Supporting information

-for-

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

Rui Wang, Shuqin Wei‡, Zeyao Li‡, Kaiyu Xue, Rui Bai, Tianlei Zhang*

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

S. NO	Caption
S4	**Fig. S1** 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
S5	**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
S6	**Table S2** Concentrations ($molecules \cdot cm^{-3}$) 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
S7	**Table S3** Zero point energy (ZPE/($kcal \cdot mol^{-1}$)), entropies (S/($kcal \cdot mol^{-1} \cdot K^{-1}$)), relative electronic energies (ΔE/($kcal \cdot mol^{-1}$)), relative energies with ZPE corrections (ΔE and $\Delta(E$ + ZPE)/($kcal \cdot mol^{-1}$)), enthalpies ($\Delta H(298)$/($kcal \cdot mol^{-1}$)), and Gibbs free energies ($\Delta G(298)$/($kcal \cdot mol^{-1}$)) 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
S8	**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.
S9	**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.

* Corresponding authorsTel: +86-0916-2641083, Fax: +86-0916-2641083
*E-mail addresses:*ztianlei88@l63.com (T. L Zhang)
‡ Shuqin Wei and Zeyao Li contributed equally to this work

S27	**Fig. S5** 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.
S28	**Fig. S6** 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.
S29	**Fig. S7** 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.
S30	**Fig. S8** 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.
S31	**Fig. S9** 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.
S32	**Fig. S10** 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.
S33	**Fig. S11** 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%
S34-S57	**Table S16** Cartesian coordinates of all molecules and clusters in the studied system.

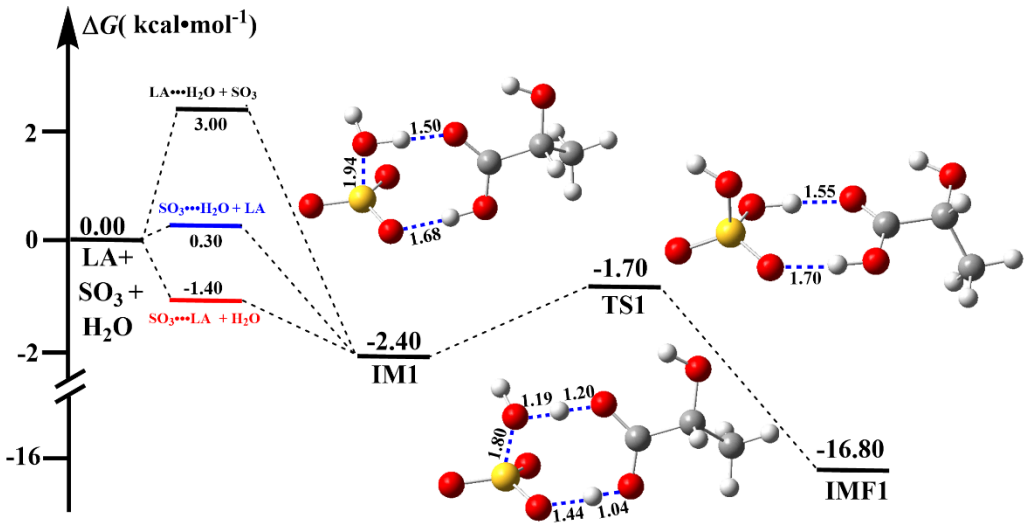

Fig. S1 Potential energy surface for the hydrolysis of SO_3 assisted by lactic acid (LA) calculated at the CCSD(T)-F12/cc-pVDZ-F12//M06-2X/6-311++G(2*df*,2*pd*) level

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 $\Delta(E + \text{ZPE})$/(kcal·mol^{-1})), enthalpies ($\Delta H(298)$/(kcal·mol^{-1})), and Gibbs free energies ($\Delta G(298)$/(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	$\Delta(E + \text{ZPE})$	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.

$$K_{eq1} = \frac{[LAS]}{[LA][SO_3]} = e^{\frac{-\Delta G}{RT}} \quad (S1)$$

$$K_{eq2} = \frac{[LAS]}{[LA][SO_3]} = e^{\frac{-\Delta G}{RT}} \quad (S2)$$

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

$$[LAS] = K_{eq1}[LA][SO_3] \quad (S3)$$

$$[LASA] = K_{eq2}[LA][SO_3] \quad (S4)$$

[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}
k'_{WM}	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}		
	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.

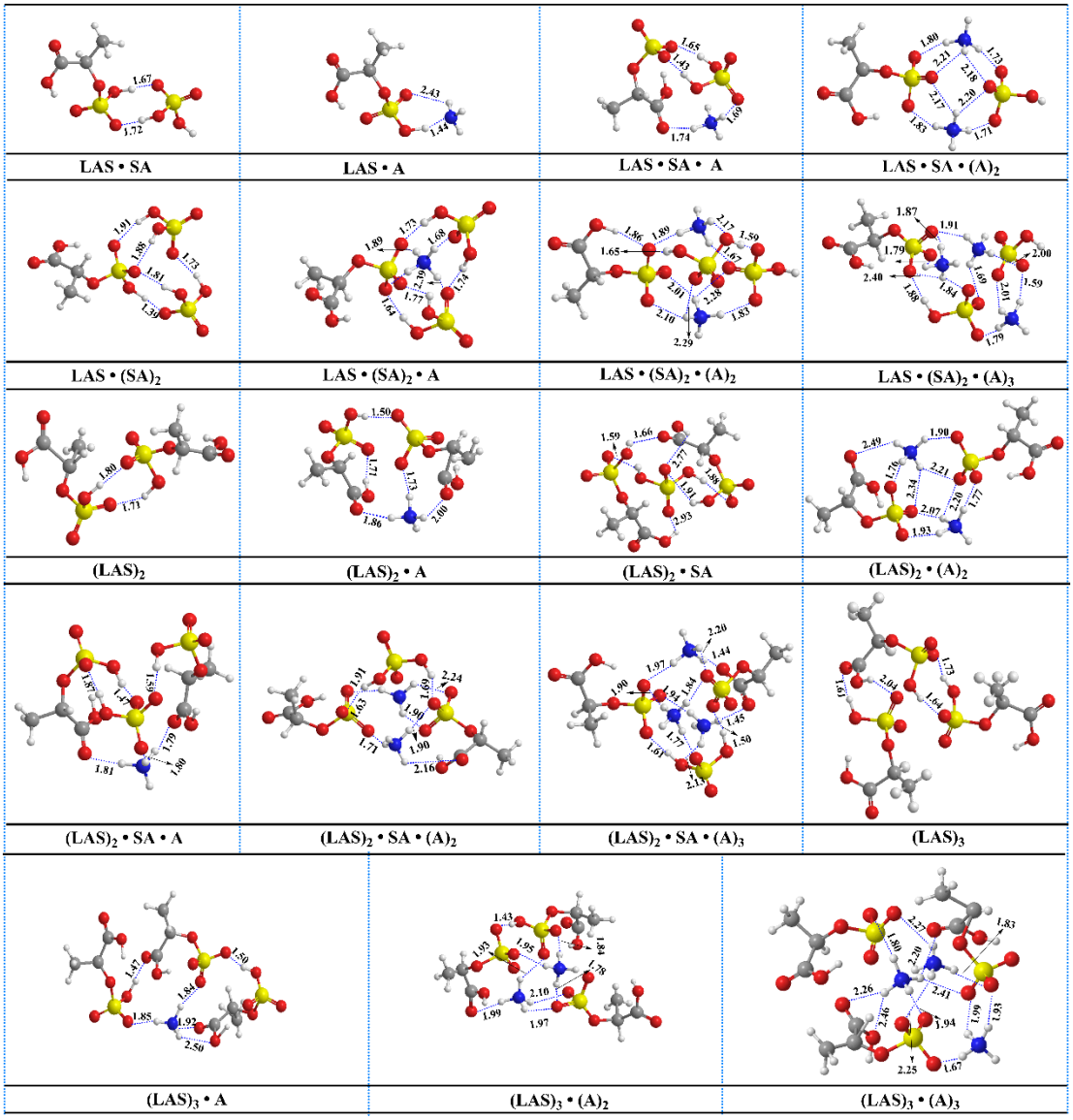

Fig. S2 Optimized structures of the most stable LAS-SA-A-based clusters, obtained at the M06-2X/6-311++G(2*df*,2*pd*) level of theory. Hydrogen bond lengths are indicated in Å (Color code: blue = nitrogen, yellow = sulfur, red = oxygen, gray = carbon, and white = hydrogen)

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.)

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}
$(SA)_2$·$(A)_2$ + 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}
$(SA)_3$·$(A)_2$ + 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}
$(LAS)_2$·$(A)_2$ + 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}
$(LAS)_3$·$(A)_2$ + 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·LAS·A + A	3.28×10^{-10}	3.06×10^{-10}	2.84×10^{-10}	2.62×10^{-10}
SA·LAS·A + SA	9.06×10^{-11}	8.45×10^{-11}	7.84×10^{-11}	7.23×10^{-11}
$(SA)_2$·A + LAS	9.05×10^{-11}	8.44×10^{-11}	7.83×10^{-11}	7.22×10^{-11}
$(SA)_2$·LAS + A	4.28×10^{-10}	3.99×10^{-10}	3.70×10^{-10}	3.42×10^{-10}
SA·LAS·$(A)_2$ + SA	1.03×10^{-11}	9.58×10^{-11}	8.89×10^{-11}	8.20×10^{-11}
$(SA)_2$·$(A)_2$ + LAS	9.27×10^{-11}	8.64×10^{-11}	8.02×10^{-11}	7.40×10^{-11}
$(SA)_2$·LAS·A + A	4.35×10^{-10}	4.06×10^{-10}	3.77×10^{-10}	3.48×10^{-10}
$(SA)_2$·LAS·$(A)_2$ + A	5.23×10^{-10}	4.88×10^{-10}	4.53×10^{-10}	4.18×10^{-10}
$(LAS)_2$·A + SA	8.95×10^{-11}	8.35×10^{-11}	7.75×10^{-11}	7.15×10^{-11}
SA·LAS·A + LAS	8.80×10^{-11}	8.21×10^{-11}	7.62×10^{-11}	7.03×10^{-11}
SA·$(LAS)_2$ + A	3.82×10^{-10}	3.56×10^{-10}	3.31×10^{-10}	3.05×10^{-10}
$(LAS)_2$·$(A)_2$ + SA	1.52×10^{-10}	1.42×10^{-10}	1.32×10^{-10}	1.22×10^{-10}
SA·LAS·$(A)_2$ + LAS	9.96×10^{-11}	9.04×10^{-11}	8.39×10^{-11}	7.74×10^{-11}
SA·$(LAS)_2$·A + A	4.20×10^{-10}	3.92×10^{-10}	3.64×10^{-10}	3.36×10^{-10}
SA·$(LAS)_2$·$(A)_2$ + 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 ($\sum y$, s^{-1}) for each cluster analyzed in the present study of LAS-SA-A system

Clusters	$\sum y$, 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}

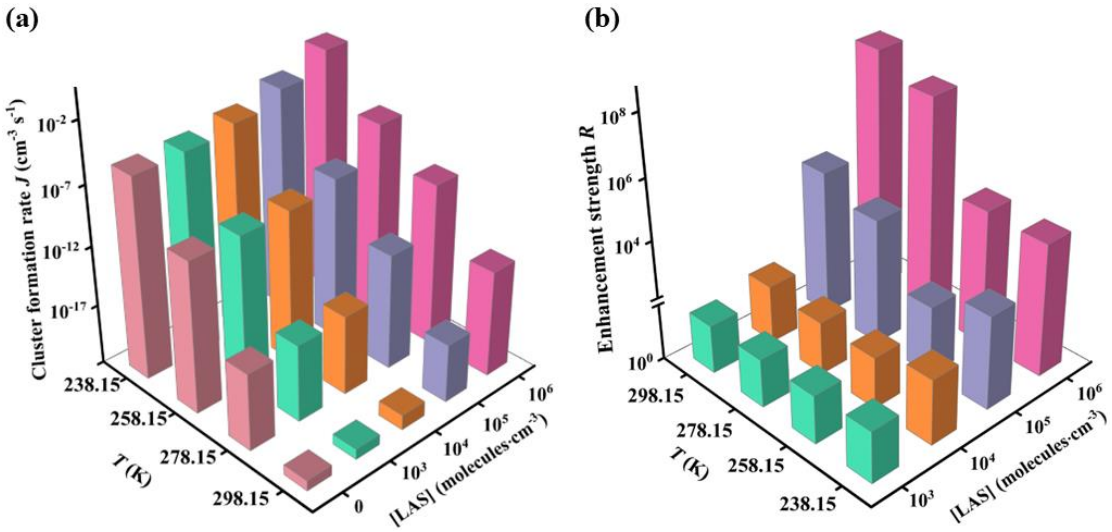

Fig. S3 (a) Cluster formation rate J and (b) enhancement factor R of LAS as functions of [LAS] (10^3 to 10^6 molecules·cm^{-3}) at temperatures of 238.15, 258.15, 278.15 and 298.15 K, with [SA] = 10^5 molecules·cm^{-3} and [A] = 10^9 molecules·cm^{-3}.

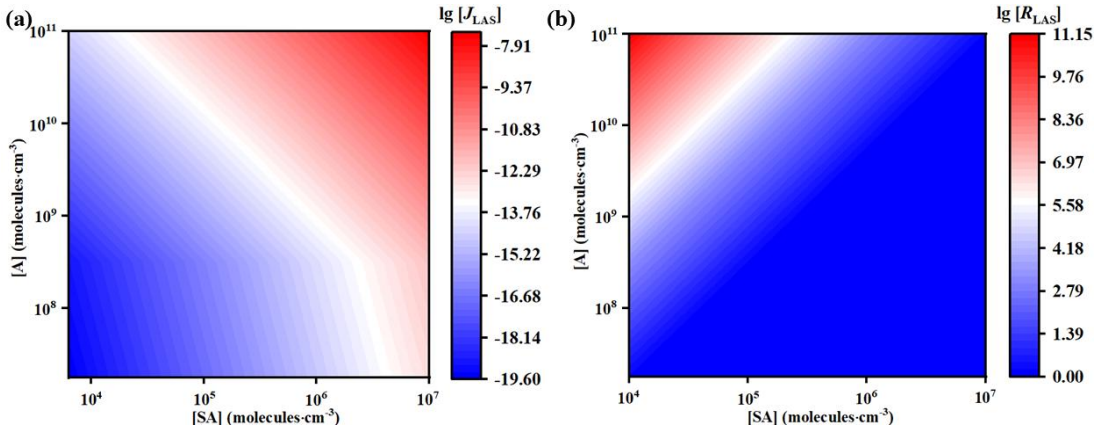

Fig. S4 (a) Cluster formation rate J and (b) enhancement factor R as functions of [SA] and [A] at [LAS] = 10^5 molecules·cm^{-3} and 278.15 K. Color bars represent the logaritmic values of lg[J_{LAS}] lg[R_{LAS}], respectively.

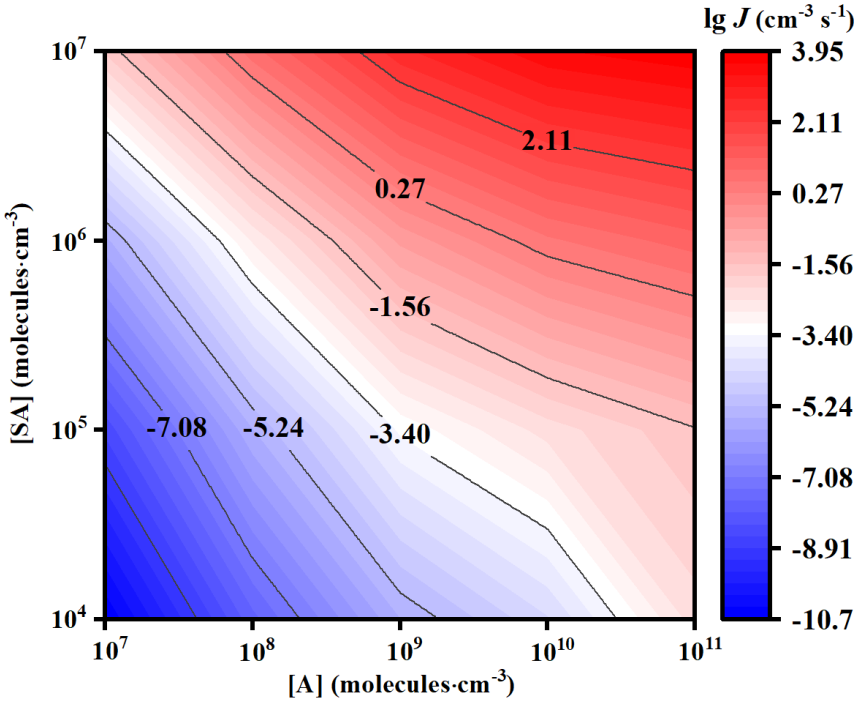

Fig. S5 Cluster formation rate (J) as a function of [SA] and [A] at [LAS]=10^5 molecules·cm^{-3} and 238.15 K. Color bars indicate $\log_{10}[J]$ values.

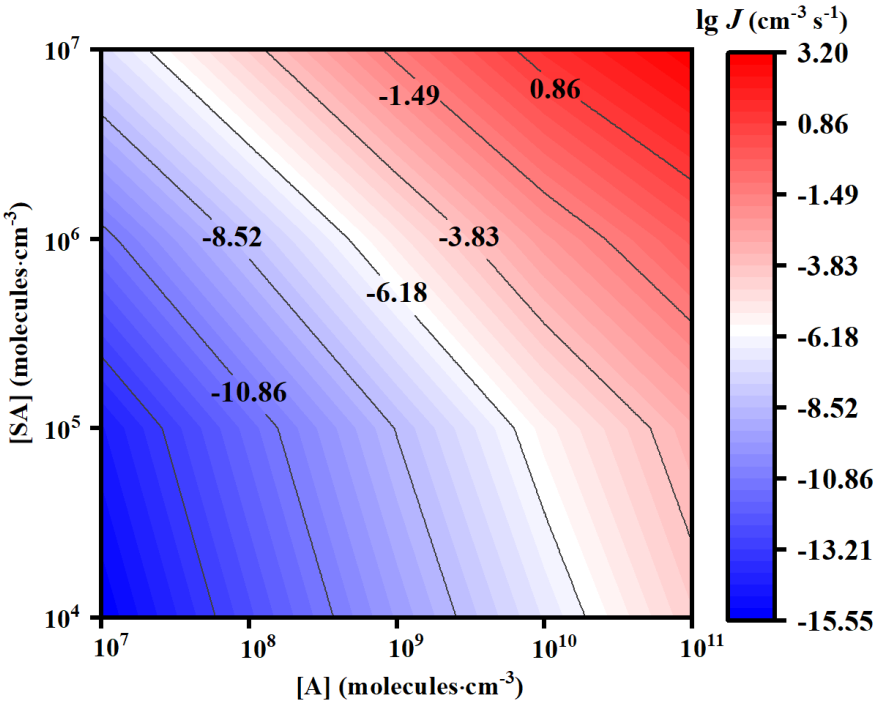

Fig. S6 Cluster formation rate (J) as a function of [SA] and [A] at [LAS]=10^5 molecules·cm^{-3} and 258.15 K. Color bars indicate $\log_{10}[J]$ values.

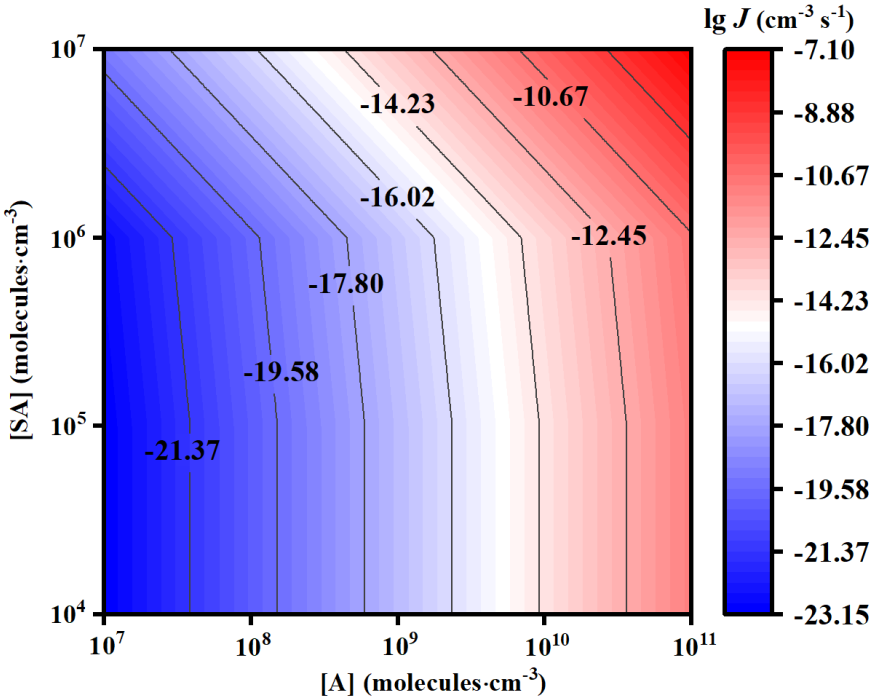

Fig. S7 Cluster formation rate (J) as a function of [SA] and [A] at [LAS]=10^5 molecules·cm^{-3} and 298.15 K. Color bars indicate $\log_{10}[J]$ values.

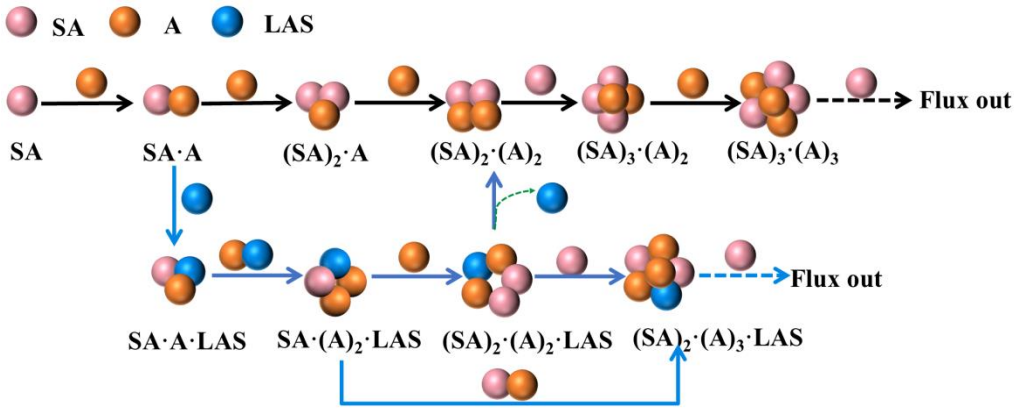

Fig. S8 Main cluster formation mechanisms in the SA-A-LAS-based system at 238.15 K, with [SA] = 10^6 molecules·cm^{-3}, [A] = 10^9 molecules·cm^{-3}, and [LAS] = 10^5 molecules·cm^{-3}. Only net fluxes contributing more than 5% to cluster growth are shown. Black arrows indicate pure SA-A-based growth pathways; blue arrows represent pathways involving LAS; green arrows denote pure LAS-A-based growth pathways.

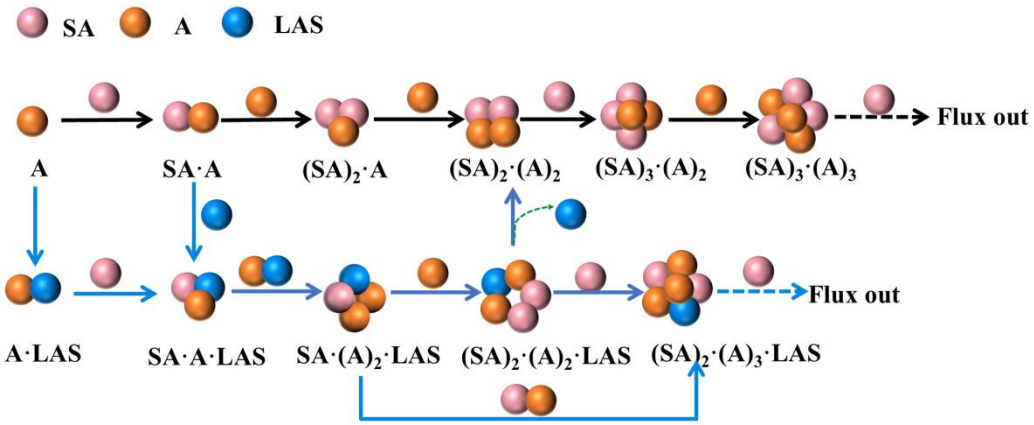

Fig. S9 Main cluster formation mechanism in the SA-A-LAS-based system at 258.15 K, with [SA] = 10^6 molecules·cm^{-3}, [A] = 10^9 molecules·cm^{-3}, and [LAS] = 10^5 molecules·cm^{-3}. Only net fluxes contributing more than 5% to cluster growth are shown. Black arrows indicate pure SA-A-based growth pathways; blue arrows represent pathways involving LAS; green arrows denote pure LAS-A-based growth pathways.

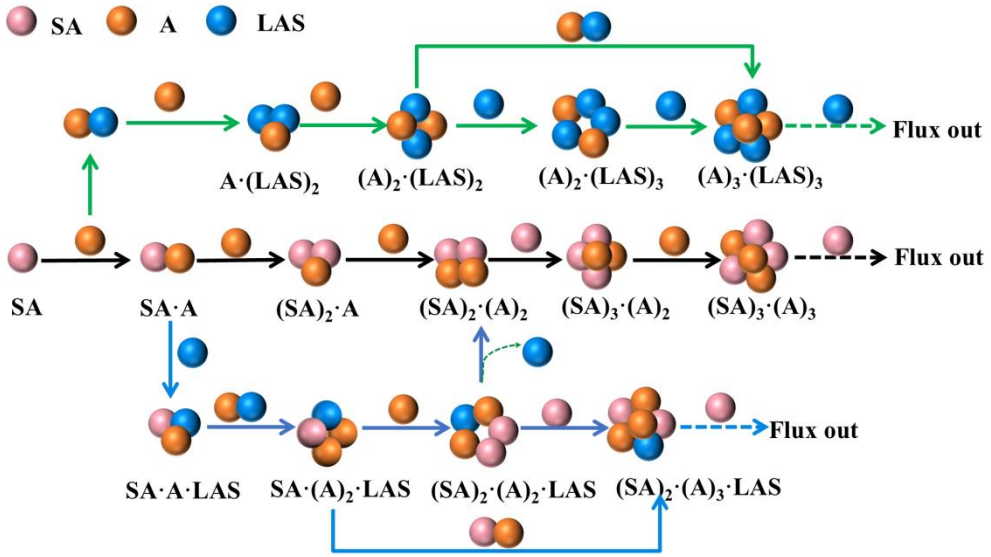

Fig. S10 Main cluster formation mechanisms in the SA-A-LAS-based system at 298.15 K, with [SA] = 10^6 molecules·cm^{-3}, [A] = 10^9 molecules·cm^{-3}, and [LAS] = 10^5 molecules·cm^{-3}. Only net fluxes contributing more than 5% to cluster growth are shown. Black arrows indicate pure SA-A-based growth pathways; blue arrows represent pathways involving LAS; green arrows denote pure LAS-A-based growth pathways.

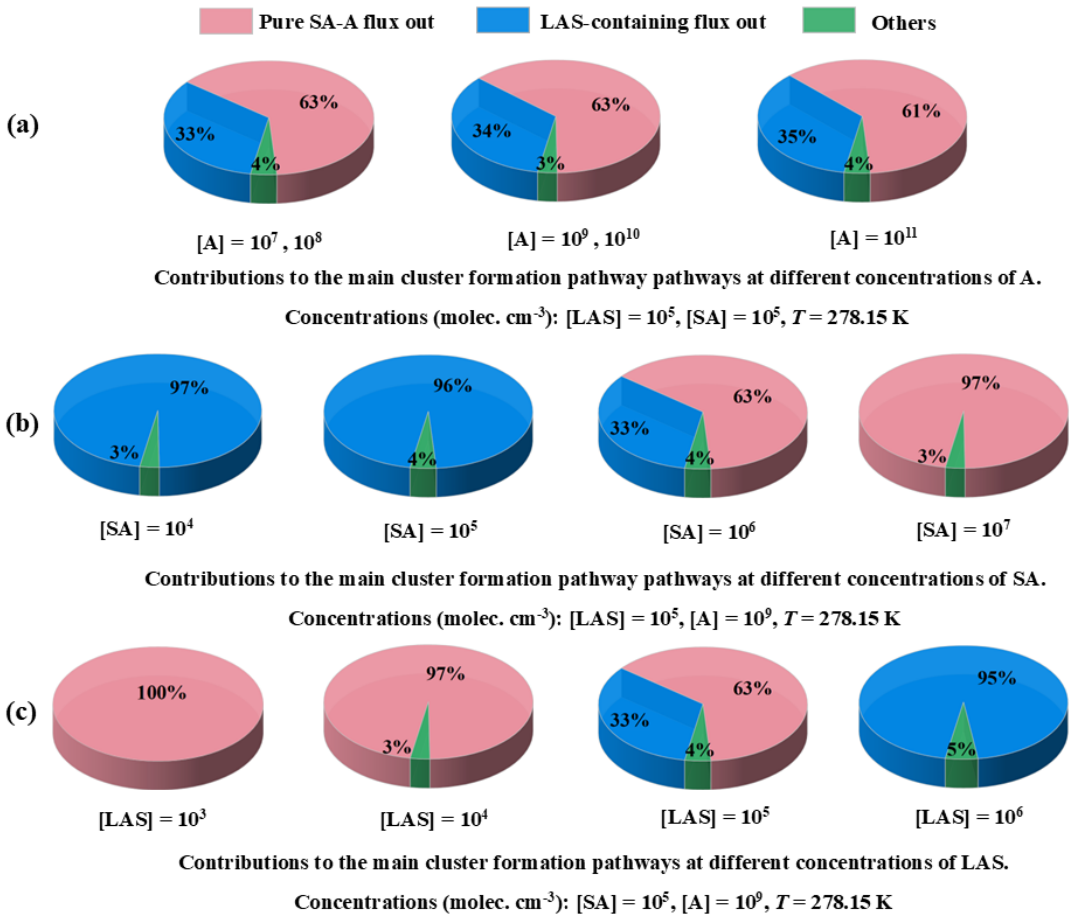

Fig. S11 The influence of (a) [A], (b) [SA] and (c) [LAS] on the relative contribution of the pure SA-A-based clustering route and the LAS participation route to the system flux is analyzed. Others in (a), (b) and (c) indicate that the route contribution of the cluster growing out of the studied system 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

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

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

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

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

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

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

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

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

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

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