-1.74321300
H	-1.13732600	-1.23961000	-3.04422900
H	0.21823700	-1.80568400	-2.19540900
S	-0.06455200	2.72561200	-0.53080200
O	-0.04785500	4.08602500	-0.92213700
O	-0.64874400	1.72545900	-1.38120900
O	-0.72154700	2.61421300	0.89639100
O	1.39733200	2.30480600	-0.18118300
H	-1.58974300	2.11178800	0.89308600
H	1.53655800	1.33998700	-0.39906800

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290

(A)<sub>2</sub>·(FSA)<sub>3</sub>

Atom	X	Y	Z
N	-0.11133900	0.24657900	-2.28896400
H	0.82895800	-0.08629700	-2.04773100
H	-0.18294700	1.22685200	-1.99200100
H	-0.28175800	0.14911400	-3.28384500
S	0.08139700	2.06744100	0.56332000
O	-0.39544000	2.37514200	1.87256700
O	0.51543200	0.65888700	0.41907100
O	-0.67437700	2.51594000	-0.57506900
C	2.29126000	2.79019200	-0.60671400
O	1.52064500	2.89950300	0.49399800
H	3.16765500	3.43567800	-0.49670300
O	2.06737500	2.09492700	-1.54901700
H	-0.80364500	-0.30930700	-1.72586000
S	-3.15708200	-1.35264700	-0.52722200
O	-3.67483200	-2.14280200	-1.59065400
O	-3.57688500	-1.66484300	0.82116000
O	-1.72160600	-1.05739200	-0.59577100
C	-3.67905300	1.17348500	-0.02743400
O	-3.85405900	0.14547100	-0.86392000
H	-4.21642800	2.04886700	-0.40686200
O	-3.04040600	1.16497000	0.98177900
H	-2.31472000	-0.95063500	1.98048600
N	-1.36613600	-0.58667900	2.17802500
H	-0.85635900	-0.64272800	1.28578500
H	-0.87118200	-1.13454600	2.87367000
H	-1.41779800	0.40307900	2.43147200
S	3.20510500	-1.11588600	-0.33809600
O	4.57086000	-1.07250000	-0.69183800
O	2.87098500	-0.02555500	0.67088900
O	2.18193400	-1.22709200	-1.33181300
C	2.00153200	-2.76533200	1.30340800
O	3.10048700	-2.48276700	0.57126600
H	2.13258000	-3.74911100	1.76309100
O	1.05323000	-2.06021800	1.44114400
H	1.85807900	0.24373200	0.62113600

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(SA)<sub>3</sub>·(A)<sub>3</sub>

Atom	X	Y	Z
S	2.61550300	-1.21713100	0.07787100
O	1.50419700	-2.11956500	0.33153900
O	3.94552200	-2.09812300	0.14786300

O	2.66374100	-0.67863000	-1.27165400
H	3.94723000	-2.59642300	0.97400000
S	-2.80519300	-0.98920500	-0.06753700
O	-2.88751900	0.34179100	0.50484700
O	-4.14297800	-1.67881400	0.45755400
O	-2.85144000	-1.05270500	-1.52017700
H	-4.26188300	-2.51704700	-0.00442200
S	-0.33046500	2.24661500	0.03312700
O	0.21614600	0.92532100	-0.34071300
O	-0.53745000	2.32266200	1.47103800
O	-1.71152100	2.40034500	-0.67450000
O	0.49429700	3.31883300	-0.51434200
H	1.96174700	2.66009600	-0.62515700
O	2.74348300	-0.20042500	1.12633500
N	-0.09442900	-0.29203800	2.17408000
N	2.82992600	2.04774500	-0.59450900
N	-0.09600400	-1.28903300	-1.85188200
H	3.67861200	2.57105100	-0.77685000
H	2.87821600	1.57373000	0.31751000
H	2.72943200	1.26102800	-1.24862100
H	-2.31296100	1.69948700	-0.30930200
H	0.20493900	-1.93442300	-1.11044700
H	0.50390300	-1.39420000	-2.66253600
H	-1.09902400	-1.41255800	-2.04950500
H	0.02767100	-0.33907600	-1.43743600
H	0.89281000	-0.35062400	1.89832100
H	-0.65647300	-0.89341900	1.53205000
H	-0.39668000	0.69889100	2.05200600
H	-0.21685000	-0.59772400	3.13279700
O	-1.69080900	-1.77318400	0.47325800

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(SA)<sub>2</sub>·(A)<sub>3</sub>·FSA

Atom	X	Y	Z
S	2.54617000	-1.61306500	0.17337400
O	2.53073400	-1.36697700	-1.25655200
O	3.45690900	-2.91890000	0.29359500
O	3.20340600	-0.57689400	0.96273600
O	1.24418100	-1.98353300	0.72922600
H	-0.06330300	-1.89373500	-0.74184800
H	3.48671000	-3.19854000	1.21636200
S	0.53066300	2.33941500	-0.17921600
O	0.17450500	2.49218600	1.22770400
O	0.77296300	0.92495900	-0.50459000

O	-0.68640100	2.81865800	-1.03655700
O	1.63632400	3.18459700	-0.60929500
H	0.15632000	1.05760800	1.94961500
H	3.03934200	0.60258500	-1.61078700
N	0.13954700	0.09425900	2.39442900
H	0.71510400	0.08969000	3.22966200
H	-0.82844200	-0.14317700	2.61268200
H	0.49563400	-0.60542600	1.71987000
N	-0.34546600	-1.35648200	-1.57066200
H	-1.35760200	-1.45842700	-1.71549200
H	-0.11532200	-0.37569100	-1.32520200
H	0.21126100	-1.64797400	-2.36726500
S	-2.61335700	-0.05628800	0.52624900
O	-2.95163800	0.67828500	1.70612200
O	-2.31535000	0.72497100	-0.66244500
O	-1.71447800	-1.17225400	0.73835200
C	-4.13486100	-1.58315700	-0.94138500
O	-4.07585500	-0.78824800	0.12364400
H	-5.15461800	-1.96391800	-1.05876800
O	-3.23553400	-1.86575600	-1.68171200
H	-1.43543700	2.19580100	-0.88160100
N	3.50117100	1.31384300	-1.03524100
H	2.86161200	2.14900800	-0.93597000
H	4.40902100	1.55980500	-1.41211400
H	3.58837200	0.84024400	-0.11885000

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296 SA·(A<sub>3</sub>)·(FSA)<sub>2</sub>

Atom	X	Y	Z
N	0.83387200	-0.43401100	2.18783400
H	1.83389100	-0.65793000	2.09210800
H	0.55630300	-0.36783400	3.16077200
H	0.60144600	0.45302000	1.68709900
S	2.70283700	-0.48528200	-0.63007100
O	2.88110700	-0.34723300	-2.03825700
O	2.72100500	0.72551700	0.16993400
O	1.68179000	-1.43461900	-0.21621700
C	4.33574600	-1.55761700	1.10917500
O	4.13897600	-1.24754600	-0.16631800
H	5.31915900	-2.02416100	1.22792800
O	3.58011800	-1.37482900	2.02297600
H	0.27895200	-1.14925000	1.70325800
S	-2.44346000	-0.75224800	0.58884300
O	-2.78436500	-0.16036100	1.85451000

O	-2.67741800	0.09593000	-0.56675100
O	-1.21277000	-1.50876600	0.54864300
C	-3.63487700	-2.70660000	-0.65158100
O	-3.62775700	-1.93907500	0.44108300
H	-4.45210500	-3.43205200	-0.58213000
O	-2.88250100	-2.63845300	-1.57915900
H	0.25793400	-1.47566400	-1.39132900
N	-0.38344300	-1.06744000	-2.08835900
H	-0.41701600	-0.04875900	-1.86347800
H	-1.31050300	-1.49358200	-1.99162100
H	0.00156300	-1.19188200	-3.01919000
S	0.00000200	2.38018500	-0.34011300
O	-0.91643900	3.50541100	-0.51249300
O	0.12099600	1.52027000	-1.50393100
O	-0.32908200	1.63241100	0.88522400
O	1.39814700	3.05241500	-0.12406800
H	-2.61835800	2.10423700	1.57133600
H	2.06716500	2.33176000	-0.11600600
N	-3.00983500	2.53990000	0.73431700
H	-2.23497100	3.10334500	0.26088200
H	-3.83550100	3.08519800	0.95075400
H	-3.22184200	1.74865900	0.10755200

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298 (A)<sub>3</sub>·(FSA)<sub>3</sub>

Atom	X	Y	Z
N	0.43250300	0.17461100	-1.90860200
H	0.10701400	1.14755100	-1.73877900
H	-0.31737800	-0.45690900	-1.59577500
H	0.61293800	0.03033900	-2.89673700
S	-2.25698800	-1.81816200	0.04075300
O	-1.44494000	-3.00259800	-0.00029100
O	-2.33250900	-1.17406200	1.33768600
O	-2.07128100	-0.89108400	-1.06173500
C	-4.85272000	-1.67047200	-0.27173300
O	-3.77813400	-2.46023900	-0.21420500
H	-5.74320400	-2.28242200	-0.44533700
O	-4.87464800	-0.48030200	-0.15658100
H	1.30592500	0.00696000	-1.37120700
S	3.70101600	-0.65750200	0.17026800
O	5.07379000	-0.31215000	0.26556000
O	3.06031900	-1.10038400	1.40161500
O	2.85804500	0.21667100	-0.62798700
C	2.65607400	-2.69384300	-1.10528300

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O	3.77598400	-2.08121800	-0.75588400
H	2.88569800	-3.59050600	-1.69151400
O	1.53798100	-2.34265500	-0.83717600
H	1.53197900	-1.72176300	1.60556600
N	0.51467200	-1.88462600	1.79271000
H	0.04921600	-0.97118800	1.69558700
H	0.35394200	-2.25282500	2.72446000
H	0.10351400	-2.51521000	1.09235900
S	-0.28232600	3.53522200	-0.18513700
O	0.32545100	4.72113900	-0.67222700
O	-1.23090200	3.63661400	0.89519200
O	-0.70156900	2.56942900	-1.21050900
C	0.96933200	1.56572600	1.06846000
O	1.05910300	2.76585000	0.54378400
H	1.89157400	1.30031300	1.59196500
O	0.01410300	0.82215900	0.99078000
H	-2.19413900	1.68039600	-0.42187000
N	-2.81105700	1.45973500	0.37213500
H	-2.96880000	2.33503000	0.86744900
H	-2.29677800	0.80508800	0.97083100
H	-3.66401200	0.97836400	0.07232500

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