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Supplement of

Unexpected enhancement of new particle formation by lactic acid sulfate resulting from SO_3 loss in forested and agricultural regions

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S42	**Fig. S18** The influence of (a) [A], (b) [SA] and (c) [LAS] on the relative contribution of the pure SA-A-based clustering route and the LAS participation route to the system flux is analyzed. Others in (a), (b) and (c) indicate that the route contribution of the cluster growing out of the studied system is less than 5%
S43-S66	**Table S16** Cartesian coordinates of all molecules and clusters in the studied system.

The specific outgoing fluxes of LAS

To quantify the contribution of LAS to SA-A nucleation, we analyzed the steady-state cluster formation fluxes (J) output by ACDC. The LAS-related nucleation fraction at a given temperature was defined as the ratio of the total formation flux of all nucleated clusters containing at least one LAS molecule to the total nucleation flux from all pathways. Specifically,

$$f_{LAS}(T) = \frac{\sum J_{out}(C_i \mid C_i \in C_{LAS})}{\sum J_{out}(C_i)} \quad \text{(S1)}$$

where $J_{out}(C_i)$ denotes the outgoing flux of cluster C_i that meets the nucleation criterion (size/composition threshold), and C_{LAS} represents the set of all nucleated clusters containing one or more LAS molecules. This metric directly reflects the proportion of new particles formed through LAS-involved pathways under steady-state conditions.

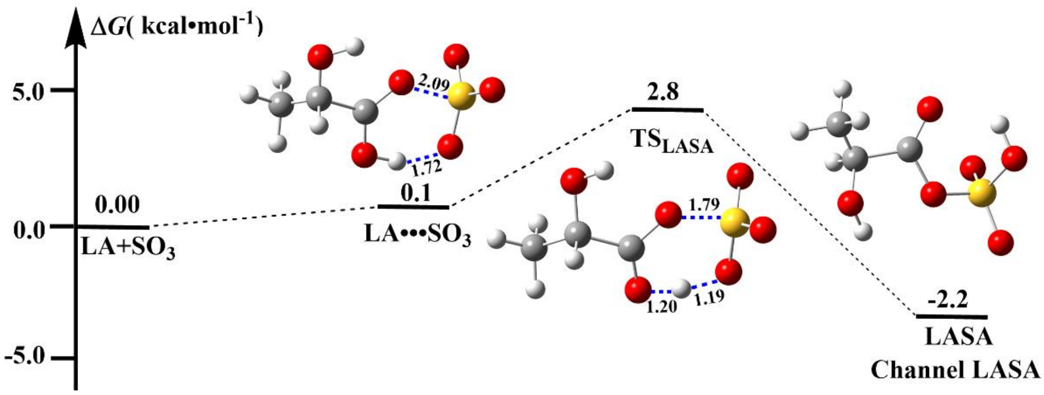

Fig. S1 Potential energy surface for the gas-phase reaction of LA(-COOH) with SO_3 at the CCSD(T)-F12/cc-pVDZ-F12//M06-2X/6-311++G(2*df*,2*pd*) of theory

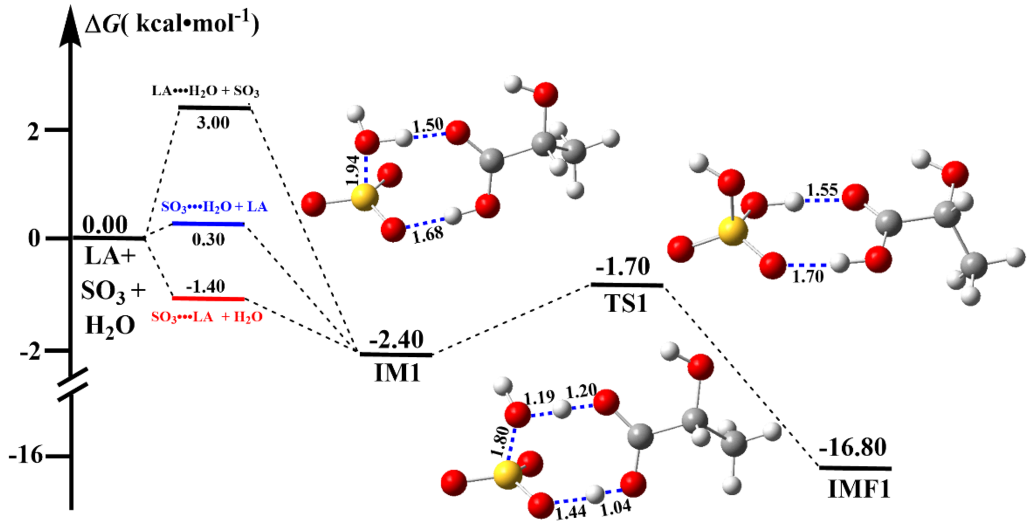

Fig. S2 Potential energy surface for the hydrolysis of SO_3 assisted by lactic acid (LA) calculated at the CCSD(T)-F12/cc-pVDZ-F12//M06-2X/6-311++G(2*df*,2*pd*) level

Table S1 Equilibrium constants ($cm^3 \cdot molecule^{-1}$) for the $SO_3 \cdots LA$, $SO_3 \cdots H_2O$ and $LA \cdots H_2O$ complexes within the temperature range of 229.7-320.0 K

T/K	$SO_3 \cdots LA$	$SO_3 \cdots H_2O$	$LA \cdots H_2O$
229.7	1.44×10^{-16}	2.70×10^{-18}	6.15×10^{-21}
259.3	7.60×10^{-18}	5.65×10^{-19}	1.34×10^{-21}
280	1.43×10^{-18}	1.77×10^{-19}	5.68×10^{-22}
290	7.08×10^{-19}	1.09×10^{-19}	3.95×10^{-22}
298	4.18×10^{-19}	7.53×10^{-20} (5.80×10^{-20})[a]	3.01×10^{-22}
300	3.68×10^{-19}	6.89×10^{-20}	2.82×10^{-22}
310	1.99×10^{-19}	4.51×10^{-20}	2.06×10^{-22}
320	1.13×10^{-19}	3.04×10^{-20}	1.54×10^{-22}

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

Table S2 Concentrations (molecules·cm^{-3}) of H_2O, $SO_3\cdots H_2O$, $LA\cdots H_2O$ and $SO_3\cdots LA$ within the temperature range of 229.7-320.0 K

T/K	H_2O[a]	$SO_3\cdots H_2O$ $[SO_3]$[b] = 10^5	$LA\cdots H_2O$ [LA][c] = 10^{12}	$SO_3\cdots LA$
229.7	4.90×10^{15}	1323.0	3.01×10^{7}	1.44×10^{1}
259.3	2.40×10^{16}	1356.0	3.22×10^{7}	7.60×10^{-1}
280	2.58×10^{17}	4566.7	1.47×10^{8}	1.43×10^{-1}
290	4.78×10^{17}	5210.2	1.89×10^{8}	7.08×10^{-2}
298	7.70×10^{17}	5798.1	2.32×10^{8}	4.18×10^{-2}
300	8.58×10^{17}	5911.6	2.42×10^{8}	3.68×10^{-2}
310	1.46×10^{18}	6584.6	3.01×10^{8}	1.99×10^{-2}
320	2.35×10^{18}	7144.0	3.62×10^{8}	1.13×10^{-2}

[a] The concentrations (molecules·cm^{-3}) of H_2O values were reported from reference (*J. Phys. Chem. A*, **2013**, *117*, 10381-10396)

[b] The values are reported from reference (*Atmos. Chem. Phys.,* **2024**; *24*:3693-3612)

[c] The values are reported from reference (*Atmos. Environ.,* **2017**; *166*:479-487)

Table S3 Zero point energy (ZPE/(kcal·mol^{-1})), entropies (S/(kcal·mol^{-1}·K^{-1})), relative electronic energies (ΔE/(kcal·mol^{-1})), relative energies with ZPE corrections (ΔE and Δ(E + ZPE)/(kcal·mol^{-1})), enthalpies (ΔH(298)/(kcal·mol^{-1})), and Gibbs free energies (ΔG(298)/(kcal·mol^{-1})) for the reaction of SO_3 with the OH group of LA, both in the absence and presence of H_2O and H_2SO_4, calculated at the CCSD(T)-F12/cc-pVDZ-F12//M06-2X/6-311++G(2*df*,2*pd*) level

Species	ZPE	ΔE	S	ΔG	Δ(E + ZPE)	ΔH
LA + SO_3	68.4	0.0	105.8	0.0	0.0	0.0
IM	70.0	1.7	75.0	5.6	-5.2	-5.1
TS	67.5	-1.5	66.4	27.9	15.7	15.2
LAS	70.4	1.6	69.3	-7.7	-19.5	-19.9
LA + SO_3 + H_2O	81.9	0.0	186.3	0.0	0.0	0.0
LA + SO_3⋯H_2O	84.2	-9.4	131.4	0.3	-7.1	-7.6
SO_3⋯LA + H_2O	83.9	-13.9	134.8	-1.4	-11.8	-12.0
LA⋯H_2O + SO_3	84.5	-8.4	61.2	3.0	-5.8	-6.5
IM_WM1	86.0	-20.4	96.5	3.5	-16.3	-17.0
TS_WM1	84.4	-12.7	84.9	11.3	-10.2	-12.2
LAS⋯H_2O	87.1	-36.2	91.5	-9.9	-31.0	-32.4
LA + SO_3 + SA	93.5	0.0	212.9	0.0	0.0	0.0
LA + SO_3⋯SA	94.7	-14.5	131.4	-3.3	-13.3	-13.1
SO_3⋯LA + SA	95.5	-13.9	134.8	-1.4	-11.8	-12.0
LA⋯SA + SO_3	94.9	-18.0	61.2	-5.5	-16.6	-16.6
IM_SA1	96.2	-29.3	96.5	-4.6	-26.6	-26.6
TS_SA1	92.3	-23.3	84.9	-1.1	-24.6	-25.3
LAS⋯SA	96.4	-34.9	91.5	-10.0	-32.0	-32.1

Table S4 Equilibrium constant (K_{eq}, cm^3 $molecule^{-1}$) and corresponding atmospheric concentrations (molecules cm^{-3}) for the formation of LAS and LASA from SO_3 and LA. Values are based on Gibbs free energy (ΔG) calculated at the CCSD(T)-F12/cc-pVDZ-F12//M06-2X/6-311++G(2*df*,2*pd*) level of theory under conditions of 278 K and 101.3 kPa

Reaction pathways	[LA][a] (molec cm^{-3})	[SO_3][b] (molec cm^{-3})	Keq (cm^3 $molec^{-1}$)	[C] (molec cm^{-3})
$(LA + SO_3)_{-OH} \rightarrow LAS$	10^{10} - 10^{12}	10^5	5.51×10^{-12}	5.51×10^{3}-5.51×10^{5}
$(LA + SO_3)_{-COOH} \rightarrow LASA$	10^{10} - 10^{12}	10^5	7.16×10^{-19}	7.16×10^{-4}-7.16×10^{-2}

Keq_1 and Keq_2 represent the equilibrium constants for the formation of LAS and LASA from the reaction of SO_3 with LA, respectively.

Keq_1 and Keq_2 are calculated using equations (S1) and (S2), respectively.

$$K_{eq1} = \frac{[LAS]}{[LA][SO_3]} = e^{\frac{-\Delta G}{RT}} \tag{S2}$$

$$K_{eq2} = \frac{[LAS]}{[LA][SO_3]} = e^{\frac{-\Delta G}{RT}} \tag{S3}$$

The equilibrium concentrations of LAS and LASA are approximately estimated using equations (S3) and (S4), respectively.

$$[LAS] = K_{eq1}[LA][SO_3] \tag{S4}$$

$$[LASA] = K_{eq2}[LA][SO_3] \tag{S5}$$

[LA] and [SO_3] represent the concentrations of LA and SO_3 monomer, respectively.

References

[a] The value was taken from reference (Li et al., ***Atmos. Environ.***, **2017**, 166, 479-487.)

[b] The value was taken from reference (Yao et al., ***Environ. Sci. Technol.***, **2020**, 7, 809-818.)

Table S5 Rate constant (k, $cm^3 \cdot molecule^{-1} \cdot s^{-1}$) for the reaction of SO_3 with LA to producing LAS, both in the absence and presence of H_2O and H_2SO_4, as well as the effective rate constants (k', s^{-1}) obtained from master equation analysis over the temperature range of 229-320 K and altitude range of 0-10 km

Altitude		0 km						5 km	10 km
T/K		280	290	298	300	310	320	259.3	229.7
$k_{Without}$		9.76×10^{-26}	1.53×10^{-25}	2.22×10^{-25}	2.43×10^{-25}	3.88×10^{-25}	6.21×10^{-25}	4.03×10^{-26}	1.35×10^{-26}
k_{WM}		1.88×10^{-16}	1.95×10^{-16}	2.00×10^{-16}	2.01×10^{-16}	2.08×10^{-16}	2.15×10^{-16}	1.74×10^{-16}	1.54×10^{-16}
k_{SA}		1.49×10^{-11}	1.32×10^{-11}	1.19×10^{-11}	1.16×10^{-11}	9.99×10^{-12}	8.51×10^{-12}	1.72×10^{-11}	2.05×10^{-11}
	20%RH	3.61×10^{-17}	3.33×10^{-17}	3.08×10^{-17}	3.11×10^{-17}	2.87×10^{-17}	2.63×10^{-17}		
	40%RH	7.21×10^{-17}	6.62×10^{-17}	6.36×10^{-17}	6.19×10^{-17}	5.75×10^{-17}	5.26×10^{-17}		
k'_{WM}	60%RH	1.08×10^{-16}	9.95×10^{-17}	9.23×10^{-17}	9.30×10^{-17}	8.63×10^{-17}	7.89×10^{-17}	1.00×10^{-20}	1.62×10^{-20}
	80%RH	1.45×10^{-16}	1.32×10^{-16}	1.27×10^{-16}	1.24×10^{-16}	1.15×10^{-16}	1.05×10^{-16}		
	100%RH	1.81×10^{-16}	1.66×10^{-16}	1.58×10^{-16}	1.55×10^{-16}	1.44×10^{-16}	1.31×10^{-16}		
k'_{SA}		2.87×10^{-16}	8.63×10^{-17}	3.43×10^{-17}	2.68×10^{-17}	8.99×10^{-18}	3.16×10^{-18}	6.10×10^{-16}	7.89×10^{-15}

k, k_{WM} and k_{SA} represent the rate constant for the reaction of SO_3 with LA to producing LAS in the absence and presence of H_2O and H_2SO_4, respectively; k'_{WM} and k'_{SA} denote the effective rate constant for this reaction in the presence of H_2O and H_2SO_4, respectively.

Table S6 Effective rate constants (k', s^{-1}) for the hydrolysis of SO_3 in the presence of *X* (*X*= LA, H_2SO_4, HNO_3, HCOOH, $H_2C_2O_4$ and NH_3) within the temperature range of 229-320 K and altitude range of 0-10 km

Altitude	0 km						5 km	10 km
T/K	280	290	298	300	310	320	259.3	229.7
k'_{SA_LA}	3.01×10^{-20}	7.35×10^{-21}	2.55×10^{-21}	1.98×10^{-21}	5.82×10^{-22}	1.85×10^{-22}	8.36×10^{-19}	2.88×10^{-16}
k'_{SA_SA}	3.51×10^{-23}	1.64×10^{-23}	9.17×10^{-24}	7.80×10^{-24}	3.97×10^{-24}	2.09×10^{-24}	2.99×10^{-21}	7.08×10^{-21}
k'_{SA_NA}	3.71×10^{-23}	1.93×10^{-23}	1.18×10^{-23}	1.04×10^{-23}	5.88×10^{-24}	3.48×10^{-24}	2.48×10^{-23}	3.60×10^{-21}
k'_{SA_FA}	4.75×10^{-22}	2.65×10^{-22}	1.70×10^{-22}	1.50×10^{-22}	8.95×10^{-23}	5.40×10^{-23}	1.90×10^{-20}	2.26×10^{-20}
k'_{SA_OA}	6.51×10^{-22}	3.03×10^{-22}	1.71×10^{-22}	1.48×10^{-22}	7.60×10^{-23}	4.06×10^{-23}	5.60×10^{-20}	2.06×10^{-20}

k'_{SA_LA}, k'_{SA_SA}, k'_{SA_NA}, k'_{SA_FA}, and k'_{SA_OA} represent the effective rate constants for the hydrolysis of SO_3 with LA, H_2SO_4, HNO_3, HCOOH, and H_2C_2O, respectively.

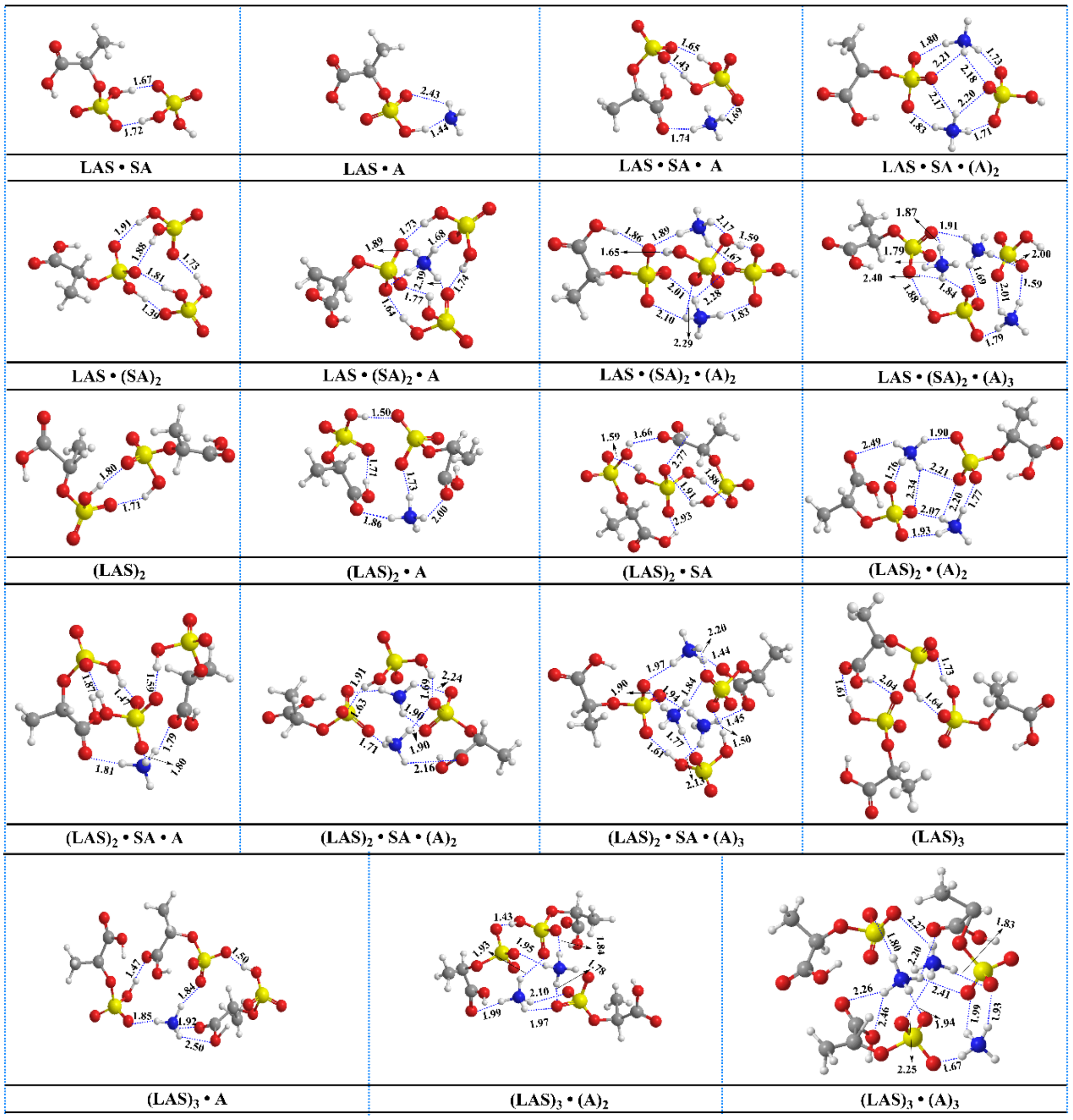

Fig. S3 Optimized structures of the most stable LAS-SA-A-based clusters, obtained at the M06-2X/6-311++G(2*df*,2*pd*) level of theory. Hydrogen bond lengths are indicated in Å (Color code: blue = nitrogen, yellow = sulfur, red = oxygen, gray = carbon, and white = hydrogen)

Table S7 The Gibbs free energy (ΔG, kcal·mol^{-1}) of LAS-SA-A-based clusters at 1 atm and temperatures of 298.15, 278.15, 258.15 and 238.15 K

Clusters	T = 298.15 K	T = 278.15 K	T = 258.15 K	T = 238.15 K
SA·A	-5.77 (-7.33)	-6.41 (-7.94)	-7.04 (-8.54)	-7.67 (-9.15)
$(SA)_2$	-8.06 (-8.42)	-8.73 (-9.10)	-9.39 (-9.77)	-10.06 (-10.45)
$(SA)_2$·A	-21.01 (-20.84)	-22.53 (-22.41)	-24.05 (-23.96)	-25.56 (-25.52)
$(SA)_2$·$(A)_2$	-26.17 (-26.55)	-28.39 (-28.81)	-30.61 (-31.04)	-32.83 (-33.28)
$(SA)_3$	-13.03 (-13.91)	-14.53 (-15.46)	-16.04 (-17.00)	-17.56 (-18.54)
$(SA)_3$·A	-28.36 (-30.19)	-30.71 (-32.52)	-33.06 (-34.85)	-35.41 (-37.17)
$(SA)_3$·$(A)_2$	-41.78 (-41.79)	-44.80 (-44.87)	-47.83 (-47.94)	-50.86 (-51.01)
$(SA)_3$·$(A)_3$	-51.75 (-52.79)	-55.61 (-56.64)	-59.47 (-60.47)	-63.34 (-64.30)
$(LAS)_2$	-3.96	-4.80	-5.64	-6.49
A·LAS	-6.59	-7.31	-8.02	-8.73
$(A)_2$·$(LAS)_2$	-32.18	-34.56	-36.94	-39.32
A·$(LAS)_2$	-21.53	-23.37	-25.21	-27.06
SA·LAS	-7.16	-7.96	-8.76	-9.57
SA·A·LAS	-19.73	-21.46	-23.20	-24.93
SA·$(A)_2$·LAS	-30.14	-32.43	-34.72	-37.01
$(LAS)_3$	-4.93	-6.78	-8.64	-10.50
SA_2·A·LAS	-31.82	-34.19	-36.56	-38.94
$(SA)_2$·$(A)_2$·LAS	-39.56	-42.86	-46.07	-49.29
$(SA)_2$·$(A)_3$·LAS	-51.56	-55.52	-59.49	-63.46
SA·$(LAS)_2$	-7.03	-8.91	-10.80	-12.69
A·$(LAS)_3$	-36.99	-39.86	-42.72	-45.58
SA·$(A)_2$·$(LAS)_2$	-38.35	-41.71	-45.08	-48.44
$(SA)_2$·LAS	-10.00	-11.71	-13.42	-15.14
SA·A·$(LAS)_2$	-32.41	-35.10	-37.78	-40.47
$(A)_2$·$(LAS)_3$	-40.05	-43.42	-46.78	-50.16
SA·$(A)_3$·$(LAS)_2$	-48.91	-53.02	-57.13	-61.25
$(A)_3$·$(LAS)_3$	-57.22	-61.41	-65.62	-69.83

*Calculated at M06-2X/6-311++G(2*df*,2*pd*) level of theory.

The values in parentheses taken from reference (***J. Phys. Chem. A*** 2020, 124: 3261-3268.)

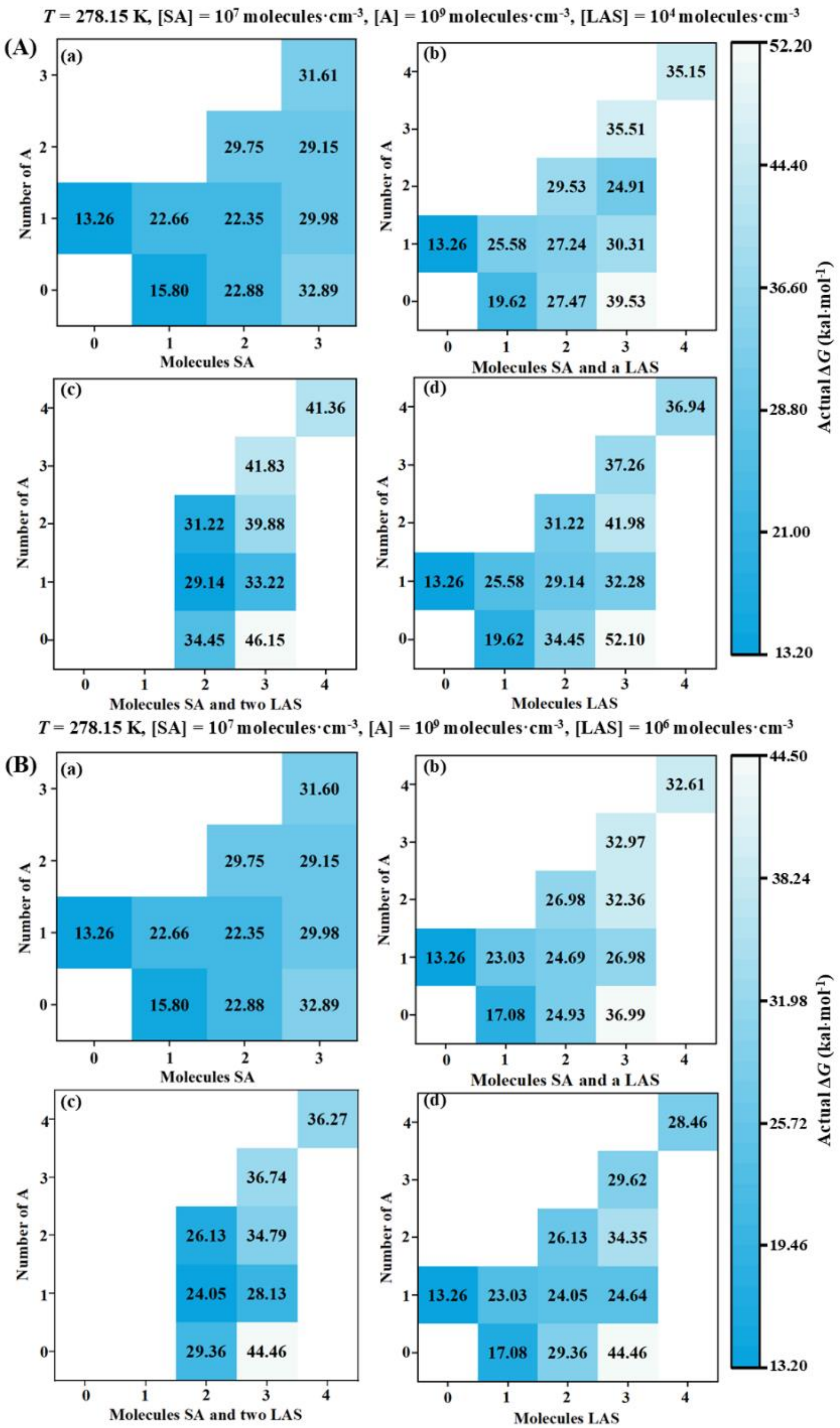

Fig. S4 A typical actual ΔG surface at 278.15 K. [SA] is the concentration of sulfuric acid monomers, [A] the concentration of ammonia monomers and [LAS] is lactic acid sulfate

Table S8 Collision coefficients (β, $cm^3 \cdot s^{-1}$) for each cluster investigated in the present study of LAS-SA-A system

Collisions	β, $cm^3 \cdot s^{-1}$			
	298.15 K	278.15 K	258.15 K	238.15 K
SA + A	1.64×10^{-10}	1.53×10^{-10}	1.42×10^{-10}	1.31×10^{-10}
SA + LAS	8.85×10^{-11}	8.01×10^{-11}	7.43×10^{-11}	6.85×10^{-11}
LAS + A	2.67×10^{-10}	2.49×10^{-10}	2.31×10^{-10}	2.13×10^{-10}
SA + SA	6.76×10^{-11}	6.30×10^{-11}	5.85×10^{-11}	5.40×10^{-11}
LAS + LAS	9.23×10^{-11}	8.61×10^{-11}	7.99×10^{-11}	7.37×10^{-11}
$(SA)_2$ + A	2.78×10^{-10}	2.60×10^{-10}	2.41×10^{-10}	2.22×10^{-10}
SA·A + SA	8.91×10^{-11}	8.31×10^{-11}	7.71×10^{-11}	7.11×10^{-11}
$(SA)_2$·A + A	2.95×10^{-10}	2.76×10^{-10}	2.56×10^{-10}	2.36×10^{-10}
$(LAS)_2$ + A	4.80×10^{-10}	4.48×10^{-10}	4.15×10^{-10}	3.83×10^{-10}
LAS·A + LAS	1.11×10^{-10}	1.03×10^{-10}	9.60×10^{-11}	8.86×10^{-11}
$(LAS)_2$·A + A	3.39×10^{-10}	3.16×10^{-10}	2.93×10^{-11}	2.71×10^{-11}
$(SA)_2$ + LAS	8.95×10^{-11}	8.35×10^{-11}	7.75×10^{-11}	7.15×10^{-11}
SA·LAS + SA	1.07×10^{-10}	9.99×10^{-11}	9.27×10^{-11}	8.55×10^{-11}
$(LAS)_2$ + SA	1.24×10^{-10}	1.15×10^{-10}	1.07×10^{-10}	9.87×10^{-11}
SA·LAS + LAS	1.02×10^{-10}	9.54×10^{-11}	8.86×10^{-11}	8.17×10^{-11}
$(SA)_2$ + SA	8.56×10^{-11}	7.98×10^{-11}	7.41×10^{-11}	6.83×10^{-11}
$(LAS)_2$ + LAS	1.12×10^{-10}	1.04×10^{-10}	9.66×10^{-11}	8.91×10^{-11}
SA + $(SA)_2$·A	8.83×10^{-11}	8.23×10^{-11}	7.64×10^{-11}	7.05×10^{-11}
$(SA)_3$ + A	3.98×10^{-10}	3.71×10^{-10}	3.45×10^{-10}	3.18×10^{-10}
$(SA)_2 \cdot (A)_2$ + SA	9.24×10^{-11}	8.62×10^{-11}	8.00×10^{-11}	7.38×10^{-11}
$(SA)_3$·A + A	3.16×10^{-10}	2.95×10^{-10}	2.74×10^{-10}	2.52×10^{-10}
$(SA)_3 \cdot (A)_2$ + A	4.16×10^{-10}	3.88×10^{-10}	3.60×10^{-10}	3.32×10^{-10}
$(LAS)_2$·A + LAS	8.42×10^{-11}	7.85×10^{-11}	7.29×10^{-11}	6.72×10^{-11}
$(LAS)_3$ + A	4.92×10^{-10}	4.59×10^{-10}	4.26×10^{-10}	3.93×10^{-10}
$(LAS)_2 \cdot (A)_2$ + LAS	1.32×10^{-10}	1.23×10^{-10}	1.14×10^{-10}	1.06×10^{-10}
$(LAS)_3$·A + A	4.94×10^{-10}	4.61×10^{-10}	4.28×10^{-10}	3.95×10^{-10}
$(LAS)_3 \cdot (A)_2$ + A	4.89×10^{-10}	4.57×10^{-10}	4.24×10^{-10}	3.91×10^{-10}
LAS·A + SA	1.09×10^{-10}	1.02×10^{-10}	9.47×10^{-11}	8.73×10^{-11}
SA·A + LAS	1.03×10^{-10}	9.96×10^{-11}	8.94×10^{-11}	8.42×10^{-11}
SA·LAS + A	3.89×10^{-10}	3.63×10^{-10}	3.37×10^{-10}	3.11×10^{-10}

$SA \cdot LAS \cdot A + A$	3.28×10^{-10}	3.06×10^{-10}	2.84×10^{-10}	2.62×10^{-10}
$SA \cdot LAS \cdot A + SA$	9.06×10^{-11}	8.45×10^{-11}	7.84×10^{-11}	7.23×10^{-11}
$(SA)_2 \cdot A + LAS$	9.05×10^{-11}	8.44×10^{-11}	7.83×10^{-11}	7.22×10^{-11}
$(SA)_2 \cdot LAS + A$	4.28×10^{-10}	3.99×10^{-10}	3.70×10^{-10}	3.42×10^{-10}
$SA \cdot LAS \cdot (A)_2 + SA$	1.03×10^{-11}	9.58×10^{-11}	8.89×10^{-11}	8.20×10^{-11}
$(SA)_2 \cdot (A)_2 + LAS$	9.27×10^{-11}	8.64×10^{-11}	8.02×10^{-11}	7.40×10^{-11}
$(SA)_2 \cdot LAS \cdot A + A$	4.35×10^{-10}	4.06×10^{-10}	3.77×10^{-10}	3.48×10^{-10}
$(SA)_2 \cdot LAS \cdot (A)_2 + A$	5.23×10^{-10}	4.88×10^{-10}	4.53×10^{-10}	4.18×10^{-10}
$(LAS)_2 \cdot A + SA$	8.95×10^{-11}	8.35×10^{-11}	7.75×10^{-11}	7.15×10^{-11}
$SA \cdot LAS \cdot A + LAS$	8.80×10^{-11}	8.21×10^{-11}	7.62×10^{-11}	7.03×10^{-11}
$SA \cdot (LAS)_2 + A$	3.82×10^{-10}	3.56×10^{-10}	3.31×10^{-10}	3.05×10^{-10}
$(LAS)_2 \cdot (A)_2 + SA$	1.52×10^{-10}	1.42×10^{-10}	1.32×10^{-10}	1.22×10^{-10}
$SA \cdot LAS \cdot (A)_2 + LAS$	9.96×10^{-11}	9.04×10^{-11}	8.39×10^{-11}	7.74×10^{-11}
$SA \cdot (LAS)_2 \cdot A + A$	4.20×10^{-10}	3.92×10^{-10}	3.64×10^{-10}	3.36×10^{-10}
$SA \cdot (LAS)_2 \cdot (A)_2 + A$	6.28×10^{-10}	5.86×10^{-10}	5.44×10^{-10}	5.02×10^{-10}

Table S9 Evaporation rates (s^{-1}) of the studied clusters in LAS-SA-A system at different temperatures of 298.15, 278.15, 258.15 and 238.15 K

Evaporation pathways	298.15 K	278.15 K	258.15 K	238.15 K
$(SA)_2 \rightarrow SA + SA$	2.03×10^{3}	2.30×10^{2}	1.84×10^{1}	9.67×10^{-1}
$(SA)_3 \rightarrow (SA)_2 + SA$	4.83×10^{5}	5.76×10^{4}	4.91×10^{3}	2.76×10^{2}
$(SA)_1{\cdot}(A)_1 \rightarrow SA + A$	2.37×10^{5}	3.73×10^{4}	4.42×10^{3}	3.65×10^{2}
$(SA)_2{\cdot}(A)_1 \rightarrow (SA)_1{\cdot}(A)_1 + SA$	1.47×10^{-2}	4.67×10^{-4}	8.68×10^{-6}	8.28×10^{-8}
$(SA)_2{\cdot}(A)_1 \rightarrow A + (SA)_2$	2.20×10^{0}	9.76×10^{-2}	2.67×10^{-3}	4.02×10^{-5}
$(SA)_3{\cdot}(A)_1 \rightarrow (SA)_2{\cdot}(A)_1 + SA$	8.84×10^{3}	8.11×10^{2}	5.09×10^{1}	1.99×10^{0}
$(SA)_3{\cdot}(A)_1 \rightarrow A + (SA)_3$	5.57×10^{-2}	1.90×10^{-3}	3.84×10^{-5}	4.03×10^{-7}
$(SA)_2{\cdot}(A)_2 \rightarrow (SA)_2{\cdot}(A)_1 + A$	1.20×10^{6}	1.80×10^{5}	2.01×10^{4}	1.55×10^{3}
$(SA)_3{\cdot}(A)_2 \rightarrow (SA)_2{\cdot}(A)_2 + SA$	8.18×10^{-3}	2.87×10^{-4}	5.95×10^{-6}	6.40×10^{-8}
$(SA)_3{\cdot}(A)_2 \rightarrow (SA)_3{\cdot}(A)_1 + A$	1.14×10^{0}	6.51×10^{-2}	2.40×10^{-3}	5.07×10^{-5}
$(SA)_3{\cdot}(A)_3 \rightarrow (SA)_3{\cdot}(A)_2 + A$	4.94×10^{2}	3.28×10^{1}	1.42×10^{0}	3.61×10^{-2}
$(SA)_1{\cdot}(LAS)_1 \rightarrow SA + LAS$	1.18×10^{4}	1.16×10^{3}	7.99×10^{1}	3.49×10^{0}
$(SA)_2{\cdot}(LAS)_1 \rightarrow (SA)_1{\cdot}(LAS)_1 + SA$	2.21×10^{7}	3.01×10^{6}	3.01×10^{5}	2.03×10^{4}
$(SA)_2{\cdot}(LAS)_1 \rightarrow LAS + (SA)_2$	8.45×10^{7}	1.00×10^{7}	8.57×10^{5}	4.84×10^{4}
$(LAS)_1{\cdot}(A)_1 \rightarrow LAS + A$	9.64×10^{4}	1.19×10^{4}	1.07×10^{3}	6.39×10^{1}
$(SA)_1{\cdot}(LAS)_1{\cdot}(A)_1 \rightarrow SA + (LAS)_1{\cdot}(A)_1$	6.28×10^{1}	2.01×10^{-2}	3.75×10^{-4}	3.60×10^{-6}

Continued table

Evaporation pathways	298.15 K	278.15 K	258.15 K	238.15 K
$(SA)_1\cdot(LAS)_1\cdot(A)_1 \rightarrow A + (SA)_1\cdot(LAS)_1$	5.87×10^{0}	2.35×10^{-1}	5.73×10^{-3}	7.52×10^{-5}
$(SA)_1\cdot(LAS)_1\cdot(A)_1 \rightarrow LAS + (SA)_1\cdot(A)_1$	1.48×10^{-1}	3.72×10^{-3}	5.26×10^{-5}	3.66×10^{-7}
$(SA)_2\cdot(LAS)_1\cdot(A)_1 \rightarrow SA + (SA)_1\cdot(A)_1\cdot(LAS)_1$	3.02×10^{0}	2.22×10^{-1}	1.07×10^{-2}	3.10×10^{-4}
$(SA)_2\cdot(LAS)_1\cdot(A)_1 \rightarrow A + (SA)_2\cdot(LAS)_1$	1.04×10^{-6}	2.24×10^{-8}	2.66×10^{-10}	1.49×10^{-12}
$(SA)_2\cdot(LAS)_1\cdot(A)_1 \rightarrow LAS + (SA)_2\cdot(A)_1$	2.64×10^{1}	1.52×10^{0}	5.60×10^{-2}	1.18×10^{-3}
$(SA)_1\cdot(LAS)_1\cdot(A)_2 \rightarrow A + (SA)_1\cdot(LAS)_1\cdot(A)_1$	1.88×10^{2}	1.95×10^{1}	1.41×10^{0}	6.54×10^{-2}
$(SA)_2\cdot(LAS)_1\cdot(A)_2 \rightarrow SA + (SA)_1\cdot(LAS)_1\cdot(A)_2$	2.68×10^{2}	1.60×10^{1}	6.16×10^{-1}	1.36×10^{-2}
$(SA)_2\cdot(LAS)_1\cdot(A)_2 \rightarrow A + (SA)_2\cdot(LAS)_1\cdot(A)_1$	1.95×10^{4}	1.65×10^{3}	9.52×10^{1}	3.37×10^{0}
$(SA)_2\cdot(LAS)_1\cdot(A)_2 \rightarrow LAS + (SA)_2\cdot(A)_2$	2.98×10^{-1}	9.70×10^{-3}	1.85×10^{-4}	1.79×10^{-6}
$(SA)_2\cdot(LAS)_1\cdot(A)_3 \rightarrow A + (SA)_2\cdot(LAS)_1\cdot(A)_2$	2.39×10^{1}	1.43×10^{0}	5.57×10^{-2}	1.26×10^{-3}
$(LAS)_2 \rightarrow LAS + LAS$	2.84×10^{6}	3.83×10^{5}	3.78×10^{4}	2.51×10^{3}
$(SA)_1\cdot(LAS)_2 \rightarrow SA + (LAS)_2$	1.71×10^{7}	1.79×10^{6}	1.30×10^{5}	6.14×10^{3}
$(SA)_1\cdot(LAS)_2 \rightarrow LAS + (SA)_1\cdot(LAS)_1$	3.18×10^{9}	4.53×10^{8}	4.76×10^{7}	3.40×10^{6}
$(LAS)_2\cdot(A)_1 \rightarrow A + (LAS)_2$	1.55×10^{-3}	2.99×10^{-5}	3.14×10^{-7}	1.54×10^{-9}
$(LAS)_2\cdot(A)_1 \rightarrow LAS + (LAS)_1\cdot(A)_1$	3.06×10^{-2}	6.43×10^{-4}	7.44×10^{-6}	4.06×10^{-8}
$(SA)_1\cdot(LAS)_2\cdot(A)_1 \rightarrow SA + (LAS)_2\cdot(A)_1$	2.29×10^{1}	1.34×10^{0}	4.99×10^{-2}	1.06×10^{-3}

Continued table

Evaporation pathways	298.15 K	278.15 K	258.15 K	238.15 K
$(SA)_1{\cdot}(LAS)_2{\cdot}(A)_1 \rightarrow A + (SA)_1{\cdot}(LAS)_2$	2.28×10^{-9}	2.46×10^{-11}	1.32×10^{-13}	2.94×10^{-16}
$(SA)_1{\cdot}(LAS)_2{\cdot}(A)_1 \rightarrow LAS + (SA)_1{\cdot}(LAS)_1{\cdot}(A)_1$	1.08×10^{0}	4.16×10^{-2}	9.59×10^{-4}	1.17×10^{-5}
$(LAS)_2{\cdot}(A)_2 \rightarrow A + (LAS)_2{\cdot}(A)_1$	1.28×10^{2}	1.34×10^{1}	9.84×10^{-1}	4.61×10^{-2}
$(SA)_1{\cdot}(LAS)_2{\cdot}(A)_2 \rightarrow SA + (LAS)_2{\cdot}(A)_2$	1.12×10^{5}	8.96×10^{3}	4.82×10^{2}	1.59×10^{1}
$(SA)_1{\cdot}(LAS)_2{\cdot}(A)_2 \rightarrow A + (SA)_1{\cdot}(LAS)_2{\cdot}(A)_1$	4.56×10^{5}	6.54×10^{4}	6.93×10^{3}	5.01×10^{2}
$(SA)_1{\cdot}(LAS)_2{\cdot}(A)_2 \rightarrow LAS + (SA)_1{\cdot}(LAS)_1{\cdot}(A)_2$	2.26×10^{3}	1.20×10^{2}	4.04×10^{0}	7.66×10^{-2}
$(SA)_1{\cdot}(LAS)_2{\cdot}(A)_3 \rightarrow A + (SA)_1{\cdot}(LAS)_2{\cdot}(A)_2$	2.79×10^{2}	1.99×10^{1}	9.47×10^{-1}	2.70×10^{-2}
$(LAS)_3 \rightarrow (LAS)_2 + LAS$	5.33×10^{8}	7.62×10^{7}	8.00×10^{6}	5.72×10^{5}
$(LAS)_3{\cdot}(A)_1 \rightarrow A + (LAS)_3$	3.74×10^{-14}	1.22×10^{-16}	1.66×10^{-19}	7.49×10^{-23}
$(LAS)_3{\cdot}(A)_1 \rightarrow LAS + (LAS)_2{\cdot}(A)_1$	9.44×10^{-3}	2.29×10^{-4}	3.11×10^{-6}	2.04×10^{-8}
$(LAS)_3{\cdot}(A)_2 \rightarrow A + (LAS)_3{\cdot}(A)_1$	6.92×10^{7}	1.93×10^{7}	4.38×10^{6}	7.74×10^{5}
$(LAS)_3{\cdot}(A)_2 \rightarrow LAS + (LAS)_2{\cdot}(A)_2$	5.51×10^{3}	3.55×10^{2}	1.49×10^{1}	3.69×10^{-1}
$(LAS)_3{\cdot}(A)_3 \rightarrow A + (LAS)_3{\cdot}(A)_2$	3.14×10^{-3}	8.64×10^{-5}	1.35×10^{-6}	1.05×10^{-8}

Table S10 Total evaporation coefficients ($\sum\gamma$, s^{-1}) for each cluster analyzed in the present study of LAS-SA-A system

Clusters	$\sum\gamma$, s^{-1}			
	298.15 K	278.15 K	258.15 K	238.15 K
SA·A	2.37×10^{5}	3.73×10^{4}	4.42×10^{3}	3.65×10^{2}
SA·LAS	1.18×10^{4}	1.16×10^{3}	7.99×10^{1}	3.49×10^{0}
A·LAS	9.64×10^{4}	1.19×10^{4}	1.07×10^{3}	6.39×10^{1}
$(SA)_2$	2.03×10^{3}	2.29×10^{2}	1.84×10^{1}	9.67×10^{-1}
$(LAS)_2$	2.84×10^{7}	3.82×10^{6}	3.78×10^{5}	2.51×10^{4}
$(SA)_2$·A	2.21×10^{0}	9.80×10^{-2}	2.68×10^{-3}	4.03×10^{-5}
$(SA)_2$·$(A)_2$	1.90×10^{0}	1.13×10^{-1}	4.33×10^{-3}	9.50×10^{-5}
A·$(LAS)_2$	3.21×10^{-2}	6.73×10^{-4}	7.75×10^{-6}	4.22×10^{-8}
$(A)_2$·$(LAS)_2$	1.28×10^{2}	1.34×10^{1}	9.84×10^{-1}	4.61×10^{-2}
$(SA)_2$·LAS	1.07×10^{8}	1.31×10^{7}	1.16×10^{6}	6.87×10^{4}
SA·$(LAS)_2$	3.20×10^{9}	4.54×10^{8}	4.77×10^{7}	3.41×10^{6}
$(SA)_3$	4.83×10^{5}	5.76×10^{4}	4.91×10^{3}	2.76×10^{2}
$(LAS)_3$	5.33×10^{8}	7.62×10^{7}	8.00×10^{6}	5.72×10^{5}
$(SA)_3$·A	8.84×10^{3}	8.11×10^{2}	5.09×10^{1}	1.99×10^{0}
$(SA)_3$·$(A)_2$	1.14×10^{0}	6.54×10^{-2}	2.40×10^{-3}	5.08×10^{-5}
$(SA)_3$·$(A)_3$	4.94×10^{2}	3.28×10^{1}	1.42×10^{0}	3.61×10^{-2}
A·$(LAS)_3$	9.44×10^{-3}	2.29×10^{-4}	3.11×10^{-6}	2.04×10^{-8}
$(A)_2$·$(LAS)_3$	6.92×10^{-5}	3.49×10^{-6}	4.38×10^{-7}	7.74×10^{-8}
$(A)_3$·$(LAS)_3$	3.14×10^{-6}	8.64×10^{-8}	1.35×10^{-9}	1.05×10^{-11}
SA·A·LAS	6.64×10^{0}	2.58×10^{-1}	6.16×10^{-3}	7.92×10^{5}
SA·$(A)_2$·LAS	1.88×10^{2}	1.95×10^{1}	1.41×10^{0}	6.54×10^{-2}
SA_2·A·LAS	2.94×10^{1}	1.74×10^{0}	$6.68 \times 10S^{-2}$	1.49×10^{-3}
$(SA)_2$·$(A)_2$·LAS	1.98×10^{4}	1.67×10^{3}	9.58×10^{1}	3.39×10^{0}
$(SA)_2$·$(A)_3$·LAS	4.79×10^{-7}	1.99×10^{-8}	1.07×10^{-9}	2.34×10^{-11}
SA·A·$(LAS)_2$	2.40×10^{1}	1.37×10^{0}	5.08×10^{-2}	1.08×10^{-3}
SA·$(A)_2$·$(LAS)_2$	5.71×10^{5}	7.45×10^{4}	7.42×10^{3}	5.16×10^{2}
SA·$(A)_3$·$(LAS)_2$	2.79×10^{2}	1.99×10^{1}	9.47×10^{-1}	2.70×10^{-2}

Table S11 Ratios ($\beta C/\sum\gamma$) between monomer molecule collisions and evaporation coefficients for each cluster involving LAS in the present study. [SA] = 1.0 × 107 molecules·cm^{-3}, [A] = 1.0 × 10^{10} molecules·cm^{-3}, [LAS] = 1.0 × 10^{10} molecules·cm^{-3}

Clusters	$\beta C/\sum\gamma$			
	298.15 K	278.15 K	258.15 K	238.15 K
Collision with SA monomer: C = [SA]				
SA·A	3.76×10^{-15}	2.23×10^{-14}	1.75×10^{-13}	1.95×10^{-12}
SA·LAS	9.08×10^{-14}	8.59×10^{-13}	1.16×10^{-11}	2.45×10^{-10}
A·LAS	1.13×10^{-14}	8.56×10^{-14}	8.86×10^{-13}	1.37×10^{-11}
$(SA)_2$	4.22×10^{-13}	3.47×10^{-12}	4.02×10^{-11}	7.07×10^{-10}
$(LAS)_2$	4.35×10^{-16}	3.01×10^{-15}	2.83×10^{-14}	3.92×10^{-13}
$(SA)_2$·A	3.99×10^{-10}	8.40×10^{-9}	2.85×10^{-7}	1.75×10^{-5}
$(SA)_2$·$(A)_2$	4.86×10^{-10}	7.60×10^{-9}	1.85×10^{-7}	7.77×10^{-6}
A·$(LAS)_2$	2.78×10^{-8}	1.24×10^{-6}	9.99×10^{-5}	1.69×10^{-2}
$(A)_2$·$(LAS)_2$	1.19×10^{-11}	1.06×10^{-10}	1.34×10^{-9}	2.64×10^{-8}
SA·A·LAS	1.36×10^{-10}	3.27×10^{-9}	1.27×10^{-7}	9.14×10^{-6}
SA·$(A)_2$·LAS	5.47×10^{-12}	4.91×10^{-11}	6.29×10^{-10}	1.25×10^{-8}
Collision with A monomer: C = [A]				
SA·LAS	3.30×10^{-11}	3.12×10^{-10}	4.22×10^{-9}	8.89×10^{-8}
$(SA)_2$	1.37×10^{-10}	1.13×10^{-9}	1.31×10^{-8}	2.30×10^{-7}
$(LAS)_2$	1.69×10^{-13}	1.17×10^{-12}	1.10×10^{-11}	1.52×10^{-10}
$(SA)_2$·A	1.33×10^{-7}	2.81×10^{-6}	9.53×10^{-5}	5.86×10^{-3}
A·$(LAS)_2$	1.05×10^{-5}	4.70×10^{-4}	3.79×10^{-2}	6.42×10^{0}
$(SA)_2$·LAS	4.01×10^{-15}	3.06×10^{-14}	3.20×10^{-13}	4.97×10^{-12}
SA·$(LAS)_2$	1.19×10^{-16}	7.84×10^{-16}	6.93×10^{-15}	8.95×10^{-14}
$(SA)_3$	8.23×10^{-13}	6.45×10^{-12}	7.02×10^{-11}	1.15×10^{-9}
$(LAS)_3$	9.23×10^{-16}	6.03×10^{-15}	5.33×10^{-14}	6.88×10^{-13}
$(SA)_3$·A	3.57×10^{-11}	3.64×10^{-10}	5.38×10^{-9}	1.27×10^{-7}
$(SA)_3$·$(A)_2$	3.63×10^{-7}	5.93×10^{-6}	1.50×10^{-4}	6.54×10^{-3}
A·$(LAS)_3$	5.23×10^{-5}	2.01×10^{-3}	1.37×10^{-1}	1.94×10^{1}
$(A)_2$·$(LAS)_3$	7.07×10^{-15}	2.37×10^{-14}	9.67×10^{-14}	5.05×10^{-13}
SA·A·LAS	4.93×10^{-8}	1.18×10^{-6}	4.61×10^{-5}	3.31×10^{-3}

$(SA)_2{\cdot}A{\cdot}LAS$	1.48×10^{-8}	2.33×10^{-7}	5.65×10^{-6}	2.33×10^{-4}
$(SA)_2{\cdot}(A)_2{\cdot}LAS$	2.64×10^{-11}	2.92×10^{-10}	4.73×10^{-9}	1.23×10^{-7}
$SA{\cdot}A{\cdot}(LAS)_2$	1.75×10^{-8}	2.85×10^{-7}	7.16×10^{-6}	3.12×10^{-4}
$SA{\cdot}(A)_2{\cdot}(LAS)_2$	1.10×10^{-12}	7.86×10^{-12}	7.33×10^{-11}	9.71×10^{-10}
Collision with LAS monomer: C = [LAS]				
$SA{\cdot}A$	4.36×10^{-17}	2.58×10^{-16}	2.02×10^{-15}	2.26×10^{-14}
$SA{\cdot}LAS$	8.68×10^{-16}	8.21×10^{-15}	1.11×10^{-13}	2.34×10^{-12}
$A{\cdot}LAS$	1.15×10^{-16}	8.68×10^{-16}	8.99×10^{-15}	1.38×10^{-13}
$(SA)_2$	4.41×10^{-15}	3.64×10^{-14}	4.20×10^{-13}	7.39×10^{-12}
$(LAS)_2$	3.93×10^{-18}	2.72×10^{-17}	2.56×10^{-16}	3.54×10^{-15}
$(SA)_2{\cdot}A$	4.09×10^{-12}	8.61×10^{-11}	2.92×10^{-9}	1.79×10^{-7}
$(SA)_2{\cdot}(A)_2$	4.88×10^{-12}	7.63×10^{-11}	1.85×10^{-9}	7.79×10^{-8}
$A{\cdot}(LAS)_2$	2.62×10^{-10}	1.17×10^{-8}	9.40×10^{-7}	1.59×10^{-4}
$(A)_2{\cdot}(LAS)_2$	1.03×10^{-13}	9.20×10^{-13}	1.16×10^{-11}	2.29×10^{-10}
$SA{\cdot}A{\cdot}LAS$	1.32×10^{-12}	3.17×10^{-11}	1.24×10^{-9}	8.88×10^{-8}
$SA{\cdot}(A)_2{\cdot}LAS$	5.17×10^{-14}	4.64×10^{-13}	5.94×10^{-12}	1.18×10^{-10}

Research has shown that it is important to consider the concentration of precursors when evaluating the cluster stability, because a larger concentration of precursors increases the collision probability for a cluster, resulting in higher stability of the cluster. Therefore, the ratio of the collision frequency to the total evaporation rate ($\beta{\cdot}C/\sum\gamma$, in Table S5) was investigated. The $\beta{\cdot}C/\sum\gamma$ increases with the decrease of temperature, this indicates that the lower temperature is more LASvorable for the formation of clusters.

Table S12 Formation rate J (cm^{-3} s^{-1}) of LAS at T = 238.15 K, with [SA] = 10^6-10^8 molecules·cm^{-3}, [A] = 10^7-10^{11} molecules·cm^{-3}, and [LAS] = 0, 10^4-10^7 molecules·cm^{-3}. SA, A and LAS denote sulfuric acid, ammonia and disulfuric acid, respectively.

[SA]	[A]	[LAS] = 0	[LAS] = 10^3	[LAS] = 10^4	[LAS] = 10^5	[LAS] = 10^6
[SA] = 10^4	[A] = 10^7	7.29×10^{-15}	2.44×10^{-14}	3.19×10^{-13}	1.79×10^{-11}	8.33×10^{-9}
[SA] = 10^4	[A] = 10^8	4.14×10^{-12}	1.93×10^{-11}	2.84×10^{-10}	1.59×10^{-8}	5.59×10^{-6}
[SA] = 10^4	[A] = 10^9	6.26×10^{-10}	3.31×10^{-9}	5.01×10^{-8}	2.81×10^{-6}	1.15×10^{-3}
[SA] = 10^4	[A] = 10^{10}	1.65×10^{-8}	4.15×10^{-8}	4.76×10^{-7}	4.41×10^{-5}	1.44×10^{-1}
[SA] = 10^4	[A] = 10^{11}	5.94×10^{-8}	1.56×10^{-7}	2.66×10^{-6}	4.72×10^{-3}	2.78×10^{1}
[SA] = 10^5	[A] = 10^7	7.36×10^{-11}	8.91×10^{-11}	2.42×10^{-10}	3.10×10^{-9}	1.47×10^{-7}
[SA] = 10^5	[A] = 10^8	4.16×10^{-8}	5.54×10^{-8}	1.91×10^{-7}	2.75×10^{-6}	1.28×10^{-4}
[SA] = 10^5	[A] = 10^9	6.24×10^{-6}	8.65×10^{-6}	3.25×10^{-5}	4.75×10^{-4}	2.06×10^{-2}
[SA] = 10^5	[A] = 10^{10}	1.63×10^{-4}	1.86×10^{-4}	4.06×10^{-4}	4.48×10^{-3}	3.52×10^{-1}
[SA] = 10^5	[A] = 10^{11}	5.85×10^{-4}	6.67×10^{-4}	1.52×10^{-3}	2.53×10^{-2}	3.07×10^{1}
[SA] = 10^6	[A] = 10^7	8.12×10^{-7}	8.26×10^{-7}	9.51×10^{-7}	2.30×10^{-6}	2.35×10^{-5}
[SA] = 10^6	[A] = 10^8	4.36×10^{-4}	4.48×10^{-4}	5.58×10^{-4}	1.75×10^{-3}	2.03×10^{-2}
[SA] = 10^6	[A] = 10^9	6.10×10^{-2}	6.30×10^{-2}	8.08×10^{-2}	2.70×10^{-1}	2.96×10^{0}
[SA] = 10^6	[A] = 10^{10}	1.48×10^{0}	1.50×10^{0}	1.65×10^{0}	3.25×10^{0}	2.56×10^{1}
[SA] = 10^6	[A] = 10^{11}	4.90×10^{0}	4.95×10^{0}	5.48×10^{0}	1.13×10^{1}	1.44×10^{2}
[SA] = 10^7	[A] = 10^7	1.48×10^{-2}	1.48×10^{-2}	1.48×10^{-2}	1.53×10^{-2}	1.95×10^{-2}
[SA] = 10^7	[A] = 10^8	5.23×10^{0}	5.24×10^{0}	5.29×10^{0}	5.76×10^{0}	1.02×10^{1}
[SA] = 10^7	[A] = 10^9	3.88×10^{2}	3.88×10^{2}	3.92×10^{2}	4.31×10^{2}	7.85×10^{2}
[SA] = 10^7	[A] = 10^{10}	3.81×10^{3}	3.82×10^{3}	3.83×10^{3}	3.97×10^{3}	5.35×10^{3}
[SA] = 10^7	[A] = 10^{11}	7.62×10^{3}	7.62×10^{3}	7.66×10^{3}	8.04×10^{3}	1.18×10^{4}

Table S13 Formation rate J ($cm^{-3}\ s^{-1}$) of LAS at T = 258.15 K, with [SA] = 10^6-10^8 molecules·cm^{-3}, [A] = 10^7-10^{11} molecules·cm^{-3}, and [LAS] = 0, 10^4-10^7 molecules·cm^{-3}. SA, A and LAS represent sulfuric acid, ammonia and disulfuric acid, respectively.

[SA]	[A]	[LAS] = 0	[LAS] = 10^3	[LAS] = 10^4	[LAS] = 10^5	[LAS] = 10^6
[SA] = 10^4	[A] = 10^7	4.70×10^{-20}	6.37×10^{-20}	3.62×10^{-19}	2.99×10^{-16}	2.16×10^{-12}
[SA] = 10^4	[A] = 10^8	4.68×10^{-17}	6.34×10^{-17}	3.59×10^{-16}	2.92×10^{-13}	2.12×10^{-9}
[SA] = 10^4	[A] = 10^9	4.42×10^{-14}	6.04×10^{-14}	3.40×10^{-13}	2.42×10^{-10}	1.71×10^{-6}
[SA] = 10^4	[A] = 10^{10}	2.79×10^{-11}	4.11×10^{-11}	2.60×10^{-10}	1.25×10^{-7}	8.41×10^{-4}
[SA] = 10^4	[A] = 10^{11}	3.77×10^{-9}	7.38×10^{-9}	7.42×10^{-8}	5.22×10^{-5}	3.50×10^{-1}
[SA] = 10^5	[A] = 10^7	4.73×10^{-16}	4.88×10^{-16}	6.39×10^{-16}	3.61×10^{-15}	2.38×10^{-12}
[SA] = 10^5	[A] = 10^8	4.70×10^{-13}	4.85×10^{-13}	6.36×10^{-13}	3.59×10^{-12}	2.32×10^{-9}
[SA] = 10^5	[A] = 10^9	4.44×10^{-10}	4.59×10^{-10}	6.06×10^{-10}	3.40×10^{-9}	1.92×10^{-6}
[SA] = 10^5	[A] = 10^{10}	2.78×10^{-7}	2.90×10^{-7}	4.09×10^{-7}	2.59×10^{-6}	1.01×10^{-3}
[SA] = 10^5	[A] = 10^{11}	3.73×10^{-5}	4.06×10^{-5}	7.31×10^{-5}	7.27×10^{-4}	4.16×10^{-1}
[SA] = 10^6	[A] = 10^7	4.95×10^{-12}	4.96×10^{-12}	5.10×10^{-12}	6.60×10^{-12}	3.57×10^{-11}
[SA] = 10^6	[A] = 10^8	4.91×10^{-9}	4.93×10^{-9}	5.06×10^{-9}	6.56×10^{-9}	3.54×10^{-8}
[SA] = 10^6	[A] = 10^9	4.59×10^{-6}	4.60×10^{-6}	4.74×10^{-6}	6.19×10^{-6}	3.35×10^{-5}
[SA] = 10^6	[A] = 10^{10}	2.69×10^{-3}	2.70×10^{-3}	2.81×10^{-3}	3.96×10^{-3}	2.49×10^{-2}
[SA] = 10^6	[A] = 10^{11}	3.37×10^{-1}	3.40×10^{-1}	3.67×10^{-1}	6.56×10^{-1}	5.92×10^{0}
[SA] = 10^7	[A] = 10^7	7.17×10^{-8}	7.17×10^{-8}	7.18×10^{-8}	7.30×10^{-8}	8.58×10^{-8}
[SA] = 10^7	[A] = 10^8	7.04×10^{-5}	7.04×10^{-5}	7.05×10^{-5}	7.16×10^{-5}	8.44×10^{-5}
[SA] = 10^7	[A] = 10^9	5.92×10^{-2}	5.92×10^{-2}	5.93×10^{-2}	6.04×10^{-2}	7.25×10^{-2}
[SA] = 10^7	[A] = 10^{10}	2.16×10^{1}	2.16×10^{1}	2.17×10^{1}	2.25×10^{1}	3.15×10^{1}
[SA] = 10^7	[A] = 10^{11}	1.40×10^{3}	1.40×10^{3}	1.41×10^{3}	1.49×10^{3}	2.26×10^{3}

Table S14 Formation rate J (cm^{-3} s^{-1}) of LAS at T = 278.15 K, with [SA] = 10^6-10^8 molecules·cm^{-3}, [A] = 10^7-10^{11} molecules·cm^{-3}, and [LAS] = 0, 10^4-10^7 molecules·cm^{-3}. SA, A and LAS denote sulfuric acid, ammonia and disulfuric acid, respectively.

[SA]	[A]	[LAS] = 0	[LAS] = 10^3	[LAS] = 10^4	[LAS] = 10^5	[LAS] = 10^6
[SA] = 10^4	[A] = 10^7	2.64×10^{-26}	4.21×10^{-26}	4.46×10^{-23}	4.31×10^{-19}	3.47×10^{-15}
[SA] = 10^4	[A] = 10^8	2.64×10^{-23}	4.21×10^{-23}	4.46×10^{-20}	4.31×10^{-16}	3.47×10^{-12}
[SA] = 10^4	[A] = 10^9	2.64×10^{-20}	4.21×10^{-20}	4.49×10^{-17}	4.34×10^{-13}	3.50×10^{-9}
[SA] = 10^4	[A] = 10^{10}	2.64×10^{-17}	4.20×10^{-17}	4.67×10^{-14}	4.52×10^{-10}	3.64×10^{-6}
[SA] = 10^4	[A] = 10^{11}	2.60×10^{-14}	3.93×10^{-14}	3.83×10^{-11}	3.70×10^{-7}	2.98×10^{-3}
[SA] = 10^5	[A] = 10^7	2.64×10^{-22}	2.71×10^{-22}	4.21×10^{-22}	4.36×10^{-19}	3.47×10^{-15}
[SA] = 10^5	[A] = 10^8	2.64×10^{-19}	2.71×10^{-19}	4.21×10^{-19}	4.36×10^{-16}	3.48×10^{-12}
[SA] = 10^5	[A] = 10^9	2.64×10^{-16}	2.71×10^{-16}	4.21×10^{-16}	4.39×10^{-13}	3.50×10^{-9}
[SA] = 10^5	[A] = 10^{10}	2.64×10^{-13}	2.71×10^{-13}	4.20×10^{-13}	4.57×10^{-10}	3.63×10^{-6}
[SA] = 10^5	[A] = 10^{11}	2.60×10^{-10}	2.67×10^{-10}	3.93×10^{-10}	3.74×10^{-7}	2.98×10^{-3}
[SA] = 10^6	[A] = 10^7	2.65×10^{-18}	2.65×10^{-18}	2.72×10^{-18}	4.20×10^{-18}	3.53×10^{-15}
[SA] = 10^6	[A] = 10^8	2.65×10^{-15}	2.65×10^{-15}	2.72×10^{-15}	4.20×10^{-15}	3.53×10^{-12}
[SA] = 10^6	[A] = 10^9	2.65×10^{-12}	2.65×10^{-12}	2.72×10^{-12}	4.20×10^{-12}	3.55×10^{-9}
[SA] = 10^6	[A] = 10^{10}	2.64×10^{-9}	2.65×10^{-9}	2.72×10^{-9}	4.19×10^{-9}	3.69×10^{-6}
[SA] = 10^6	[A] = 10^{11}	2.60×10^{-6}	2.61×10^{-6}	2.67×10^{-6}	3.92×10^{-6}	3.04×10^{-3}
[SA] = 10^7	[A] = 10^7	2.71×10^{-14}	2.71×10^{-14}	2.71×10^{-14}	2.78×10^{-14}	4.17×10^{-14}
[SA] = 10^7	[A] = 10^8	2.71×10^{-11}	2.71×10^{-11}	2.71×10^{-11}	2.78×10^{-11}	4.17×10^{-11}
[SA] = 10^7	[A] = 10^9	2.71×10^{-8}	2.71×10^{-8}	2.71×10^{-8}	2.78×10^{-8}	4.17×10^{-8}
[SA] = 10^7	[A] = 10^{10}	2.69×10^{-5}	2.69×10^{-5}	2.70×10^{-5}	2.77×10^{-5}	4.14×10^{-5}
[SA] = 10^7	[A] = 10^{11}	2.58×10^{-2}	2.58×10^{-2}	2.59×10^{-2}	2.65×10^{-2}	3.83×10^{-2}

Table S15 The formation rate J (cm^{-3} s^{-1}) of LAS at T = 298.15 K, with [SA] = 10^6-10^8 molecules·cm^{-3}, [A] = 10^7-10^{11} molecules·cm^{-3}, and [LAS] = 0, 10^4-10^7 molecules·cm^{-3}. SA, A and LAS represent sulfuric acid, ammonia and disulfuric acid, respectively.

[SA]	[A]	[LAS] = 0	[LAS] = 10^3	[LAS] = 10^4	[LAS] = 10^5	[LAS] = 10^6
[SA] = 10^4	[A] = 10^7	6.98×10^{-32}	1.75×10^{-31}	7.49×10^{-28}	7.44×10^{-24}	7.06×10^{-20}
[SA] = 10^4	[A] = 10^8	6.98×10^{-29}	1.75×10^{-28}	7.49×10^{-25}	7.44×10^{-21}	7.06×10^{-17}
[SA] = 10^4	[A] = 10^9	6.98×10^{-26}	1.75×10^{-25}	7.49×10^{-22}	7.44×10^{-18}	7.06×10^{-14}
[SA] = 10^4	[A] = 10^{10}	6.98×10^{-23}	1.75×10^{-22}	7.50×10^{-19}	7.44×10^{-15}	7.07×10^{-11}
[SA] = 10^4	[A] = 10^{11}	6.98×10^{-20}	1.75×10^{-19}	7.53×10^{-16}	7.47×10^{-12}	7.09×10^{-8}
[SA] = 10^5	[A] = 10^7	6.98×10^{-28}	7.17×10^{-28}	1.75×10^{-27}	7.45×10^{-24}	7.06×10^{-20}
[SA] = 10^5	[A] = 10^8	6.98×10^{-25}	7.17×10^{-25}	1.75×10^{-24}	7.45×10^{-21}	7.06×10^{-17}
[SA] = 10^5	[A] = 10^9	6.98×10^{-22}	7.17×10^{-22}	1.75×10^{-21}	7.45×10^{-18}	7.06×10^{-14}
[SA] = 10^5	[A] = 10^{10}	6.98×10^{-19}	7.17×10^{-19}	1.75×10^{-18}	7.46×10^{-15}	7.07×10^{-11}
[SA] = 10^5	[A] = 10^{11}	6.98×10^{-16}	7.17×10^{-16}	1.75×10^{-15}	7.49×10^{-12}	7.09×10^{-8}
[SA] = 10^6	[A] = 10^7	6.98×10^{-24}	7.00×10^{-24}	7.17×10^{-24}	1.74×10^{-23}	7.08×10^{-20}
[SA] = 10^6	[A] = 10^8	6.98×10^{-21}	7.00×10^{-21}	7.17×10^{-21}	1.74×10^{-20}	7.08×10^{-17}
[SA] = 10^6	[A] = 10^9	6.98×10^{-18}	7.00×10^{-18}	7.17×10^{-18}	1.74×10^{-17}	7.08×10^{-14}
[SA] = 10^6	[A] = 10^{10}	6.98×10^{-15}	7.00×10^{-15}	7.17×10^{-15}	1.74×10^{-14}	7.08×10^{-11}
[SA] = 10^6	[A] = 10^{11}	6.98×10^{-12}	7.00×10^{-12}	7.17×10^{-12}	1.75×10^{-11}	7.11×10^{-8}
[SA] = 10^7	[A] = 10^7	6.99×10^{-20}	6.99×10^{-20}	7.01×10^{-20}	7.18×10^{-20}	1.71×10^{-19}
[SA] = 10^7	[A] = 10^8	6.99×10^{-17}	6.99×10^{-17}	7.01×10^{-17}	7.18×10^{-17}	1.71×10^{-16}
[SA] = 10^7	[A] = 10^9	6.99×10^{-14}	6.99×10^{-14}	7.01×10^{-14}	7.18×10^{-14}	1.71×10^{-13}
[SA] = 10^7	[A] = 10^{10}	6.99×10^{-11}	6.99×10^{-11}	7.01×10^{-11}	7.18×10^{-11}	1.71×10^{-10}
[SA] = 10^7	[A] = 10^{11}	6.99×10^{-8}	6.99×10^{-8}	7.01×10^{-8}	7.18×10^{-8}	1.71×10^{-7}

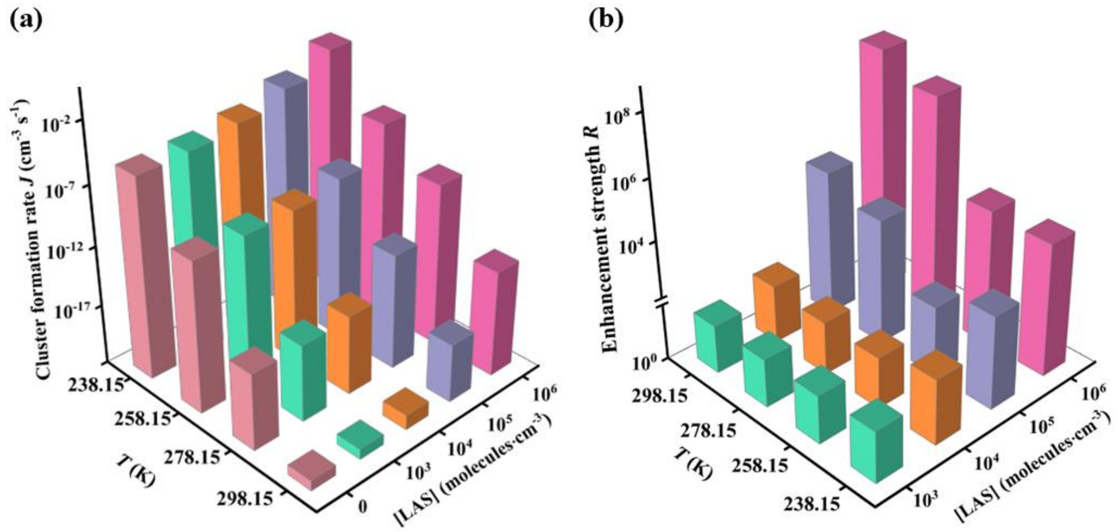

Fig. S5 (a) Cluster formation rate J and (b) enhancement factor R of LAS as functions of [LAS] (10^3 to 10^6 molecules·cm^{-3}) at temperatures of 238.15, 258.15, 278.15 and 298.15 K, with [SA] = 10^5 molecules·cm^{-3} and [A] = 10^9 molecules·cm^{-3}.

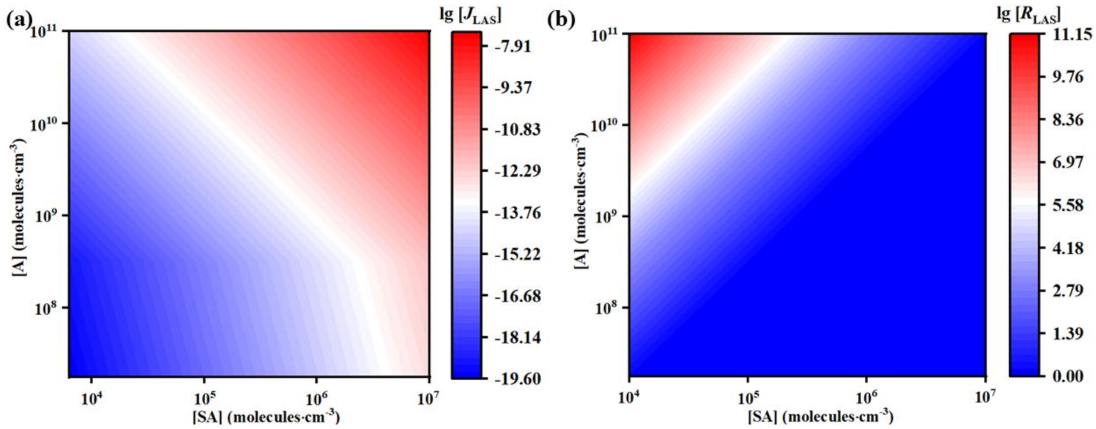

Fig. S6 (a) Cluster formation rate J and (b) enhancement factor R as functions of [SA] and [A] at [LAS] = 10^5 molecules·cm^{-3} and 278.15 K. Color bars represent the values of lg[J_{LAS}] and lg[R_{LAS}], respectively.

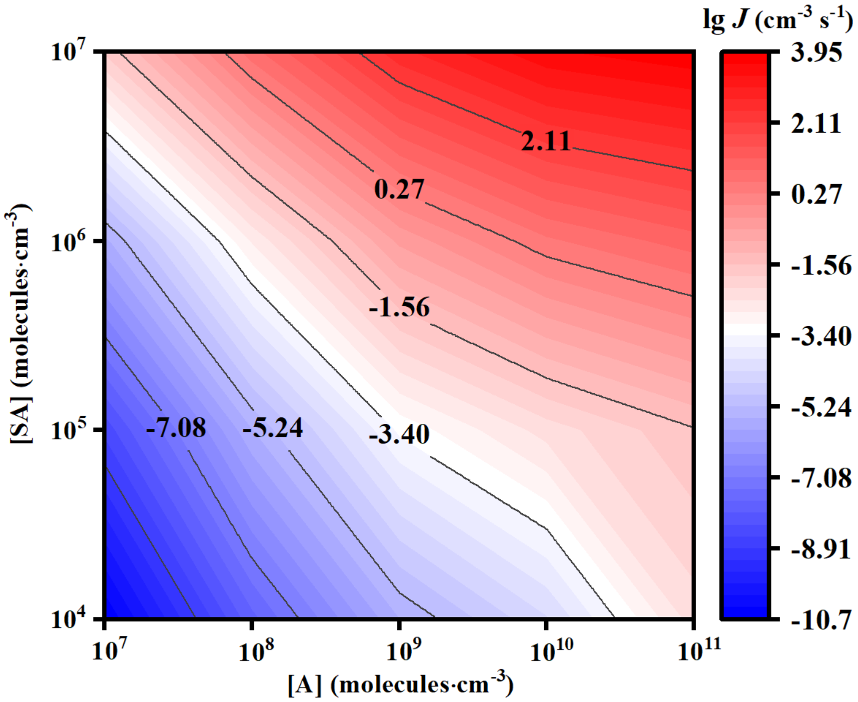

Fig. S7 Cluster formation rate (J) as a function of [SA] and [A] at [LAS]=10^5 molecules·cm^{-3} and 238.15 K. Color bars indicate $\log_{10}[J]$ values.

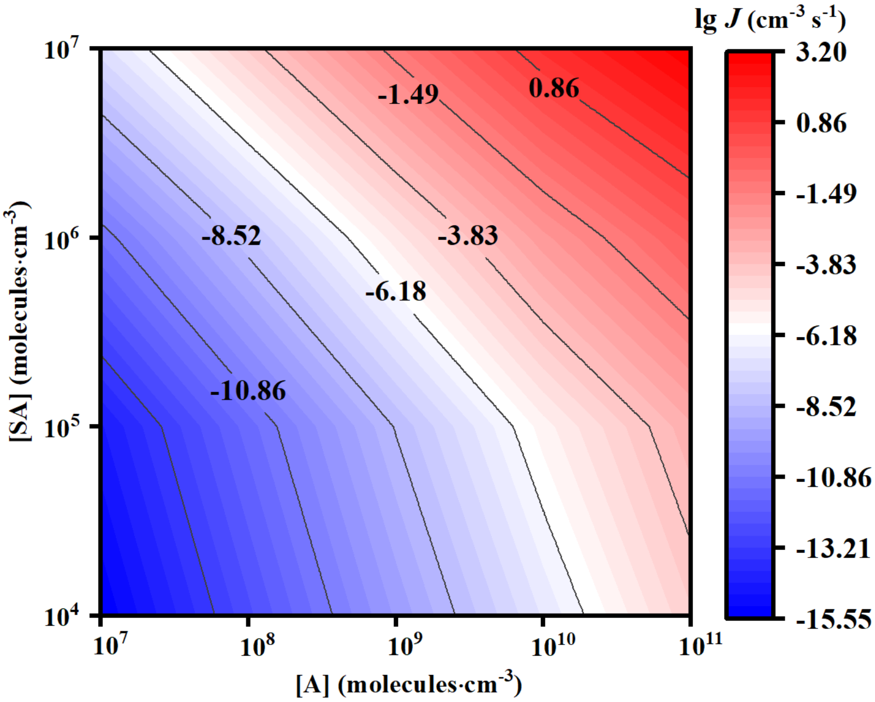

Fig. S8 Cluster formation rate (J) as a function of [SA] and [A] at [LAS]=10^5 molecules·cm^{-3} and 258.15 K. Color bars indicate $\log_{10}[J]$ values.

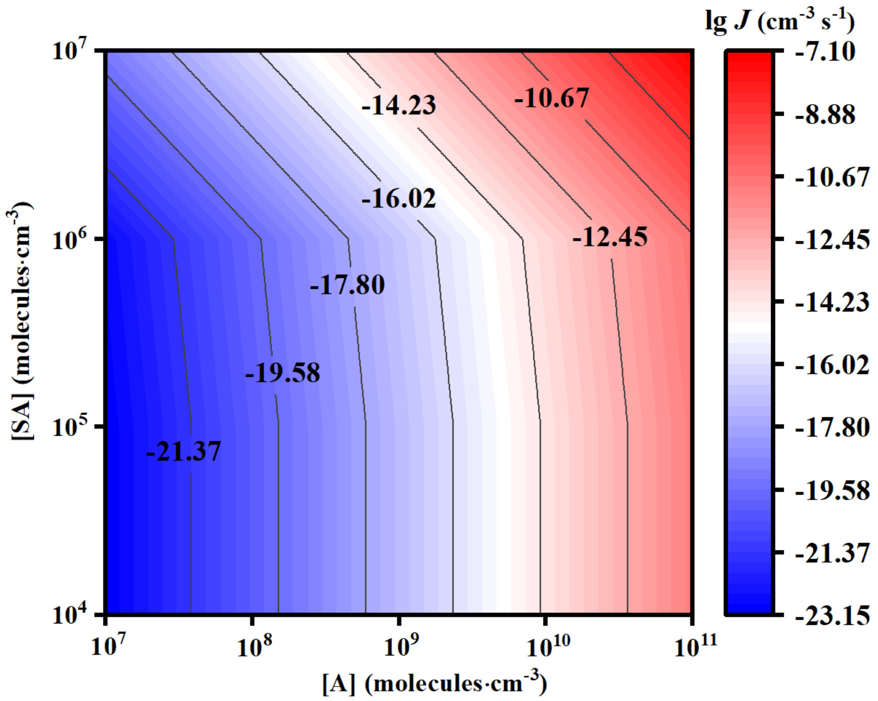

Fig. S9 Cluster formation rate (*J*) as a function of [SA] and [A] at [LAS]=10^5 molecules·cm^{-3} and 298.15 K. Color bars indicate $\log_{10}[J]$ values.

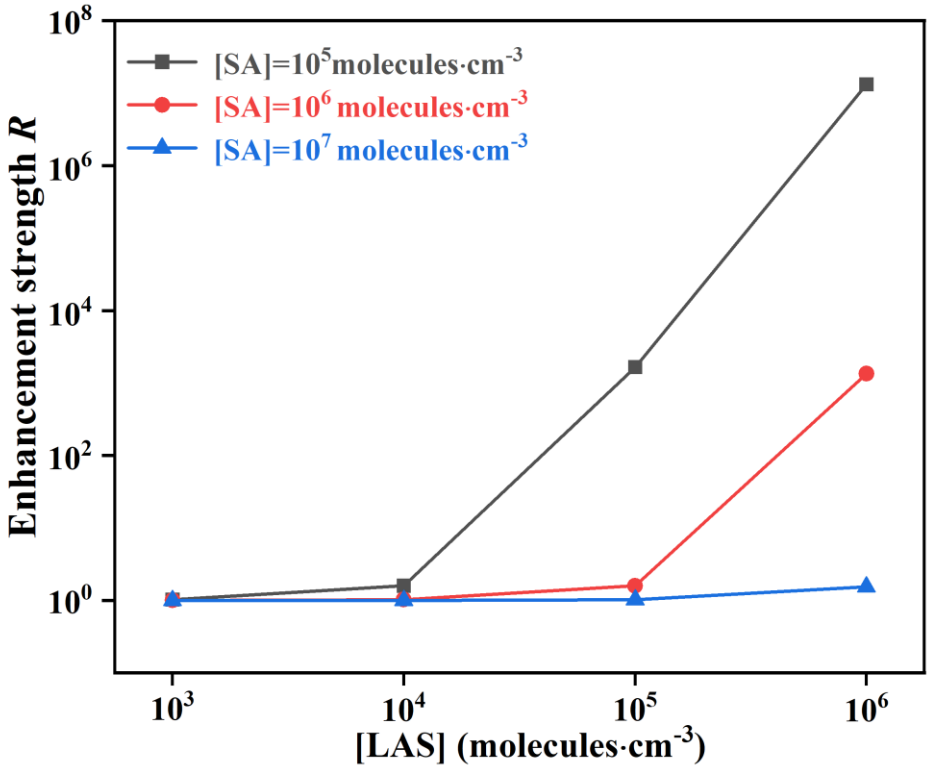

Fig. S10 Enhancement factor R as functions of [SA] and [LAS] at [A] = 10^9 molecules·cm^{-3} and 278.15 K.

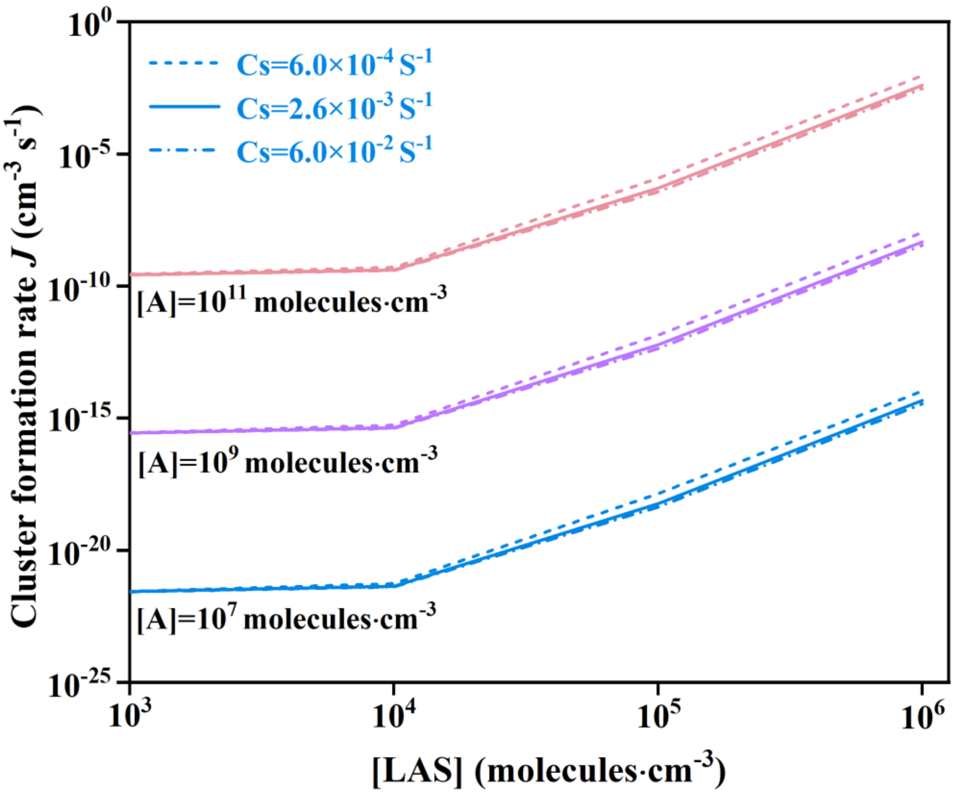

Fig. S11 The formation rate J (cm^{-3} s^{-1}) of LAS at varying consentrations of A and different condensation sink (CS) values in the SA-A-LAS-based system where T = 278.15 K, [SA] = 10^5 molecules cm^{-3}, [LAS] = 10^3 ~ 10^6 molecules cm^{-3}. CS = 6×10^{-4} s^{-1} (dotted lines), 2.6×10^{-3} s^{-1} (solid lines) and 6×10^{-2} s^{-1} (dash-dotted lines)

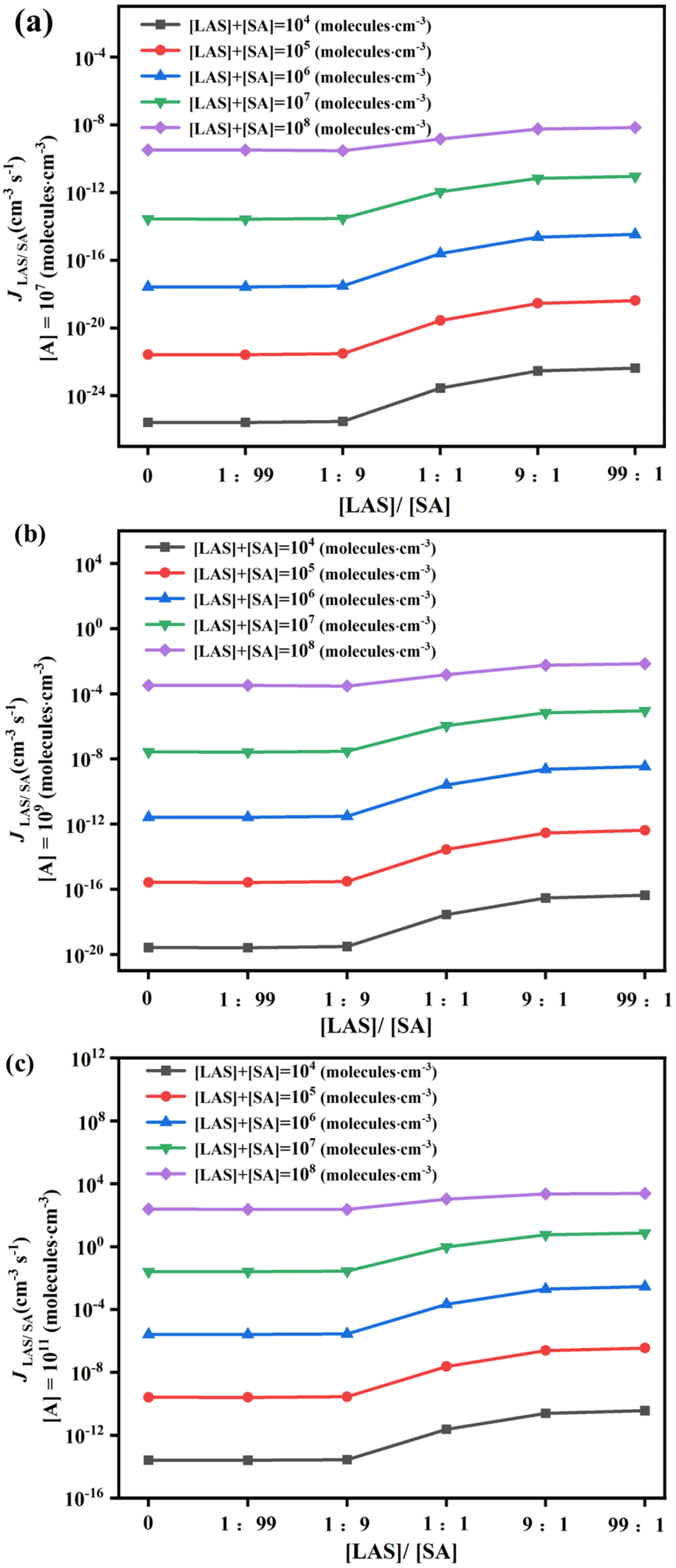

Fig. S12 Particle formation rates (J, $cm^{-3}\cdot s^{-1}$) with varying ratios of [LAS]:[SA] at 278.15 K under different A concentrations ((a)10^7 molecules·cm^{-3}, (b)10^9 molecules·cm^{-3}, (c)10^{11} molecules·cm^{-3}). [LAS] + [SA] = 10^4-10^8 molecules·cm^{-3}

The observed concentration dependence indicates that the LAS-driven nucleation process becomes particularly significant in environments with moderate to high LAS concentrations and relatively low SA levels. Therefore, in the LAS-SA-A ternary nucleation system, LAS is likely to function as an "acid" molecule, exhibiting a competitive effect. To evaluate the competitive interactions between LAS and SA molecules, another set of ACDC simulations was conducted, considering different ratios of the concentrations of LAS and SA ([LAS]/[SA]) and varying the total concentration of LAS and SA. Fig. S12 shows the variation of $J_{LAS/SA}$ with the total concentrations of SA and LAS at A concentrations of 10^7, 10^9, and 10^{11} molecules·cm^{-3}.

As shown in Fig. S12(a), at lower atmospheric concentration of A (10^7 molecules·cm^{-3}), the formation rate $J_{LAS/SA}$ increases with the substitution percentage. At a 50% substitution rate ([LAS]:[SA] = 1:1), $J_{LAS/SA}$ sharply increases to 1.46×10^{-9} cm^{-3}·s^{-1}, which is larger by 1-2 orders of magnitude than the value at unsubstituted condition. At a 99% substitution rate ([LAS]:[SA] = 99:1), $J_{LAS/SA}$ reaches its maximum value of 6.99×10^{-9} cm^{-3}·s^{-1}, which is 1-3 orders of magnitude greater than the value under non-substituted conditions. These results indicate that, at lower atmospheric concentrations of A, the enhancing effect of LAS on the SA-A group particle formation rate increases with the substitution percentage. At intermediate (10^9 molecules·cm^{-3}) and higher concentrations (10^{11} molecules·cm^{-3}) of atmospheric A, the $J_{LAS/SA}$ at a 99% substitution rate ([LAS]:[SA] = 99:1) reaches its maximum value. Compared to the $J_{LAS/SA}$ under non-substituted conditions, the value at a 99% substitution rate is increased by one order of magnitude. In contrast, urban and industrial environments, which typically have high SA concentrations, favor SA-A self-aggregation nucleation, thereby reducing the relative contribution of LAS.

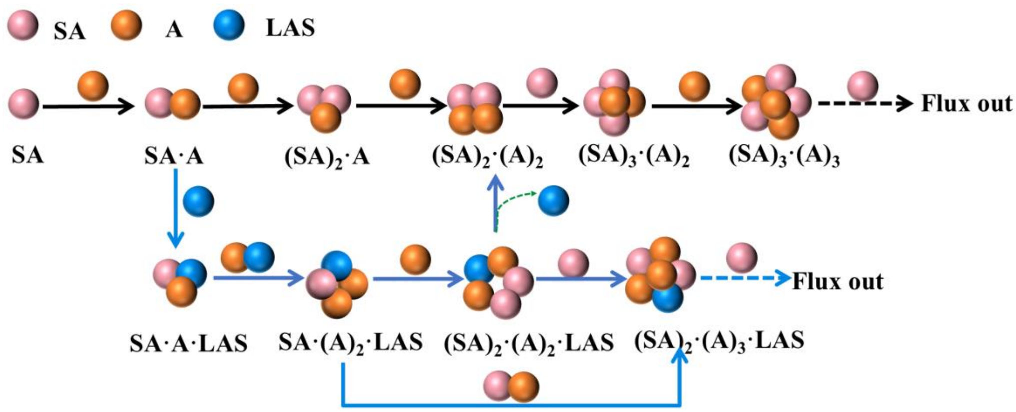

Fig. S13 Main cluster formation mechanisms in the SA-A-LAS-based system at 238.15 K, with [SA] = 10^6 molecules·cm^{-3}, [A] = 10^9 molecules·cm^{-3}, and [LAS] = 10^5 molecules·cm^{-3}. Only net fluxes contributing more than 5% to cluster growth are shown. Black arrows indicate pure SA-A-based growth pathways; blue arrows represent pathways involving LAS; green arrows denote pure LAS-A-based growth pathways.

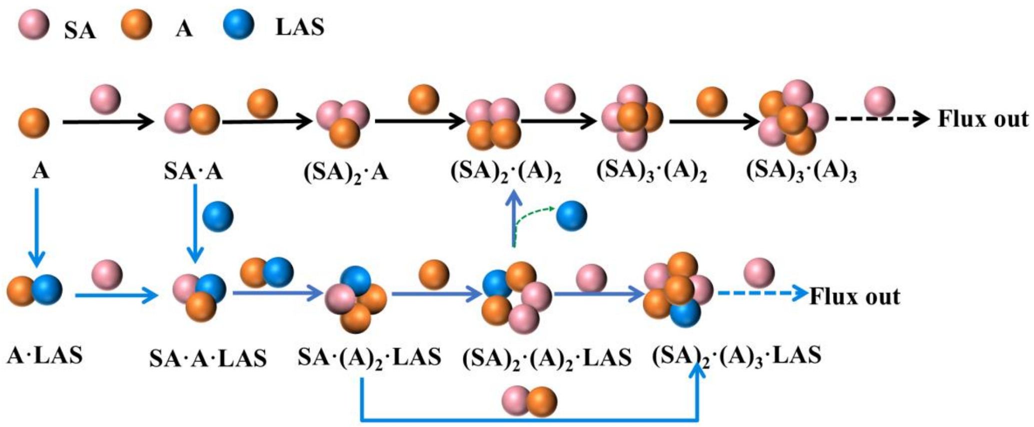

Fig. S14 Main cluster formation mechanism in the SA-A-LAS-based system at 258.15 K, with [SA] = 10^6 molecules·cm^{-3}, [A] = 10^9 molecules·cm^{-3}, and [LAS] = 10^5 molecules·cm^{-3}. Only net fluxes contributing more than 5% to cluster growth are shown. Black arrows indicate pure SA-A-based growth pathways; blue arrows represent pathways involving LAS; green arrows denote pure LAS-A-based growth pathways.

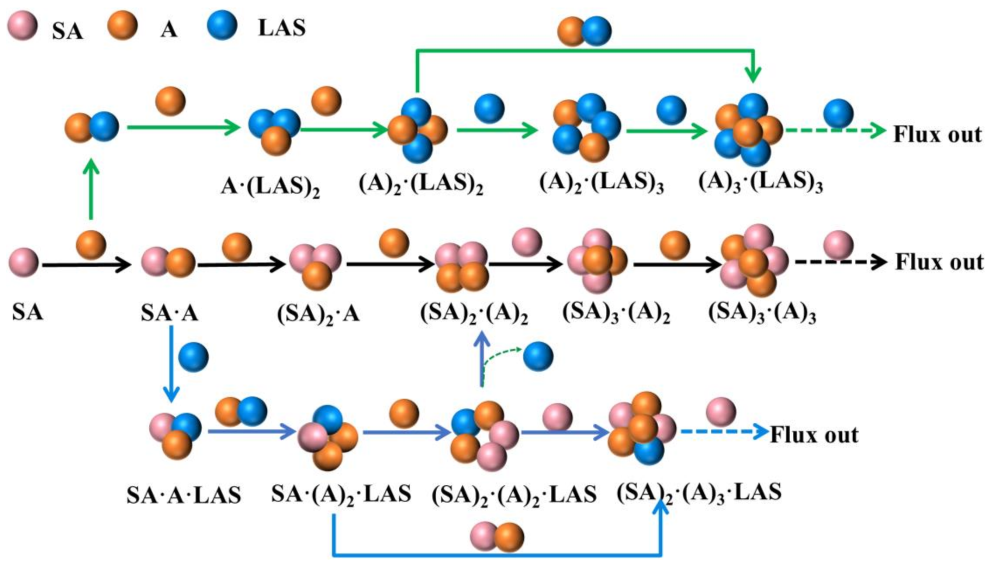

Fig. S15 Main cluster formation mechanisms in the SA-A-LAS-based system at 298.15 K, with [SA] = 10^6 molecules·cm^{-3}, [A] = 10^9 molecules·cm^{-3}, and [LAS] = 10^5 molecules·cm^{-3}. Only net fluxes contributing more than 5% to cluster growth are shown. Black arrows indicate pure SA-A-based growth pathways; blue arrows represent pathways involving LAS; green arrows denote pure LAS-A-based growth pathways.

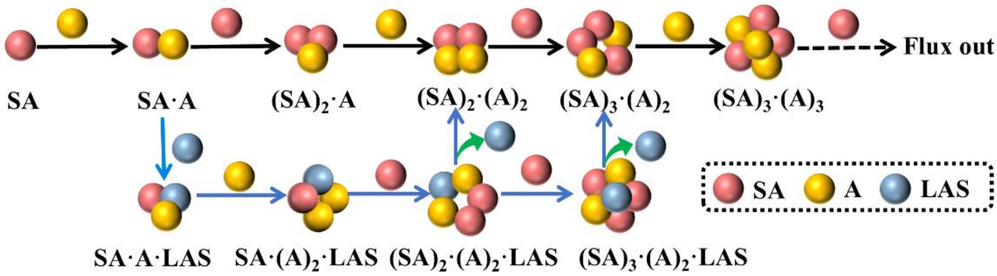

Fig. S16 Main cluster formation mechanisms in the SA-A-LAS-based system at 278.15 K, with [SA] = 9.25×10^6 molecules·cm^{-3}, [A] = 10^9 molecules·cm^{-3}, and [LAS] = 10^4 molecules·cm^{-3}. Only net fluxes contributing more than 5% to cluster growth are shown. Black arrows indicate pure SA-A-based growth pathways; blue arrows represent pathways involving LAS; green arrows denote pure LAS-A-based growth pathways.

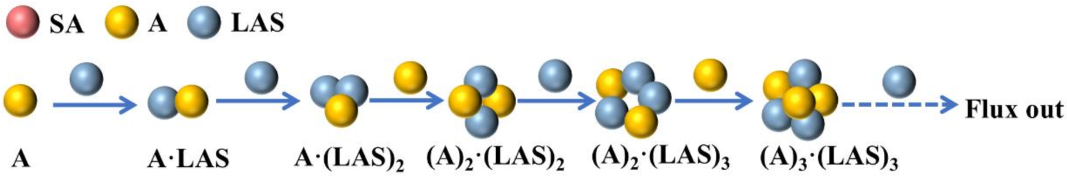

Fig. S17 Main cluster formation mechanisms in the SA-A-LAS-based system at 278.15 K, with [SA] = 10^6 molecules·cm^{-3}, [A] = 10^9 molecules·cm^{-3}, and [LAS] = 1.77×10^6 molecules·cm^{-3}. Only net fluxes contributing more than 5% to cluster growth are shown. Black arrows indicate pure SA-A-based growth pathways; blue arrows represent pathways involving LAS; green arrows denote pure LAS-A-based growth pathways.

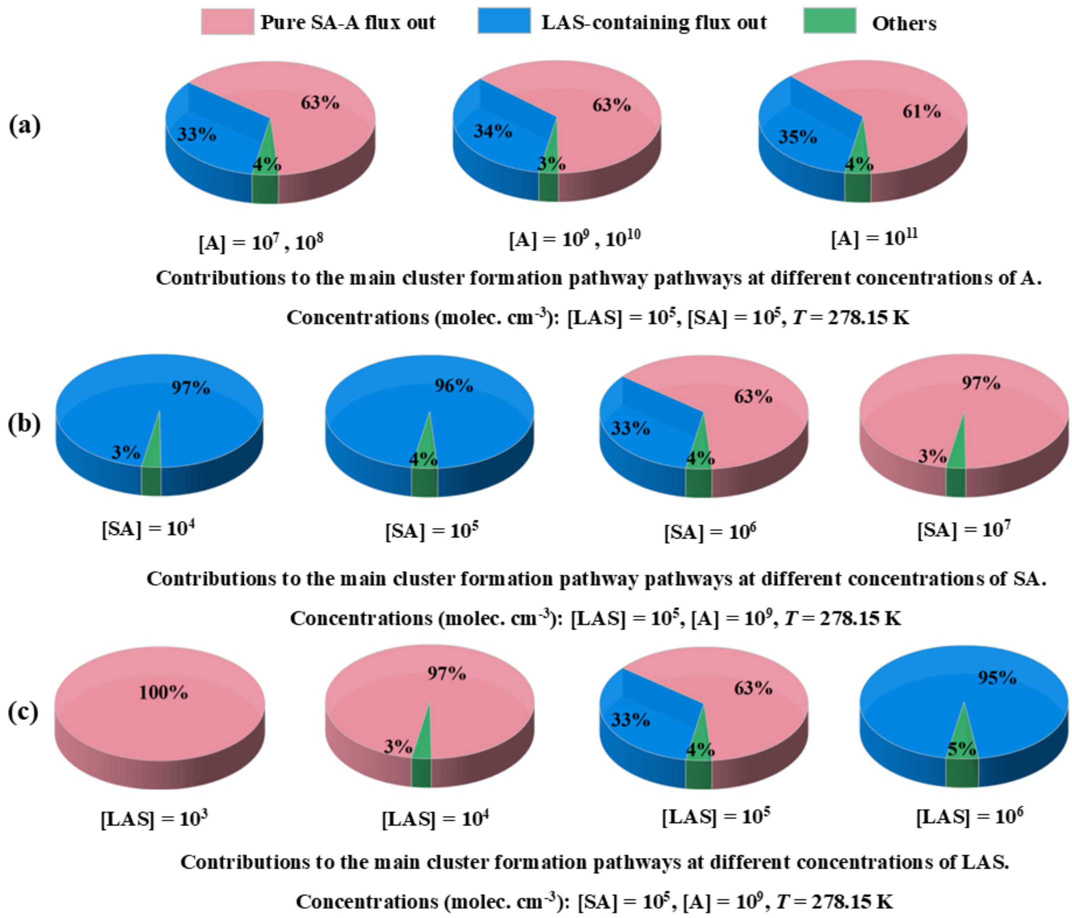

Fig. S18 The influence of (a) [A], (b) [SA] and (c) [LAS] on the relative contribution of the pure SA-A-based clustering route and the LAS participation route to the system flux is analyzed. Others in (a), (b) and (c) indicate that the route contribution of the cluster growing out of the studied system is less than 5%

Table S16 Cartesian coordinates of all molecules and clusters in the studied system.

SA:

Atoms	X	Y	Z
S	-0.00000100	0.00000200	-0.15847400
O	0.66569900	-1.06446300	-0.82038600
O	-0.66570900	1.06448600	-0.82034800
O	1.02252900	0.68572000	0.84196700
O	-1.02251900	-0.68574400	0.84196100
H	1.69063500	0.03522600	1.09500600
H	-1.69062200	-0.03525700	1.09502400

A:

Atoms	X	Y	Z
N	0.00000000	0.11333800	0.00000000
H	-0.93914000	-0.26450400	0.00000000
H	0.46957000	-0.26443200	0.81335400
H	0.46957000	-0.26443200	-0.81335400

LAS:

Atoms	X	Y	Z
C	-2.17748100	-0.37870600	0.11480900
O	-3.16213200	-0.06777000	0.71067000
H	-1.23527000	-1.56295200	-1.02996700
O	-2.10331000	-1.49601300	-0.61366400
C	-0.94088600	0.51766900	0.14960700
C	-1.22992800	1.87167700	-0.46428000
H	-0.35448000	2.50926300	-0.37402400
H	-1.48996200	1.75827400	-1.51560500
H	-2.06808700	2.32278800	0.06153100
H	-0.64595800	0.61017600	1.19456600
O	1.50255800	-0.86126600	1.31709200
O	1.81128900	1.32530000	0.38919500
O	2.41465100	-0.70755400	-0.95236200
O	0.11832100	-0.15320500	-0.58703300
S	1.59732500	-0.01418700	-0.02264600
H	1.67531200	-1.79033100	1.11383500

$(SA)_1 \cdot (A)_1$:

Atoms	X	Y	Z
S	-0.59849900	-0.11290900	0.09133500
O	0.10965700	-0.06479400	1.33359500
O	-1.76408700	-0.91246900	-0.08540000
O	0.39367800	-0.42172400	-1.05079200

O	-1.01109700	1.40357600	-0.19963600
H	1.37106100	-0.22193300	-0.72476200
H	-1.75621000	1.39602100	-0.81277800
N	2.72845100	0.04170600	-0.05392700
H	3.17388500	0.91971000	-0.29060600
H	3.41309400	-0.69669300	-0.16028100
H	2.44978300	0.08078400	0.92241700

$(SA)_1 \cdot (LAS)_1$:

Atoms	X	Y	Z
S	-2.96546200	0.53642400	-0.09103300
O	-3.89956300	1.58279600	-0.27951900
O	-2.33737200	0.21287600	-1.47624300
O	-3.71868500	-0.80232600	0.28709300
O	-1.92551200	0.63783100	0.89748800
H	-4.55783600	-0.84541700	-0.19166200
H	-0.76861400	-0.44818600	1.44463500
O	-0.43943900	-1.57610900	-0.80357100
O	0.04576600	-1.00594900	1.53512700
O	1.71700200	-2.16774500	0.28035600
O	1.14723600	0.13383200	-0.34429900
S	0.61936400	-1.27177400	0.11568400
C	3.51317900	0.68004000	-0.29899900
C	2.18526600	0.77228800	0.46507000
H	2.28852100	0.21773000	1.40055000
H	-1.59867700	-0.43286300	-1.36315100
O	4.20141700	1.63927200	-0.46940400
H	3.23678200	-1.21731000	-0.46397800
O	3.86575700	-0.53014900	-0.73063300
C	1.75432600	2.19333100	0.71489700
H	2.52127800	2.70527200	1.29053400
H	1.63235000	2.71593900	-0.23112100
H	0.81427700	2.20185500	1.26281000

$(SA)_1 \cdot (LAS)_1 \cdot (A)_1$:

Atoms	X	Y	Z
S	2.31631600	-0.71154000	-0.34042500
O	1.87018700	-0.60614000	1.16838500
O	2.56814600	-2.05971700	-0.70082800
O	3.36043300	0.28038100	-0.46184000
O	1.09040500	-0.13623900	-1.09371000
H	2.73717400	1.72327500	0.17984800
H	0.28707000	-0.81059200	-1.12655000

N	2.19361900	2.43055200	0.73147900
H	1.34374900	2.73503100	0.20634300
H	2.77511400	3.22537000	0.97732200
H	1.85774300	1.95938700	1.57232200
C	-0.82723300	1.82741200	0.09721900
O	-0.28470900	2.77543700	-0.42797300
H	-0.80928600	0.56406600	1.54371100
O	-0.47853100	1.46259200	1.32008200
C	-1.92190000	1.05496000	-0.62825200
C	-3.07805800	1.98924900	-0.95019300
H	-3.82258200	1.44203200	-1.52207300
H	-3.53514900	2.35135300	-0.03086800
H	-2.71567800	2.83346200	-1.53111900
H	-1.47784400	0.67594700	-1.54956800
O	-0.68731700	-1.19485800	1.32848800
O	-0.93386000	-1.55495500	-1.05844400
O	-2.65227200	-2.39795200	0.48388300
O	-2.44682900	-0.01630100	0.14302300
S	-1.64364000	-1.43632500	0.22574600
H	0.95947100	-0.99507800	1.27397500

$(SA)_1 \cdot (LAS)_1 \cdot (A)_2$:

Atoms	X	Y	Z
S	-1.02460600	0.26704700	0.02376600
O	-0.11367700	0.27314500	1.15359400
O	-2.46437200	0.41776700	0.69229400
O	-0.85501800	1.39453000	-0.88254200
O	-1.06270800	-1.02892100	-0.67629700
H	0.37804400	-1.99511700	-0.07923300
H	1.19920400	-3.06102400	0.94399500
N	1.23277000	-2.16064500	0.47870300
H	1.27652700	-1.39456500	1.16090800
H	2.09325800	-2.06556600	-0.10851500
H	1.55503400	1.70222100	0.88598200
N	1.58922400	2.33286400	0.07646500
H	0.69911300	2.19282300	-0.43611900
H	1.69644500	3.29691100	0.37162700
S	3.76089700	-0.13572500	-0.12325100
O	2.95700700	0.03664500	1.07775800
O	5.25659600	-0.21465000	0.43899900
O	3.51419600	-1.40460700	-0.80513000
O	3.72148300	1.01840900	-1.01743200
H	5.85316000	-0.32960500	-0.31074500
H	2.40833700	2.01505500	-0.48787700

C	-3.59263300	0.53231300	-0.20747500
H	-3.22224400	0.65813200	-1.22808600
C	-4.39148600	-0.77615700	-0.15276200
O	-5.58160300	-0.78872400	-0.03856700
O	-3.68044400	-1.89630500	-0.27032900
H	-2.73593500	-1.70216200	-0.40843400
C	-4.41664900	1.72450100	0.20905700
H	-5.29252200	1.80266400	-0.43011400
H	-4.75382700	1.60368200	1.23631800
H	-3.81629200	2.62760500	0.12417300

$(SA)_1 \cdot (LAS)_2$:

Atoms	X	Y	Z
S	0.08600700	0.78431500	1.67156300
O	1.43997800	0.43758200	2.41142200
O	0.13451700	0.20282900	0.34165000
O	-0.15641400	2.18176700	1.75735500
O	-0.85723700	-0.03118700	2.56222300
H	-0.42920000	3.45026000	-0.87035300
H	-1.38746100	-0.71428300	2.04917100
C	-1.90481200	2.29486600	-0.81292100
O	-2.59585000	3.06064800	-0.21886400
H	1.10627800	1.25080500	-0.93285500
O	-0.64766900	2.57130500	-1.21267600
C	-2.35308200	0.90281300	-1.24688300
C	-3.58822200	0.97971600	-2.11638800
H	-3.91030200	-0.01791200	-2.40752500
H	-4.38721400	1.47556300	-1.56939600
H	-3.36043500	1.55100600	-3.01582800
H	-1.52979200	0.38805600	-1.73507200
O	-2.10226900	-1.88809800	-1.13706400
O	-4.29826800	-1.54424700	-0.22745500
O	-2.34464900	-1.74073800	1.29455400
O	-2.61935900	0.23751100	0.01037000
S	-2.92975200	-1.31075000	0.04622900
H	-1.22384700	-2.24909300	-0.84973900
C	1.20027100	-2.25634200	-0.10172600
O	0.33122400	-2.82371700	-0.71889400
H	1.85006800	-1.60085400	1.55764500
O	1.23213000	-2.26555800	1.21472700
C	2.34475500	-1.58548600	-0.84724500
C	3.43443800	-2.58322600	-1.19096900
H	4.22860200	-2.07148200	-1.73039000
H	3.84469600	-3.02370100	-0.28368600

H	3.02080600	-3.37120800	-1.81724100
H	1.91935400	-1.13427400	-1.74027700
O	3.15312800	1.71080100	0.61660500
O	1.93484300	1.20298500	-1.45976400
O	4.28957500	0.83816100	-1.42423800
O	2.86689300	-0.56153300	0.02161000
S	3.17087000	0.89078400	-0.55849400
H	2.13976900	1.01539400	2.04108500

$(SA)_1\cdot(LAS)_2\cdot(A)_1$:

Atoms	X	Y	Z
S	0.22739100	1.04348200	1.77213400
O	0.50542700	0.76337100	0.33598700
O	-1.07259000	0.51605600	2.16843300
O	0.45536100	2.43099600	2.08636200
O	1.32851900	0.25905000	2.58971500
H	0.71848600	3.27659900	0.51108100
H	1.29165500	-0.68413900	2.34153100
N	1.01983900	3.49631700	-0.45647400
H	1.93029300	3.02848500	-0.60421700
H	1.10866700	4.49897800	-0.58476400
H	0.31632600	3.10920700	-1.11422200
C	3.07833800	0.81527400	-0.85876200
O	3.34786500	1.90840700	-0.42565700
H	2.23160400	-0.24873300	-2.18468300
O	2.43825600	0.68045700	-2.00762500
C	3.49558500	-0.43712400	-0.10094400
C	5.00921500	-0.53337000	-0.03216700
H	5.28644600	-1.39038700	0.57612100
H	5.42645500	-0.65641400	-1.03028500
H	5.40578900	0.37517200	0.41419000
H	3.07053500	-0.35232800	0.89801800
O	0.59348100	-1.34711100	-0.98897900
O	1.50723100	-2.10716600	1.13830200
O	1.58912300	-3.54919700	-0.89079900
O	3.01299600	-1.62379700	-0.75146500
S	1.61604000	-2.27460900	-0.28542100
H	0.44893100	-0.51248700	-0.40609000
C	-1.72041800	1.80308600	-1.15822600
O	-0.97305500	2.23538000	-2.00314500
H	-2.43315200	1.92762400	0.59534500
O	-1.90235700	2.45763300	-0.02290600
C	-2.48312100	0.50624100	-1.36829400
C	-3.36028500	0.57726100	-2.60455200

H	-3.84005100	-0.38730400	-2.74894100
H	-4.12280400	1.34411400	-2.47768500
H	-2.74887200	0.81748300	-3.47124800
H	-1.73708700	-0.28539900	-1.46914000
O	-1.89245500	-1.49148500	0.76291800
O	-3.63221700	-2.08298100	-0.76814600
O	-4.22602500	-1.14465500	1.46935200
O	-3.27666100	0.28670100	-0.19333400
S	-3.37014200	-1.23502100	0.34262700
H	-1.60378500	-0.79780300	1.42642500

$(SA)_1 \cdot (LAS)_2 \cdot (A)_2$:

Atoms	X	Y	Z
S	2.30007100	-0.48114800	-0.29249300
O	1.16803100	-1.36655000	-0.04847100
O	3.46300200	-1.49385200	-0.66436800
O	2.10142100	0.38391300	-1.45336100
O	2.73647100	0.23060400	0.91147100
H	1.25142100	0.17092700	2.11228100
S	-2.62384600	-0.07549600	1.06120200
O	-1.65310500	-1.15420300	0.85232900
O	-4.03546100	-0.85969600	1.13546000
O	-2.47245500	0.62076000	2.30617300
O	-2.75250600	0.77154000	-0.14081000
H	-1.41468100	0.10170400	-1.32664800
H	-0.06343900	-0.80752400	1.83537400
N	0.39568900	-0.21119700	2.54455900
H	-0.26868500	0.54296200	2.73806600
H	0.60603200	-0.74392100	3.38217300
H	-0.13119700	-0.95464000	-1.09132300
N	-0.85866000	-0.64039100	-1.77451500
H	-0.41169500	-0.28879900	-2.61686300
H	-1.49702100	-1.41262700	-1.97820900
C	-4.92348200	-0.79936600	0.01034500
H	-5.15733000	0.23670900	-0.22012700
C	5.64893100	-1.32721900	0.45215400
C	-4.31693900	-1.39756100	-1.25661300
O	-4.74928900	-1.14710100	-2.33919600
O	6.75811700	-1.77002600	0.38630900
O	5.08736000	-0.98566700	1.60842500
H	4.22549200	-0.55256000	1.46975500
O	-3.29190400	-2.26117600	-1.10513800
H	-2.97959500	-2.29452600	-0.18655400
S	-0.05848100	2.70810600	-0.17114100

O	0.01714400	1.53641300	0.67058100
O	0.71591300	3.85361300	0.13567500
O	-1.54352600	3.14093100	-0.30877600
O	0.23053000	2.20925800	-1.63695300
H	-2.11704800	2.34248600	-0.19073600
H	1.02213600	1.60388900	-1.58494500
C	4.84600400	-1.08284100	-0.82863000
H	5.22974800	-1.79393800	-1.55385600
C	5.05970300	0.33636200	-1.33070600
H	6.13229400	0.47792900	-1.45357200
H	4.56608000	0.48162100	-2.28748300
H	4.68589400	1.07663200	-0.62542900
C	-6.17047800	-1.57131700	0.39923900
H	-6.62175100	-1.11390300	1.27625600
H	-6.87747200	-1.54631400	-0.42712200
H	-5.92265700	-2.60682900	0.62802700

(SA)$_1$·(LAS)$_2$·(A)$_3$:

Atoms	X	Y	Z
S	-2.01468200	-0.01002900	0.54238000
O	-1.13682300	-0.38763600	1.61920100
O	-3.45417800	-0.07744600	1.20633600
O	-1.81982900	1.33452800	0.00781200
O	-2.03490600	-0.99300400	-0.56776200
H	-1.27326300	0.03502400	-1.98104900
S	2.24017100	-0.90522400	-1.58390700
O	1.31706900	-1.64241300	-2.44400500
O	2.88375000	-2.09161300	-0.71155300
O	3.29586500	-0.17582900	-2.21457200
O	1.46139800	-0.09471000	-0.60769200
H	2.17033200	0.43817300	2.72821700
H	0.11953000	-0.28569400	-2.81897500
N	-0.57275100	0.45376600	-2.60759900
H	-0.11027200	1.23061900	-2.09679500
H	-1.00644300	0.80869600	-3.45372100
H	1.08752500	1.79876000	2.47068000
N	1.17241500	0.88775100	2.92138200
H	0.99162600	0.97461100	3.91531800
H	0.47233300	0.26412000	2.50343200
C	3.73632300	-1.65879100	0.36664900
H	4.35248800	-0.82808500	0.02535100
C	-4.69351300	0.08829000	0.47362100
H	-5.36341100	0.51320600	1.21517000
C	-5.30405100	-1.26381900	0.09370800

C	2.88829700	-1.18810800	1.54925600
O	3.34936500	-0.23493400	2.21329000
O	-6.48976700	-1.41128300	0.13024300
O	-4.48059100	-2.22423900	-0.31959800
H	-3.56390100	-1.90376900	-0.38397800
O	1.80764800	-1.77786800	1.80669800
H	0.96828000	-2.38430200	0.81562300
S	1.11264000	3.15816100	-0.17282600
O	0.51217500	2.75557200	-1.42486000
O	1.60230900	4.47529000	-0.00355900
O	2.23796900	2.16493800	0.20658600
O	0.04208800	2.89571700	0.96027100
H	2.01428900	1.23355900	-0.15024900
H	-0.68770400	2.31467100	0.60854000
N	0.21785800	-2.82879200	0.11591400
H	0.64779400	-2.95618800	-0.80092300
H	-0.56947500	-2.18425800	0.00693800
H	-0.11846900	-3.71631600	0.47388000
C	4.59077600	-2.84471000	0.76266000
H	5.20044600	-3.16122800	-0.08051800
H	5.24046700	-2.56102800	1.58878100
H	3.95649900	-3.67128900	1.08005200
C	-4.63442700	0.99903500	-0.74220100
H	-4.26400100	1.98257900	-0.46871800
H	-3.99819800	0.58468100	-1.52255700
H	-5.64794800	1.08590800	-1.12957200

(LAS)$_1$·(A)$_1$:

Atoms	X	Y	Z
S	-0.95896800	-0.52691700	0.22557200
O	-1.53721700	0.24939500	1.28622500
O	0.15580100	0.34525100	-0.48790600
O	-0.35577600	-1.78571800	0.56120300
O	-1.93785000	-0.68347100	-0.92192900
H	-2.77483500	0.00133000	-0.80148700
H	-3.61568100	1.20539000	0.46678300
N	-3.84934300	0.91228000	-0.47782100
H	-4.76348700	0.47649500	-0.46185600
H	-3.89935600	1.73456600	-1.06698100
C	1.31592400	0.68811200	0.30891400
H	1.11875700	0.42964500	1.35354200
C	2.50987000	-0.15236700	-0.16660900
O	3.58140700	0.34126900	-0.35759000
O	2.29230500	-1.45300700	-0.32195000

H	1.38806400	-1.71401500	-0.07373500
C	1.56576800	2.16786800	0.16743100
H	2.45088300	2.44307000	0.73510900
H	1.74092200	2.41710100	-0.87712700
H	0.70489300	2.71971500	0.53851600

$(SA)_2$:

Atoms	X	Y	Z
S	-2.04390900	0.06786900	-0.12274300
O	-1.06625300	-0.09101600	-1.16405200
O	-3.34418400	0.55364400	-0.40365000
O	-2.13867600	-1.37002600	0.53377700
H	-2.91688700	-1.40825700	1.10624100
O	-1.45210400	0.94146800	1.01741400
H	-0.49514200	0.71878700	1.13904200
O	1.06633900	0.09030600	1.16418700
S	2.04395700	-0.06787700	0.12273000
O	1.45244500	-0.94153800	-1.01753300
O	3.34450900	-0.55305800	0.40337700
O	2.13790700	1.37020200	-0.53350800
H	0.49539600	-0.71919700	-1.13906000
H	2.91599500	1.40893500	-1.10610600

$(SA)_2\cdot(A)_1$:

Atoms	X	Y	Z
S	-1.76935400	-0.34962900	-0.05233400
O	-1.08309000	0.19932200	1.13239500
O	-0.99133900	-1.38502800	-0.71189200
O	-3.08817800	-1.06570200	0.47333200
H	-2.85599800	-1.95590400	0.76522200
O	-2.27997700	0.71341300	-0.90168300
H	-1.42705000	2.08769400	-0.46598000
O	1.40271700	1.05968200	-0.57216200
S	2.07096100	-0.10538600	-0.01797900
O	1.43094700	-0.40517200	1.36903000
O	3.47799500	-0.09578500	0.12290300
O	1.68380500	-1.33472400	-0.89139100
H	0.44412500	-0.22362400	1.33583000
H	0.69729500	-1.39466700	-0.95091500
N	-0.68484100	2.68352600	-0.01796800
H	0.20742800	2.15665900	-0.15300600
H	-0.88739000	2.72499600	0.97772000
H	-0.63328600	3.61236300	-0.42234600

$(SA)_2\cdot(LAS)_1$:

Atoms	X	Y	Z
S	-1.00918500	-0.16501900	-0.38605900
O	-0.31250800	-0.40709000	0.86726100
O	-2.32964300	-0.99478800	-0.39954800
O	-1.35625700	1.21696600	-0.62586600
O	-0.29215000	-0.76398800	-1.56520400
H	0.57894300	-1.29521800	-1.30362300
S	1.65543300	2.37287900	0.21999500
O	0.60965500	3.25119000	-0.53722300
O	2.77924500	3.17900000	0.49259100
O	0.94353100	2.03648100	1.57668500
O	1.78553600	1.12423000	-0.50788200
H	0.42594600	1.21420200	1.47923400
H	-0.15099800	2.69518400	-0.79284000
S	2.82729800	-1.92728100	-0.07504100
O	3.71140500	-0.73995400	-0.53382800
O	3.66499000	-3.03988900	0.13335000
O	2.23670400	-1.44509600	1.29189900
O	1.70129700	-2.07088200	-0.99198100
H	1.31946900	-1.13054200	1.16839900
H	3.16630900	0.07752600	-0.60671300
C	-3.32736600	-0.67857000	0.62799000
H	-2.89894000	0.04890500	1.32156200
C	-4.53024800	-0.02432500	-0.06478300
O	-4.25973500	0.94779000	-0.93596900
H	-3.31259500	1.13239000	-1.00322000
O	-5.64599500	-0.35171900	0.19606100
C	-3.68502200	-1.95859300	1.33501900
H	-4.44947600	-1.75265200	2.07982700
H	-4.08578900	-2.67754700	0.62406300
H	-2.80239700	-2.37059800	1.81887300

$(SA)_2\cdot(LAS)_1\cdot(A)_1$:

Atoms	X	Y	Z
S	-1.01176800	-0.32132900	0.45902000
O	-0.99580800	0.79003800	1.43164100
O	-2.41248100	-1.03043700	0.59614300
O	-0.93923500	0.16438000	-0.91867500
O	-0.06029100	-1.35389400	0.81173300
H	0.57319300	0.38562000	2.40650500
H	2.08770000	1.02099800	2.66987000
N	1.53322700	0.16835600	2.71571500
H	1.95208900	-0.50980600	2.03727000

H	1.53665200	-0.22053700	3.65395600
S	1.23244500	2.60022700	-0.36501500
O	0.75108900	2.12867300	-1.76931800
O	2.05317600	3.73458400	-0.53911100
O	-0.06795700	3.02271900	0.37711500
O	1.75060800	1.42712100	0.33330600
H	-0.50330500	2.22140200	0.77867000
H	0.15246000	1.35574400	-1.65640200
C	-3.59891900	-0.22229200	0.35616800
H	-3.29856900	0.82119400	0.23581500
C	-4.23777400	-0.68228400	-0.96088100
O	-3.41347600	-0.83099500	-1.99672200
H	-2.50077900	-0.59351000	-1.77219300
O	-5.41385500	-0.86380000	-1.05374000
S	3.00235900	-1.85985900	-0.31564900
O	4.13052800	-2.53890800	-0.82519000
O	2.99035900	-1.41135600	1.06401800
O	1.76316300	-2.77248300	-0.55876700
O	2.70712200	-0.60955800	-1.20874600
H	0.97181000	-2.36176100	-0.14394300
H	2.41151000	0.14489700	-0.65269500
C	-4.52435800	-0.38339600	1.53458100
H	-5.43458600	0.18377800	1.35867000
H	-4.79269500	-1.43037400	1.65662500
H	-4.03388200	-0.02160100	2.43544500

$(SA)_2$·$(LAS)_1$·$(A)_2$:

Atoms	X	Y	Z
S	-1.57453400	-0.61085800	0.21592700
O	-0.69478400	-1.62406000	-0.32728300
O	-3.03170300	-1.17116700	-0.08431400
O	-1.46848700	-0.36443200	1.63474200
O	-1.51151500	0.64782400	-0.59554400
H	-0.06202400	0.17889600	-1.71535800
H	0.72933300	-0.29498000	-3.11981600
N	0.85296800	0.01456000	-2.16068500
H	1.36784600	-0.71874500	-1.60848600
H	1.39876800	0.87782200	-2.13012800
H	0.85647200	-1.93818900	0.91538900
N	1.13549300	-1.69866800	1.87780100
H	0.47382900	-0.97608000	2.18037200
H	1.08736600	-2.51661100	2.47592500
S	3.58679100	-1.01330300	-0.33194100
O	2.39099500	-1.73966800	-0.75971800

O	4.76638600	-1.92305800	-0.90013800
O	3.73506200	0.27827300	-1.01099200
O	3.75183000	-0.95386700	1.10760100
H	5.60712700	-1.55505300	-0.60014000
H	2.09807700	-1.31955600	1.82653400
C	-4.15466000	-0.41551200	0.43327400
H	-3.77935900	0.39065400	1.06864200
C	-4.89194200	0.22223200	-0.75032500
O	-6.08299600	0.20433400	-0.83943200
O	-4.12361700	0.82801400	-1.65671300
H	-3.18605700	0.79179200	-1.40397000
C	-5.03448600	-1.34923400	1.22548400
H	-5.91167300	-0.81209300	1.57689300
H	-5.36591900	-2.17221000	0.59567600
H	-4.47655700	-1.73873500	2.07402600
S	1.34609900	2.09409000	0.60083200
O	1.18477000	0.66394700	0.73511000
O	1.87811800	2.85682500	1.66897300
O	-0.01746700	2.69900400	0.16560500
O	2.18989100	2.31758900	-0.70986200
H	-0.64436200	1.95871000	-0.06253900
H	2.90888400	1.61288700	-0.72481400

$(SA)_2{\cdot}(LAS)_1{\cdot}(A)_3$:

Atoms	X	Y	Z
S	-2.11642300	-0.47143800	-0.34478100
O	-0.98003500	0.42927500	-0.49321600
O	-3.35791600	0.46555400	-0.67216800
O	-2.09346000	-1.56352500	-1.30531200
O	-2.29681300	-0.92592700	1.04002600
H	-0.54051800	-0.81729100	1.78376000
H	0.76345400	0.23260500	1.48484700
N	0.48109200	-0.71619700	1.81854100
H	0.94171100	-1.39096500	1.18386600
H	0.85044700	-0.86112700	2.75294800
H	-0.44299300	-1.59473500	-2.00052700
N	0.55375800	-1.37922400	-2.18781400
H	1.16381500	-1.86203500	-1.49900800
H	0.81511400	-1.62702600	-3.13611400
S	1.65859000	2.08211300	-0.39995200
O	2.74168500	3.03269500	-0.55856800
O	1.81889500	0.90089300	-1.27806700
O	1.45780600	1.69622100	0.99386500
O	0.36096200	2.81488700	-0.89931400

H	0.70145900	-0.37205900	-2.01531300
H	-0.38298700	2.18852800	-0.79332900
S	3.41621500	-1.65058200	0.34062900
O	4.43644000	-2.64099900	0.43389800
O	3.85680100	-0.69633400	-0.86044400
O	2.06867800	-2.15137500	-0.01670300
O	3.29317500	-0.74905500	1.50987700
H	3.11411400	-0.06250100	-1.04975800
H	4.93044200	1.96872600	1.83096000
C	-4.73208200	0.03180100	-0.50854600
H	-5.26345500	0.60241300	-1.26415600
C	-5.30788200	0.49066000	0.83409600
O	-6.44459800	0.86018100	0.89555400
O	-4.52652700	0.41556200	1.90602100
H	-3.67020700	-0.00096800	1.69789200
N	4.54878300	1.53249300	0.99742500
H	5.30409900	1.21956100	0.39135100
H	3.95600800	2.21306700	0.47831000
H	3.97765600	0.66627700	1.26194900
C	-4.98332800	-1.45427100	-0.71209500
H	-4.65190800	-1.76560100	-1.69854100
H	-4.47071900	-2.05598800	0.03626200
H	-6.05605200	-1.61545900	-0.62112400

$(SA)_2 \cdot (A)_2$:

Atoms	X	Y	Z
S	-1.98527000	0.06019200	-0.13165900
O	-1.94585100	1.50267600	-0.36384000
O	-3.45405200	-0.40805400	-0.56585500
O	-1.13262500	-0.71715500	-1.02373000
O	-1.81953100	-0.29404000	1.27183000
H	-0.62436700	2.25190300	0.39887800
H	-4.09523900	0.12722600	-0.08324700
S	2.12696800	-0.08241900	-0.14556000
O	2.09058800	-1.50978000	-0.48429900
O	1.26111100	0.67174000	-1.26380700
O	1.35759200	0.13089400	1.11037600
O	3.39844000	0.56508400	-0.18341300
H	0.88841600	-2.12928700	0.29737900
H	0.41650000	0.18667900	-1.37934900
N	0.00229300	-2.43548200	0.82047900
H	-0.66962700	-2.77720000	0.13741100
H	0.20663700	-3.13890300	1.52129200
H	-0.41772000	-1.59386800	1.24705100
N	0.30232200	2.48478500	0.82193500

H	0.20060800	3.09063400	1.62797400
H	0.76220000	1.53887400	1.07762200
H	0.88775300	2.92351600	0.11548800

$(LAS)_2$:

Atoms	X	Y	Z
S	2.17738500	1.71207100	0.04051600
O	1.12522700	1.55094600	-0.93198900
O	2.92354500	2.90596300	0.13335300
O	1.59640500	1.35833200	1.44509300
H	0.73646300	0.88521900	1.35297600
O	-0.71617800	0.04350900	1.00764500
S	-1.19359800	-0.34879600	-0.29708200
O	-1.49110700	0.94391700	-1.13264900
O	-0.46812900	-1.30700900	-1.04747900
H	-0.65180400	1.44680000	-1.21328300
O	3.23103200	0.56117800	-0.19790300
C	2.74051500	-0.80187600	-0.34514100
H	1.75990500	-0.88993300	0.12550200
C	2.66651200	-1.17449300	-1.80851800
H	2.33431700	-2.20658800	-1.88720800
H	1.95375800	-0.52877700	-2.31470800
H	3.64693500	-1.07419700	-2.27147200
C	3.67933700	-1.72747600	0.43020200
O	3.51118400	-2.90748700	0.40289200
O	4.66469900	-1.15938800	1.12667800
H	4.64650000	-0.20111900	1.01446500
O	-2.66204500	-0.87214300	-0.15900500
C	-3.58498900	-0.11572400	0.68728000
H	-3.16762500	0.87554300	0.86276900
C	-3.79693800	-0.86217000	1.98374200
H	-4.16318300	-1.86751000	1.78357600
H	-2.85945100	-0.91991100	2.53178400
H	-4.53562300	-0.32836400	2.57643200
C	-4.89024500	0.08622200	-0.08330300
O	-4.91894600	-0.29459600	-1.36016700
H	-4.07781700	-0.69073100	-1.61641800
O	-5.82670300	0.58431100	0.46041700

$(LAS)_2·(A)_1$:

Atoms	X	Y	Z
N	-1.38743300	2.56247600	-1.11254600
H	-1.11570400	1.56264700	-1.00769900

H	-1.39042500	2.81812400	-2.09469700
H	-2.32663400	2.65597800	-0.70920300
C	-3.51882800	0.46028500	-0.29528400
O	-3.72174800	1.53752600	0.20266100
H	-2.84193000	-0.50815600	-1.79219800
O	-3.23087300	0.36975300	-1.59436800
C	-3.55883900	-0.85852100	0.49890400
C	-4.47453300	-0.74090500	1.69230200
H	-4.45176100	-1.67129900	2.25433900
H	-4.14954100	0.07950600	2.32695000
H	-5.49310400	-0.54544600	1.36130700
H	-3.86886000	-1.66265100	-0.16945400
O	-1.64602900	-1.80351600	-1.27678800
O	-0.09580500	-2.12076800	0.61124700
O	-0.58371100	0.11409900	-0.21224700
O	-2.25463500	-1.17224700	1.00775300
S	-1.05127600	-1.26479000	-0.06895800
H	-0.67767700	3.10382600	-0.59275300
C	1.44267700	2.04914700	0.04065600
O	0.85336700	3.01235000	0.47672900
H	1.73288100	0.88405400	-1.45420300
O	1.44366300	1.80418200	-1.25627000
C	2.14652700	1.07409600	0.98189000
C	2.67258100	1.76651700	2.22026000
H	3.09956900	1.02347900	2.88896200
H	3.44087500	2.48793400	1.94876800
H	1.86088500	2.28725100	2.72030600
H	1.39261900	0.33072800	1.25026100
O	2.40773400	-1.83219100	0.76550800
O	4.35170700	-1.45487800	-0.64148000
O	2.07701800	-0.79822600	-1.40619300
O	3.26084400	0.43318000	0.34039900
S	3.04833700	-0.98936000	-0.35339800
H	1.39809100	-1.93472800	0.64684600

$(LAS)_2{\cdot}(A)_2$:

Atoms	X	Y	Z
S	1.99076300	-0.26995700	-0.01608100
O	1.06518500	-0.18054100	1.09838500
O	3.39620900	-0.56222700	0.68074200
O	1.73215700	-1.36436300	-0.93478700
O	2.17182300	1.02668300	-0.70276400
H	1.02949200	2.17420000	0.01556900
S	-2.48694300	1.18831700	-0.18077000

O	-1.80678400	0.72484900	1.03255800
O	-4.06321800	0.95512200	0.14559800
O	-2.34564200	2.60828300	-0.40163600
O	-2.20644900	0.33690700	-1.33149600
H	-1.38211700	-1.13079900	-0.79544600
H	-0.00929400	1.74426500	1.22045300
N	0.31109700	2.55173000	0.66783700
H	-0.51802600	2.90736300	0.16886700
H	0.71437500	3.26506200	1.26635200
H	-0.77310700	-1.35125100	0.71428500
N	-0.92417700	-1.83120600	-0.17872600
H	0.00427200	-2.06140900	-0.55903400
H	-1.53986600	-2.63482700	-0.06617800
C	-4.67708500	-0.21400900	-0.41052100
H	-4.56932700	-0.20936800	-1.49178700
C	4.52104100	-0.81690000	-0.19384800
H	4.15671300	-0.92537500	-1.21855700
C	5.45398200	0.39934200	-0.14737000
C	-4.01560200	-1.49553500	0.08968800
O	-3.98589700	-2.50199800	-0.56062800
O	6.63396200	0.29112400	0.01057800
O	4.87021500	1.58493100	-0.32242800
H	3.91437400	1.48679500	-0.48421900
O	-3.48147300	-1.46606900	1.31693300
H	-3.36989800	-0.55494600	1.63060600
C	5.20209000	-2.08180000	0.26436200
H	6.07009200	-2.27846500	-0.35992000
H	5.53902400	-1.97203200	1.29289400
H	4.50360000	-2.91261800	0.19415100
C	-6.13591100	-0.18619300	0.00493100
H	-6.60056700	0.72042100	-0.37514700
H	-6.64629200	-1.05363900	-0.40902100
H	-6.22478800	-0.20183900	1.09006700

$(SA)_3$:

Atoms	X	Y	Z
S	0.18420700	1.32393500	-0.06376700
O	-0.07936000	0.10716800	-0.82066100
O	1.39800700	2.00440600	-0.38233900
H	3.14082500	1.28744900	-0.26099000
O	0.10569000	0.98656800	1.45256900
O	-0.98458100	2.30188300	-0.20416000
O	3.84751100	0.61578000	-0.20963100
S	3.21853700	-0.78586500	0.09265400

O	4.28365900	-1.69798000	0.24204700
O	2.45805400	-1.13840400	-1.23559500
O	-2.42809800	-1.23933200	-1.05481200
H	1.54850400	-0.78495900	-1.20456200
H	-1.54697200	-0.80010800	-1.02022800
O	2.22430200	-0.62726900	1.12872700
O	-3.14850800	0.85895200	-0.03329700
H	0.83423300	0.35176300	1.64307800
H	-1.85406100	1.81303500	-0.13777100
O	-4.69254100	-1.07332300	-0.27731300
S	-3.39617800	-0.55768800	-0.04537800
O	-2.86112400	-1.05091600	1.35730700
H	-3.21168800	-1.93354200	1.54158600

$(SA)_3\cdot(A)_1$:

Atoms	X	Y	Z
N	-0.05211300	0.36418400	2.52190300
H	-0.92755600	0.12725200	2.01514500
H	0.68571800	-0.26724900	2.17260800
H	-0.17637200	0.26155400	3.52356900
S	1.04454400	1.98710900	-0.14967300
O	0.01432600	0.94579400	-0.25027600
O	1.18648800	2.51744400	1.18192900
H	0.25092500	1.31832300	2.27297400
O	2.28773900	1.53703100	-0.79797900
S	-2.88805200	-0.41028000	-0.10672100
O	-2.09182900	-1.31312400	-1.10220300
O	-2.60422400	1.03669900	-0.62118600
O	-4.26847400	-0.65812400	-0.28224700
O	-2.28587500	-0.56146200	1.20144900
H	-1.18385800	-1.49514600	-0.77402800
H	-1.63424400	1.20617500	-0.54124200
S	1.71019900	-1.67137900	-0.07241700
O	2.64617700	-2.94041800	-0.09412700
O	2.21949100	-0.87609000	-1.26375400
O	0.36866200	-2.14623400	-0.29036100
O	2.00304300	-0.99324000	1.15997500
H	2.25779700	-3.60894600	-0.67355300
H	2.27424200	0.16766700	-1.06122400
O	0.55138200	3.22674600	-1.01383800
H	0.73583400	3.05370200	-1.94565100

$(SA)_3\cdot(A)_2$:

Atoms	X	Y	Z
N	-0.01391100	-2.02910600	0.09508700
H	-0.79103400	-2.12376000	-0.57703900
H	0.90622900	-1.89330600	-0.36185700
H	0.00286700	-2.83367600	0.71419700
N	-2.34000200	1.89261200	1.66553800
H	-3.28613700	2.12031200	1.37052500
H	-2.13842600	2.28527800	2.57903200
H	-2.25952800	0.85603500	1.67417800
S	-3.06529100	-0.81069700	-0.12581900
O	-2.56171300	-1.82565200	-1.03489300
O	-3.03586500	0.54056100	-0.68687500
O	-2.47187000	-0.85825100	1.21058100
H	-1.35514400	0.64468300	-1.42148100
S	0.28498600	1.50837900	-0.40397500
O	-0.37821800	0.55379400	-1.48066700
O	1.58420500	1.83817700	-0.93390000
O	-0.62624700	2.63465600	-0.22908200
O	0.35152700	0.70345900	0.84302400
H	-0.20623800	-1.17664500	0.63776300
H	-1.66285700	2.26087600	0.93407800
O	-4.60054000	-1.15742900	0.15004700
H	-5.03265300	-1.31487500	-0.69892800
S	3.47070300	-0.69508500	0.14000000
O	3.93041100	0.65534800	-0.48074000
O	2.72519900	-0.27812200	1.45312300
O	4.62312800	-1.42530600	0.51468700
O	2.49349700	-1.28510700	-0.75106500
H	3.12836200	1.15677900	-0.77049200
H	1.85747300	0.16316500	1.23843100

$(SA)_3{\cdot}(A)_3$:

Atoms	X	Y	Z
S	2.58494200	-1.22685200	0.07734200
O	1.45675300	-2.11414600	0.31629000
O	3.90450900	-2.13428500	0.14732000
O	2.65420800	-0.67743100	-1.26903400
H	3.87404700	-2.64740900	0.96356700
S	-2.77710800	-0.99140100	-0.06139000
O	-2.81933800	0.30525400	0.59155900
O	-4.12571200	-1.68896100	0.44644800
O	-2.85360300	-0.96982800	-1.51658600
H	-4.27944700	-2.47120300	-0.09589400
S	-0.32071600	2.26002000	0.04013600

O	0.26019100	0.94246700	-0.30433500
O	-0.58275500	2.34615600	1.46776200
O	-1.68810400	2.38192400	-0.72166300
O	0.49842400	3.34009600	-0.50193200
H	1.99382600	2.65725700	-0.60436900
O	2.72524300	-0.22226000	1.13903900
N	-0.11804700	-0.30897500	2.15759400
N	2.84524600	2.03284600	-0.56068800
N	-0.10298200	-1.23859700	-1.88739400
H	3.70742500	2.54320100	-0.71550300
H	2.86213400	1.54461600	0.34571700
H	2.74630400	1.25564000	-1.22653500
H	-2.29560100	1.70954800	-0.33204400
H	0.18146200	-1.89274100	-1.14639700
H	0.49325600	-1.35461000	-2.69936000
H	-1.10864900	-1.34274800	-2.08295200
H	0.04044300	-0.29492700	-1.47126000
H	0.87512300	-0.32564200	1.89523600
H	-0.64294200	-0.92655900	1.50307400
H	-0.46159600	0.66466700	2.04175300
H	-0.24381500	-0.62909700	3.11147800
O	-1.66798600	-1.82839000	0.41132200

(LAS)$_3$:

Atoms	X	Y	Z
S	1.71625600	-0.87209900	-0.29588100
O	1.35378100	-0.20623100	0.93146000
O	1.08986200	-2.09656100	-0.63071900
O	1.64700700	0.14683900	-1.46642600
H	1.22201800	0.98279500	-1.16273000
O	0.84077700	2.50690600	-0.43717800
S	0.28887800	2.98002300	0.80643900
O	-0.22429300	1.75545500	1.63281800
O	1.02571000	3.86052700	1.62794600
H	0.22300300	0.91830400	1.33344600
O	3.25961100	-1.18443800	-0.26065000
C	4.24571300	-0.11632900	-0.36555700
H	4.13599100	0.32315400	-1.35702800
C	4.12308600	0.93554200	0.71622400
H	5.01629300	1.55422800	0.67658200
H	3.25070000	1.56393600	0.55419400
H	4.05240500	0.46913500	1.69717500
C	5.61909600	-0.79506100	-0.33543200
O	6.60903600	-0.13165000	-0.30302300

O	5.65233900	-2.12623500	-0.37952200
H	4.75958100	-2.49152800	-0.39408400
O	-1.09308600	3.69896300	0.52557000
C	-1.91762200	3.28158700	-0.58464500
H	-1.29689500	2.78928000	-1.33230600
C	-2.57898700	4.52484200	-1.14738200
H	-3.15572100	5.02986500	-0.37464000
H	-1.81563200	5.20153400	-1.52210100
H	-3.24155400	4.23614700	-1.95912400
C	-2.95766900	2.25911600	-0.15866100
O	-3.00827500	1.84276200	1.08714800
H	-2.23816200	2.13103300	1.59749900
O	-3.73411100	1.83388000	-0.98424000
C	-2.83519200	-3.94707400	0.61554400
O	-2.81974700	-5.13995100	0.65495600
H	-3.82152700	-2.30273200	0.57885700
O	-3.97322900	-3.25231500	0.66088700
C	-1.51736600	-3.17618900	0.54981700
C	-0.69295800	-3.43802400	1.79349000
H	0.26112200	-2.92490700	1.70992300
H	-1.21873100	-3.08681200	2.68034100
H	-0.52927800	-4.50908900	1.88158400
H	-0.98893800	-3.48757900	-0.34737000
O	-3.45603200	-0.75155000	-0.86011000
O	-1.62843700	-1.91263400	-1.96304500
O	-1.22239500	0.23878500	-0.77760600
O	-1.73120700	-1.74035600	0.49264200
S	-1.91558600	-1.01601700	-0.90309000
H	-3.67452800	0.22469600	-0.88737400

(LAS)$_3$·(A)$_1$:

Atoms	X	Y	Z
N	-0.65609000	1.69085700	2.53100300
H	-0.81547300	1.69688300	1.50534700
H	-0.55105600	0.71245300	2.83429700
H	0.19547000	2.21807700	2.72383200
C	2.33179200	2.32255800	0.32099700
O	1.66553900	2.84804600	1.16807300
H	3.70615800	1.03257600	-0.10423400
O	3.39798400	1.58384100	0.64221600
C	2.05840200	2.49679500	-1.17202800
C	2.62586800	3.81954400	-1.64841200
H	2.41855100	3.94355000	-2.70832400
H	2.16667600	4.63392000	-1.09173800

H	3.70351400	3.83858900	-1.49199400
H	2.48569700	1.66215000	-1.72977800
O	0.74024700	0.34494600	-0.34832800
O	-0.62438400	0.70686600	-2.33690100
O	-1.28553800	1.69553300	-0.20656600
O	0.64810000	2.55097300	-1.38439100
S	-0.20104100	1.23558900	-1.04923600
H	-1.49479900	2.08757300	2.95657400
C	-3.34602800	0.65166400	1.40119300
O	-3.51941500	1.68992000	1.98546800
H	-2.26021100	-0.93580300	1.24556200
O	-2.51954700	-0.25939900	1.89752400
C	-4.05093600	0.37829400	0.07368300
C	-5.50300300	0.80716700	0.12798800
H	-5.95297200	0.67858000	-0.85316700
H	-6.04661600	0.20310900	0.85211900
H	-5.55756500	1.85100300	0.42434800
H	-3.50995400	0.94913500	-0.68079500
O	-2.80203400	-0.63851200	-2.36017700
O	-3.31586800	-2.88987900	-1.57365600
O	-1.63826300	-1.48001000	-0.40177300
O	-4.03842000	-1.01953600	-0.27622400
S	-2.86080800	-1.61571800	-1.16378900
H	-1.93573000	-0.10932600	-2.36075900
C	1.13344200	-0.95945000	2.26810600
O	0.06727800	-1.16117400	2.78942500
H	2.55165400	0.29700900	1.92071200
O	1.80477700	0.15454800	2.52770100
C	1.75535600	-1.98274400	1.33084200
C	2.22484400	-3.21308300	2.08246000
H	2.64412800	-3.92671100	1.37652500
H	2.98703600	-2.94280000	2.81147600
H	1.37839400	-3.66483000	2.59508700
H	0.99231500	-2.22908100	0.59359600
O	1.83064300	-1.65428500	-1.51495700
O	3.82249800	-2.87986800	-0.98477900
O	3.93367100	-0.41213700	-1.21222800
O	2.86577200	-1.32169700	0.69120200
S	3.22109700	-1.60558200	-0.83923700
H	1.29672700	-0.85055100	-1.22151800

$(LAS)_3 \cdot (A)_2$:

Atoms	X	Y	Z
S	1.78985500	-1.47957300	-0.37487300

O	0.55632300	-2.22297700	-0.09143600
O	2.87891800	-2.64320500	-0.37292200
O	1.79962100	-0.84859300	-1.67762300
O	2.14937300	-0.58366600	0.73131600
H	-0.04159400	-0.05822200	2.06603400
S	-3.19470900	-0.11521100	1.36259800
O	-2.15493500	-0.44749700	0.39430000
O	-4.53140000	-0.86020800	0.82394600
O	-3.00900700	-0.68388300	2.67054100
O	-3.52181400	1.31652600	1.33199500
H	-1.78211700	-1.15908900	-2.69364200
H	-0.02961000	-1.61089900	1.47429800
N	-0.16247100	-1.04727400	2.33640900
H	-1.11530800	-1.15651600	2.70336700
H	0.54369800	-1.30150000	3.02036700
H	-1.02823700	-0.16479400	-1.56137900
N	-0.94611500	-1.02421000	-2.11967800
H	-0.07168700	-0.96228600	-2.64482400
H	-0.82403500	-1.78165700	-1.43712800
C	-4.88464800	-0.53934000	-0.52618300
H	-4.71616300	0.51935900	-0.71871300
C	4.30121800	-2.37368100	-0.45209700
H	4.69398000	-3.24802400	-0.96272800
C	4.93440600	-2.38927300	0.94171800
C	-4.01208300	-1.32691700	-1.49306600
O	-3.76714800	-0.93759300	-2.60386700
O	5.99402700	-2.91569000	1.11894000
O	4.28204700	-1.75896700	1.91644500
H	3.48553200	-1.31094000	1.57072100
O	-3.56093500	-2.50644000	-1.06861900
H	-3.73773700	-2.59792700	-0.12148600
O	-1.85118100	2.57749300	-0.00281700
O	-0.32548800	1.72781700	1.70355300
O	0.04631200	1.16474200	-0.64792700
O	0.29507500	3.48164000	0.06442600
S	-0.43559000	2.12141800	0.32214500
C	2.37745300	3.38665100	-1.30853100
C	1.75464900	3.59350100	0.08142500
H	1.89047300	4.64817600	0.29480100
H	-2.56101200	2.07846600	0.59336400
O	3.01015300	4.27369900	-1.80285500
H	1.70979200	1.57091500	-1.41020500
O	2.28265300	2.19375500	-1.88716300
C	-6.34529800	-0.90090300	-0.72256200
H	-6.95669700	-0.30255800	-0.05190200

H	-6.63398800	-0.69811000	-1.75205500
H	-6.50909400	-1.95572500	-0.50674300
C	2.43818000	2.73865900	1.12971900
H	2.03882500	2.95905000	2.11671300
H	2.33018200	1.67387100	0.92665200
H	3.49913700	2.98686800	1.11319200
C	4.70097100	-1.11351300	-1.20520100
H	5.78904200	-1.08172400	-1.22851200
H	4.31822200	-1.13660300	-2.22132800
H	4.33352400	-0.21213700	-0.71712900

$(LAS)_3\cdot(A)_3$:

Atoms	X	Y	Z
S	-0.50159100	2.94509000	-0.63015500
O	0.32460500	1.93109300	0.03970600
O	-1.79787100	3.14859600	0.31936600
O	0.11867600	4.26306400	-0.57022800
O	-0.98807700	2.52977200	-1.92308200
H	0.23144800	1.04057200	-3.09181700
S	-0.99267700	-2.01483600	-0.85023100
O	-1.10329300	-0.55662200	-0.65696500
O	-2.51407600	-2.50422900	-1.05613600
O	-0.34440400	-2.37333300	-2.08780700
O	-0.50991600	-2.67363100	0.35411300
H	0.25765600	-1.36372600	1.33823400
S	3.55758700	0.43030200	-0.29810600
O	3.13036500	1.29972000	-1.39881900
O	2.74394700	-0.94305900	-0.61383100
O	4.96133100	0.08702500	-0.30722800
O	3.05450700	0.87441800	0.99804400
H	2.49340200	2.77808600	0.84309600
H	0.46357800	0.28419300	1.06780800
N	0.51678400	-0.46016300	1.77662800
H	1.46724900	-0.52003000	2.14066000
H	-0.16143700	-0.25358100	2.51040900
H	1.60579300	0.67241600	-2.19384500
N	0.68082300	0.33988800	-2.50589000
H	0.74257800	-0.57195300	-2.95840000
H	0.06265400	0.20897100	-1.67660100
H	1.68430600	3.98555000	-0.03546000
N	2.61713700	3.55445400	0.17938300
H	2.95957900	3.08008300	-0.66698000
H	3.29196600	4.23008700	0.52092100
C	-3.38944900	-2.35206700	0.07847300

H	-2.80254500	-2.14968800	0.97447100
C	-4.30569900	-1.14474200	-0.10529500
O	-5.20239000	-0.92023000	0.65349900
O	-4.05874300	-0.34619400	-1.14981800
H	-3.28047100	-0.67229700	-1.62122000
C	-2.58696900	1.96420800	0.53592200
H	-2.48612900	1.28449800	-0.30612300
C	-2.07218900	1.23524800	1.76632600
O	-1.28130600	1.93889700	2.58912100
H	-1.10926200	2.80173200	2.18527500
O	-2.34913500	0.09620800	2.02042200
C	3.40353700	-2.15782400	-0.17985300
H	4.39113000	-2.17738500	-0.63721900
C	3.53335300	-2.11601700	1.35538700
O	2.61678600	-2.39863700	2.07742200
O	4.71117000	-1.74102900	1.84557700
H	5.22536300	-1.28448100	1.16044600
C	-4.18765000	-3.62974400	0.23585000
H	-4.90697800	-3.50691900	1.04142000
H	-4.72159600	-3.85552300	-0.68598800
H	-3.51264300	-4.45047900	0.46612500
C	-4.03584300	2.37022700	0.72091500
H	-4.63271900	1.48291300	0.92755900
H	-4.13329400	3.07904500	1.54264700
H	-4.39275800	2.83237600	-0.19615300
C	2.56658200	-3.32774500	-0.63003800
H	3.09378000	-4.25159100	-0.39403600
H	1.60438300	-3.33148100	-0.12695700
H	2.40885000	-3.27377800	-1.70509300