Supporting information

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Reaction of SO_3 with H_2SO_4 and Its Implication for Aerosol Particle Formation in the Gas Phase and at the Air-Water Interface

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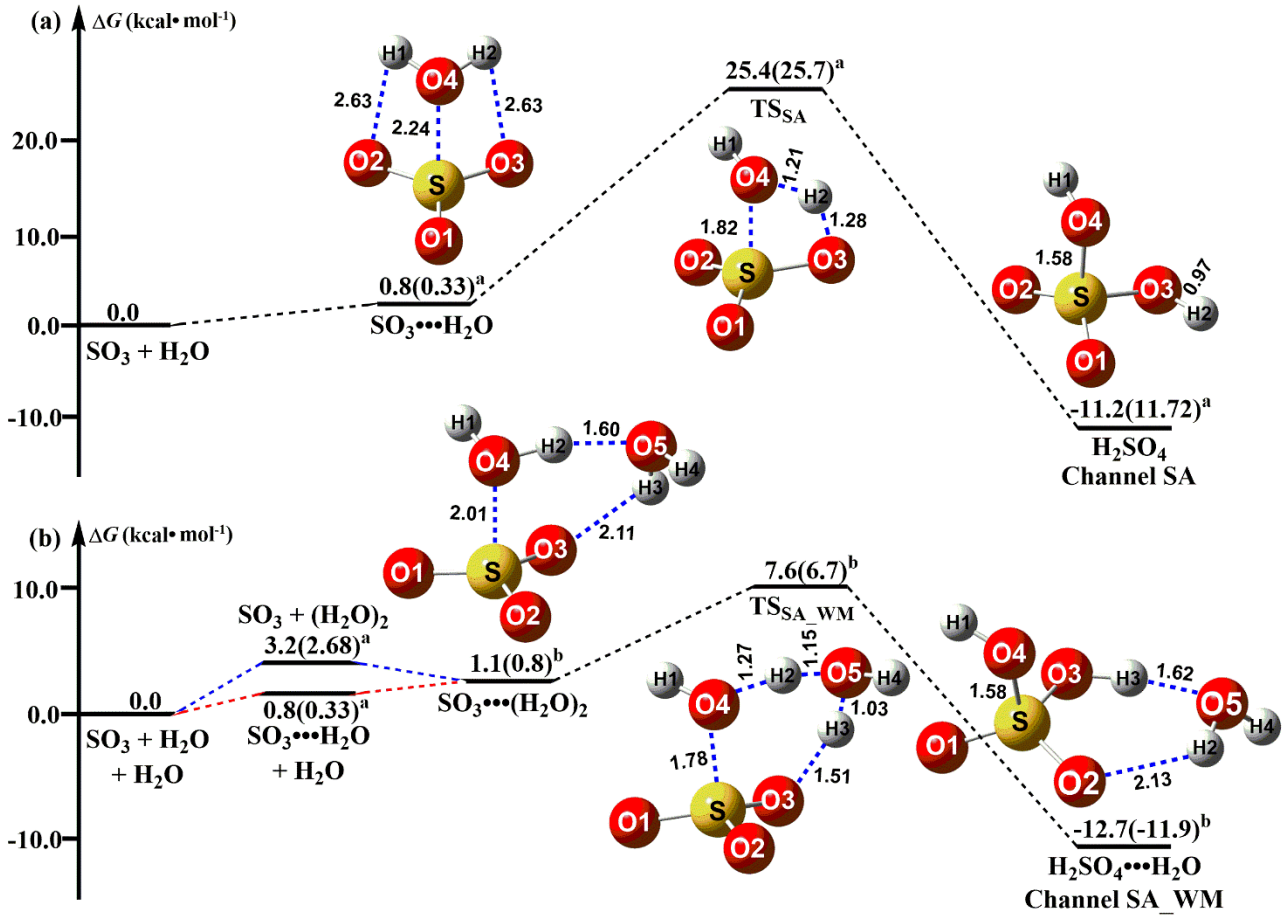

Fig. S1 Schematic energy diagrams for the formation of H_2SO_4 from the $SO_3 + H_2O$ reaction without and with H_2O at the CCSD(T)-F12/cc-pVDZ-F12//M06-2X/6-311++G(2*df*,2*pd*) level of theory

[a] The value was taken from reference (***Chem. Phys. Lett.***, **2013**, 581, 26-29.)

[b] The value was taken from reference (***J. Phys. Chem. A***, **2021**, 123, 3131–3141.)

Table S1 Relative energies (ΔE and $\Delta(E + ZPE)$/(kcal·mol^{-1})), enthalpies (ΔH/(kcal·mol^{-1})), entropy (S(298 K)/(cal·mol^{-1}·K^{-1})) and free energies (ΔG(298 K)/(kcal·mol^{-1})) for the reactants, intermediates, transition states and products involved in the reaction of $SO_3 + H_2SO_4$ without and with H_2O along with the hydrolysis reaction of SO_3 without and with H_2O

Species	ZPE	ΔE	S	ΔG	$\Delta(E+ZPE)$	ΔH
$SO_3 + H_2SO_4$	33.1	0.0	133.5	0.0	0.0	0.0
$SO_3\cdots H_2SO_4$	34.6	-14.3	93.8	-1.6	-12.9	-13.4
TS_{DSA}	32.9	-11.6	87.1	0.7	-11.9	-13.1
$H_2S_2O_7$	35.4	-21.6	89.5	-7.0	-19.4	-20.2
$SO_3 + H_2SO_4 + H_2O$	46.7	0.0	178.6	0.0	0.0	0.0
$SO_3\cdots H_2O + H_2SO_4$	24.0	-9.4	77.9	0.8	-7.0	-7.6
$H_2SO_4\cdots H_2O + SO_3$	40.9	-12.4	87.0	-1.9(-1.82)[a]	-10.2	-10.9
IM_{DSA_WM}'	49.3	-18.0	119.4	2.1	-15.4	-15.6
TS_{DSA_WM}'	49.2	-18.0	112.8	3.3	-15.6	-16.3
$SO_3\cdots H_2SO_4\cdots H_2O$	49.8	-27.8	104.5	-4.0	-24.7	-26.1
TS_{DSA_WM}	49.3	-27.5	99.9	-3.5	-24.9	-26.9
$H_2S_2O_7\cdots H_2O$	50.7	-34.6	102.8	-9.5	-30.6	-32.1
$SO_3 + H_2O$	21.6	0.0	106.2	0.0	0.0	0.0
$SO_3\cdots H_2O$	24.0	-9.4	77.9	0.8(0.33)[b] (0.62)[c]	-7.0	-7.6
TS_{SA}	22.3	15.7	70.4	25.4 (25.7)[b]	16.4	14.7
H_2SO_4	25.2	-23.6	71.8	-11.2(-10.72)[b]	-20.0	-21.4
$SO_3 + H_2O + H_2O$	35.2	0.0	151.3	0.0	0.0	0.0
$SO_3\cdots H_2O + H_2O$	24.0	-9.4	77.9	0.8(0.33)[b] (0.62)[c]	-7.0	-7.6
$SO_3 + (H_2O)_2$	29.5	-5.0	68.6	3.2(2.68)[b]	-2.7	-3.3
$SO_3\cdots(H_2O)_2$	40.7	-21.6	87.4	1.1(0.8)[d]	-16.0	-17.9
TS_{SA_WM}	39.1	-14.5	80.1	7.6(6.7)[d]	-10.6	-13.6
$H_2SO_4\cdots H_2O$	41.0	-36.0	85.5	-12.7(-11.9)[d]	-30.2	-32.3

[a] The value was taken from reference (Long, B., Tan, X. F., Chang, C. R., Zhao, W. X., Long, Z. W., Ren, D. S., and Zhang, W. J.: Theoretical studies on gas-phase reactions of sulfuric acid catalyzed hydrolysis of formaldehyde and formaldehyde with sulfuric acid and $H_2SO_4\cdots H_2O$ complex, J. Phys. Chem. A 117, 5106-5116, 2013.)

[b] The value was taken from reference (Long, B., Chang, C. R., Long, Z. W., Wang, Y. B., Tan, X. F., and Zhang, W. J.: Nitric acid catalyzed hydrolysis of SO_3 in the formation of sulfuric acid: A theoretical study, Chem. Phys. Lett., 581, 26-29, 2013.)

[c] The value was taken from reference (Long, B., Long, Z. W., Wang, Y. B., Tan, X. F., Han, Y. W., Long, C. W., Qin, S. J., and Zhang, W. J.: Formic acid catalyzed gas-phase reaction of H_2O with SO_3 and the reverse reaction: A theoretical study, ChemPhysChem, 13, 323-329, 10.1002/cphc.201100558, 2012.)

[d] The value was taken from reference (Sarkar, S., Oram, B. K., and Bandyopadhyay, B.: Influence of ammonia and water on the fate of sulfur trioxide in the troposphere: theoretical investigation of sulfamic acid and sulfuric acid formation pathways, J. Phys. Chem. A, 123, 3131-3141, 2019.)

Table S2 Equilibrium constants ($cm^3 \cdot molecule^{-1}$) for $SO_3 \cdots H_2SO_4$, $SO_3 \cdots H_2O$, $H_2SO_4 \cdots H_2O$ and $(H_2O)_2$ within the temperature range of 280-320 K

T/K	$SO_3 \cdots H_2SO_4$	$SO_3 \cdots H_2O$	$H_2SO_4 \cdots H_2O$	$(H_2O)_2$
280	2.54×10^{-18}	2.45×10^{-20}	3.00×10^{-118}	2.86×10^{-22}
290	1.15×10^{-18}	1.59×10^{-20}	2.66×10^{-19}	2.42×10^{-22}
298	6.33×10^{-19}	1.14×10^{-20} (6.44×10^{-20})[a]	1.67×10^{-19} (5.16×10^{-20})[b]	2.14×10^{-22} (2.34×10^{-21})[c]
300	5.48×10^{-19}	1.06×10^{-20}	1.49×10^{-19}	2.08×10^{-22}
310	2.75×10^{-19}	7.25×10^{-21}	8.68×10^{-20}	1.80×10^{-22}
320	1.44×10^{-20}	5.10×10^{-21}	5.24×10^{-20}	1.58×10^{-22}

[a] The value was taken from reference (Long, B., Long, Z. W., Wang, Y. B., Tan, X. F., Han, Y. W., Long, C. W., Qin, S. J., and Zhang, W. J.: Formic Acid Catalyzed Gas-Phase Reaction of H_2O with SO_3 and the Reverse Reaction: A Theoretical Study, ChemPhysChem, 13, 323-329, 10.1002/cphc.201100558, 2012.)

[b] The value was taken from reference (Wang, R., Wen, M., Chen, X., Mu, R., Zeng, Z., Chai, G., Lily, M., Wang, Z., and Zhang, T.: Atmospheric Chemistry of CH_2OO: The Hydrolysis of CH_2OO in Small Clusters of Sulfuric Acid, J. Phys. Chem. A, 125, 2642-2652, 10.1021/acs.jpca.1c02006, 2021.)

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

Table S3 Concentrations (molecules·cm^{-3}) of H_2O and H_2SO_4 within the temperature range of 280-320 K

Catalysts	RH	280 K	290 K	298 K	300 K	310 K	320 K
H_2O	20%RH[a]	5.16×10^{16}	9.60×10^{16}	1.50×10^{17}	1.72×10^{17}	2.92×10^{17}	4.70×10^{17}
	40%RH[a]	1.03×10^{17}	1.91×10^{17}	3.10×10^{17}	3.43×10^{17}	5.84×10^{17}	9.40×10^{17}
	60%RH[a]	1.55×10^{17}	2.87×10^{17}	4.50×10^{17}	5.15×10^{17}	8.77×10^{17}	1.41×10^{18}
	80%RH[a]	2.07×10^{17}	3.82×10^{17}	6.20×10^{17}	6.86×10^{17}	1.17×10^{18}	1.88×10^{18}
	100%RH[a]	2.58×10^{17}	4.78×10^{17}	7.70×10^{17}	8.58×10^{17}	1.46×10^{18}	2.35×10^{18}
H_2SO_4	[SA][b] = 10^6	3.90×10^6	3.80×10^6	3.70×10^6	3.60×10^6	3.50×10^6	3.40×10^6
	[SA][c] = 10^7	5.00×10^7	5.00×10^7	5.00×10^7	5.00×10^7	5.00×10^7	5.00×10^7
	[SA][b] = 10^8	3.90×10^8	3.80×10^8	3.70×10^8	3.60×10^8	3.50×10^8	3.40×10^8
$H_2SO_4 \cdots H_2O$	[SA][e] = 10^6	20%RH	6.03×10^5	5.76×10^5	5.42×10^5	5.39×10^5	5.10×10^5
		40%RH	1.20×10^6	1.15×10^6	1.12×10^6	1.07×10^6	1.02×10^6
		60%RH	1.81×10^6	1.72×10^6	1.63×10^6	1.61×10^6	1.53×10^6
		80%RH	2.42×10^6	2.29×10^6	2.24×10^6	2.15×10^6	2.04×10^6
		100%RH	3.01×10^6	2.87×10^6	2.78×10^6	2.69×10^6	2.55×10^6
	[SA][c] = 10^7	20%RH	7.73×10^6	7.58×10^6	7.33×10^6	7.48×10^6	7.29×10^6
		40%RH	1.54×10^7	1.51×10^7	1.51×10^7	1.49×10^7	1.46×10^7
		60%RH	2.32×10^7	2.27×10^7	2.20×10^7	2.24×10^7	2.19×10^7
		80%RH	3.10×10^7	3.02×10^7	3.03×10^7	2.98×10^7	2.92×10^7
		100%RH	3.86×10^7	3.77×10^7	3.76×10^7	3.73×10^7	3.64×10^7
	[SA][e] = 10^8	20%RH	6.03×10^7	5.76×10^7	5.42×10^7	5.39×10^7	5.10×10^7
		40%RH	1.20×10^8	1.15×10^8	1.12×10^8	1.07×10^8	1.02×10^8
		60%RH	1.81×10^8	1.72×10^8	1.63×10^8	1.61×10^8	1.53×10^8
		80%RH	2.42×10^8	2.29×10^8	2.24×10^8	2.15×10^8	2.04×10^8
		100%RH	3.01×10^8	2.87×10^8	2.78×10^8 (2.40×10^7)[c] (1.11×10^8)[d]	2.69×10^8	2.55×10^8

[a] The values were reported from reference (Anglada, J. M., Hoffman, G. J., Slipchenko, L. V., M. Costa, M., Ruiz-Lopez, M. F., and Francisco, J. S.: Atmospheric significance of water clusters and ozone-water complexes, J. Phys. Chem. A, 117, 10381-10396, 2013.)

[b] The values were taken from reference (Liu, J., Fang, S., Wang, Z., Yi, W., Tao, F. M., and Liu, J. Y.: Hydrolysis of sulfur dioxide in small clusters of sulfuric acid: Mechanistic and kinetic study, Environ. Sci. Technol., 49, 13112-13120, 2015.)

[c] The values were taken from reference (Liu, L., Zhong, J., Vehkamäki, H., Kurtén, T., Du, L., Zhang, X., Francisco, J. S., and Zeng, X. C.: Unexpected quenching effect on new particle formation from the atmospheric reaction of methanol with SO_3, Proc. Natl. Acad. Sci. U.S.A., 116, 24966-24971, 2019.)

[d] The values were taken from reference (Wang, R., Wen, M., Chen, X., Mu, R., Zeng, Z., Chai, G., Lily, M., Wang, Z., and Zhang, T.: Atmospheric Chemistry of CH_2OO: The Hydrolysis of CH_2OO in Small Clusters of Sulfuric Acid, J. Phys. Chem. A, 125, 2642-2652, 10.1021/acs.jpca.1c02006, 2021.)

Part 1 The calculation details of high-pressure-limit (HPL) rate constants

The VRC-VTST calculations were carried out with the potential surface obtained by using CCSD(T)-F12/cc-pVDZ-F12//M06-2X/6-311++G(2*df*,2*pd*) and were performed by variationally minimizing the rate constant with respect to the distance *s* between pivot points and with respect to the location of the pivot points. Specifically, using two pivot points produces a single-faceted dividing surface for the SO_3 + H_2SO_4 reaction without and with H_2O. Such as, using two pivot points produces a single-faceted dividing surface for the reaction of SO_3 + H_2SO_4. One pivot point is located at a distance *d* from the center of mass (COM) of SO_3, where the vector connecting the pivot point with SO_3's COM is perpendicular to the SO_3 plane, and the other pivot point is located at a distance *d* from the COM of catalyst H_2SO_4, where the vector connecting the pivot point with catalyst H_2SO_4's COM is perpendicular to catalyst H_2SO_4 plane. The lengths of these vectors are fixed successively at 0.2 Å. The reaction coordinate *s* is the distance between a pivot point on one reactant and a pivot point on the other reactant. The distance *s* between pivot points is varied from 2.5 to 8.0 Å for SO_3 + H_2SO_4 in each case with a 0.2 Å grid increment. The details of the VRC-VTST calculations can be seen in the supporting information of reference (Bao et al., 2016).

Reference

Bao, J. L.; Zhang, X.; Truhlar, D. G.: Barrierless association of CF_2 and dissociation of C_2F_4 by variational transition-state theory and system-specific quantum Rice-Ramsperger-Kassel theory, Proc. Natl. Acad. Sci. U. S. A., 113, 13606-13611, 2016

Table S4 The high-pressure limiting rate constants ($cm^3 \cdot molecule^{-1} \cdot s^{-1}$) for the reactants to pre-reactive complex process in the SO_3 + H_2SO_4 reaction without and with H_2O, and the hydrolysis of SO_3 without and with H_2O calculated by the master equation within the temperature range of 280-320 K

T(K)	$SO_3 + H_2SO_4 \rightarrow SO_3\cdots H_2SO_4$	$SO_3 + H_2SO_4\cdots H_2O \rightarrow IM_{DSA\_WM\_a}'$	$SO_3\cdots H_2O + H_2SO_4 \rightarrow SO_3\cdots H_2SO_4\cdots H_2O$
280	9.75×10^{-11}	1.69×10^{-10}	7.23×10^{-11}
290	9.93×10^{-11}	1.72×10^{-10}	7.35×10^{-11}
298	1.01×10^{-10}	1.75×10^{-10}	7.46×10^{-11}
300	1.01×10^{-10}	1.75×10^{-10}	7.48×10^{-11}
310	1.03×10^{-10}	1.78×10^{-10}	7.60×10^{-11}
320	1.04×10^{-10}	1.81×10^{-10}	7.73×10^{-11}
T(K)	$SO_3 + H_2O \rightarrow SO_3\cdots H_2O$	$SO_3\cdots H_2O + H_2O \rightarrow SO_3\cdots (H_2O)_2$	
280	1.45×10^{-10}	2.24×10^{-10}	
290	1.47×10^{-10}	2.28×10^{-10}	
298	1.49×10^{-10}	2.32×10^{-10}	
300	1.50×10^{-10}	2.32×10^{-10}	
310	1.52×10^{-10}	2.36×10^{-10}	
320	1.55×10^{-10}	2.40×10^{-10}	

Part 2 The details of Master Equation Solver for Multi-Energy Well Reactions

The rate constants for the SO_3 + H_2SO_4 reaction without and with H_2O within the temperature range of 280-320 K were calculated by using the Master Equation Solver for Multi-Energy Well Reactions (MESMER) (Miller and Klippenstein, 2006). Specifically, as for the SO_3 + H_2SO_4 reaction without and with H_2O, the barrierless bimolecular reaction steps were evaluated by using Inverse Laplace Transform (ILT) method (Horváth et al., 2020), whereas the rate determining steps were obtained by employing the RRKM theory. The ILT methods and RRKM theory can be respectively expressed in Eq. (S1)-Eq. (S2).

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

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

In Eq. (S1) and Eq. (S2), $W(E\text{-}E_0)$ is the rovibrational sum of states (SOS) at the optimized transition state (TS) geometry, E_0 is the reaction threshold energy, h is Planck's constant, $\rho(E)$ is the density of rovibrational states of the reactant, and $Q(\beta)$ is the corresponding canonical partition function. Moreover, the electronic geometries, vibrational frequencies, and rotational constants were calculated at the M06-2X/6-311+G(2*df*,2*pd*) level; single-point energy calculations were refined at the CCSD(T)-F12/cc-pVDZ-F12 level for the modeling. The one-dimensional asymmetric Eckart potential was used to treat the tunneling effect in the RRKM calculation. In addition, the Lennard-Jones (L-J) parameters ε/k_B = 71.4 K and σ = 3.798 Å were used for N_2, while ε/k_B = 420.08 K and σ = 2.89 Å were estimated for H_2SO_4 and its isomer.

Reference

Horváth, G., Horváth, I., Almousa, S. A. D., and Telek, M.: Numerical inverse Laplace transformation using concentrated matrix exponential distributions, Perform. Evaluation, 137, 102067, 2020.

Miller, J. A., and Klippenstein, S. J.: Master equation methods in gas phase chemical kinetics, J. Phys. Chem. A, 110, 10528-10544, 2006.

Table S5 Rate constants ($cm^3 \cdot molecule^{-1} \cdot s^{-1}$) for the $SO_3 + H_2SO_4$ reaction with H_2O and the hydrolysis of SO_3 without and with H_2O within the temperature range of 280-320 K

Channel	*T*/K	280	290	298	300	310	320
Channel DSA_WM	$k_{DSA\_WM\_o}$	3.35×10^{-11}	3.53×10^{-11}	3.27×10^{-11}	3.19×10^{-11}	2.73×10^{-11}	2.29×10^{-11}
	$k_{DSA\_WM\_s}$	1.33×10^{-11}	1.13×10^{-11}	9.87×10^{-12}	9.53×10^{-12}	7.95×10^{-12}	6.59×10^{-12}
Channel SA	k_{SA}	6.22×10^{-24} (8.0×10^{-24})[a]	8.07×10^{-24} (1.1×10^{-23})[a]	1.02×10^{-23} (1.4×10^{-23})[a]	1.08×10^{-23} (1.4×10^{-23})[a]	1.49×10^{-23} (2.0×10^{-23})[a]	2.11×10^{-23} (3.0×10^{-23})[a]
Channel SA_WM	k_{SA_WM}	1.37×10^{-12}	1.17×10^{-12}	1.04×10^{-12} (4.08×10^{-12})[a]	1.01×10^{-12}	8.67×10^{-13}	7.49×10^{-13}

$k_{DSA\_WM\_o}$ and $k_{DSA\_WM\_s}$ are respectively the rate constants for the formation of $H_2S_2O_7$ from the reaction of $SO_3 + H_2SO_4$ with H_2O occurring through one-step and stepwise routes; k_{SA} and k_{SA_WM} are respectively the rate constants for the formation of H_2SO_4 without and with H_2O.

[a] The value was taken from reference (Bandyopadhyay, B., Kumar, P., and Biswas, P.: Ammonia Catalyzed Formation of Sulfuric Acid in Troposphere: The Curious Case of a Base Promoting Acid Rain, J. Phys. Chem. A, 121, 3101-3108, 10.1021/acs.jpca.7b01172, 2017.)

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

Part 3 Calculations of effective rate constants

Usually, the effective rate constants (k') is considered to be the relative efficiency of many atmospheric reactions (Liu et al., 2019; Sun et al., 2016; Ali et al., 2018; Ali et al., 2019) with water vapor. To better understand the competition between $H_2S_2O_7$ and H_2SO_4 formation in the atmospheric environment, it is necessary to compare the effective rate constants in different reaction. For the $H_2S_2O_7$ formation, the k' for the H_2O-assisted reaction (Channels DSA_WM) can be respectively expressed as:

$$k'_{DSA\_WM\_o} = k_{DSA\_WM\_o} \times K_{eq1} \times [H_2O] \quad (S3)$$

$$k'_{DSA\_WM\_s} = k_{DSA\_WM\_s} \times K_{eq2} \times [H_2O] \quad (S4)$$

In above formula, $k_{DSA\_WM\_o}$ and $k_{DSA\_WM\_s}$ were respectively denoted the bimolecular rate coefficient for Channels DSA_WM_o, DSA_WM_s and SA_WM; $[H_2O]$ and $[H_2SO_4]$ were respectively represented the concentration of H_2O and H_2SO_4 listed in Table S3; K_{eq1} and K_{eq2} is the equilibrium constant for the formation of complex $SO_3\cdots H_2O$ and $H_2SO_4\cdots H_2O$ shown in Table S2.

Reference

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Table S6 The rate ratio between the $SO_3 + H_2SO_4$ reaction and the hydrolysis of SO_3 within the temperature range of 280-320 K

RH	$[H_2SO_4]$	280	290	298	300	310	320
20%RH	10^6	3.30×10^{-7}	1.40×10^{-8}	7.48×10^{-8}	5.98×10^{-8}	2.80×10^{-8}	1.41×10^{-9}
	10^7	4.23×10^{-6}	1.84×10^{-6}	1.01×10^{-6}	8.30×10^{-7}	4.00×10^{-7}	2.07×10^{-7}
	10^8	3.30×10^{-5}	1.40×10^{-5}	7.48×10^{-6}	5.98×10^{-6}	2.80×10^{-6}	1.41×10^{-7}
40%RH	10^6	1.05×10^{-7}	4.48×10^{-8}	2.25×10^{-8}	1.91×10^{-8}	8.90×10^{-9}	4.45×10^{-9}
	10^7	1.35×10^{-6}	5.90×10^{-7}	3.04×10^{-7}	2.65×10^{-7}	1.27×10^{-7}	6.54×10^{-8}
	10^8	1.05×10^{-5}	4.48×10^{-6}	2.25×10^{-6}	1.91×10^{-6}	8.90×10^{-7}	4.45×10^{-7}
60%RH	10^6	5.65×10^{-8}	2.41×10^{-8}	1.28×10^{-8}	1.03×10^{-8}	4.79×10^{-9}	2.39×10^{-9}
	10^7	7.24×10^{-7}	3.17×10^{-7}	1.72×10^{-7}	1.43×10^{-7}	6.84×10^{-8}	3.51×10^{-8}
	10^8	5.65×10^{-6}	2.41×10^{-6}	1.28×10^{-6}	1.03×10^{-6}	4.79×10^{-7}	2.39×10^{-7}
80%RH	10^6	3.73×10^{-8}	1.60×10^{-8}	8.05×10^{-9}	6.82×10^{-9}	3.16×10^{-9}	1.57×10^{-9}
	10^7	4.78×10^{-7}	2.10×10^{-7}	1.09×10^{-7}	9.47×10^{-8}	4.52×10^{-8}	2.32×10^{-8}
	10^8	3.73×10^{-6}	1.60×10^{-6}	8.05×10^{-7}	6.82×10^{-7}	3.16×10^{-7}	1.57×10^{-7}
100%RH	10^6	2.75×10^{-8}	1.17×10^{-8}	5.98×10^{-9}	5.01×10^{-9}	2.33×10^{-9}	1.16×10^{-9}
	10^7	3.53×10^{-7}	1.55×10^{-7}	8.08×10^{-8}	6.96×10^{-8}	3.33×10^{-8}	1.70×10^{-8}
	10^8	2.75×10^{-6}	1.17×10^{-6}	5.98×10^{-7}	5.01×10^{-7}	2.33×10^{-7}	1.16×10^{-7}

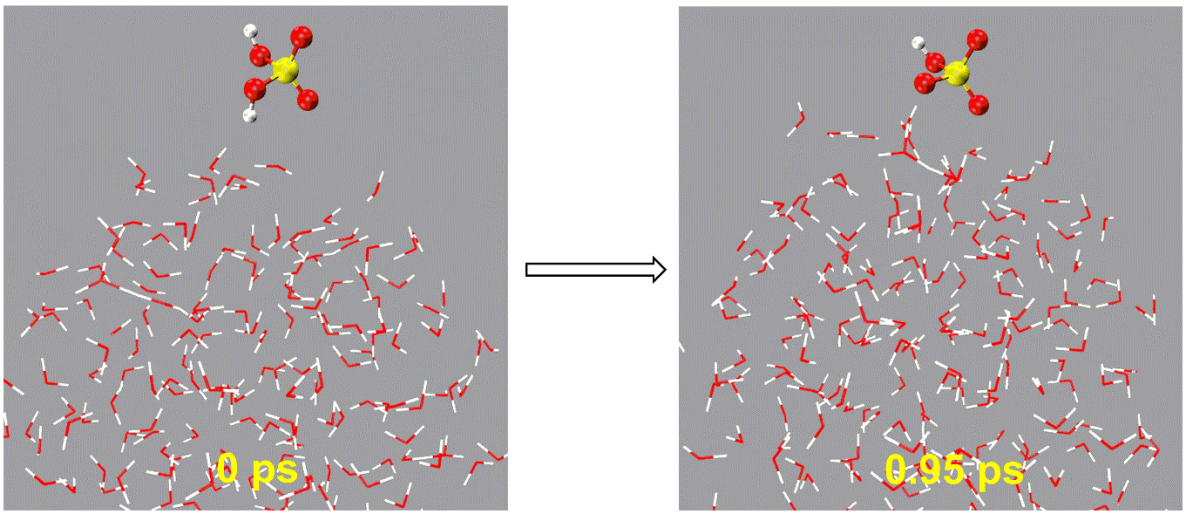

Fig. S2 Snapshot structures taken from the BOMD simulations of H_2SO_4 reaction at the air-water interface. The white, red and yellow spheres represent H, O and S atoms, respectively.

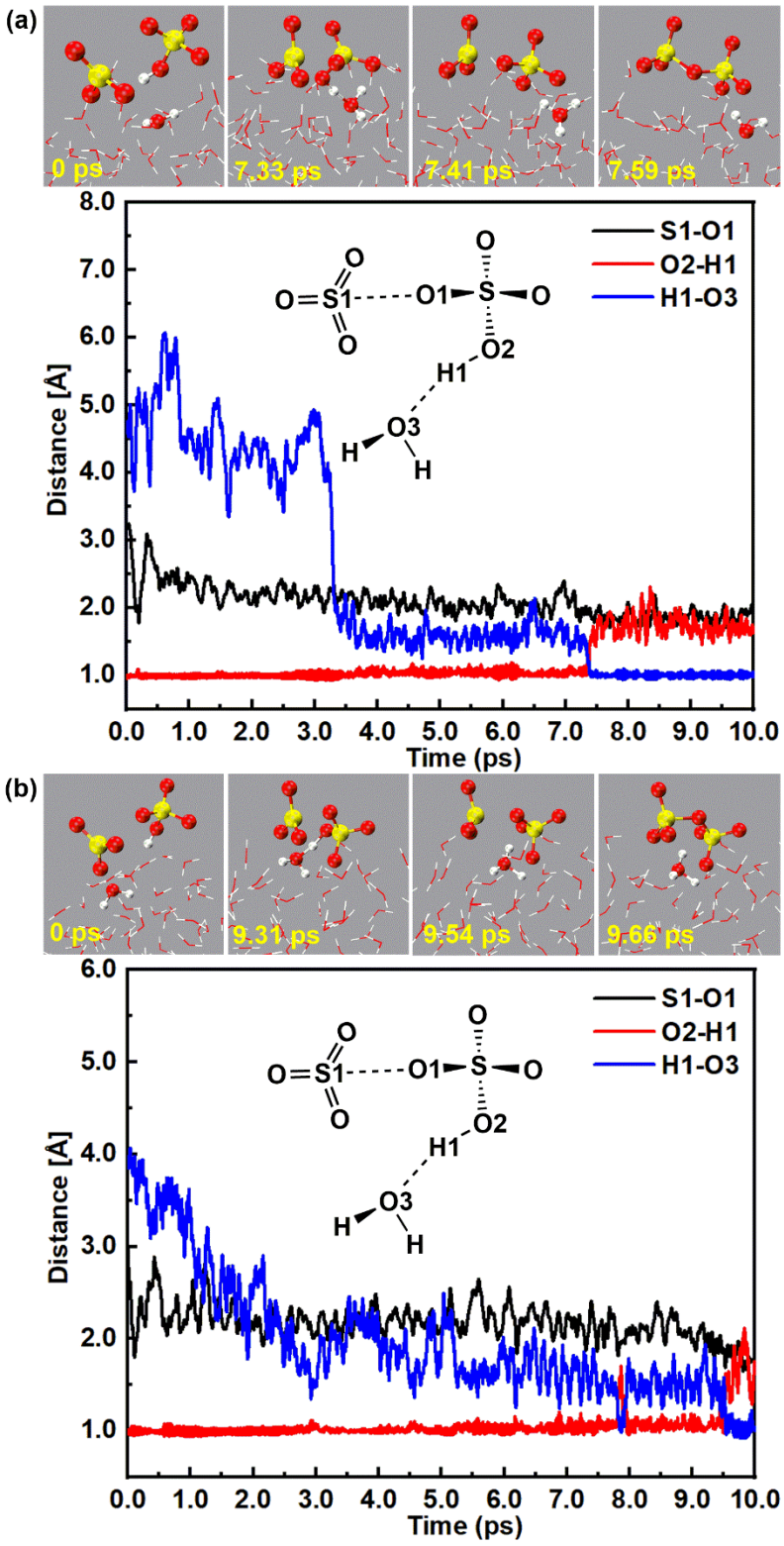

Fig. S3 Two BOMD trajectories and snapshots for H_2O-induced the formation of $S_2O_7^{2-}$•••H_3O^+ ion pair from the reaction of SO_3 with HSO_4^- at the air-water interface (Top panel: Snapshot structures taken from the BOMD simulations, which illustrate H_2O-induced the formation of $S_2O_7^{2-}$•••H_3O^+ ion pair from the reaction of SO_3 with HSO_4^- at the air-water interface. Lower panel: time evolution of key bond distances (S-O1, O2-H1, and O3-H1) involved in the induced mechanism.)

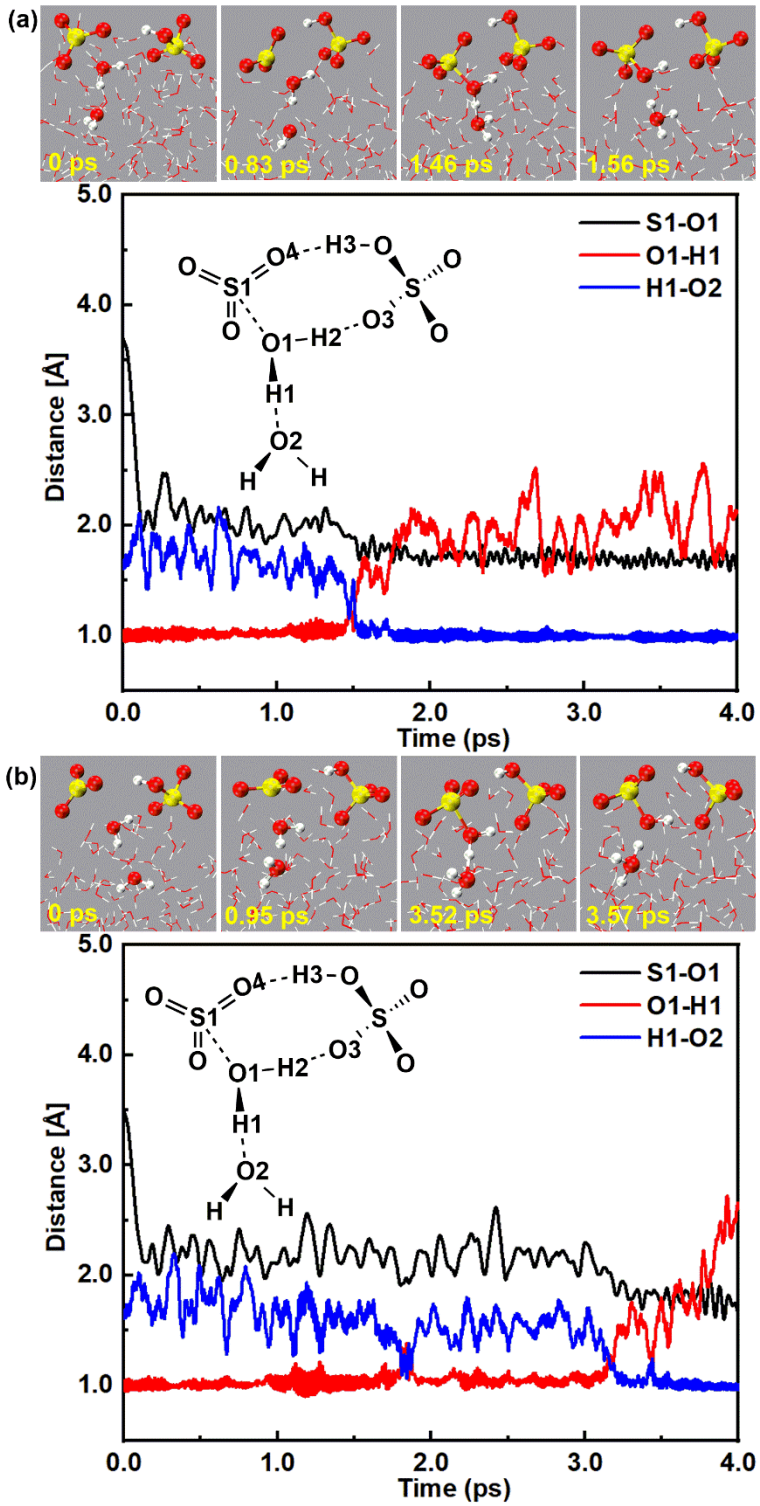

Fig. S4 Two BOMD trajectories and snapshots for the direct HSO_4^--mediated formation of $HSO_4^-\cdots H_3O^+$ ion pair at the air water interface (Top panel: Snapshot structures taken from the BOMD simulations, which illustrate the direct HSO_4^--mediated formation of $HSO_4^-\cdots H_3O^+$ ion pair at the air water interface. Lower panel: time evolution of key bond distances (S1-O1, O1-H1 and H1-O2) involved in the hydration mechanism.)

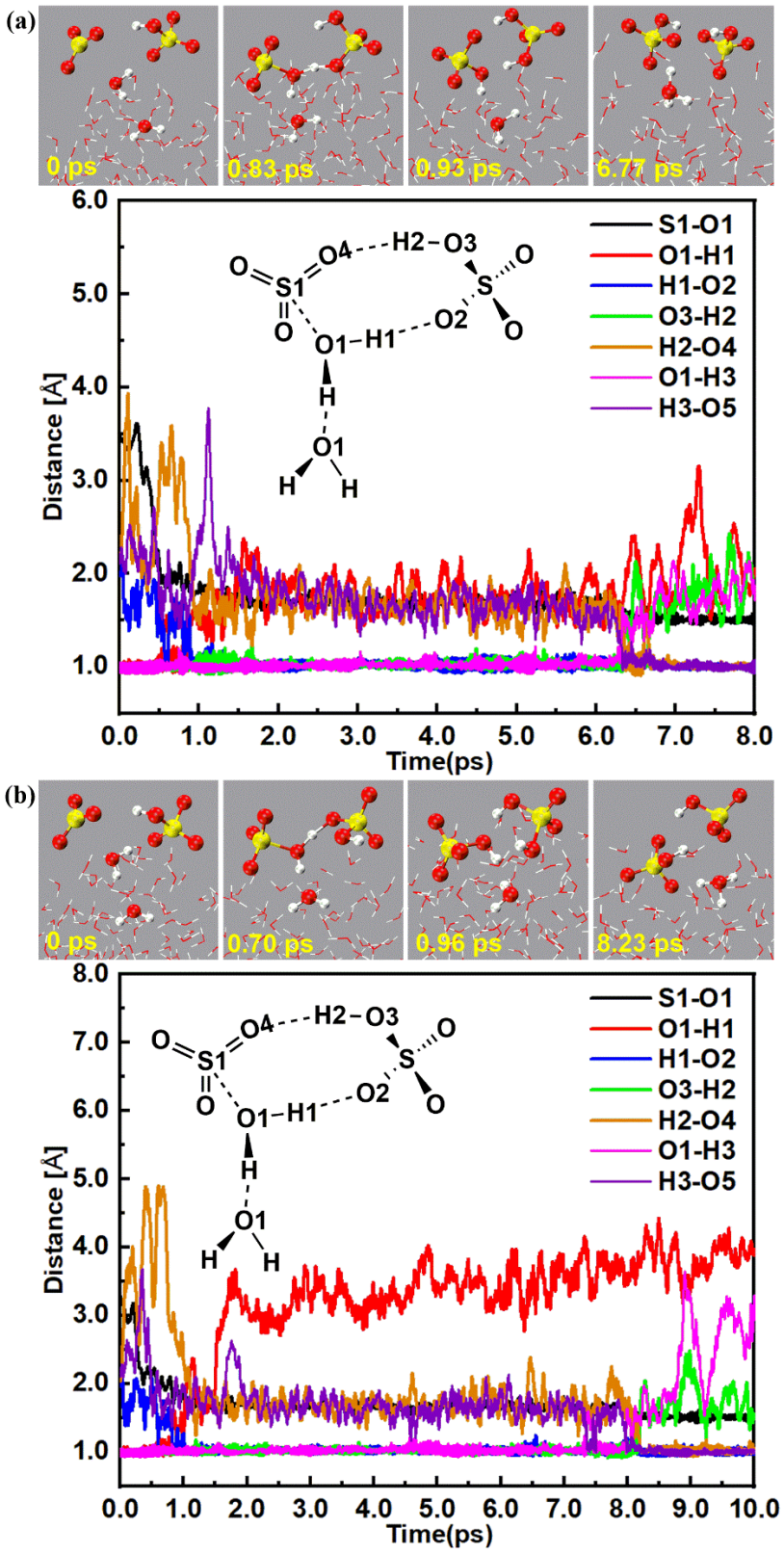

Fig. S5 Two BOMD trajectories and snapshots for the indirect HSO_4^--mediated formation of $HSO_4^-\cdots H_3O^+$ ion pair at the air water interface (Top panel: Snapshot structures taken from the BOMD simulations, which illustrate the indirect HSO_4^--mediated formation of $HSO_4^-\cdots H_3O^+$ ion pair at the air water interface. Lower panel: time evolution of key bond distances (S1-O1, O1-H1 and H1-O2) involved in the hydration mechanism.)

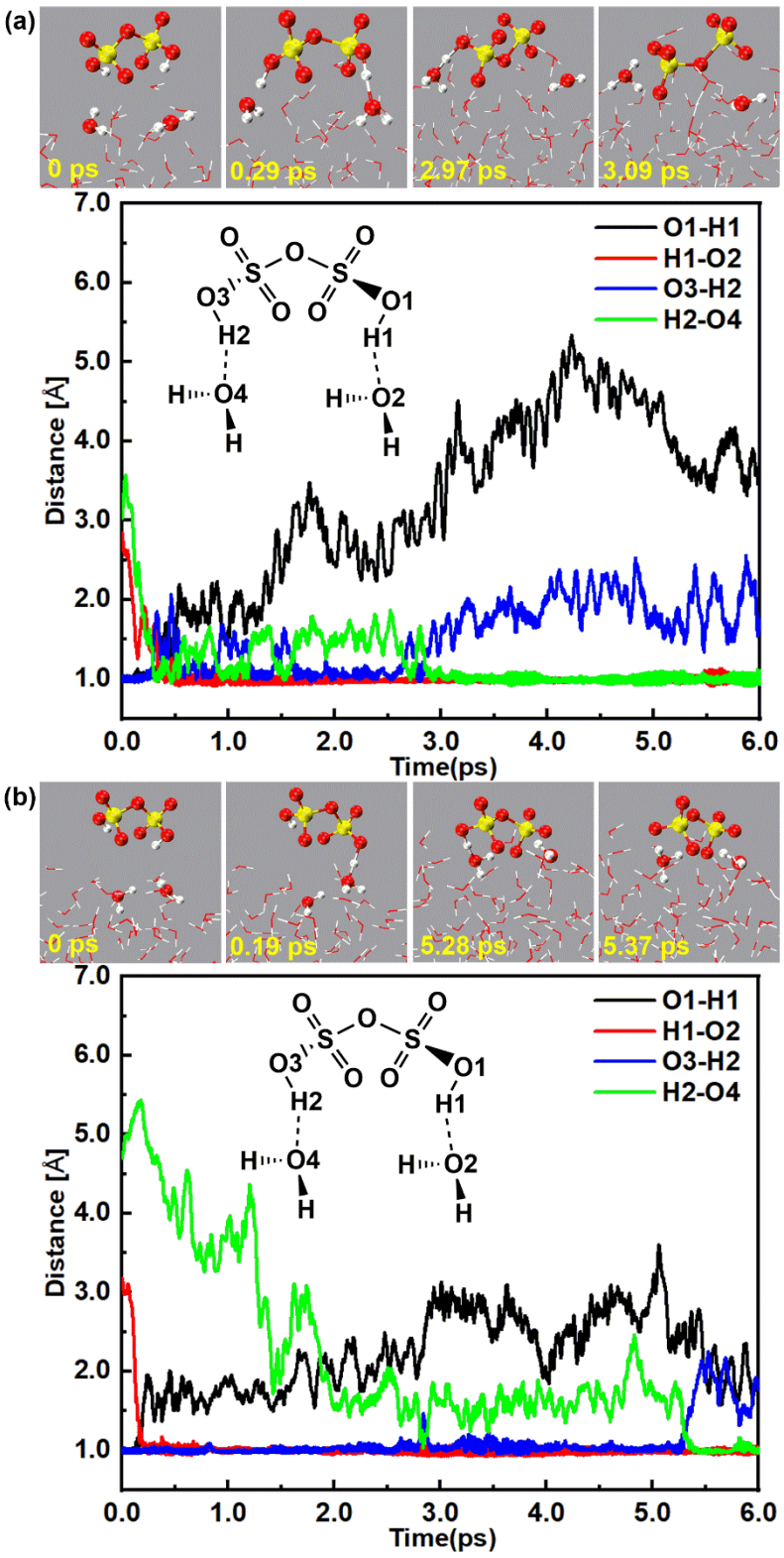

Fig. S6 Two BOMD trajectories and snapshots for the deprotonation of $H_2S_2O_7$ at the air water interface (Top panel: Snapshot structures taken from the BOMD simulations, which illustrate the deprotonation of $H_2S_2O_7$ at the air water interface. Lower panel: time evolution of key bond distances (O1-H1, H1-O2, O3-H2 and H2-O4) involved in the hydration mechanism.)

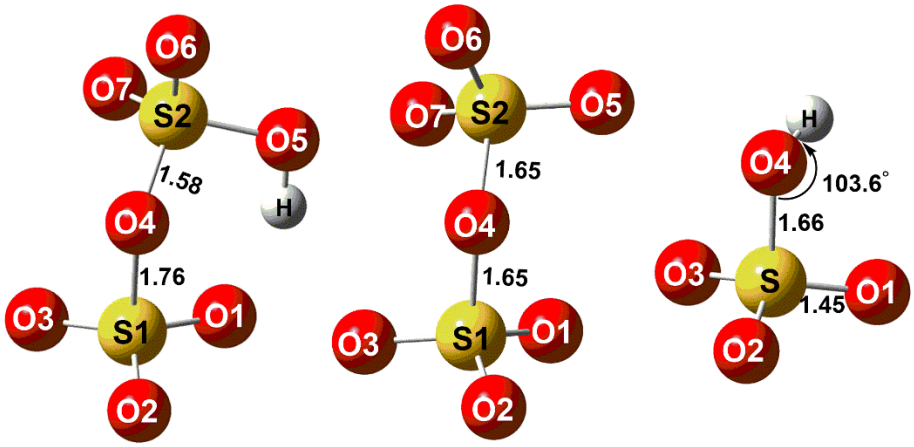

Fig. S7 The optimized geometrical structures of $HS_2O_7^-$, $S_2O_7^{2-}$ and HSO_4^- ion at M06-2X/6-311++G(2*df*,2*pd*) level of theory

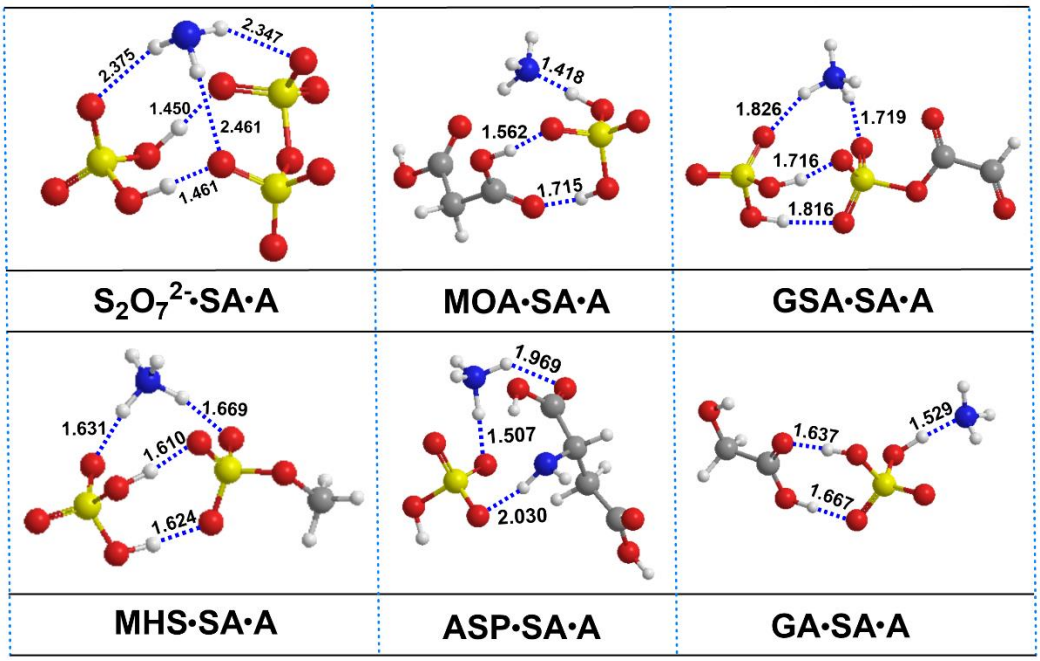

Fig. S8 The most stable configurations of the $(SA)_1(A)_1(Acid)_1$ clusters identified at the M06-2X/6-311++G (2*df*,2*pd*) level of theory. SA^-, SA, A, MOA, GSA, MHS, ASP and GA are respectively $HS_2O_4^-$, H_2SO_4, NH_3, $HOOCCH_2COOH$, $HOCCOOSO_3H$, CH_3OSO_3H, $HOOCC(H)NH_2COOH$ and $HOCH_2COOH$.The lengths of hydrogen bonds are given in Å. (blue = nitrogen, yellow = sulfur, red = oxygen, gray = carbon, and white = hydrogen.)

Table S7 Gibbs free energy (ΔG, kcal·mol^{-1}), equilibrium constant (K_{eq}, cm^3·molecule^{-1}) and the concentrations of SA, SO_3 and DSA computed at the CCSD(T)-F12/cc-pVDZ-F12//M06-2X/6-311++G(2*df*,2*pd*) level of theory

ΔG	T (K)	K_{eq}	[SA]/(molecules·cm^{-3})	[SO_3]/(molecules·cm^{-3})	[DSA]/(molecules·cm^{-3})
	218.15	6.79×10^{-10}			6.79×10^{3}
	238.15	1.55×10^{-11}			6.06×10^{2}
-7.0	258.15	6.44×10^{-13}	(1.00×10^{8})[a]	(1.00×10^{5})[b]	2.51×10^{1}
	278.18	4.25×10^{-14}			1.66×10^{0}
	298.15	4.07×10^{-15}			1.59×10^{-1}

[a] The values were taken from reference (Liu, J., Fang, S., Wang, Z., Yi, W., Tao, F.-M., and Liu, J.-y.: Hydrolysis of sulfur dioxide in small clusters of sulfuric acid: Mechanistic and kinetic study, Environ. Sci. Technol., 49, 13112-13120, 2015.)

[b] The values were taken from reference (Yao, L., Fan, X., Yan, C., Kurtén, T., Daellenbach, K. R., Li, C., Wang, Y., Guo, Y., Dada, L., Rissanen, M. P., Cai, J., Tham, Y. J., Zha, Q., Zhang, S., Du, W., Yu, M., Zheng, F., Zhou, Y., Kontkanen, J., Chan, T., Shen, J., Kujansuu, J. T., Kangasluoma, J., Jiang, J., Wang, L., Worsnop, D. R., Petäjä, T., Kerminen, V. M., Liu, Y., Chu, B., He, H., Kulmala, M., and Bianchi, F.: Unprecedented ambient sulfur trioxide (SO_3) detection: Possible formation mechanism and atmospheric implications, Environ. Sci. Technol. Lett., 7, 809-818, 10.1021/acs.estlett.0c00615, 2020.)

The equilibrium constant of $H_2S_2O_7$ within the temperature range of 218.15 - 298.15 K was 6.79×10^{-10} - 4.07×10^{-15} cm^3·molecule^{-1}. Taking into account typical tropospheric concentration of H_2SO_4 (1.00×10^{8} molecules·cm^{-3}) and SO_3 (1.00×10^{5} molecules·cm^{-3}), it is estimated that the atmospheric concentration of the $H_2S_2O_7$ is $1.59 \times 10^{-1} \times 10^{1}$-$6.79 \times 10^{3}$ molecules·cm^{-3} within the temperature range of 218.15 - 298.15 K.

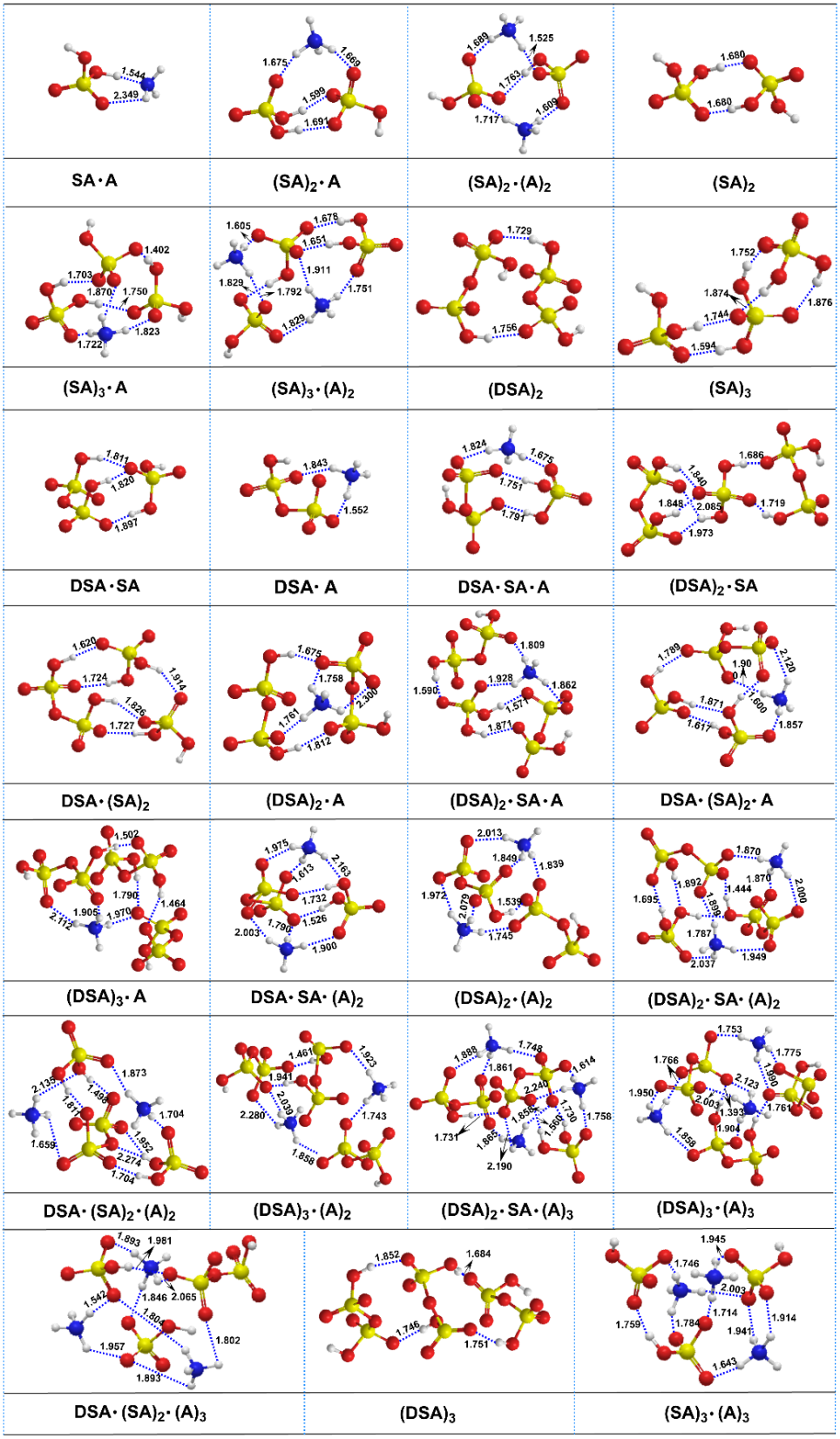

Fig. S9 The most stable configurations of the DSA-SA-A-based clusters identified at the M06-2X/6-311++G(2*df*,2*pd*) level of theory. DSA, SA, A are the shorthand for disulfuric acid, sulfuric acid and ammonia, respectively. The lengths of hydrogen bonds are given in Å. (blue = nitrogen, yellow = sulfur, red = oxygen, gray = carbon, and white = hydrogen.)

Table S8 The Gibbs free energy ΔG (kcal·mol$^{-1)}$ of formation of all clusters at pressure of 1 atm and the temperature range of 218.15-298.15 K, calculated at DLPNO-CCSD(T)/aug-cc-pVTZ//M06-2X/6-311++G(2*df*,2*pd*) level of theory

Clusters	T = 298.15 K	T = 278.15 K	T = 258.15 K	T = 238.15 K	T = 218.15 K
$(DSA)_2$	-5.0	-5.8	-6.7	-7.5	-8.4
$(DSA)_3$	-4.6	-6.2	-7.9	-9.6	-11.3
$(SA)_1{\cdot}(DSA)_1$	-4.7	-5.5	-6.3	-7.2	-8.0
$(SA)_1{\cdot}(DSA)_2$	-8.8	-10.4	-12.1	-13.7	-16.0
$(SA)_2{\cdot}(DSA)_1$	-6.8	-8.6	-10.4	-12.2	-14.0
$(DSA)_1{\cdot}(A)_1$	-15.3	-16.1	-16.9	-17.6	-18.4
$(DSA)_2{\cdot}(A)_1$	-24.8	-26.4	-28.0	-29.7	-31.3
$(DSA)_3{\cdot}(A)_1$	-32.3	-34.8	-37.4	-40.0	-42.5
$(DSA)_2{\cdot}(A)_2$	-41.9	-44.3	-46.7	-49.1	-51.5
$(SA)_1{\cdot}(DSA)_1{\cdot}(A)_1$	-25.9	-27.4	-29.0	-30.5	-32.0
$(SA)_1{\cdot}(DSA)_2{\cdot}(A)_1$	-32.8	-35.3	-37.8	-40.3	-43.3
$(SA)_2{\cdot}(DSA)_1{\cdot}(A)_1$	-31.9	-34.2	-36.6	-38.9	-41.3
$(SA)_1{\cdot}(DSA)_1{\cdot}(A)_2$	-37.9	-40.3	-42.8	-45.2	-47.7
$(SA)_1{\cdot}(DSA)_2{\cdot}(A)_2$	-49.1	-52.4	-55.7	-59.0	-62.3
$(SA)_2{\cdot}(DSA)_1{\cdot}(A)_2$	-48.4	-51.7	-55.0	-58.3	-61.6
$(SA)_2{\cdot}(DSA)_1{\cdot}(A)_3$	-61.3	-65.2	-69.1	-73.0	-77.0
$(SA)_1{\cdot}(DSA)_2{\cdot}(A)_3$	-73.9	-77.9	-81.8	-85.8	-89.8
$(DSA)_3{\cdot}(A)_3$	-69.5	-73.6	-77.6	-81.7	-85.8
$(DSA)_3{\cdot}(A)_2$	-51.6	-54.8	-58.1	-61.4	-64.7
$(SA)_2$	-7.8 (-8.4)	-8.6 (-9.1)	-9.1 (-9.8)	-9.8 (-10.5)	-10.5 (-11.1)
$(SA)_3$	-12.5 (-13.9)	-14.0 (-15.5)	-15.7 (-17.0)	-17.1 (-18.5)	-18.7 (-20.1)
$(SA)_1{\cdot}(A)_1$	-5.7 (-7.3)	-6.3 (-7.9)	-7.0 (-8.5)	-7.6 (-9.2)	-8.3 (-9.8)
$(SA)_2{\cdot}(A)_1$	-20.5 (-20.8)	-22.0 (-22.4)	-23.5 (-24.0)	-25.1 (-25.5)	-26.6 (-27.1)
$(SA)_2{\cdot}(A)_2$	-26.6 (-26.6)	-28.9 (-28.8)	-31.1 (-31.0)	-33.4 (-33.28)	-35.6 (-35.5)
$(SA)_3{\cdot}(A)_1$	-27.4 (-30.2)	-29.8 (-32.5)	-32.2 (-34.8)	-34.6 (-37.1)	-37.2 (-39.5)
$(SA)_3{\cdot}(A)_2$	-40.5 (-41.8)	-43.6 (-44.9)	-46.7 (-47.9)	-49.8 (-51.0)	-52.9 (-54.1)
$(SA)_3{\cdot}(A)_3$	-51.2 (-52.8)	-55.0 (-56.6)	-58.9 (-60.5)	-62.8 (-64.3)	-66.7 (-68.1)

The values in parentheses were taken from (Zhang, H., Kupiainen-Määttä, O., Zhang, X., Molinero, V., Zhang, Y., and Li, Z.: The enhancement mechanism of glycolic acid on the formation of atmospheric sulfuric acid–ammonia molecular clusters, J. Chem. Phys., 146, 184308, 10.1063/1.4982929, 2017.)

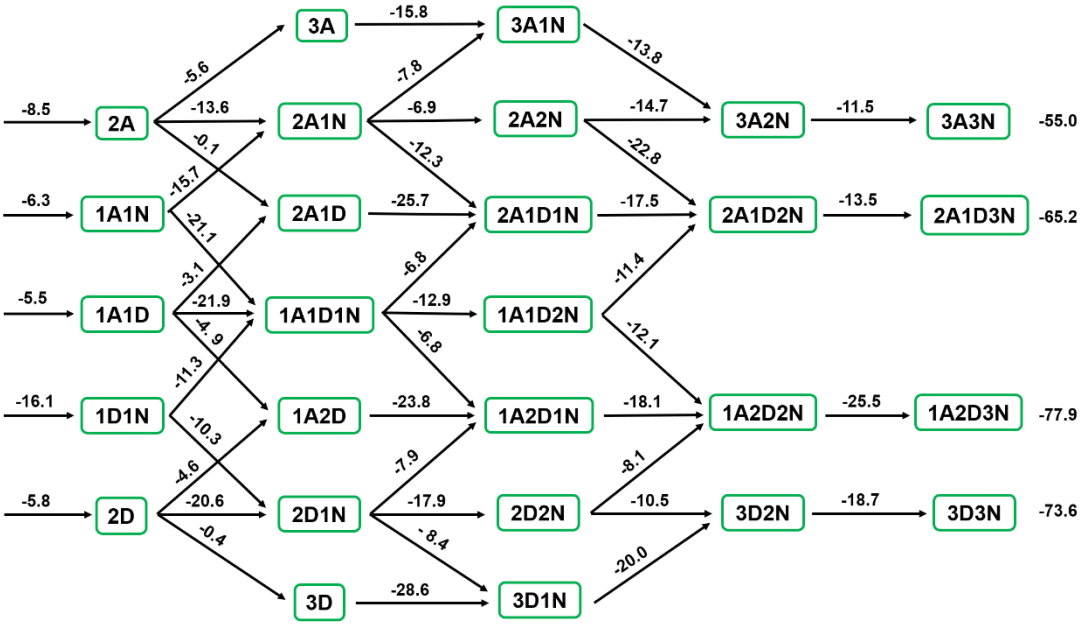

Fig. S10 The Gibbs free energy (kcal·mol^{-1}) diagram of $(DSA)_x(SA)_y(A)_z$ ($z \leq x + y \leq 3$) clusters at 278.15K and 1 atm. "A" refers to sulfuric acid, "D" refers to disulfuric acid and "N" refers to ammonia

Part 4 Collision coefficients and evaporation coefficients

The collision rate coefficient $\beta_{i,j}$ between clusters i and j was calculated using hard-sphere collision theory (Chapman and Cowling, 1990) in Eq. (S5).

$$\beta_{i,j} = \pi(r_i + r_j)^2 \sqrt{\frac{8k_B T}{\pi\mu}} \quad \text{(S5)}$$

Where r_i is the radius of cluster i, defined as the sum of distance between the two farthest atom in cluster i and half of the van der Waals radii of these two atoms and given by Multiwfn_3.7 software (Lu and Chen, 2012); k_B is the Boltzmann constant; T is the temperature and $\mu = m_i \cdot m_j/(mi + mj)$ is the reduced mass.

The evaporation coefficient $\gamma_{(i+j)\to i}$ was computed using the corresponding collision coefficients and the Gibbs free energies of formation of the clusters as show in Eq. (S6).

$$\gamma_{(i+j)\to i} = \beta_{i,j} \frac{p_{ref}}{k_B T} \exp\left(\frac{\Delta G_{i+j} - \Delta G_i - \Delta G_j}{k_B T}\right) \quad \text{(S6)}$$

Where p_{ref} is the reference pressure (1 atm in current study) at which the Gibbs free energies have been calculated, and ΔG_{i+j} is the Gibbs free energy of formation of cluster $i+j$ from monomers i and j.

Reference

Chapman, S., and Cowling, T. G.: The mathematical theory of non-uniform gases: an account of the kinetic theory of viscosity, thermal conduction and diffusion in gases, Cambridge university press, 1990.

Lu, T., and Chen, F.: Multiwfn: A multifunctional wavefunction analyzer, J. Comput. Chem., 33, 580-592, https://doi.org/10.1002/jcc.22885, 2012.

Part 5 Boundary conditions and concentration range

The maximum number of acid or basic molecules in the studied system is three. Whether a cluster is allowed to leave the size range under study depends on the boundary conditions. The boundary conditions in the ACDC require that the smallest clusters outside of the simulated system should be very stable so that not to evaporate back immediately (McGrath et al., 2012). Only clusters allowed to grow out of the studied system can be considered to contribute to the clusters' formation rate. For the atmospheric new particle formation (NPF), the stability of the corresponding cluster could be determined by comparing the collision rate and evaporation rate. The results from the studied clusters show that the collision rate coefficients are on the same order of magnitude (10^{-10}~10^{-11} molecules^{-1} cm^3 s^{-1}, shown in Table S9). Based on cluster volatilization rate (shown in Table S10) and the formation Gibbs free energy of the clusters (shown in Table S8), the cluster boundary conditions simulated in this study were set as $(SA)_4 \cdot (A)_3$ and $SA \cdot (A)_3 \cdot (DSA)_3$

According to field observations, the concentration of SA and A was respectively set in a range of $10^6 \sim 10^8$ molecules·cm^{-3} and $10^7 \sim 10^{11}$ molecules cm^{-3} (Almeida et al., 2013; Kuang et al., 2008; Bouo et al., 2011; Zhang et al., 2018). As the prediction in Table S7, the concentration of DSA is set to $10^1 \sim 10^3$ molecules cm^{-3}. Besides, the temperature was set to be 218.15~278.15 K, which span most regions of the troposphere and the polluted atmospheric boundary layer.

Reference

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Table S9 Collision coefficients (β, $cm^3 \cdot s^{-1}$) for each cluster in the present study

Collisions	β, $cm^3 \cdot s^{-1}$				
	298.15 K	278.15 K	258.15 K	238.15 K	218.15 K
SA + A	1.65×10^{-10}	1.54×10^{-10}	1.43×10^{-10}	1.32×10^{-10}	1.20×10^{-10}
SA + DSA	7.02×10^{-11}	6.55×10^{-11}	6.08×10^{-11}	5.61×10^{-11}	5.14×10^{-11}
DSA + A	2.15×10^{-10}	2.00×10^{-10}	1.86×10^{-10}	1.71×10^{-10}	1.57×10^{-10}
SA + SA	6.81×10^{-11}	6.35×10^{-11}	5.90×10^{-11}	5.44×10^{-11}	4.98×10^{-11}
DSA + DSA	6.40×10^{-11}	5.97×10^{-11}	5.54×10^{-11}	5.11×10^{-11}	4.68×10^{-11}
$(SA)_2$ + A	3.03×10^{-10}	2.83×10^{-10}	2.62×10^{-10}	2.42×10^{-10}	2.22×10^{-10}
SA·A + SA	8.90×10^{-11}	8.31×10^{-11}	7.71×10^{-11}	7.11×10^{-11}	6.51×10^{-11}
$(SA)_2$·A + A	2.81×10^{-10}	2.62×10^{-10}	2.43×10^{-10}	2.25×10^{-10}	2.06×10^{-10}
$(DSA)_2$ + A	3.25×10^{-10}	3.03×10^{-10}	2.81×10^{-10}	2.59×10^{-10}	2.38×10^{-10}
DSA·A + DSA	6.95×10^{-11}	6.48×10^{-11}	6.01×10^{-11}	5.55×10^{-11}	5.08×10^{-11}
$(DSA)_2$·A + A	3.37×10^{-10}	3.15×10^{-10}	2.92×10^{-10}	2.70×10^{-10}	2.47×10^{-10}
$(SA)_2$ + DSA	8.05×10^{-11}	7.51×10^{-11}	6.97×10^{-11}	6.43×10^{-11}	5.89×10^{-11}
SA·DSA + SA	8.62×10^{-11}	8.04×10^{-11}	7.46×10^{-11}	6.89×10^{-11}	6.31×10^{-11}
$(DSA)_2$ + SA	8.65×10^{-11}	8.07×10^{-11}	7.49×10^{-11}	6.91×10^{-11}	6.33×10^{-11}
SA·DSA + DSA	7.13×10^{-11}	6.65×10^{-11}	6.17×10^{-11}	5.69×10^{-11}	5.21×10^{-11}
$(SA)_2$ + SA	9.26×10^{-11}	8.64×10^{-11}	8.02×10^{-11}	7.40×10^{-11}	6.77×10^{-11}
$(DSA)_2$ + DSA	6.88×10^{-11}	6.42×10^{-11}	5.96×10^{-11}	5.50×10^{-11}	5.04×10^{-11}
SA + $(SA)_2$·A	8.48×10^{-11}	7.91×10^{-11}	7.34×10^{-11}	6.78×10^{-11}	6.21×10^{-11}
$(SA)_3$ + A	3.93×10^{-10}	3.67×10^{-10}	3.41×10^{-10}	3.14×10^{-10}	2.88×10^{-10}
$(SA)_2$·$(A)_2$ + SA	9.26×10^{-11}	8.64×10^{-11}	8.02×10^{-11}	7.40×10^{-11}	6.78×10^{-11}
$(SA)_3$·A + A	3.13×10^{-10}	2.92×10^{-10}	2.71×10^{-10}	2.50×10^{-10}	2.29×10^{-10}
$(SA)_3$·$(A)_2$ + A	4.08×10^{-10}	3.80×10^{-10}	3.53×10^{-10}	3.26×10^{-10}	2.98×10^{-10}
$(DSA)_2$·A + DSA	7.00×10^{-11}	6.53×10^{-11}	6.06×10^{-11}	5.59×10^{-11}	5.12×10^{-11}
$(DSA)_3$ + A	4.90×10^{-10}	4.57×10^{-10}	4.24×10^{-10}	3.91×10^{-10}	3.58×10^{-10}
$(DSA)_2$·$(A)_2$ + DSA	7.76×10^{-11}	7.24×10^{-11}	6.72×10^{-11}	6.20×10^{-11}	5.68×10^{-11}
$(DSA)_3$·A + A	4.17×10^{-10}	3.89×10^{-10}	3.61×10^{-10}	3.33×10^{-10}	3.05×10^{-10}
$(DSA)_3$·$(A)_2$ + A	4.78×10^{-10}	4.46×10^{-10}	4.14×10^{-10}	3.82×10^{-10}	3.50×10^{-10}
DSA·A + SA	7.85×10^{-11}	7.32×10^{-11}	6.79×10^{-11}	6.27×10^{-11}	5.74×10^{-11}
SA·A + DSA	8.60×10^{-11}	8.02×10^{-11}	7.44×10^{-11}	6.87×10^{-11}	6.29×10^{-11}
SA·DSA + A	3.06×10^{-10}	2.86×10^{-10}	2.65×10^{-10}	2.45×10^{-10}	2.24×10^{-10}
SA·DSA·A + A	3.03×10^{-10}	2.83×10^{-10}	2.62×10^{-10}	2.42×10^{-10}	2.22×10^{-10}
SA·DSA·A + SA	8.43×10^{-11}	7.87×10^{-11}	7.30×10^{-11}	6.74×10^{-11}	6.17×10^{-11}

$(SA)_2 \cdot A + DSA$	7.33×10^{-11}	6.84×10^{-11}	6.35×10^{-11}	5.86×10^{-11}	5.36×10^{-11}
$(SA)_2 \cdot DSA + A$	3.80×10^{-10}	3.54×10^{-10}	3.29×10^{-10}	3.03×10^{-10}	2.78×10^{-10}
$SA \cdot DSA \cdot (A)_2 + SA$	8.09×10^{-11}	7.55×10^{-11}	7.00×10^{-11}	6.46×10^{-11}	5.92×10^{-11}
$(SA)_2 \cdot (A)_2 + DSA$	7.83×10^{-11}	7.30×10^{-11}	6.78×10^{-11}	6.25×10^{-11}	5.73×10^{-11}
$(SA)_2 \cdot DSA \cdot A + A$	3.25×10^{-10}	3.03×10^{-10}	2.82×10^{-10}	2.60×10^{-10}	2.38×10^{-10}
$(SA)_2 \cdot DSA \cdot (A)_2 + A$	4.22×10^{-10}	3.93×10^{-10}	3.65×10^{-10}	3.37×10^{-10}	3.08×10^{-10}
$(DSA)_2 \cdot A + SA$	8.88×10^{-11}	8.28×10^{-11}	7.69×10^{-11}	7.09×10^{-11}	6.49×10^{-11}
$SA \cdot DSA \cdot A + DSA$	6.92×10^{-11}	6.46×10^{-11}	5.99×10^{-11}	5.53×10^{-11}	5.06×10^{-11}
$SA \cdot (DSA)_2 + A$	3.31×10^{-10}	3.08×10^{-10}	2.86×10^{-10}	2.64×10^{-10}	2.42×10^{-10}
$(DSA)_2 \cdot (A)_2 + SA$	1.00×10^{-10}	9.34×10^{-11}	8.67×10^{-11}	8.00×10^{-11}	7.33×10^{-11}
$SA \cdot DSA \cdot (A)_2 + DSA$	6.61×10^{-11}	6.17×10^{-11}	5.72×10^{-11}	5.28×10^{-11}	4.84×10^{-11}
$SA \cdot (DSA)_2 \cdot A + A$	4.19×10^{-10}	3.91×10^{-10}	3.63×10^{-10}	3.35×10^{-10}	3.06×10^{-10}
$SA \cdot (DSA)_2 \cdot (A)_2 + A$	3.84×10^{-10}	3.58×10^{-10}	3.32×10^{-10}	3.06×10^{-10}	2.81×10^{-10}

Table S10 Evaporation rates (s^{-1}) of the studied clusters at different temperatures of 298.15, 278.15, 258.15, 238.15 and 218.15 K

Evaporation pathways	298.15 K	278.15 K	258.15 K	238.15 K	218.15 K
$(SA)_2 \rightarrow SA + SA$	3.36×10^{3} (2.89×10^{3})	3.81×10^{2} (3.14×10^{2})	3.07×10^{1} (2.46×10^{1})	1.61×10^{0} (1.23×10^{0})	4.91×10^{-2} (3.51×10^{-2})
$(SA)_3 \rightarrow (SA)_2 + SA$	7.99×10^{5} (1.22×10^{6})	9.55×10^{4} (1.34×10^{5})	8.20×10^{3} (1.05×10^{4})	4.64×10^{2} (5.40×10^{2})	1.54×10^{1} (1.58×10^{1})
$(SA)_1\cdot(A)_1 \rightarrow SA + A$	2.67×10^{5} (4.76×10^{4})	4.19×10^{4} (6.70×10^{3})	4.92×10^{3} (7.09×10^{2})	4.03×10^{2} (5.01×10^{1})	2.08×10^{1} (2.17×10^{0})
$(SA)_2\cdot(A)_1 \rightarrow (SA)_1\cdot(A)_1 + SA$	3.32×10^{-2} (1.48×10^{0})	1.08×10^{-3} (5.23×10^{-2})	2.07×10^{-5} (1.12×10^{-3})	2.05×10^{-7} (3.33×10^{-4})	8.64×10^{-10} (6.20×10^{-8})
$(SA)_2\cdot(A)_1 \rightarrow A + (SA)_2$	3.72×10^{0} (1.60×10^{1})	1.68×10^{-1} (7.31×10^{-1})	4.69×10^{-3} (2.11×10^{-2})	7.20×10^{-5} (1.25×10^{-5})	5.16×10^{-7} (2.51×10^{-6})
$(SA)_3\cdot(A)_1 \rightarrow (SA)_2\cdot(A)_1 + SA$	1.63×10^{4} (1.85×10^{3})	1.53×10^{3} (1.56×10^{2})	9.93×10^{1} (8.72×10^{0})	4.02×10^{0} (3.00×10^{-1})	4.95×10^{-2} (5.39×10^{-3})
$(SA)_3\cdot(A)_1 \rightarrow A + (SA)_3$	1.07×10^{-1} (3.12×10^{-2})	3.81×10^{-3} (1.09×10^{-3})	8.04×10^{-5} (2.25×10^{-5})	8.84×10^{-7} (2.37×10^{-7})	2.34×10^{-9} (1.19×10^{-9})
$(SA)_2\cdot(A)_2 \rightarrow (SA)_2\cdot(A)_1 + A$	2.02×10^{5} (1.37×10^{6})	2.71×10^{4} (2.07×10^{5})	2.65×10^{3} (2.32×10^{4})	1.75×10^{2} (1.80×10^{3})	7.05×10^{0} (8.49×10^{1})
$(SA)_3\cdot(A)_2 \rightarrow (SA)_2\cdot(A)_2 + SA$	1.61×10^{-1} (9.75×10^{-2})	6.34×10^{-3} (3.53×10^{-3})	1.51×10^{-4} (7.48×10^{-5})	1.90×10^{-6} (8.44×10^{-7})	1.06×10^{-8} (4.16×10^{-9})
$(SA)_3\cdot(A)_2 \rightarrow (SA)_3\cdot(A)_1 + A$	2.04×10^{0} (7.26×10^{1})	1.14×10^{-1} (4.73×10^{0})	4.10×10^{-3} (2.02×10^{-1})	8.43×10^{-5} (5.11×10^{-3})	1.55×10^{-6} (6.61×10^{-5})
$(SA)_3\cdot(A)_3 \rightarrow (SA)_3\cdot(A)_2 + A$	1.49×10^{2}	9.81×10^{0}	4.22×10^{-1}	1.07×10^{-2}	1.36×10^{-4} (2.93×10^{-4})
$(SA)_1\cdot(DSA)_1 \rightarrow SA + DSA$	6.68×10^{5}	8.27×10^{4}	7.35×10^{3}	4.32×10^{2}	1.50×10^{1}
$(SA)_2\cdot(DSA)_1 \rightarrow (SA)_1\cdot(DSA)_1 + SA$	5.71×10^{7}	8.04×10^{6}	8.34×10^{5}	5.91×10^{4}	2.57×10^{3}
$(SA)_2\cdot(DSA)_1 \rightarrow DSA + (SA)_2$	1.03×10^{10}	1.58×10^{9}	1.81×10^{8}	1.43×10^{7}	7.11×10^{5}
$(DSA)_1\cdot(A)_1 \rightarrow DSA + A$	2.96×10^{-2}	1.17×10^{-3}	2.82×10^{-5}	3.64×10^{-7}	2.13×10^{-9}
$(SA)_1\cdot(DSA)_1\cdot(A)_1 \rightarrow SA + (DSA)_1\cdot(A)_1$	3.67×10^{1}	2.48×10^{0}	1.10×10^{-1}	2.85×10^{-3}	3.77×10^{-5}
$(SA)_1\cdot(DSA)_1\cdot(A)_1 \rightarrow A + (SA)_1\cdot(DSA)_1$	2.08×10^{-6}	4.49×10^{-8}	5.37×10^{-10}	3.07×10^{-12}	6.83×10^{-15}
$(SA)_1\cdot(DSA)_1\cdot(A)_1 \rightarrow DSA + (SA)_1\cdot(A)_1$	3.41×10^{-6}	5.83×10^{-8}	5.28×10^{-10}	2.17×10^{-12}	3.23×10^{-15}
$(SA)_2\cdot(DSA)_1\cdot(A)_1 \rightarrow A + (SA)_2\cdot(DSA)_1$	3.61×10^{-9}	6.26×10^{-11}	5.77×10^{-13}	2.42×10^{-15}	3.70×10^{-18}
$(SA)_2\cdot(DSA)_1\cdot(A)_1 \rightarrow DSA + (SA)_2\cdot(A)_1$	7.26×10^{0}	4.28×10^{-1}	1.62×10^{-2}	3.49×10^{-4}	3.71×10^{-6}
$(SA)_1\cdot(DSA)_1\cdot(A)_2 \rightarrow A + (SA)_1\cdot(DSA)_1\cdot(A)_1$	1.18×10^{1}	5.29×10^{-1}	1.47×10^{-2}	2.25×10^{-4}	1.60×10^{-6}
$(SA)_2\cdot(DSA)_1\cdot(A)_2 \rightarrow SA + (SA)_1\cdot(DSA)_1\cdot(A)_2$	3.89×10^{1}	2.29×10^{0}	8.64×10^{-2}	1.87×10^{-3}	1.99×10^{-5}
$(SA)_2\cdot(DSA)_1\cdot(A)_2 \rightarrow A + (SA)_2\cdot(DSA)_1\cdot(A)_1$	6.55×10^{-3}	1.54×10^{-4}	2.02×10^{-6}	1.28×10^{-8}	3.24×10^{-11}
$(SA)_2\cdot(DSA)_1\cdot(A)_2 \rightarrow DSA + (SA)_2\cdot(A)_2$	2.17×10^{-7}	2.25×10^{-9}	1.14×10^{-11}	2.36×10^{-14}	1.57×10^{-17}
$(SA)_2\cdot(DSA)_1\cdot(A)_3 \rightarrow A + (SA)_2\cdot(DSA)_1\cdot(A)_2$	3.08×10^{0}	2.14×10^{-1}	9.81×10^{-3}	2.68×10^{-4}	3.78×10^{-6}
$(DSA)_2 \rightarrow DSA + DSA$	3.56×10^{5}	4.18×10^{4}	3.50×10^{3}	1.93×10^{2}	6.20×10^{0}
$(SA)_1\cdot(DSA)_2 \rightarrow SA + (DSA)_2$	$3.3. \times 10^{6}$	5.05×10^{5}	5.72×10^{4}	4.46×10^{3}	5.62×10^{1}

$(SA)_1 \cdot (DSA)_2 \rightarrow DSA + (SA)_1 \cdot (DSA)_1$	1.59×10^{6}	2.31×10^{5}	2.46×10^{4}	1.80×10^{3}	2.10×10^{1}
$(DSA)_2 \cdot (A)_1 \rightarrow A + (DSA)_2$	2.52×10^{-5}	5.47×10^{-7}	6.55×10^{-9}	3.73×10^{-11}	8.24×10^{-14}
$(DSA)_2 \cdot (A)_1 \rightarrow DSA + (DSA)_1 \cdot (A)_1$	2.18×10^{2}	1.40×10^{1}	5.83×10^{-1}	1.41×10^{-2}	1.72×10^{-4}
$(SA)_1 \cdot (DSA)_2 \cdot (A)_1 \rightarrow SA + (DSA)_2 \cdot (A)_1$	2.70×10^{3}	2.24×10^{2}	1.26×10^{1}	4.32×10^{-1}	2.04×10^{-3}
$(SA)_1 \cdot (DSA)_2 \cdot (A)_1 \rightarrow A + (SA)_1 \cdot (DSA)_2$	3.09×10^{-8}	3.64×10^{-10}	2.16×10^{-12}	5.41×10^{-15}	4.47×10^{-18}
$(SA)_1 \cdot (DSA)_2 \cdot (A)_1 \rightarrow DSA + (SA)_1 \cdot (DSA)_1 \cdot (A)_1$	1.41×10^{4}	1.11×10^{3}	5.89×10^{1}	1.89×10^{0}	8.19×10^{-3}
$(DSA)_2 \cdot (A)_2 \rightarrow A + (DSA)_2 \cdot (A)_1$	2.13×10^{-3}	6.68×10^{-5}	1.22×10^{-6}	1.15×10^{-8}	4.57×10^{-11}
$(SA)_1 \cdot (DSA)_2 \cdot (A)_2 \rightarrow SA + (DSA)_2 \cdot (A)_2$	1.51×10^{4}	1.25×10^{3}	7.09×10^{1}	2.45×10^{0}	4.58×10^{-2}
$(SA)_1 \cdot (DSA)_2 \cdot (A)_2 \rightarrow A + (SA)_1 \cdot (DSA)_2 \cdot (A)_1$	2.01×10^{-3}	6.02×10^{-5}	1.05×10^{-6}	9.21×10^{-9}	3.41×10^{-11}
$(SA)_1 \cdot (DSA)_2 \cdot (A)_2 \rightarrow DSA + (SA)_1 \cdot (DSA)_1 \cdot (A)_2$	1.17×10^{1}	6.51×10^{-1}	2.30×10^{-2}	4.60×10^{-4}	4.45×10^{-6}
$(SA)_1 \cdot (DSA)_2 \cdot (A)_3 \rightarrow A + (SA)_1 \cdot (DSA)_2 \cdot (A)_2$	5.72×10^{-9}	8.55×10^{-11}	6.65×10^{-13}	2.28×10^{-15}	2.76×10^{-18}
$(DSA)_3 \rightarrow (DSA)_2 + DSA$	3.48×10^{9}	8.08×10^{8}	1.49×10^{8}	2.05×10^{7}	1.94×10^{6}
$(DSA)_3 \cdot (A)_1 \rightarrow A + (DSA)_3$	3.97×10^{-11}	2.74×10^{-13}	8.73×10^{-16}	1.06×10^{-18}	3.78×10^{-22}
$(DSA)_3 \cdot (A)_1 \rightarrow DSA + (DSA)_2 \cdot (A)_1$	3.50×10^{3}	2.58×10^{2}	1.26×10^{1}	3.67×10^{-1}	5.59×10^{-3}
$(DSA)_3 \cdot (A)_2 \rightarrow A + (DSA)_3 \cdot (A)_1$	7.22×10^{-5}	1.94×10^{-6}	2.95×10^{-8}	2.22×10^{-10}	6.77×10^{-13}
$(DSA)_3 \cdot (A)_2 \rightarrow DSA + (DSA)_2 \cdot (A)_2$	1.78×10^{2}	1.16×10^{1}	4.90×10^{-1}	1.21×10^{-2}	1.49×10^{-4}
$(DSA)_3 \cdot (A)_3 \rightarrow A + (DSA)_3 \cdot (A)_2$	8.19×10^{-4}	2.23×10^{-5}	3.46×10^{-7}	2.67×10^{-9}	8.48×10^{-12}

*The values in parentheses were taken from (Liu, J., Liu, L., Rong, H., and Zhang, X.: The potential mechanism of atmospheric new particle formation involving amino acids with multiple functional groups, Phys. Chem. Chem. Phys., 23, 10184-10195, 10.1039/D0CP06472F, 2021.)

Table S11 Total evaporation coefficients ($\sum\gamma$, s^{-1}) for each cluster in the present study

Clusters	$\sum\gamma$, s^{-1}				
	298.15 K	278.15 K	258.15 K	238.15 K	218.15 K
SA·A	2.67×10^{5}	4.19×10^{4}	4.92×10^{3}	4.03×10^{2}	2.08×10^{1}
SA·DSA	6.68×10^{5}	8.27×10^{4}	7.35×10^{3}	4.32×10^{2}	1.50×10^{1}
A·DSA	2.96×10^{-2}	1.17×10^{-3}	2.82×10^{-5}	3.64×10^{-7}	2.13×10^{-9}
$(SA)_2$	3.36×10^{3}	3.81×10^{2}	3.07×10^{1}	1.61×10^{0}	4.91×10^{-2}
$(DSA)_2$	3.56×10^{5}	4.18×10^{4}	3.50×10^{3}	1.93×10^{2}	6.20×10^{0}
$(SA)_2$·A	$3.75E \times 10^{0}$	1.69×10^{-1}	4.71×10^{-3}	7.22×10^{-5}	5.17×10^{-7}
$(SA)_2$·$(A)_2$	2.02×10^{5}	2.71×10^{4}	2.65×10^{3}	1.75×10^{2}	7.05×10^{0}
A·$(DSA)_2$	2.18×10^{2}	1.40×10^{1}	5.83×10^{-1}	1.41×10^{-2}	1.72×10^{-4}
$(A)_2$·$(DSA)_2$	2.13×10^{-3}	6.68×10^{-5}	1.22×10^{-6}	1.15×10^{-8}	4.57×10^{-11}
$(SA)_2$·DSA	1.03×10^{10}	1.59×10^{9}	1.82×10^{8}	1.44×10^{7}	7.14×10^{5}
SA·$(DSA)_2$	4.90×10^{6}	7.36×10^{5}	8.18×10^{4}	6.26×10^{3}	7.72×10^{1}
$(SA)_3$	7.99×10^{5}	9.55×10^{4}	8.20×10^{3}	4.64×10^{2}	1.54×10^{1}
$(DSA)_3$	3.48×10^{9}	8.08×10^{8}	1.49×10^{8}	2.05×10^{7}	1.94×10^{6}
$(SA)_3$·A	1.63×10^{4}	1.53×10^{3}	9.93×10^{1}	4.02×10^{0}	4.95×10^{-2}
$(SA)_3$·$(A)_2$	2.20×10^{0}	1.21×10^{-1}	4.25×10^{-3}	8.62×10^{-5}	1.56×10^{-6}
$(SA)_3$·$(A)_3$	1.49×10^{2}	9.81×10^{0}	4.22×10^{-1}	1.07×10^{-2}	1.36×10^{-4}
A·$(DSA)_3$	3.50×10^{3}	2.58×10^{2}	1.26×10^{1}	3.67×10^{-1}	5.59×10^{-3}
$(A)_2$·$(DSA)_3$	1.45×10^{3}	9.80×10^{1}	4.28×10^{0}	1.08×10^{-1}	1.41×10^{-3}
$(A)_3$·$(DSA)_3$	2.70×10^{-3}	7.59×10^{-5}	1.22×10^{-6}	9.82×10^{-9}	3.24×10^{-11}
SA·A·DSA	3.67×10^{1}	2.48×10^{0}	1.10×10^{-1}	2.85×10^{-3}	3.77×10^{-5}
SA·$(A)_2$·DSA	1.18×10^{1}	5.29×10^{-1}	1.47×10^{-2}	2.25×10^{-4}	1.60×10^{-6}
SA_2·A·DSA	7.84×10^{4}	8.84×10^{3}	7.06×10^{2}	3.67×10^{1}	1.10×10^{0}
$(SA)_2$·$(A)_2$·DSA	3.89×10^{1}	2.29×10^{0}	8.64×10^{-2}	1.87×10^{-3}	1.99×10^{-5}
$(SA)_2$·$(A)_3$·DSA	4.23×10^{8}	1.27×10^{8}	3.16×10^{7}	6.14×10^{6}	8.75×10^{5}
SA·A·$(DSA)_2$	1.68×10^{4}	1.34×10^{3}	7.14×10^{1}	2.32×10^{0}	1.02×10^{-2}
SA·$(A)_2$·$(DSA)_2$	1.51×10^{4}	1.26×10^{3}	7.09×10^{1}	2.46×10^{0}	4.58×10^{-2}
SA·$(A)_3$·$(DSA)_2$	5.72×10^{-9}	8.55×10^{-11}	6.65×10^{-13}	2.28×10^{-15}	2.76×10^{-18}

Table S12 The generated enhancement strength R of DSA at the conditions of T = 218.15 K, [SA] = 10^6 - 10^8 molecules·cm^{-3}, [A] = 10^7 - 10^{11} molecules·cm^{-3}, and [DSA] = 10^1 - 10^3 molecules·cm^{-3}

[SA]	[A]	[DSA] = 10^1	[DSA] = 10^2	[DSA] = 10^3
[SA] = 10^6	[A] = 10^7	1.00×10^0	1.00×10^0	1.00×10^0
[SA] = 10^6	[A] = 10^8	1.00×10^0	1.00×10^0	1.00×10^0
[SA] = 10^6	[A] = 10^9	1.00×10^0	1.00×10^0	1.00×10^0
[SA] = 10^6	[A] = 10^{10}	1.00×10^0	1.00×10^0	1.16×10^0
[SA] = 10^6	[A] = 10^{11}	1.00×10^0	1.03×10^0	2.48×10^1
[SA] = 10^7	[A] = 10^7	1.00×10^0	1.00×10^0	1.00×10^0
[SA] = 10^7	[A] = 10^8	1.00×10^0	1.00×10^0	1.00×10^0
[SA] = 10^7	[A] = 10^9	1.00×10^0	1.00×10^0	1.00×10^0
[SA] = 10^7	[A] = 10^{10}	1.00×10^0	1.00×10^0	1.00×10^0
[SA] = 10^7	[A] = 10^{11}	1.00×10^0	1.01×10^0	1.01×10^0
[SA] = 10^8	[A] = 10^7	1.00×10^0	1.00×10^0	1.00×10^0
[SA] = 10^8	[A] = 10^8	1.00×10^0	1.00×10^0	1.00×10^0
[SA] = 10^8	[A] = 10^9	1.00×10^0	1.00×10^0	1.00×10^0
[SA] = 10^8	[A] = 10^{10}	1.00×10^0	1.00×10^0	1.00×10^0
[SA] = 10^8	[A] = 10^{11}	1.00×10^0	1.00×10^0	1.00×10^0

Table S13 The generated enhancement strength R of DSA at the conditions of T = 238.15 K, [SA] = 10^6-10^8 molecules·cm^{-3}, [A] = 10^7-10^{11} molecules·cm^{-3}, and [DSA] = 10^1-10^3 molecules·cm^{-3}

[SA]	[A]	[DSA] = 10^1	[DSA] = 10^2	[DSA] = 10^3
[SA] = 10^6	[A] = 10^7	1.00×10^0	1.00×10^0	1.03×10^0
[SA] = 10^6	[A] = 10^8	1.00×10^0	1.00×10^0	1.03×10^0
[SA] = 10^6	[A] = 10^9	1.00×10^0	1.00×10^0	1.07×10^0
[SA] = 10^6	[A] = 10^{10}	1.00×10^0	1.00×10^0	2.31×10^0
[SA] = 10^6	[A] = 10^{11}	1.00×10^0	1.26×10^0	1.91×10^2
[SA] = 10^7	[A] = 10^7	1.00×10^0	1.00×10^0	1.02×10^0
[SA] = 10^7	[A] = 10^8	1.00×10^0	1.00×10^0	1.02×10^0
[SA]=10^7	[A] = 10^9	1.00×10^0	1.00×10^0	1.02×10^0
[SA] = 10^7	[A] = 10^{10}	1.00×10^0	1.00×10^0	1.02×10^0
[SA] = 10^7	[A] = 10^{11}	1.00×10^0	1.00×10^0	1.17×10^0
[SA] = 10^8	[A] = 10^7	1.00×10^0	1.00×10^0	1.00×10^0
[SA] = 10^8	[A] = 10^8	1.00×10^0	1.00×10^0	1.00×10^0
[SA] = 10^8	[A] = 10^9	1.00×10^0	1.00×10^0	1.00×10^0
[SA] = 10^8	[A] = 10^{10}	1.00×10^0	1.00×10^0	1.00×10^0
[SA] = 10^8	[A] = 10^{11}	1.00×10^0	1.00×10^0	1.00×10^0

Table S14 The generated enhancement strength R of DSA at the conditions of T = 258.15 K, [SA] = 10^6-10^8 molecules·cm^{-3}, [A] = 10^7-10^{11} molecules·cm^{-3}, and [DSA] = 10^1-10^3 molecules·cm^{-3}.

[SA]	[A]	[DSA] = 10^1	[DSA] = 10^2	[DSA] = 10^3
[SA] = 10^6	[A] = 10^7	1.00×10^0	1.02×10^0	1.93×10^1
[SA] = 10^6	[A] = 10^8	1.00×10^0	1.02×10^0	2.12×10^1
[SA] = 10^6	[A] = 10^9	1.00×10^0	1.06×10^0	4.14×10^1
[SA] = 10^6	[A] = 10^{10}	1.00×10^0	1.33×10^0	2.75×10^2
[SA] = 10^6	[A] = 10^{11}	1.00×10^0	5.56×10^0	3.29×10^3
[SA] = 10^7	[A] = 10^7	1.00×10^0	1.00×10^0	1.03×10^0
[SA] = 10^7	[A] = 10^8	1.00×10^0	1.00×10^0	1.05×10^0
[SA] = 10^7	[A] = 10^9	1.00×10^0	1.02×10^0	1.18×10^0
[SA] = 10^7	[A] = 10^{10}	1.00×10^0	1.04×10^0	1.57×10^0
[SA] = 10^7	[A] = 10^{11}	1.00×10^0	1.05×10^0	3.84×10^0
[SA] = 10^8	[A] = 10^7	1.00×10^0	1.00×10^0	1.01×10^0
[SA] = 10^8	[A] = 10^8	1.00×10^0	1.00×10^0	1.01×10^0
[SA] = 10^8	[A] = 10^9	1.00×10^0	1.00×10^0	1.05×10^0
[SA] = 10^8	[A] = 10^{10}	1.00×10^0	1.01×10^0	1.06×10^0
[SA] = 10^8	[A] = 10^{11}	1.00×10^0	1.00×10^0	1.04×10^0

Table S15 The generated enhancement strength R of DSA at the conditions of T = 278.15 K, [SA] = 10^6 - 10^8 molecules·cm^{-3}, [A] = 10^7 - 10^{11} molecules·cm^{-3}, and [DSA] = 10^1 - 10^3 molecules·cm^{-3}.

[SA]	[A]	[DSA] = 10^1	[DSA] = 10^2	[DSA] = 10^3
[SA] = 10^6	[A] = 10^7	8.90×10^0	7.90×10^3	7.90×10^6
[SA] = 10^6	[A] = 10^8	8.90×10^0	7.91×10^3	7.90×10^6
[SA] = 10^6	[A] = 10^9	8.93×10^0	7.93×10^3	7.91×10^6
[SA] = 10^6	[A] = 10^{10}	9.18×10^0	8.16×10^3	7.96×10^6
[SA] = 10^6	[A] = 10^{11}	1.17×10^1	1.05×10^4	8.34×10^6
[SA] = 10^7	[A] = 10^7	1.01×10^0	6.92×10^0	5.92×10^3
[SA] = 10^7	[A] = 10^8	1.01×10^0	6.93×10^0	5.92×10^3
[SA] = 10^7	[A] = 10^9	1.01×10^0	6.95×10^0	5.93×10^3
[SA] = 10^7	[A] = 10^{10}	1.01×10^0	7.16×10^0	6.01×10^3
[SA] = 10^7	[A] = 10^{11}	1.01×10^0	9.34×10^0	6.59×10^3
[SA] = 10^8	[A] = 10^7	1.00×10^0	1.00×10^0	2.54×10^0
[SA] = 10^8	[A] = 10^8	1.00×10^0	1.00×10^0	2.54×10^0
[SA] = 10^8	[A] = 10^9	1.00×10^0	1.00×10^0	2.56×10^0
[SA] = 10^8	[A] = 10^{10}	1.00×10^0	1.01×10^0	2.70×10^0
[SA] = 10^8	[A] = 10^{11}	1.00×10^0	1.05×10^0	4.26×10^0

Table S16 The generated enhancement strength R of DSA at the conditions of T = 298.15 K, [SA] = 10^6 - 10^8 molecules·cm^{-3}, [A] = 10^7 - 10^{11} molecules·cm^{-3}, and [DSA] = 10^1 - 10^3 molecules·cm^{-3}.

[SA]	[A]	[DSA] = 10^1	[DSA] = 10^2	[DSA] = 10^3
[SA] = 10^6	[A] = 10^7	2.01×10^4	2.01×10^7	2.00×10^{10}
[SA] = 10^6	[A] = 10^8	2.01×10^4	2.01×10^7	2.01×10^{10}
[SA] = 10^6	[A] = 10^9	2.01×10^4	2.01×10^7	2.01×10^{10}
[SA] = 10^6	[A] = 10^{10}	2.01×10^4	2.01×10^7	2.01×10^{10}
[SA] = 10^6	[A] = 10^{11}	2.07×10^4	2.06×10^7	2.03×10^{10}
[SA] = 10^7	[A] = 10^7	1.65×10^1	1.55×10^4	1.55×10^7
[SA] = 10^7	[A] = 10^8	1.65×10^1	1.55×10^4	1.55×10^7
[SA] = 10^7	[A] = 10^9	1.65×10^1	1.55×10^4	1.55×10^7
[SA] = 10^7	[A] = 10^{10}	1.66×10^1	1.56×10^4	1.55×10^7
[SA] = 10^7	[A] = 10^{11}	1.70×10^1	1.59×10^4	1.57×10^7
[SA] = 10^8	[A] = 10^7	1.00×10^0	5.73×10^0	4.73×10^3
[SA] = 10^8	[A] = 10^8	1.00×10^0	5.73×10^0	4.73×10^3
[SA] = 10^8	[A] = 10^9	1.00×10^0	5.73×10^0	4.73×10^3
[SA] = 10^8	[A] = 10^{10}	1.00×10^0	5.74×10^0	4.73×10^3
[SA] = 10^8	[A] = 10^{11}	1.00×10^0	5.85×10^0	4.76×10^3

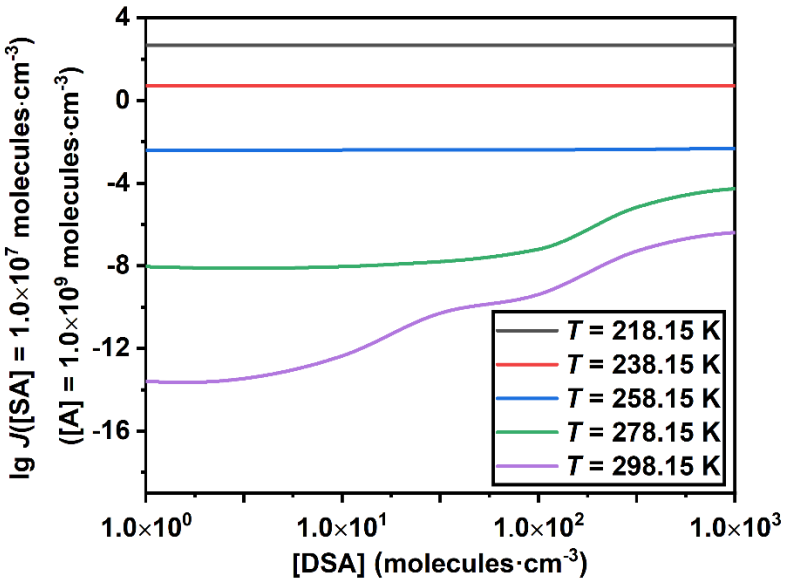

Fig. S11 The logarithms of the formation rate of DSA (lg *J*) as a function of [DSA] from 10^0 to 10^3 molecules·cm^{-3} under different temperatures (218.15, 238.15, 258.15, 278.15 and 298.15 K) where [SA] = 10^7 molecules·cm^{-3} and [A] = 10^9 molecules·cm^{-3}.

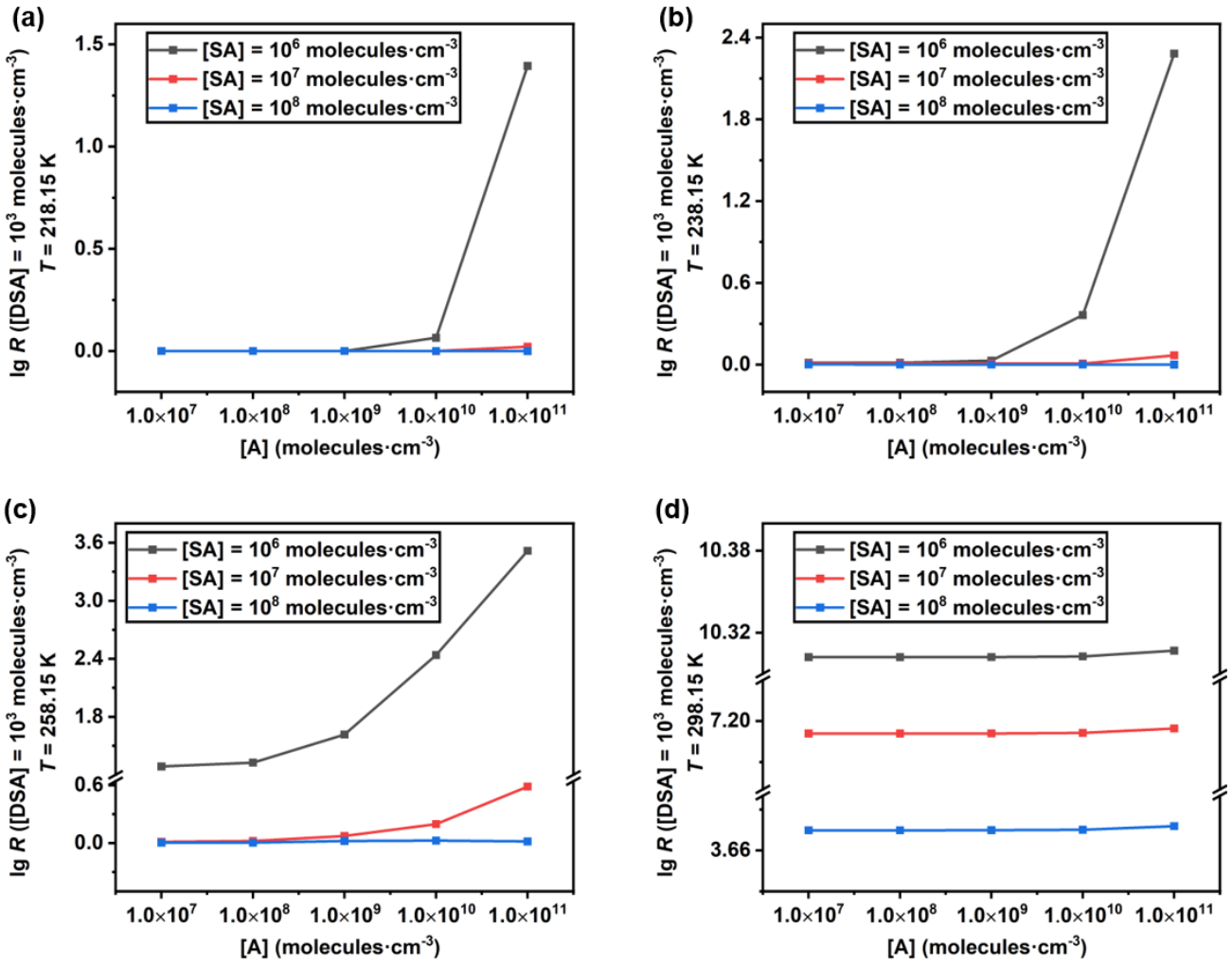

Fig. S12 The logarithms of the enhancement strength of DSA (lg *R*) as a function of [A] from 10^7 to 10^{11} molecules cm^{-3} and [DSA] = 10^3 molecules·cm^{-3} under different [SA] = 10^6 ~ 10^8 molecules·cm^{-3} *T* = (a) 218.15 K, (b) 238.15 K, (c) 258.15 K and (d) 298.15 K.

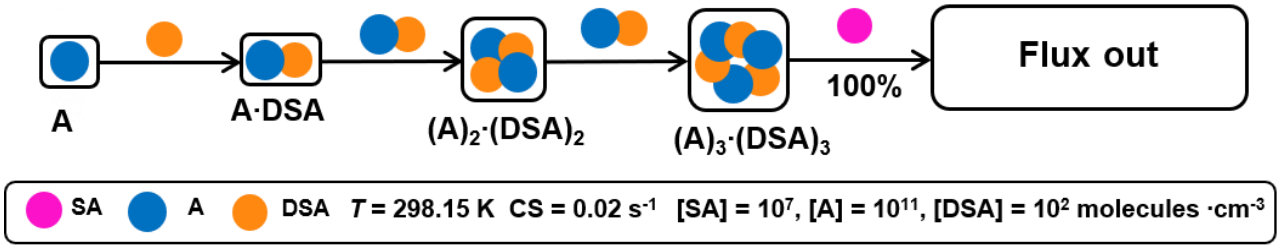

Fig. S13 The main pathways of clusters growing out of the research system under the conditions where T = 298.15 K, [SA] = 10^7 molecules·cm^{-3}, [A] = 10^{11} molecules·cm^{-3}, and [DSA] = 10^3 molecules·cm^{-3}.

Table S17. Cartesian coordinates of all molecules and clusters in the studied system.

SA:

Atoms	X	Y	Z
S	-0.00000100	-0.00000100	-0.15756700
O	0.67306500	0.67306500	-0.81983600
O	-0.67307500	-0.67307500	-0.81979800
O	1.01736800	1.01736800	0.84358200
O	-1.01735800	-1.01735800	0.84357500
H	1.70169100	1.70169100	1.07043800
H	-1.70167800	-1.70167800	1.07045700

A:

Atoms	X	Y	Z
N	0.00000000	0.11911400	0.00000000
H	-0.93235000	-0.27807200	0.00000000
H	0.46617500	-0.27786300	0.80753900
H	0.46617500	-0.27786300	-0.80753900

DSA:

Atoms	X	Y	Z
S	-1.43510900	-0.13598100	0.03492700
O	-2.38705700	-0.43102000	1.02932100
O	-1.24778700	-0.89230600	-1.14721200
O	-1.54051800	1.38764200	-0.28976900
S	1.38684600	0.12449200	0.06491400
O	1.11188700	1.05840000	-0.97277300
O	1.64540800	-1.25084900	-0.64070300
O	2.34997600	0.33819800	1.07741600
O	0.01087600	-0.15789900	0.86275800
H	-0.84560200	1.61939600	-0.93204600
H	2.07552800	-1.85290200	-0.01771400

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

Atoms	X	Y	Z
S	-0.59732600	-0.11330300	0.09028200
O	0.11386900	-0.09250800	1.33053100
O	-1.77725300	-0.88882800	-0.09102500
O	0.38323700	-0.42810500	-1.05987100
O	-0.97903500	1.41306500	-0.18279600
H	1.35885500	-0.23109000	-0.73760300
H	-1.72492000	1.42300400	-0.79399800
N	2.71575100	0.04051200	-0.05360200
H	3.15679600	0.92252300	-0.28222700

H	3.40929600	-0.69086300	-0.14794300
H	2.42039100	0.07670700	0.91776700

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

Atoms	X	Y	Z
S	-2.47894500	-0.27718400	-0.07642800
O	-1.96942000	-0.69986700	1.32142600
O	-3.71936500	-0.91541600	-0.30294600
O	-1.39496600	-0.39448700	-1.03015800
O	-2.68689900	1.27963100	0.02947600
H	0.13413900	-1.35148000	-1.27363600
H	-3.55012600	1.46532400	0.42365200
S	1.71348900	-1.27742400	0.10594200
O	2.93138800	-1.97706900	0.17828500
O	1.10381000	-1.47119600	-1.31475600
O	0.67953600	-1.42141800	1.07950900
S	1.13845700	1.55591000	0.08489700
O	0.10562700	1.27156800	1.02340900
O	0.55626500	1.50979600	-1.35863100
O	1.99771500	2.66524800	0.18881000
O	2.17216200	0.28353900	0.05759200
H	-0.99604700	-0.58635500	1.38700300
H	-0.27344600	0.98808800	-1.36114300

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

Atoms	X	Y	Z
N	0.13203900	-0.69865100	2.57081600
H	-0.09820600	0.24085300	2.88663600
H	0.94687800	-0.61472500	1.91851700
H	0.36650600	-1.29661600	3.35702000
S	-1.36558700	-1.43866900	-0.41236900
O	-1.93814100	-2.27300500	-1.40003200
O	-2.05721700	-1.34463300	0.88102700
O	0.07046500	-1.46827700	-0.22323000
S	-1.64689100	1.38540600	-0.13002500
O	-0.51624200	1.25992200	0.76902000
O	-2.95619100	1.18333900	0.69692800
O	-1.78524200	2.53966300	-0.92557400
O	-1.64573200	0.12543300	-1.08303700
H	-0.67833000	-1.06704400	2.04175900
H	-2.98291100	0.24564200	0.98396400
S	2.84196800	0.16905200	-0.13063300
O	4.17836600	0.57355300	-0.33440900
O	2.40700700	-0.23359000	1.19157800

O	2.54895000	-0.98628800	-1.13465400
O	1.88912300	1.31567200	-0.60376200
H	1.63256100	-1.30885000	-0.99865200
H	1.05622000	1.30436200	-0.08737600

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

Atoms	X	Y	Z
N	0.18558600	-0.42777500	2.69341100
H	0.42446900	0.41891100	2.13776300
H	0.22002000	-0.23493600	3.68889300
H	-0.77044100	-0.65607300	2.38916300
S	1.50115100	-1.38977600	-0.01360500
O	1.96564300	-1.72651000	-1.33444200
O	0.06199800	-1.08823200	0.00995300
O	1.91464000	-2.21104900	1.09420700
S	1.56569400	1.50356200	-0.05508300
O	0.35142500	1.60111000	0.79620900
O	1.20883500	1.38127000	-1.45768000
O	2.59905500	2.41327900	0.28396600
O	2.20419300	0.04782600	0.39472500
H	0.83092700	-1.18798700	2.43214500
H	0.21262400	0.35027500	-2.19677800
N	-0.21950900	-0.47968000	-2.68577800
H	0.42816900	-1.25280800	-2.47932300
H	-1.13410900	-0.66252500	-2.26849900
H	-0.29905600	-0.31804400	-3.68415100
S	-2.73864200	0.13718200	0.13240900
O	-2.33692000	-0.04611600	1.50407700
O	-4.06757200	0.49138800	-0.19509100
O	-2.44593300	-1.22129500	-0.64152200
O	-1.75846000	1.12418900	-0.55316500
H	-1.57732400	-1.54280100	-0.31762000
H	-0.92428500	1.29579400	0.01554000

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

Atoms	X	Y	Z
S	-0.13767500	-0.19715200	0.54525800
O	-0.42207900	-0.86585500	-0.82014700
O	1.04200900	-0.83307100	1.05116300
O	-1.32800500	-0.19667000	1.36133700
O	0.13514300	1.29151800	0.24366200
H	-2.91156200	-1.13032000	1.55389200
H	1.03801800	1.39817800	-0.15275000
S	-4.24938800	-1.33970400	-0.04918500
O	-5.44989800	-2.06032700	-0.17755700

O	-3.87733800	-1.24265900	1.46229700
O	-3.07393000	-1.64456800	-0.79753900
S	-3.65868400	1.46022300	-0.45922500
O	-2.48142200	1.03228800	-1.14047400
O	-3.32838200	1.69077400	1.04492400
O	-4.47160300	2.51468100	-0.91136100
O	-4.69233600	0.19551500	-0.37449900
H	-1.35522900	-0.72140200	-1.09153900
H	-2.50681500	1.21314800	1.27796200
S	3.72256900	1.38395500	0.20360800
O	3.64169600	2.20232700	1.34451500
O	2.62269000	1.26632800	-0.71430700
O	5.01531700	1.72818200	-0.57990200
S	4.25886000	-1.36865400	-0.29821200
O	4.98229300	-0.86284300	-1.41906500
O	2.81420000	-1.62226000	-0.77565200
O	4.75478800	-2.39492500	0.52939100
O	4.04465200	-0.10690900	0.75229600
H	5.18141100	1.04151100	-1.25808700
H	2.16089400	-1.55201000	-0.03802000

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

Atoms	X	Y	Z
N	-1.03477100	-1.42131200	2.23680900
H	-1.12479800	-1.61683800	3.22835100
H	-1.02403900	-0.40937600	2.05950300
H	-0.13593600	-1.76980700	1.87236500
S	-2.19075800	-1.64299100	-0.90140900
O	-2.28576800	-2.33434400	-2.13022700
O	-2.92530400	-2.18564200	0.24468400
O	-0.88408400	-1.14090100	-0.49689600
S	-3.68951300	0.63285700	-0.05946400
O	-2.70238300	0.72145300	0.99671100
O	-4.85219400	-0.29167500	0.41526500
O	-4.23884800	1.81821000	-0.58951400
O	-3.05939400	-0.19546700	-1.24856300
H	-1.80709100	-1.83095200	1.69067400
H	-4.48747100	-1.19327100	0.53514400
S	0.15228100	1.95387800	0.53584900
O	1.27606900	2.82182300	0.32007600
O	0.26759000	0.92056200	1.52846900
O	-0.25845800	1.33727700	-0.81415400
O	-1.02023000	2.91465900	0.88504600
H	-0.46549600	0.35646300	-0.72440200
H	-1.82682100	2.37519200	1.01264400

S	2.70599300	-1.36719900	0.84693600
O	1.53748600	-2.07068700	1.25335000
O	3.48880900	-0.61750600	1.75521000
O	3.56491500	-2.40057400	0.05893500
S	3.31947100	0.57499500	-1.12424400
O	4.51717300	-0.19412300	-1.22251200
O	3.56072300	1.67250700	-0.08237600
O	2.60229600	1.03068700	-2.24998800
O	2.20362900	-0.38844900	-0.34690900
H	4.30165600	-1.92828500	-0.37622400
H	2.71759900	2.19893600	0.06872900

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

Atoms	X	Y	Z
N	2.39985100	-2.97995600	0.60863900
H	2.17249700	-2.21230000	1.25885300
H	2.57937300	-3.84211400	1.11296400
H	1.60459000	-3.08625700	-0.04273300
S	3.31532100	-0.21618600	-0.95088900
O	3.58748000	0.62663000	-2.08297800
O	1.98642200	-0.80122700	-0.93595000
O	4.34509900	-1.10208900	-0.48385400
S	2.33992100	0.78348200	1.55891700
O	2.53468400	-0.55602700	2.03829900
O	0.88097200	0.87157200	0.98400900
O	2.56748000	1.90201600	2.39036100
O	3.20779200	1.01301900	0.25964700
H	3.23400600	-2.65890000	0.09906500
H	0.47258700	-0.07798300	0.88607700
N	0.81514100	1.54421200	-2.05391900
H	0.65845800	2.21477100	-1.29197200
H	0.30450100	1.87433700	-2.86894500
H	1.81990700	1.42934000	-2.25445900
S	-0.70849400	-1.79353700	-0.45413700
O	-0.07798500	-3.01896600	-0.85366300
O	-0.27175700	-1.31509900	0.86688700
O	-0.83967000	-0.74372800	-1.42950700
S	-3.47843400	-1.35259700	0.22474100
O	-3.52221500	-0.25603700	-0.69939800
O	-3.05481600	-0.80518700	1.62040800
O	-4.57870700	-2.21569500	0.38950700
O	-2.26460300	-2.32654000	-0.16495100
H	0.42797600	0.62807900	-1.77000500
H	-2.60391400	0.05457400	1.51595600
S	-1.88607500	2.69154700	-0.16408000

O	-0.65403000	3.41090800	-0.29487200
O	-3.12494300	3.33110600	0.05919000
O	-1.69047700	1.63600100	1.01999500
O	-1.93571200	1.76832800	-1.42330600
H	-0.73585700	1.59045200	1.23386600
H	-2.51499400	0.98098000	-1.27315900

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

Atoms	X	Y	Z
N	-2.51999000	-2.10255300	1.68586100
H	-2.66179000	-1.94588000	0.67966300
H	-2.88384800	-3.00536300	1.96981700
H	-1.51136500	-2.01395400	1.90962400
S	-2.73989300	1.10681500	1.23034100
O	-2.38587200	2.48758500	1.45205300
O	-1.65059400	0.29235300	0.71447900
O	-3.53154300	0.46062000	2.24748400
S	-3.81546900	0.17596300	-1.25519500
O	-3.67324900	-1.13779200	-0.69403000
O	-2.54198900	0.54713500	-2.06140500
O	-4.93861000	0.50740900	-2.04414200
O	-3.80396100	1.25309900	-0.07405800
H	-3.02102900	-1.32637600	2.14822300
H	-1.71148000	0.16036600	-1.69197600
N	4.28888900	-2.20923500	-0.37897100
H	3.90506700	-2.44111100	-1.29262600
H	5.08427200	-2.79218000	-0.14274400
H	4.54173900	-1.20721700	-0.38478000
S	1.10942300	-1.46982700	1.37569600
O	0.15094400	-1.78817000	2.40158700
O	1.42114800	-0.04776800	1.23348500
O	2.29522500	-2.30630200	1.39074000
S	0.69839600	-1.26214200	-1.47194400
O	2.15541900	-1.04750100	-1.39728200
O	0.00674800	0.01401300	-1.54204200
O	0.26632900	-2.29456200	-2.34625300
O	0.29343300	-1.87714900	0.02076000
H	3.50472000	-2.30252900	0.32175800
H	0.05203000	2.06645500	-0.77843200
N	0.15956600	2.27891000	0.21401300
H	0.36619600	1.36859900	0.65698600
H	0.94159700	2.91453100	0.35014800
H	-0.72450100	2.63213900	0.61640100
S	3.81394200	1.73522600	-0.19005900
O	4.59950600	0.52861500	-0.11261600

O	4.41694100	2.96511800	-0.53974200
O	3.12055100	1.96111700	1.20416100
O	2.60644900	1.47467000	-1.13553900
H	2.67064600	1.12637400	1.46726000
H	2.43113500	0.47981800	-1.23816300

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

Atoms	X	Y	Z
N	1.39103700	2.49577300	0.05425100
H	0.36403100	2.43206600	0.07924100
H	1.70913000	3.36997100	-0.34808000
H	1.75204800	2.36086900	0.99506100
S	1.23309500	-0.70744200	-0.02208000
O	1.74993600	-2.02510400	0.01713200
O	1.05815300	0.00463100	1.24344400
O	1.75554200	0.17671500	-1.05951900
S	-1.52632100	0.03673600	-0.12635900
O	-1.06629500	1.37280200	-0.39993600
O	-1.61646800	-0.16517600	1.42380200
O	-2.72809900	-0.42868500	-0.69974800
O	-0.38253900	-0.98851200	-0.52357100
H	1.67058800	1.62863800	-0.51876000
H	-0.70326600	-0.10404300	1.77497600

$(SA)_2$:

Atoms	X	Y	Z
S	-2.01322700	-0.06909400	0.12032000
O	-1.03993500	0.02070700	1.17305600
O	-3.33344600	-0.50822700	0.37973100
O	-2.03861500	1.38798500	-0.49770200
H	-2.80898000	1.47208500	-1.07474100
O	-1.44840100	-0.93353400	-1.03975000
H	-0.49362800	-0.70536900	-1.17055400
O	1.03990200	-0.02023300	-1.17304000
S	2.01323800	0.06911400	-0.12030200
O	1.44861400	0.93342700	1.03995600
O	3.33355800	0.50799300	-0.37963200
O	2.03830500	-1.38810900	0.49739500
H	0.49378000	0.70547900	1.17068500
H	2.80879500	-1.47259300	1.07421100

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

Atoms	X	Y	Z
S	-1.75156900	-0.35106400	-0.05309700

O	-1.08755700	0.22332400	1.13077400
O	-0.97588400	-1.41957800	-0.65807100
O	-3.09267400	-1.03007100	0.46440300
H	-2.87930000	-1.91566500	0.78109800
O	-2.22526600	0.68973700	-0.94849600
H	-1.40930200	2.07376900	-0.49615300
O	1.36347800	1.03234300	-0.60427700
S	2.05584200	-0.10297800	-0.02123500
O	1.42781100	-0.37315300	1.37706700
O	3.46255300	-0.06302900	0.11092600
O	1.68407300	-1.36217100	-0.85448200
H	0.44072100	-0.19621900	1.34104900
H	0.69686100	-1.43307500	-0.90284700
N	-0.68866100	2.67273600	-0.01622200
H	0.21057600	2.15515800	-0.14127600
H	-0.92046500	2.68070400	0.97367200
H	-0.63909600	3.61164500	-0.39543300

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

Atoms	X	Y	Z
S	-0.38040400	2.37720100	-0.13492600
O	0.95898800	2.43967100	-0.65606200
O	-1.01498400	3.53934700	0.35802100
O	-0.44607500	1.24514500	0.94980400
O	-1.23762100	1.73931800	-1.28917300
H	0.45992400	0.91391300	1.14848700
H	-2.16452700	1.66024100	-0.98698100
S	3.03468600	-0.04900600	0.38831200
O	4.36227200	-0.37422900	0.71647800
O	2.10425900	0.44800300	1.35549600
O	2.99023300	0.81161800	-0.88013400
S	0.86885900	-1.78465100	-0.33732000
O	0.53272600	-0.55361100	-1.23971400
O	0.23489600	-1.62448100	0.94063200
O	0.77924400	-3.01106800	-1.02731300
O	2.43502400	-1.49119900	-0.17509300
H	2.17795700	1.39648200	-0.87701700
H	-1.39391400	-1.26302900	1.38570900
S	-2.96705500	-0.64644500	0.14770400
O	-3.36927100	0.71968200	0.16497100
O	-2.35708900	-1.08137700	1.50688100
O	-2.10529400	-1.10763400	-0.91020900
O	-4.29625200	-1.47255000	0.13445800
H	-0.44432900	-0.46082900	-1.30637800
H	-4.10093900	-2.41344200	0.02347800

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

Atoms	X	Y	Z
N	-2.03199700	1.98480500	-1.64025700
H	-1.40392200	1.17426900	-1.74782000
H	-1.53675100	2.66815700	-1.04061700
H	-2.25526800	2.38840900	-2.54470100
S	-2.59331100	-0.03211400	1.00826000
O	-3.13042900	-0.41251300	2.25993300
O	-3.43575700	-0.15204100	-0.17559500
O	-1.79000600	1.18171000	0.95612300
S	-1.06821400	-1.75031000	-0.69886200
O	-0.83454200	-0.61428400	-1.53861000
O	-2.38448600	-2.46812600	-1.12841000
O	-0.08021100	-2.76573000	-0.57650200
O	-1.39196900	-1.26092000	0.76403200
H	-2.86794900	1.63509300	-1.16362500
H	-3.11850900	-1.82768600	-1.02985200
S	0.99253100	2.58597200	-0.06545800
O	2.31430600	3.06556300	0.07615000
O	-0.13468500	3.47523500	-0.12881100
O	0.76055700	1.55675500	1.10954800
O	0.83323900	1.68485500	-1.33551900
H	-0.21588200	1.35518400	1.17860100
H	1.37762100	0.85706100	-1.23959500
S	2.92117500	-1.17009800	0.17926700
O	2.11734600	-0.52247000	-0.83473000
O	4.32691400	-1.04191600	0.16236900
O	2.57646400	-2.68366900	0.17346500
O	2.33759300	-0.74343400	1.57442000
H	1.63178400	-2.79781200	-0.05997800
H	1.90330300	0.12639500	1.49517100

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

Atoms	X	Y	Z
N	0.37554800	-1.94641900	-1.19044400
H	1.10152200	-1.78793200	-0.45780800
H	0.49176900	-2.87550900	-1.58466100
H	-0.56877500	-1.85210700	-0.78569300
S	0.01581700	1.31307000	-1.30660200
O	-0.27709000	2.72030900	-1.27608500
O	-1.17174400	0.48116700	-1.11612100
O	0.90357700	0.82369400	-2.34019100
S	0.31077000	0.68614600	1.50570400
O	-0.32304200	-0.62580800	1.37308800

O	-0.64625700	1.74801000	1.74019400
O	1.49705000	0.71297700	2.31264800
O	0.95896800	0.98338000	0.01051100
H	0.49603500	-1.23497000	-1.91794500
H	-2.03214000	2.09923600	0.89843200
N	-2.72325200	2.43947000	0.18581000
H	-2.14321900	2.79726600	-0.58475100
H	-3.27583900	1.63896600	-0.13185000
H	-3.32038800	3.16488700	0.56963900
S	-3.41466400	-1.30065100	0.07381000
O	-2.37658300	-2.17078600	-0.41370200
O	-4.67380900	-1.80520200	0.46861500
O	-3.71357400	-0.22862500	-1.07018900
O	-2.83273700	-0.40995400	1.20157200
H	-2.86015200	-0.04355200	-1.50688500
H	-1.81381500	-0.52518900	1.27121100
S	3.66868100	-0.79997200	0.02627400
O	2.50831000	-1.54112300	0.47078700
O	4.92447100	-1.44102500	-0.06521800
O	3.78546500	0.46683400	0.91790700
O	3.37802700	-0.22512800	-1.40741800
H	2.97442700	0.56466400	1.47705500
H	2.56660500	0.31564000	-1.45246500

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

Atoms	X	Y	Z
S	-1.80849800	-1.01399400	1.02474100
O	-0.54273300	-1.58061900	0.58457100
O	-2.15158000	-0.11014500	-0.36807300
O	-2.91535200	-1.92415700	1.14355100
O	-1.66344800	-0.03750700	2.07929300
H	0.10055600	0.11328700	2.41451400
H	1.48544900	-0.43593600	3.21530000
N	1.13424800	0.05518400	2.40052800
H	1.54080900	0.99730700	2.30895300
H	1.40510500	-0.43611500	1.52817400
H	5.13196300	0.54475400	-0.22677100
N	4.23247000	0.99212800	-0.36818300
H	3.43218600	0.27879700	-0.29620900
H	4.00222100	1.69398800	0.34514400
H	0.83981600	-0.90516900	-2.26305100
N	0.27505000	-0.10532700	-1.94439400
H	-0.52814700	0.07914700	-2.53904700
H	-0.05264100	-0.35783800	-1.00606300
S	2.56157100	-2.02383300	-0.47451600

O	2.19644000	-0.61865600	-0.08319200
O	3.97940400	-2.22043500	-0.40538000
O	1.94156800	-2.91038100	0.69375600
O	1.88028700	-2.38416200	-1.70168600
H	0.97260000	-2.85702100	0.62166600
H	0.86658600	0.73570200	-1.83018600
S	1.38361100	2.60826200	0.07654500
O	0.83332600	3.92721700	0.10887600
O	1.89358600	2.14005400	-1.21373700
O	2.32460900	2.28321700	1.16224600
O	0.13333700	1.59669600	0.36321000
H	4.16749000	1.44454800	-1.27605700
H	-0.65278500	2.12465900	0.55465700
O	-4.19406000	0.99054300	0.45010500
S	-3.66425200	0.35803100	-0.70272000
O	-4.35878500	-1.01987600	-0.95511300
H	-4.23211000	-1.57151500	-0.15602900
O	-3.54789600	1.00596800	-1.95785900

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

Atoms	X	Y	Z
S	-1.99375600	0.03950600	-0.14679700
O	-1.96770800	1.49843900	-0.07048200
O	-3.42358600	-0.32337200	-0.76178300
O	-1.06994700	-0.54333200	-1.10365000
O	-1.92152200	-0.59640400	1.16575700
H	-0.60468900	2.18376200	0.65313600
H	-4.09078700	0.17534600	-0.27653000
S	2.10772600	-0.06533300	-0.21735300
O	1.97293600	-1.43365000	-0.71671300
O	1.24928600	0.86001100	-1.20138700
O	1.39488600	0.04212900	1.09037500
O	3.41196200	0.51312500	-0.22105800
H	0.78789600	-2.09192900	0.15000000
H	0.39594100	0.39985400	-1.36649500
N	0.14396100	-2.41317300	0.93378300
H	-0.18316600	-3.36112700	0.78560100
H	0.68671400	-2.34759800	1.79018800
H	-0.66121400	-1.75146700	1.00977700
N	0.35234900	2.40999100	1.00848400
H	0.31970800	3.00004000	1.83116400
H	0.83110500	1.45569800	1.19383700
H	0.87614100	2.85816600	0.26091400

$(DSA)_2$:

Atoms	X	Y	Z
S	-1.41878100	1.52046200	0.51265300
O	-2.69600800	1.97749800	0.90202900
O	-0.39509500	2.40403200	0.05763000
O	-0.75177200	0.64196100	1.62143800
S	-2.65392900	-0.79452000	-0.54100600
O	-2.73115000	-1.07079200	0.85848300
O	-1.80259400	-1.85627700	-1.27089700
O	-3.78153000	-0.49664300	-1.32645800
O	-1.57710700	0.46231900	-0.69698500
H	-1.38737800	-0.03921100	1.91527500
H	-1.03860300	-2.10977000	-0.70346300
S	1.43272500	-1.42786500	0.61381900
O	0.20872500	-2.15792100	0.53160200
O	1.89523500	-0.87495500	1.82812300
O	2.52147400	-2.31436100	-0.06327000
S	2.44729400	0.86296800	-0.70395500
O	3.67656900	0.18828700	-0.45870600
O	2.18502300	1.79960000	0.49286900
O	2.11650400	1.45421600	-1.94014200
O	1.23916000	-0.25844100	-0.48932200
H	3.36139800	-1.81848000	-0.08343700
H	1.28815800	2.20254100	0.39631900

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

Atoms	X	Y	Z
N	0.28528300	-0.68180100	2.62406700
H	-0.59378800	-1.13366900	2.31464700
H	0.27206000	-0.49647800	3.62203400
H	1.08812700	-1.25863900	2.37430700
S	2.45668400	0.93644500	0.59608300
O	3.40054900	1.94222600	0.28413100
O	2.88064400	-0.20857200	1.38851400
O	1.12728500	1.39851800	1.01624900
S	1.59351700	-1.22494400	-1.03439800
O	0.55866300	-1.39660200	-0.03502300
O	2.83912900	-2.06307100	-0.60091300
O	1.30960300	-1.50589800	-2.38480900
O	2.14918600	0.25504200	-0.93662500
H	0.41679800	0.19733500	2.08473200
H	3.18096000	-1.68329900	0.23376100
S	-2.62296000	-0.90586300	0.49237100
O	-3.99582000	-0.64698900	0.31863500
O	-2.14273900	-1.62725200	1.63872500
O	-2.07298100	-1.52366700	-0.81588400

S	-1.62075800	1.49496400	-0.72878600
O	-0.69288400	0.85266600	-1.58919300
O	-0.96024200	2.64782100	0.05389400
O	-2.91553400	1.88093100	-1.12983600
O	-1.77844600	0.47042000	0.60248800
H	-1.09207600	-1.59167200	-0.75677100
H	-0.04463700	2.37114300	0.31995000

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

Atoms	X	Y	Z
N	-1.06283000	-1.26663900	-2.50840500
H	-1.03918100	-0.27055900	-2.23900800
H	-0.93182000	-1.37741500	-3.50867400
H	-0.31890200	-1.75008900	-1.97521000
S	-2.88270300	-0.93204000	0.22299100
O	-3.46280900	-1.35269200	1.47136300
O	-1.44198300	-1.10220700	0.14781000
O	-3.57241900	-1.23958000	-0.99990400
S	-2.05086500	1.78124200	-0.28564000
O	-1.74922600	1.32294100	-1.61454500
O	-0.76685900	1.62319600	0.59530600
O	-2.59651700	3.06573600	-0.06175900
O	-3.05509900	0.76889200	0.41330200
H	-1.98732000	-1.60247400	-2.21041200
H	-0.07675000	1.04680300	0.12022500
N	-1.01628000	-0.40345700	2.75278200
H	-1.11800500	0.53300700	2.34765300
H	-0.77687200	-0.34249400	3.73772300
H	-1.90170500	-0.91090200	2.60434400
S	1.45886600	-1.03894800	-0.09597300
O	1.15452900	-2.15175700	-0.95485600
O	0.99445000	0.25561700	-0.64545200
O	1.20086400	-1.20109900	1.31265500
S	3.85701600	0.43994700	0.16932600
O	3.21297600	0.98589600	1.31245400
O	3.53451600	1.31556600	-1.09382700
O	5.23236900	0.12652400	0.12019500
O	3.09922200	-0.94489200	-0.23284300
H	-0.25515200	-0.86263700	2.20874100
H	2.57035800	1.44710200	-1.12645100S

$(SA)_3$:

Atoms	X	Y	Z
S	0.16483700	1.30605100	-0.06336500
O	-0.10407000	0.08451900	-0.80968300
O	1.37746300	1.98145900	-0.39595600
H	3.11822700	1.29813100	-0.24755100
O	0.10199300	0.97627800	1.45441800
O	-1.00412300	2.28075600	-0.20277700
O	3.82969200	0.63311300	-0.17992300
S	3.19659800	-0.77206100	0.08974300
O	4.25644700	-1.69047600	0.22901900
O	2.44151500	-1.08907800	-1.24922900
O	-2.42010200	-1.31989300	-1.02508800
H	1.52576000	-0.75359300	-1.20077100
H	-1.54359000	-0.87259000	-1.03690100
O	2.19850800	-0.63473100	1.12400800
O	-3.16961700	0.85361300	-0.19755800
H	0.83407900	0.33942600	1.63195900
H	-1.87447800	1.78339100	-0.18874100
O	-4.64837000	-1.13962700	-0.15465900
S	-3.36281200	-0.56330400	-0.04568500
O	-2.73563400	-0.88198700	1.36909700
H	-3.02757700	-1.75731700	1.65756900

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

Atoms	X	Y	Z
N	-0.04172000	0.31393500	2.50407500
H	-0.90969100	0.06818900	1.98691100
H	0.71310500	-0.29441000	2.15097000
H	-0.17125100	0.19382600	3.50277600
S	1.01542600	1.97849500	-0.14077200
O	-0.00526000	0.92850100	-0.23378200
O	1.18656600	2.48449400	1.19635500
H	0.24693700	1.27641200	2.27050300
O	2.24337900	1.55803500	-0.83387100
S	-2.86205700	-0.43166700	-0.10848500
O	-2.02181500	-1.23225400	-1.15389300
O	-2.63228000	1.05375200	-0.53246700
O	-4.23147800	-0.71882200	-0.30442500
O	-2.26109000	-0.64315900	1.19033600
H	-1.13058000	-1.44136000	-0.79715800
H	-1.66222100	1.22940700	-0.48893400
S	1.72178700	-1.63935800	-0.07740200
O	2.65109800	-2.91101100	-0.14869600
O	2.16645600	-0.85899500	-1.30276100
O	0.37004900	-2.12000700	-0.20621800

O	2.07535500	-0.93817900	1.12542500
H	2.14919700	-3.63570300	-0.54219400
H	2.22674400	0.18299300	-1.10444000
O	0.47811700	3.22500900	-0.96825000
H	0.67455700	3.08467700	-1.90245400

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

Atoms	X	Y	Z
N	0.04080800	0.04080800	0.08780100
H	-0.76321900	-0.76321900	-0.54706000
H	0.93979000	0.93979000	-0.41363000
H	0.08931200	0.08931200	0.74907100
N	-2.34151400	-2.34151400	1.67098900
H	-3.28639200	-3.28639200	1.34957300
H	-2.17630400	-2.17630400	2.58799900
H	-2.22980100	-2.22980100	1.68130600
S	-3.01773500	-3.01773500	-0.12741300
O	-2.49434500	-2.49434500	-1.04838500
O	-2.99705800	-2.99705800	-0.66645800
O	-2.44011400	-2.44011400	1.21337500
H	-1.33804100	-1.33804100	-1.42890100
S	0.27373000	0.27373000	-0.39748000
O	-0.35916500	-0.35916500	-1.49334800
O	1.58046200	1.58046200	-0.89844300
O	-0.64753600	-0.64753600	-0.22470400
O	0.32340100	0.32340100	0.84468800
H	-0.13168800	-0.13168800	0.59204600
H	-1.66304700	-1.66304700	0.95201500
O	-4.55140600	-4.55140600	0.11903600
H	-4.94495500	-4.94495500	-0.73381900
S	3.42424600	3.42424600	0.12698000
O	3.89261900	3.89261900	-0.32505500
O	2.62104500	2.62104500	1.44668900
O	4.56295900	4.56295900	0.47398200
O	2.48760400	2.48760400	-0.85833400
H	3.09999000	3.09999000	-0.64371300
H	1.79771600	1.79771600	1.24585300

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

Atoms	X	Y	Z
S	2.60141600	-1.19585400	0.09028500
O	1.48413400	-2.08386400	0.36783500
O	3.92882800	-2.09122400	0.15651500
O	2.64333500	-0.67818000	-1.26933200

H	3.92528500	-2.56696900	0.99505500
S	-2.73331100	-1.02693500	0.00470300
O	-2.78264800	0.26465500	0.66745400
O	-4.06497900	-1.75400600	0.51531200
O	-2.83320700	-0.99509200	-1.44855000
H	-4.30626800	-2.41338000	-0.14407300
S	-0.34333100	2.24129800	0.02140700
O	0.26545600	0.92835600	-0.28703000
O	-0.60525300	2.36316200	1.44529000
O	-1.71298000	2.30527000	-0.74363100
O	0.44986700	3.32229000	-0.55386900
H	1.94532200	2.65273900	-0.68157200
O	2.75488900	-0.16732100	1.12583000
N	-0.07985100	-0.27110800	2.17282900
N	2.80483500	2.03905400	-0.63408200
N	-0.08936400	-1.27196600	-1.83994300
H	3.65956600	2.54992200	-0.82231000
H	2.84235300	1.58042200	0.28701900
H	2.70046200	1.23535100	-1.26789800
H	-2.30374600	1.63719400	-0.32205100
H	0.20145100	-1.90642500	-1.08397800
H	0.51392500	-1.39430700	-2.64518600
H	-1.09237500	-1.39308200	-2.03483900
H	0.03941600	-0.31894800	-1.44051300
H	0.91162700	-0.26388400	1.90403900
H	-0.59002500	-0.90705900	1.52372800
H	-0.45080700	0.69119800	2.04875500
H	-0.19333800	-0.58822500	3.12877200
O	-1.60662500	-1.84665700	0.45914400

$(DSA)_3$:

Atoms	X	Y	Z
S	0.20058700	-1.09702200	-1.15759400
O	-0.75267800	-1.23915500	-2.18655000
O	1.41227700	-1.85381200	-1.13531800
O	0.61345500	0.37737400	-0.92256800
S	-0.65836100	-0.58956900	1.57248700
O	-0.96210400	0.75850000	1.24735200
O	0.77513700	-0.71673600	2.11662200
O	-1.54732800	-1.36272000	2.37363400
O	-0.58860700	-1.48732000	0.21606500
H	-0.16170800	0.97743800	-1.06934500
H	1.27191500	0.13194600	1.97015700
S	3.16751900	1.44593000	0.66771900
O	2.11537600	1.54845200	1.62857800

O	3.09683700	2.04295000	-0.61014100
O	4.47876400	1.84417900	1.40927300
S	4.47540600	-0.76257600	-0.53237500
O	5.54265900	0.17809900	-0.57016500
O	3.70722500	-0.64915700	-1.86685400
O	4.62866300	-2.09812000	-0.10838500
O	3.34601500	-0.15791000	0.52269500
H	5.23016800	1.73824800	0.79697400
H	2.88860200	-1.19670800	-1.80949100
S	-2.98114400	1.49977200	-0.86663300
O	-1.70753200	1.67676000	-1.48070000
O	-3.40748300	2.24270700	0.25560300
O	-4.02611000	1.56313900	-2.02210500
S	-4.31055300	-0.72598200	0.27882700
O	-5.45430200	-0.01498400	-0.18075800
O	-4.04308800	-0.27092900	1.73470100
O	-4.13280000	-2.11690900	0.12305200
O	-3.01137400	-0.09004300	-0.51251800
H	-4.90978200	1.38516300	-1.65097100
H	-3.27849100	-0.75983900	2.11165600

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

Atoms	X	Y	Z
N	0.23627200	-1.96073500	-0.71711400
H	0.83135000	-1.22419300	-1.11189500
H	-0.47464300	-2.24639700	-1.39057000
H	0.84398700	-2.72280400	-0.41636300
S	2.99428800	-1.48147900	1.19230900
O	3.76092700	-1.69912900	2.35965600
O	2.97618200	-2.50494100	0.15723500
O	1.65954800	-0.91023800	1.36184900
S	3.73770700	0.04348500	-1.10731600
O	2.32973500	0.00638000	-1.45803700
O	4.43420500	-1.21505500	-1.70193400
O	4.49012600	1.18658900	-1.44125800
O	3.86007400	-0.19336100	0.44978000
H	-0.24547700	-1.57048500	0.10341800
H	4.05873700	-2.00721700	-1.26167300
S	-0.48334000	1.55748600	-1.35759100
O	-1.49019000	2.53697800	-1.24910900
O	-0.65340400	0.31538200	-2.03458400
O	0.83077100	2.24481400	-1.79209600
S	0.01972700	2.04173200	1.42562100
O	0.90228500	3.08888000	1.08400800
O	0.56881200	1.04469200	2.43433600

O	-1.32676800	2.37093800	1.82356100
O	-0.09671100	1.01675700	0.15251600
H	1.54102900	1.56537600	-1.84574600
H	1.12685400	0.27775100	2.03071400
S	-3.44921300	-0.97270500	-1.36363300
O	-2.57837800	-2.10286000	-1.27881300
O	-3.54011100	-0.14399100	-2.49453500
O	-4.89306500	-1.38041200	-0.94914900
S	-2.82890800	-0.63503300	1.37361800
O	-3.87627900	-1.58120200	1.57208600
O	-3.10315200	0.61193200	2.19430100
O	-1.46587100	-1.04753600	1.46941300
O	-3.03189700	0.01798200	-0.12242900
H	-4.87209300	-1.81925600	-0.07695900
H	-2.36253400	1.31580500	2.08637700

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

Atoms	X	Y	Z
N	-0.66041100	-0.35858300	2.45263400
H	-0.30164800	0.60118200	2.51435900
H	0.13690500	-1.01375200	2.54886000
H	-1.38635500	-0.52973500	3.14244300
S	-1.08763400	-2.42013500	-0.81829300
O	-0.92506100	-3.58220100	-1.60844000
O	-0.86045500	-2.52573600	0.61572200
O	-0.77571200	-1.13423700	-1.37235000
S	-3.63437000	-1.56988600	0.31981100
O	-2.93540100	-0.28391100	0.50457700
O	-3.31331600	-2.40553400	1.60697800
O	-5.03221700	-1.52992000	0.13787400
O	-2.93960200	-2.33469900	-0.81200200
H	-1.04527300	-0.49920600	1.51155700
H	-2.40339600	-2.76174800	1.49687500
S	0.20530000	2.89462700	0.88943800
O	1.33714400	2.94939200	0.04788300
O	0.25296000	2.44757400	2.24293500
O	-0.47544400	4.30079600	0.80227100
S	-1.89470000	2.50362500	-1.01860100
O	-2.85501800	3.33046000	-0.37814900
O	-2.42405800	1.15660600	-1.45459100
O	-1.02185200	3.01980200	-2.01885500
O	-0.91574300	1.93183600	0.22655000
H	-1.33788000	4.30929600	1.24666100
H	-2.69974100	0.53578500	-0.65607200
N	1.03465500	0.82325900	-2.03991000

H	1.99624500	0.81698700	-2.37849300
H	0.58203500	1.72379100	-2.20998000
H	0.48427800	0.06373300	-2.44290500
S	1.98658500	-1.16394100	0.77541700
O	1.74077900	-1.79002200	2.04717000
O	2.01465000	-2.00086400	-0.40316200
O	1.23499400	0.07459300	0.60205500
S	4.46328600	-0.37101000	-0.34654800
O	3.66416400	0.38622300	-1.26134800
O	4.67308900	-1.81475700	-0.90706300
O	5.70869100	0.10406900	0.11341300
O	3.58026100	-0.66051100	0.96366800
H	1.08766400	0.63388100	-1.01491300
H	3.78917200	-2.21710600	-1.02815300

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

Atoms	X	Y	Z
N	-4.05000800	2.05521800	0.68059200
H	-3.51014800	1.42083700	1.29826600
H	-4.55280800	2.75404100	1.21663400
H	-3.38727800	2.49070700	0.02183800
S	-3.70982800	-0.79855400	-0.86879100
O	-3.66545400	-1.69780000	-1.98856500
O	-2.76191800	0.30192500	-0.92989400
O	-4.99946600	-0.42280700	-0.34966700
S	-2.19912800	-1.18221100	1.52852400
O	-2.92812600	-0.05873700	2.06711100
O	-0.90602200	-0.76319600	0.90343800
O	-1.98048700	-2.29294200	2.42532700
O	-3.04115800	-1.82073900	0.33668500
H	-4.68990400	1.43023600	0.17066800
H	-0.79618900	0.61522700	0.73434400
N	-0.77890000	-1.27179600	-2.07383100
H	-0.63766100	-1.47892800	-1.07740500
H	-0.00235800	-1.68416000	-2.59828100
H	-1.69853700	-1.62968500	-2.35914900
S	-0.68175800	2.36840500	-0.60726100
O	-1.86423600	3.14656200	-0.81611300
O	-0.72484300	1.67789900	0.75509400
O	-0.21230200	1.49259200	-1.63105400
S	2.01698600	3.16437800	-0.02098600
O	2.40645300	2.09568000	-0.86715700
O	1.92740500	2.67623700	1.45088900
O	2.60206900	4.44669600	-0.03629300
O	0.42311600	3.50710000	-0.33158100

H	-0.77981000	-0.24798400	-2.15438400
H	1.88253400	1.69281500	1.46370400
N	0.77094500	-2.44957600	2.36645400
H	0.94880600	-2.77060300	1.39942200
H	-0.24778300	-2.51949200	2.55866400
H	1.33412300	-2.97011600	3.03025900
S	3.17416700	-0.52117500	0.62509800
O	4.31012800	0.31723600	0.61852700
O	3.47541800	-1.90225100	1.33214900
O	1.97394100	-0.05823100	1.29584500
S	2.24319400	-2.53933000	-1.24683200
O	1.09604000	-2.68755800	-0.36751100
O	3.37940900	-3.35653200	-0.91858700
O	1.91850000	-2.32776700	-2.62215400
O	2.83816600	-0.93693100	-0.84147900
H	1.04413800	-1.46166300	2.35613700
H	3.86739000	-2.53385600	0.69063500