Supporting information

-for-

Mechanistic Insights into Nitric Sulfuric Acid Formation and Its Enhancement of Sulfuric Acid-Ammonia Nucleation under Severe Urban Pollution

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	10^{11} molecules·cm^{-3}. The concentrations of NSA and SA are collectively maintained constant (10^4-10^8 molecules·cm^{-3})
S37-S50	**Table S16** Cartesian coordinates of all molecules and clusters in the studied system

Table S1 The Gibbs free energies of formation (ΔG) for SA·A, SA·NSA and A·NSA clusters were calculated at 278.15K using different theoretical schemes for potential energy surface corrections

Cluster	DLPNO-CCSD(T) aug-cc-pVDZ cc-pVDZ/C VeryTightSCF PModel TightPNO	CCSD(T)-F12/RI cc-pVDZ-F12 cc-pVDZ-F12-CABS cc-pVTZ/C VeryTightSCF PModel
	kcal·mol^{-1}	
SA·A	-6.25	-6.03
SA·NSA	-6.06	-4.93
A·NSA	-10.24	-9.68

To validate the accuracy of single-point energy calculations at the DLPNO-CCSD(T)/aug-cc-pVDZ level, the results obtained at this level were compared with those from CCSD(T)-F12/cc-pVDZ-F12 calculations. In terms of relative energy, the two sets of results showed good agreement with an error less than 2 kcal·mol^{-1}, demonstrating the reliability of DLPNO-CCSD(T)/aug-cc-pVDZ for predicting reaction energy barriers. Therefore, the DLPNO-CCSD(T)/aug-cc-pVDZ method was employed to calculate the single-point energies of all clusters in the aerosol.

Part S1 Atmospheric concentrations of NSA under different SO_3 and NA scenarios

The steady-state concentration of NSA was calculated using the calculated equilibrium constant listed in Eq. S1.

$$K_{eq} = \frac{[NSA]}{[SO_3][NA]} \tag{S1}$$

where K_{eq} (4.21×10^{-19} $cm^3 \cdot molecule^{-1}$) is the equilibrium constant of NSA with respect to SO_3 and NA (Long et al., 2022); [SO_3], [SA] and [NSA] are the concentrations of SO_3, H_2SO_4, and O_2NOSO_3H, respectively. Although sulfur trioxide concentrations at different altitudes remain poorly constrained, experimental observations indicate that SO_3 levels can reach ~ 10^6 $molecules \cdot cm^{-3}$ in the troposphere (Yao et al., 2020). As water vapor concentrations decrease markedly with increasing altitude, SO_3 concentrations are expected to be higher in the stratosphere than in the troposphere (Long et al., 2022) and may further increase under geoengineered injections of SO_2 or SO_3. In addition, atmospheric nitric acid (HNO_3) concentrations in heavily polluted regions, such as the North China Plain, can reach 10^{11}-10^{12} molecules cm^{-3}, providing favorable conditions for its participation in aerosol nucleation and growth. Accordingly, NSA concentrations were evaluated using SO_3 levels ranging from 10^7 to 10^{14} molecules cm^{-3} and HNO_3 concentrations from 10^8 to 10^{12} $molecules \cdot cm^{-3}$.

Reference:

Long, B., Xia, Y., Bao, J. L., Carmona-García, J., Gómez Martín, J. C., Plane, J. M. C., Saiz-Lopez, A., Roca-Sanjuán, D., and Francisco, J. S.: Reaction of SO_3 with $HONO_2$ and Implications for Sulfur Partitioning in the Atmosphere, J. Am. Chem. Soc., 144, 9172-9177, 10.1021/jacs.2c03499, 2022.

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.

Table S2 The rate coefficients for the reactions of SO_3 + HNO_3, SO_3 + HCOOH, SO_3 + C_6H_5COOH and NH_3-catalyzed SO_3 + NH_3, H_2O-catalyzed hydrolysis of SO_3 over the temperature range of 280-320K

T (K)	SO_3 + HNO_3	SO_3 + HCOOH	SO_3 + C_6H_5COOH	NH_3-catalyzed SO_3 + NH_3	H_2O-catalyzed hydrolysis of SO_3
280	1.42×10^{-13}	2.06×10^{-18}	7.70×10^{-12}	5.90×10^{-10}	2.37397×10^{-12}
290	1.16×10^{-13}	1.98×10^{-18}	8.04×10^{-12}	4.80×10^{-10}	2.29731×10^{-12}
298	9.94×10^{-14}	1.93×10^{-18}	8.27×10^{-12}	4.10×10^{-10}	2.37382×10^{-12}
300	9.58×10^{-14}	1.91×10^{-18}	8.32×10^{-12}	4.00×10^{-10}	2.29718×10^{-12}
310	8.06×10^{-14}	1.84×10^{-18}	8.47×10^{-12}	3.30×10^{-10}	2.31204×10^{-12}
320	6.87×10^{-14}	1.54×10^{-18}	8.43×10^{-12}	2.70×10^{-10}	2.37397×10^{-12}

Table S3 Rate ratios for SO_3 + HNO_3 reaction (v_{R1}) relative to the SO_3 + HCOOH reaction (v_{R2}) over the temperature range of 280-320K

T (K)	HNO_3	HCOOH	v_{R1}/v_{R2}	T (K)	HNO_3	HCOOH	v_{R1}/v_{R2}
280	1×10^{9}	1×10^{9}	6.89×10^{4}	290	1×10^{9}	1×10^{9}	5.86×10^{4}
		1×10^{10}	6.89×10^{3}			1×10^{10}	5.86×10^{3}
		1×10^{11}	6.89×10^{2}			1×10^{11}	5.86×10^{2}
		1×10^{12}	6.89×10^{1}			1×10^{12}	5.86×10^{1}
	1×10^{10}	1×10^{9}	6.89×10^{5}		1×10^{10}	1×10^{9}	5.86×10^{5}
		1×10^{10}	6.89×10^{4}			1×10^{10}	5.86×10^{4}
		1×10^{11}	6.89×10^{3}			1×10^{11}	5.86×10^{3}
		1×10^{12}	6.89×10^{2}			1×10^{12}	5.86×10^{2}
	1×10^{11}	1×10^{9}	6.89×10^{6}		1×10^{11}	1×10^{9}	5.86×10^{6}
		1×10^{10}	6.89×10^{5}			1×10^{10}	5.86×10^{5}
		1×10^{11}	6.89×10^{4}			1×10^{11}	5.86×10^{4}
		1×10^{12}	6.89×10^{3}			1×10^{12}	5.86×10^{3}
	1×10^{12}	1×10^{9}	6.89×10^{7}		1×10^{12}	1×10^{9}	5.86×10^{7}
		1×10^{10}	6.89×10^{6}			1×10^{10}	5.86×10^{6}
		1×10^{11}	6.89×10^{5}			1×10^{11}	5.86×10^{5}
		1×10^{12}	6.89×10^{4}			1×10^{12}	5.86×10^{4}
298	1×10^{9}	1×10^{9}	5.15×10^{4}	300	1×10^{9}	1×10^{9}	5.02×10^{4}
		1×10^{10}	5.15×10^{3}			1×10^{10}	5.02×10^{3}
		1×10^{11}	5.15×10^{2}			1×10^{11}	5.02×10^{2}
		1×10^{12}	5.15×10^{1}			1×10^{12}	5.02×10^{1}
	1×10^{10}	1×10^{9}	5.15×10^{5}		1×10^{10}	1×10^{9}	5.02×10^{5}
		1×10^{10}	5.15×10^{4}			1×10^{10}	5.02×10^{4}
		1×10^{11}	5.15×10^{3}			1×10^{11}	5.02×10^{3}
		1×10^{12}	5.15×10^{2}			1×10^{12}	5.02×10^{2}
	1×10^{11}	1×10^{9}	5.15×10^{6}		1×10^{11}	1×10^{9}	5.02×10^{6}
		1×10^{10}	5.15×10^{5}			1×10^{10}	5.02×10^{5}
		1×10^{11}	5.15×10^{4}			1×10^{11}	5.02×10^{4}
		1×10^{12}	5.15×10^{3}			1×10^{12}	5.02×10^{3}
	1×10^{12}	1×10^{9}	5.15×10^{7}		1×10^{12}	1×10^{9}	5.02×10^{7}
		1×10^{10}	5.15×10^{6}			1×10^{10}	5.02×10^{6}
		1×10^{11}	5.15×10^{5}			1×10^{11}	5.02×10^{5}
		1×10^{12}	5.15×10^{4}			1×10^{12}	5.02×10^{4}
310	1×10^{9}	1×10^{9}	4.38×10^{4}	320	1×10^{9}	1×10^{9}	4.46×10^{4}
		1×10^{10}	4.38×10^{3}			1×10^{10}	4.46×10^{3}
		1×10^{11}	4.38×10^{2}			1×10^{11}	4.46×10^{2}
		1×10^{12}	4.38×10^{1}			1×10^{12}	4.46×10^{1}
	1×10^{10}	1×10^{9}	4.38×10^{5}		1×10^{10}	1×10^{9}	4.46×10^{5}
		1×10^{10}	4.38×10^{4}			1×10^{10}	4.46×10^{4}
		1×10^{11}	4.38×10^{3}			1×10^{11}	4.46×10^{3}
		1×10^{12}	4.38×10^{2}			1×10^{12}	4.46×10^{2}
	1×10^{11}	1×10^{9}	4.38×10^{6}		1×10^{11}	1×10^{9}	4.46×10^{6}
		1×10^{10}	4.38×10^{5}			1×10^{10}	4.46×10^{5}
		1×10^{11}	4.38×10^{4}			1×10^{11}	4.46×10^{4}
		1×10^{12}	4.38×10^{3}			1×10^{12}	4.46×10^{3}
	1×10^{12}	1×10^{9}	4.38×10^{7}		1×10^{12}	1×10^{9}	4.46×10^{7}
		1×10^{10}	4.38×10^{6}			1×10^{10}	4.46×10^{6}
		1×10^{11}	4.38×10^{5}			1×10^{11}	4.46×10^{5}
		1×10^{12}	4.38×10^{4}			1×10^{12}	4.46×10^{4}

Table S4 Rate ratios for SO_3 + HNO_3 reaction (v_{R1}) relative to the SO_3 + C_6H_5COOH reaction (v_{R3}) over the temperature range of 280-320K

T (K)	HNO_3	C_6H_5COOH	v_{R1}/v_{R3}	T (K)	HNO_3	C_6H_5COOH	v_{R1}/v_{R3}
280	1×10^{9}	1×10^{9}	1.84×10^{0}	290	1×10^{9}	1×10^{9}	1.44×10^{0}
		1×10^{10}	1.84×10^{-1}			1×10^{10}	1.44×10^{-1}
		1×10^{11}	1.84×10^{-2}			1×10^{11}	1.44×10^{-2}
		1×10^{12}	1.84×10^{-3}			1×10^{12}	1.44×10^{-3}
	1×10^{10}	1×10^{9}	1.84×10^{1}		1×10^{10}	1×10^{9}	1.44×10^{1}
		1×10^{10}	1.84×10^{0}			1×10^{10}	1.44×10^{0}
		1×10^{11}	1.84×10^{-1}			1×10^{11}	1.44×10^{-1}
		1×10^{12}	1.84×10^{-2}			1×10^{12}	1.44×10^{-2}
	1×10^{11}	1×10^{9}	1.84×10^{2}		1×10^{11}	1×10^{9}	1.44×10^{2}
		1×10^{10}	1.84×10^{1}			1×10^{10}	1.44×10^{1}
		1×10^{11}	1.84×10^{0}			1×10^{11}	1.44×10^{0}
		1×10^{12}	1.84×10^{-1}			1×10^{12}	1.44×10^{-1}
	1×10^{12}	1×10^{9}	1.84×10^{3}		1×10^{12}	1×10^{9}	1.44×10^{3}
		1×10^{10}	1.84×10^{2}			1×10^{10}	1.44×10^{2}
		1×10^{11}	1.84×10^{1}			1×10^{11}	1.44×10^{1}
		1×10^{12}	1.84×10^{0}			1×10^{12}	1.44×10^{0}
298	1×10^{9}	1×10^{9}	1.20×10^{0}	300	1×10^{9}	1×10^{9}	1.15×10^{0}
		1×10^{10}	1.20×10^{-1}			1×10^{10}	1.15×10^{-1}
		1×10^{11}	1.20×10^{-2}			1×10^{11}	1.15×10^{-2}
		1×10^{12}	1.20×10^{-3}			1×10^{12}	1.15×10^{-3}
	1×10^{10}	1×10^{9}	1.20×10^{1}		1×10^{10}	1×10^{9}	1.15×10^{1}
		1×10^{10}	1.20×10^{0}			1×10^{10}	1.15×10^{0}
		1×10^{11}	1.20×10^{-1}			1×10^{11}	1.15×10^{-1}
		1×10^{12}	1.20×10^{-2}			1×10^{12}	1.15×10^{-2}
	1×10^{11}	1×10^{9}	1.20×10^{2}		1×10^{11}	1×10^{9}	1.15×10^{2}
		1×10^{10}	1.20×10^{1}			1×10^{10}	1.15×10^{1}
		1×10^{11}	1.20×10^{0}			1×10^{11}	1.15×10^{0}
		1×10^{12}	1.20×10^{-1}			1×10^{12}	1.15×10^{-1}
	1×10^{12}	1×10^{9}	1.20×10^{3}		1×10^{12}	1×10^{9}	1.15×10^{3}
		1×10^{10}	1.20×10^{2}			1×10^{10}	1.15×10^{2}
		1×10^{11}	1.20×10^{1}			1×10^{11}	1.15×10^{1}
		1×10^{12}	1.20×10^{0}			1×10^{12}	1.15×10^{0}
310	1×10^{9}	1×10^{9}	9.52×10^{-1}	320	1×10^{9}	1×10^{9}	8.15×10^{-1}
		1×10^{10}	9.52×10^{-2}			1×10^{10}	8.15×10^{-2}
		1×10^{11}	9.52×10^{-3}			1×10^{11}	8.15×10^{-3}
		1×10^{12}	9.52×10^{-4}			1×10^{12}	8.15×10^{-4}
	1×10^{10}	1×10^{9}	9.52×10^{0}		1×10^{10}	1×10^{9}	8.15×10^{0}
		1×10^{10}	9.52×10^{-1}			1×10^{10}	8.15×10^{-1}
		1×10^{11}	9.52×10^{-2}			1×10^{11}	8.15×10^{-2}
		1×10^{12}	9.52×10^{-3}			1×10^{12}	8.15×10^{-3}
	1×10^{11}	1×10^{9}	9.52×10^{1}		1×10^{11}	1×10^{9}	8.15×10^{1}
		1×10^{10}	9.52×10^{0}			1×10^{10}	8.15×10^{0}
		1×10^{11}	9.52×10^{-1}			1×10^{11}	8.15×10^{-1}
		1×10^{12}	9.52×10^{-2}			1×10^{12}	8.15×10^{-2}
	1×10^{12}	1×10^{9}	9.52×10^{2}		1×10^{12}	1×10^{9}	8.15×10^{2}
		1×10^{10}	9.52×10^{1}			1×10^{10}	8.15×10^{1}
		1×10^{11}	9.52×10^{0}			1×10^{11}	8.15×10^{0}
		1×10^{12}	9.52×10^{-1}			1×10^{12}	8.15×10^{-1}

Table S5 Rate ratios for SO_3 + HNO_3 reaction (v_{R1}) relative to the NH_3-catalyzed SO_3 + NH_3 reaction (v_{R4}) over the temperature range of 280-320K

T (K)	HNO_3	NH_3	v_{R1}/v_{R4}	T (K)	HNO_3	NH_3	v_{R1}/v_{R4}
280	1×10^{9}	1×10^{9}	2.41×10^{0}	290	1×10^{9}	1×10^{9}	2.42×10^{0}
		1×10^{10}	2.41×10^{-1}			1×10^{10}	2.42×10^{-1}
		1×10^{11}	2.41×10^{-2}			1×10^{11}	2.42×10^{-2}
		1×10^{12}	2.41×10^{-3}			1×10^{12}	2.42×10^{-3}
	1×10^{10}	1×10^{9}	2.41×10^{1}		1×10^{10}	1×10^{9}	2.42×10^{1}
		1×10^{10}	2.41×10^{0}			1×10^{10}	2.42×10^{0}
		1×10^{11}	2.41×10^{-1}			1×10^{11}	2.42×10^{-1}
		1×10^{12}	2.41×10^{-2}			1×10^{12}	2.42×10^{-2}
	1×10^{11}	1×10^{9}	2.41×10^{2}		1×10^{11}	1×10^{9}	2.42×10^{2}
		1×10^{10}	2.41×10^{1}			1×10^{10}	2.42×10^{1}
		1×10^{11}	2.41×10^{0}			1×10^{11}	2.42×10^{0}
		1×10^{12}	2.41×10^{-1}			1×10^{12}	2.42×10^{-1}
	1×10^{12}	1×10^{9}	2.41×10^{3}		1×10^{12}	1×10^{9}	2.42×10^{3}
		1×10^{10}	2.41×10^{2}			1×10^{10}	2.42×10^{2}
		1×10^{11}	2.41×10^{1}			1×10^{11}	2.42×10^{1}
		1×10^{12}	2.41×10^{0}			1×10^{12}	2.42×10^{0}
298	1×10^{9}	1×10^{9}	2.42×10^{0}	300	1×10^{9}	1×10^{9}	2.40×10^{0}
		1×10^{10}	2.42×10^{-1}			1×10^{10}	2.40×10^{-1}
		1×10^{11}	2.42×10^{-2}			1×10^{11}	2.40×10^{-2}
		1×10^{12}	2.42×10^{-3}			1×10^{12}	2.40×10^{-3}
	1×10^{10}	1×10^{9}	2.42×10^{1}		1×10^{10}	1×10^{9}	2.40×10^{1}
		1×10^{10}	2.42×10^{0}			1×10^{10}	2.40×10^{0}
		1×10^{11}	2.42×10^{-1}			1×10^{11}	2.40×10^{-1}
		1×10^{12}	2.42×10^{-2}			1×10^{12}	2.40×10^{-2}
	1×10^{11}	1×10^{9}	2.42×10^{2}		1×10^{11}	1×10^{9}	2.40×10^{2}
		1×10^{10}	2.42×10^{1}			1×10^{10}	2.40×10^{1}
		1×10^{11}	2.42×10^{0}			1×10^{11}	2.40×10^{0}
		1×10^{12}	2.42×10^{-1}			1×10^{12}	2.40×10^{-1}
	1×10^{12}	1×10^{9}	2.42×10^{3}		1×10^{12}	1×10^{9}	2.40×10^{3}
		1×10^{10}	2.42×10^{2}			1×10^{10}	2.40×10^{2}
		1×10^{11}	2.42×10^{1}			1×10^{11}	2.40×10^{1}
		1×10^{12}	2.42×10^{0}			1×10^{12}	2.40×10^{0}
310	1×10^{9}	1×10^{9}	2.44×10^{0}	320	1×10^{9}	1×10^{9}	2.54×10^{0}
		1×10^{10}	2.44×10^{-1}			1×10^{10}	2.54×10^{-1}
		1×10^{11}	2.44×10^{-2}			1×10^{11}	2.54×10^{-2}
		1×10^{12}	2.44×10^{-3}			1×10^{12}	2.54×10^{-3}
	1×10^{10}	1×10^{9}	2.44×10^{1}		1×10^{10}	1×10^{9}	2.54×10^{1}
		1×10^{10}	2.44×10^{0}			1×10^{10}	2.54×10^{0}
		1×10^{11}	2.44×10^{-1}			1×10^{11}	2.54×10^{-1}
		1×10^{12}	2.44×10^{-2}			1×10^{12}	2.54×10^{-2}
	1×10^{11}	1×10^{9}	2.44×10^{2}		1×10^{11}	1×10^{9}	2.54×10^{2}
		1×10^{10}	2.44×10^{1}			1×10^{10}	2.54×10^{1}
		1×10^{11}	2.44×10^{0}			1×10^{11}	2.54×10^{0}
		1×10^{12}	2.44×10^{-1}			1×10^{12}	2.54×10^{-1}
	1×10^{12}	1×10^{9}	2.44×10^{3}		1×10^{12}	1×10^{9}	2.54×10^{3}
		1×10^{10}	2.44×10^{2}			1×10^{10}	2.54×10^{2}
		1×10^{11}	2.44×10^{1}			1×10^{11}	2.54×10^{1}
		1×10^{12}	2.44×10^{0}			1×10^{12}	2.54×10^{0}

Table S6 Rate ratios for $SO_3 + H_2O$ reaction (v_{R1}) relative to the H_2O-catalyzed hydrolysis of SO_3 reaction (v_{R5}) over the temperature range of 280-320K

T (K)	HNO_3	H_2O	v_{R1}/v_{R5}	T (K)	HNO_3	H_2O	v_{R1}/v_{R5}
280	1×10^{9}	20%	5.79×10^{-4}	290	1×10^{9}	20%	3.97×10^{-4}
		40%	1.45×10^{-4}			40%	9.97×10^{-5}
		60%	6.43×10^{-5}			60%	4.42×10^{-5}
		80%	3.61×10^{-5}			80%	2.49×10^{-5}
	1×10^{10}	20%	5.79×10^{-3}		1×10^{10}	20%	3.97×10^{-3}
		40%	1.45×10^{-3}			40%	9.97×10^{-4}
		60%	6.43×10^{-4}			60%	4.42×10^{-4}
		80%	3.61×10^{-4}			80%	2.49×10^{-4}
	1×10^{11}	20%	5.79×10^{-2}		1×10^{11}	20%	3.97×10^{-2}
		40%	1.45×10^{-2}			40%	9.97×10^{-3}
		60%	6.43×10^{-3}			60%	4.42×10^{-3}
		80%	3.61×10^{-3}			80%	2.49×10^{-3}
	1×10^{12}	20%	5.79×10^{-1}		1×10^{12}	20%	2.49×10^{-2}
		40%	1.45×10^{-1}			40%	3.97×10^{0}
		60%	6.43×10^{-2}			60%	9.97×10^{-1}
		80%	3.61×10^{-2}			80%	4.42×10^{-1}
	1×10^{13}	20%	5.79×10^{0}		1×10^{13}	20%	2.49×10^{-1}
		40%	1.45×10^{0}			40%	3.97×10^{-4}
		60%	6.43×10^{-1}			60%	9.97×10^{-5}
		80%	3.61×10^{-1}			80%	4.42×10^{-5}
298	1×10^{9}	20%	3.05×10^{-4}	300	1×10^{9}	20%	3.05×10^{-4}
		40%	7.38×10^{-5}			40%	7.38×10^{-5}
		60%	3.39×10^{-5}			60%	3.39×10^{-5}
		80%	1.85×10^{-5}			80%	1.85×10^{-5}
	1×10^{10}	20%	3.05×10^{-3}		1×10^{10}	20%	3.05×10^{-3}
		40%	7.38×10^{-4}			40%	7.38×10^{-4}
		60%	3.39×10^{-4}			60%	3.39×10^{-4}
		80%	1.85×10^{-4}			80%	1.85×10^{-4}
	1×10^{11}	20%	3.05×10^{-2}		1×10^{11}	20%	3.05×10^{-2}
		40%	7.38×10^{-3}			40%	7.38×10^{-3}
		60%	3.39×10^{-3}			60%	3.39×10^{-3}
		80%	1.85×10^{-3}			80%	1.85×10^{-3}
	1×10^{12}	20%	3.05×10^{-1}		1×10^{12}	20%	3.05×10^{-1}
		40%	7.38×10^{-2}			40%	7.38×10^{-2}
		60%	3.39×10^{-2}			60%	3.39×10^{-2}
		80%	1.85×10^{-2}			80%	1.85×10^{-2}
	1×10^{13}	20%	3.05×10^{0}		1×10^{13}	20%	3.05×10^{0}
		40%	7.38×10^{-1}			40%	7.38×10^{-1}
		60%	3.39×10^{-1}			60%	3.39×10^{-1}
		80%	1.85×10^{-1}			80%	1.85×10^{-1}
310	1×10^{9}	20%	2.78×10^{-4}	320	1×10^{9}	20%	2.04×10^{-4}
		40%	6.98×10^{-5}			40%	5.10×10^{-5}
		60%	3.10×10^{-5}			60%	2.44×10^{-5}
		80%	1.75×10^{-5}			80%	1.27×10^{-5}
	1×10^{10}	20%	2.78×10^{-3}		1×10^{10}	20%	2.04×10^{-3}
		40%	6.98×10^{-4}			40%	5.10×10^{-4}
		60%	3.10×10^{-4}			60%	2.44×10^{-4}
		80%	1.75×10^{-4}			80%	1.27×10^{-4}
	1×10^{11}	20%	2.78×10^{-2}		1×10^{11}	20%	2.04×10^{-2}
		40%	6.98×10^{-3}			40%	5.10×10^{-3}
		60%	3.10×10^{-3}			60%	2.44×10^{-3}
		80%	1.75×10^{-3}			80%	1.27×10^{-3}
	1×10^{12}	20%	2.78×10^{-1}		1×10^{12}	20%	2.04×10^{-1}

	40%	6.98×10^{-2}		40%	5.10×10^{-2}
	60%	3.10×10^{-2}		60%	2.44×10^{-2}
	80%	1.75×10^{-2}		80%	1.27×10^{-2}
1×10^{13}	20%	2.78×10^{0}	1×10^{13}	20%	2.04×10^{0}
	40%	6.98×10^{-1}		40%	5.10×10^{-1}
	60%	3.10×10^{-1}		60%	2.44×10^{-1}
	80%	1.75×10^{-1}		80%	1.27×10^{-1}

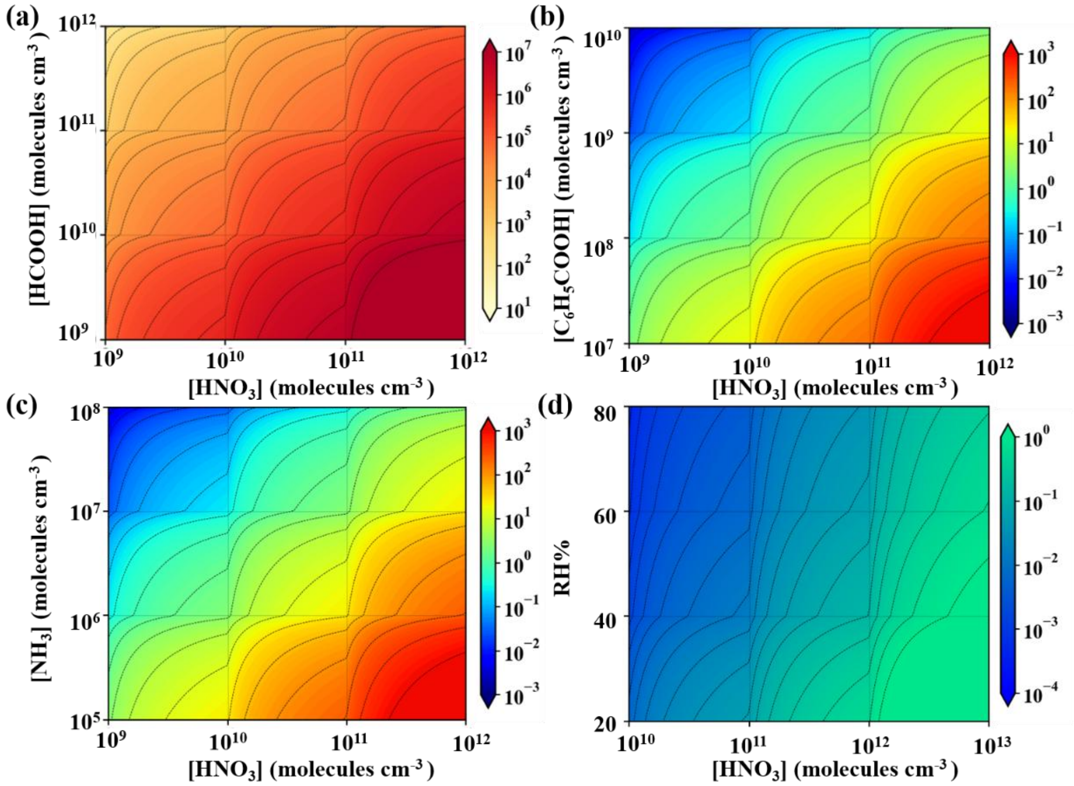

Fig. S1 Rate ratios of v_{R1}/v_{R2} (a), v_{R1}/v_{R3} (b), v_{R1}/v_{R4} (c) and v_{R1}/v_{R5} (d) at 280 K

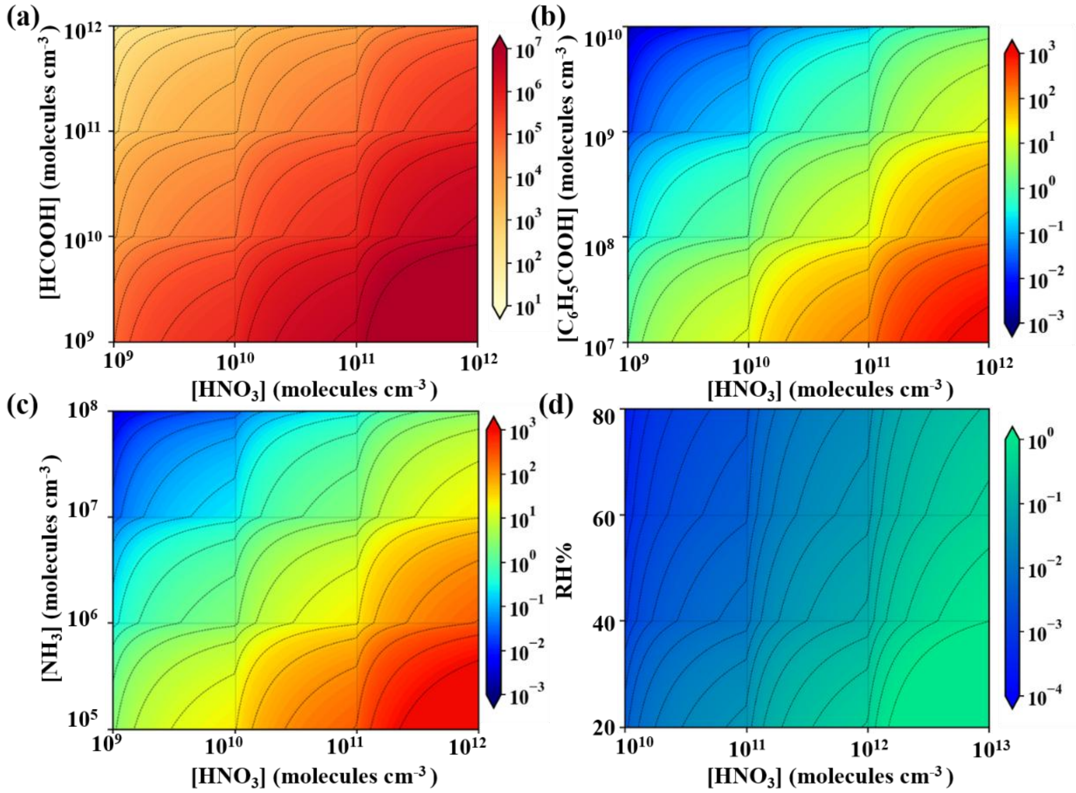

Fig. S2 Rate ratios of v_{R1}/v_{R2} (a), v_{R1}/v_{R3} (b), v_{R1}/v_{R4} (c) and v_{R1}/v_{R5} (d) at 290 K

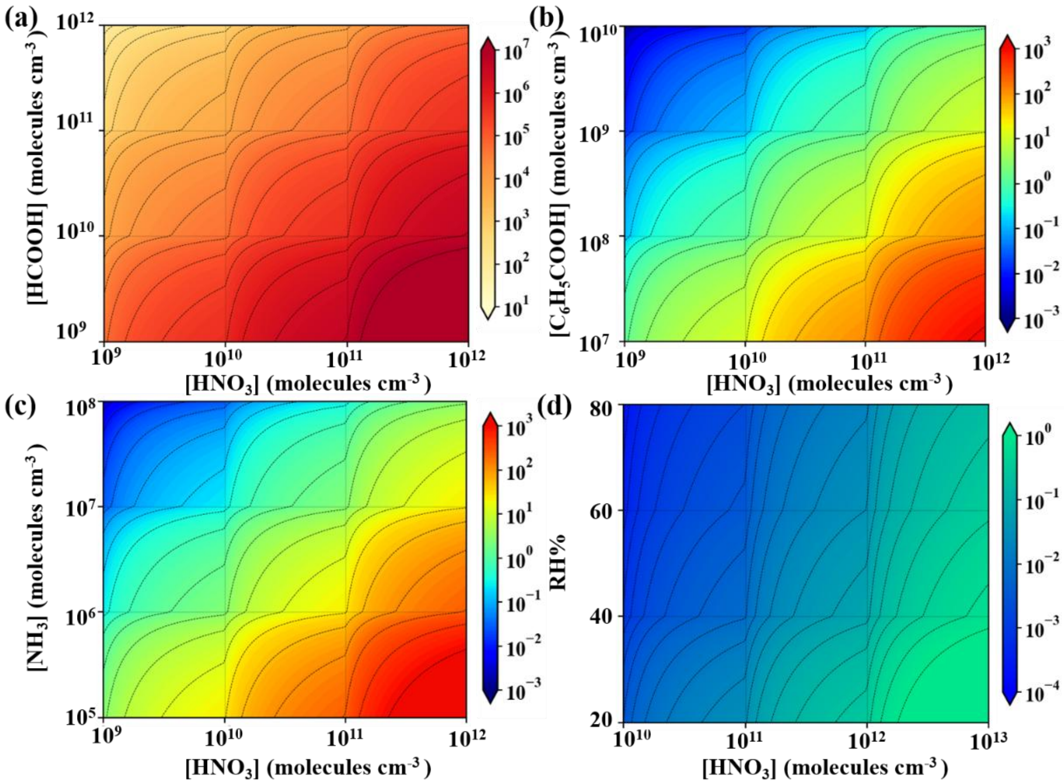

Fig. S3 Rate ratios of v_{R1}/v_{R2} (a), v_{R1}/v_{R3} (b), v_{R1}/v_{R4} (c) and v_{R1}/v_{R5} (d) at 300 K

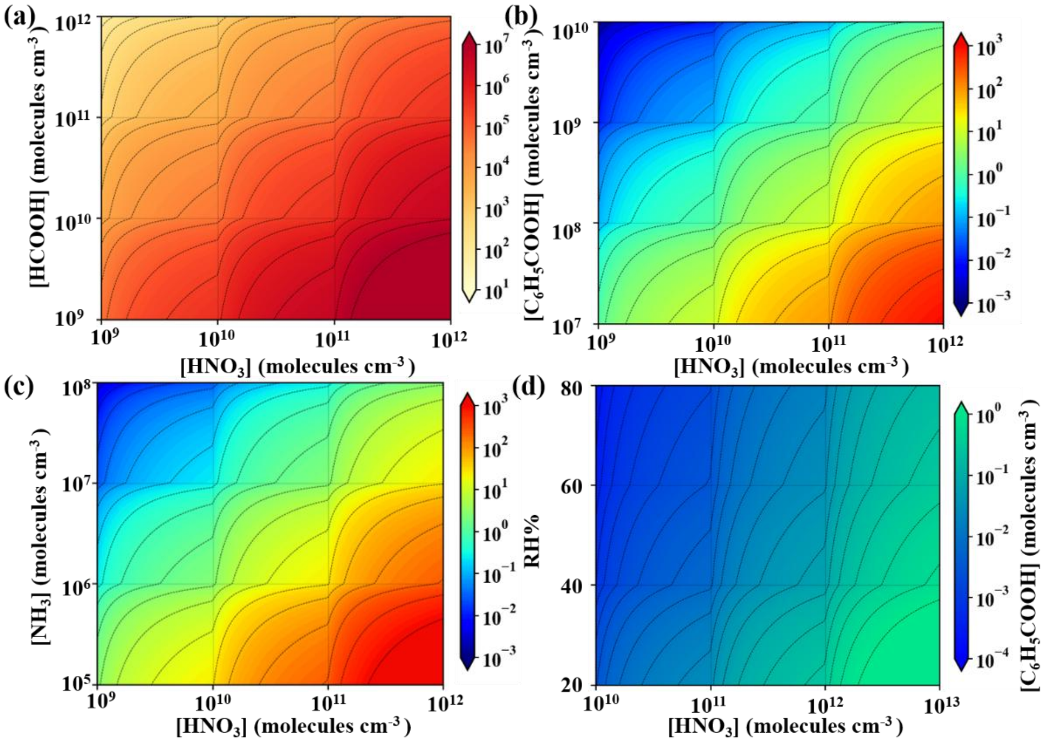

Fig. S4 Rate ratios of v_{R1}/v_{R2} (a), v_{R1}/v_{R3} (b), v_{R1}/v_{R4} (c) and v_{R1}/v_{R5} (d) at 310 K

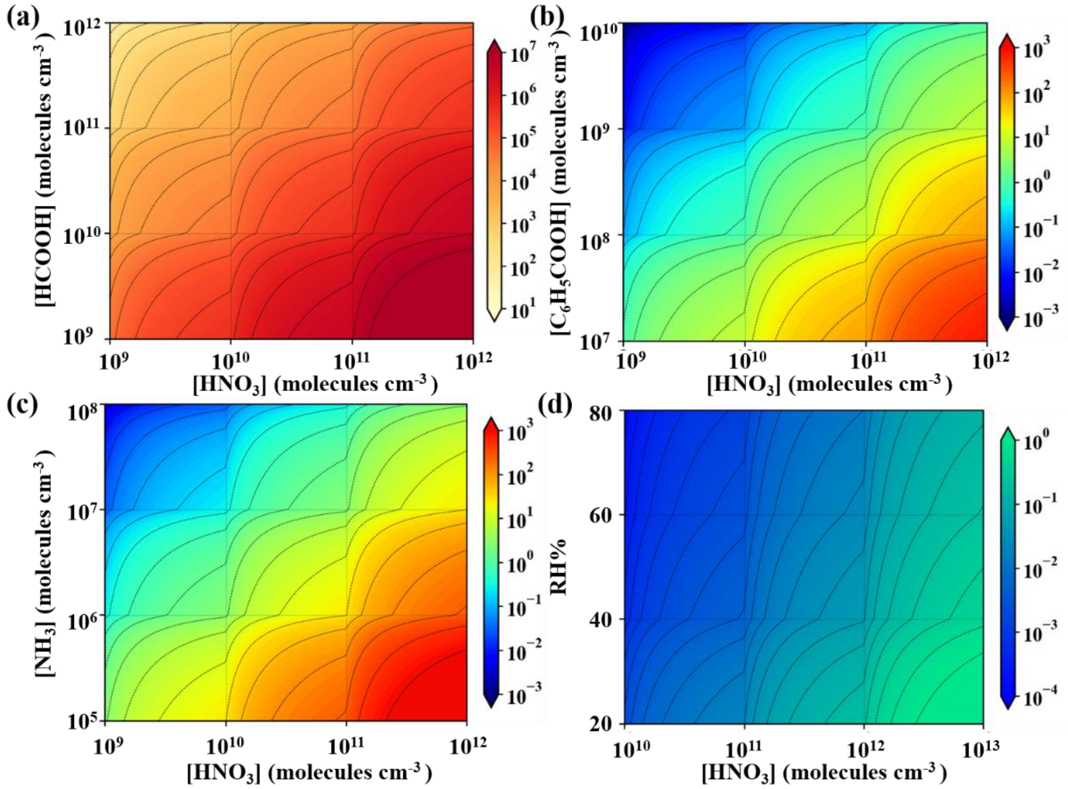

Fig. S5 Rate ratios of v_{R1}/v_{R2} (a), v_{R1}/v_{R3} (b), v_{R1}/v_{R4} (c) and v_{R1}/v_{R5} (d) at 320 K

Part S2 Collision coefficients and evaporation coefficients

The collision coefficients $\beta_{i,j}$, which characterize the interactions between clusters i and j, can be determined using the hard-sphere collision theory:

$$\beta_{i,j} = \pi(r_i + r_j)^2 \sqrt{\frac{8k_B T}{\pi\mu}} \tag{S2}$$

In Eq. (S2), r_i is the radius of cluster i, which is calculated using the Multiwfn 3.8 program; k_B denotes the Boltzmann constant; T represents the temperature and $\mu = m_i \times m_j/(m_i + m_j)$ signifies the reduced mass. The radius of a cluster is defined as half the sum of the maximum distance between any two corresponding atoms within the cluster, as determined by the Multiwfn 3.8 program, and the van der Waals radii of these constituent atoms.

Evaporation coefficient $\gamma_{(i+j)\to i}$ was calculated by utilizing the relevant collision coefficients and the Gibbs free energies associated with cluster formation, which can be written in Eq. (S3):

$$\gamma_{(i+j)\to i} = \beta_{i,j} \frac{P_{ref}}{k_B T} \exp\left(\frac{\Delta G_{i+j} - \Delta G_i - \Delta G_j}{k_B T}\right) \tag{S3}$$

In Eq. (3), P_{ref} denotes the reference pressure, corresponding to the standard pressure of 1 atm at which the formation free energies were computed, and ΔG_{i+j} signifies the Gibbs free energy of formation of cluster $i + j$, derived from its constituent monomers.

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.

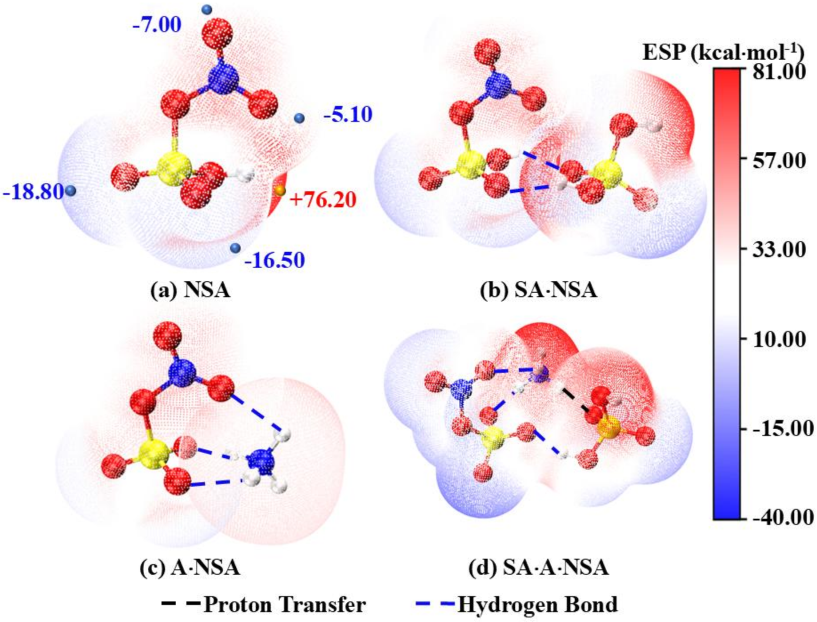

Fig. S6 ESP-mapped molecular vdW surface of (a) NSA, (b) SA·NSA, (c) A·NSA and (d) SA·A·NSA at M06-2X/6-311++G(2*df*,2*pd*) level of theory. Color coding: blue = nitrogen, red = oxygen, yellow = sulfur and white = hydrogen. The black line represents the proton transfer, and the blue line represents the hydrogen bond

The stability of molecular clusters relies on strong interactions among nucleation precursors. The possible binding sites of NSA with SA and A were examined by analyzing the electrostatic potential (ESP) mapped onto the van der Waals surfaces. As illustrated in Fig. S6, the hydrogen atom in the $-SO_3H$ group in NSA exhibits the most positive ESP value (+ 76.20 kcal·mol^{-1}), identifying it is a strong HB donor. In contrast, the oxygen atoms in both the $-SO_3H$ and $-ONO_2$ groups serve as potential HB acceptors due to their high electronegativity. Similarly, in SA and A, hydrogen atoms show positive ESP values (donors), while oxygen and nitrogen atoms show negative ESP values (acceptors). Therefore, when NSA interacts with SA or A, stable clusters can form through one, two or even three proton-transfer events. For instance, in the ternary $(SA)_1{\cdot}(A)_1{\cdot}(NSA)_1$ cluster (Fig. S6 (d)), one proton is transferred and three strong hydrogen bonds are established, underscoring the role of NSA in enhancing stability via intermolecular proton transfer and hydrogen bonding.

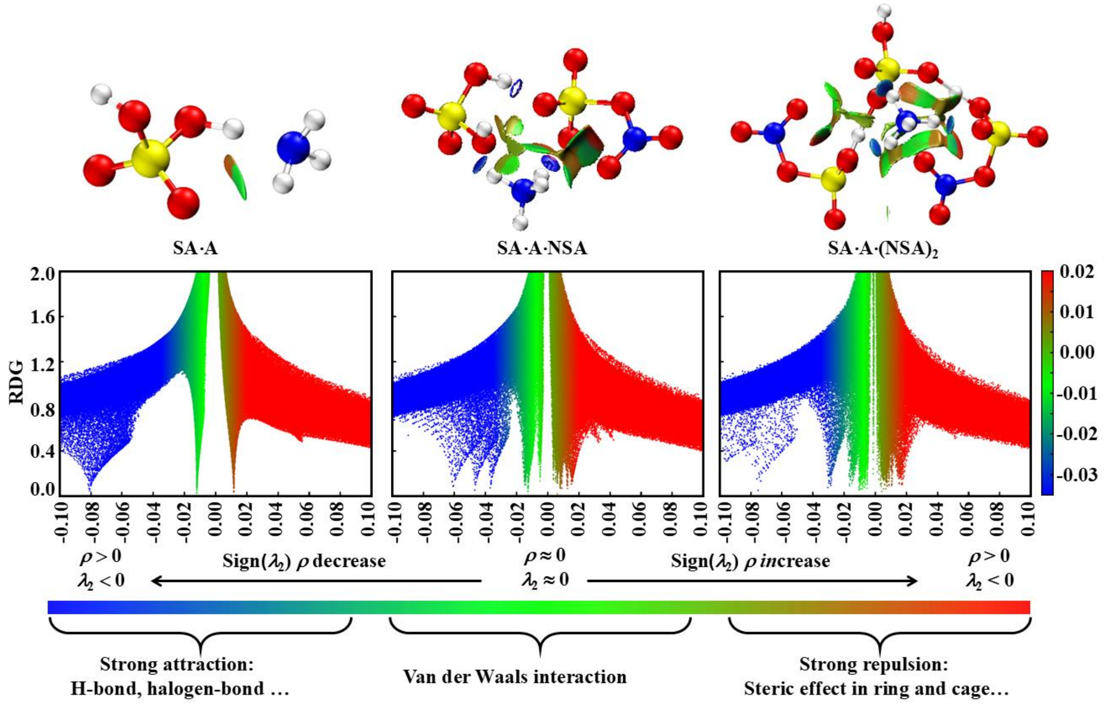

Fig. S7 RDG color-filled maps and isosurface of the SA·A, SA·A·NSA and SA·A·$(NSA)_2$ clusters

The reduced density gradient (RDG) method was applied to characterize intermolecular interactions within the binary SA·A cluster as well as in the ternary SA·A·NSA and SA·A·$(NSA)_2$ clusters. The RDG scatter plot (Fig. S7) reveal a prominent blue spike at negative values of sign(λ_2)ρ, which corresponds to strong attractive non-covalent interactions such as hydrogen bonds. Regions in green represent van der Waals interactions, while red areas indicate steric repulsion. The accompanying molecular configurations (top row of Fig. S7) clearly illustrate these attractive and van der Waals interactions. Quantitatively, the SA·A·NSA cluster exhibits two additional blue spikes compared to the binary SA·A system. Moreover, in the SA·A·$(NSA)_2$ cluster, the primary blue spike shifts further leftward relative to that in SA·A·NSA. These results confirm that the incorporation of NSA strengthens the hydrogen-bonding network within the SA-A-NSA system.

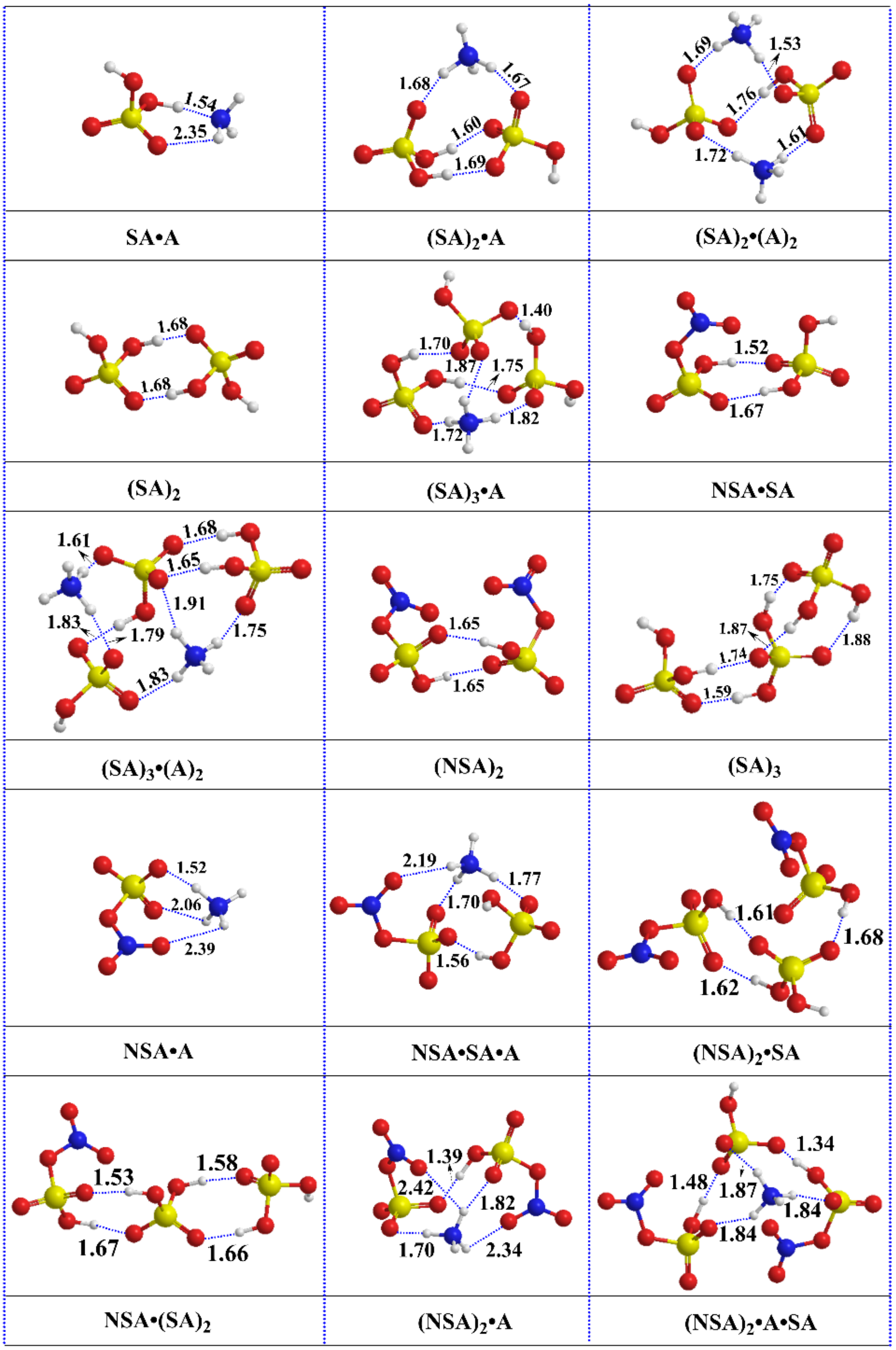

Fig. S8 The most stable configurations of the NSA-SA-A-based clusters identified at the M06-2X/6-311++G(2*df*,2*pd*) level of theory. The lengths of hydrogen bonds are given in Å (Color code: blue = nitrogen, yellow = sulfur, red = oxygen, gray = carbon and white = hydrogen)

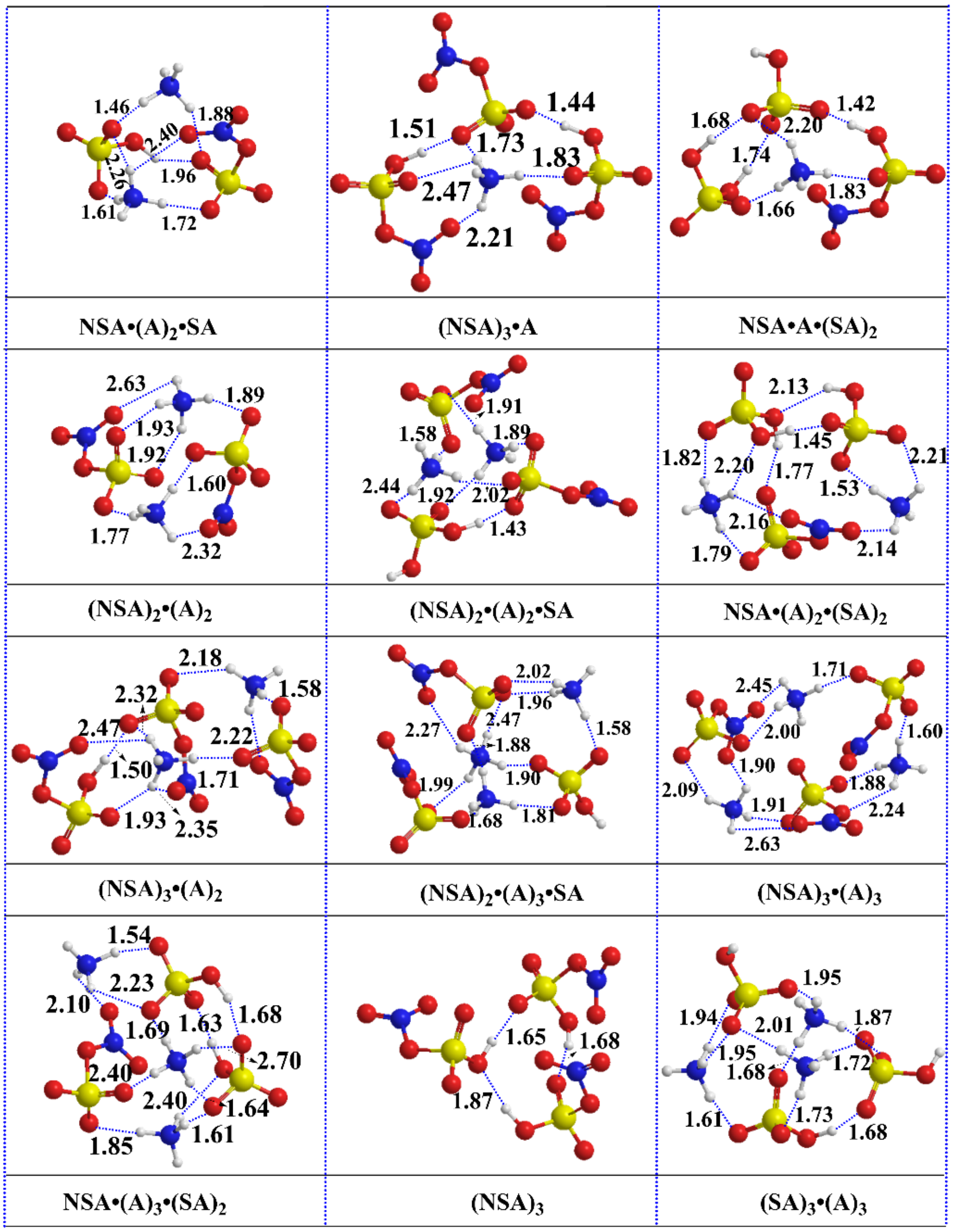

Fig. S9 The most stable configurations of the NSA-SA-A-based clusters identified at the M06-2X/6-311++G(2*df*,2*pd*) level of theory. The lengths of hydrogen bonds are given in Å (Color code: blue = nitrogen, yellow = sulfur, red = oxygen, gray = carbon and white = hydrogen)

Table S7 Gibbs free energy of cluster formation, ΔG (kcal·mol^{-1}), for all clusters at pressure of 1 atm and temperatures ranges of 298.15, 288.15, 278.15, 268.15 and 258.15 K

Clusters	T = 298.15 K	T = 288.15 K	T = 278.15 K	T = 268.15 K	T = 258.15 K
SA·A	-5.61	-5.93	-6.25 (-7.94)	-6.56	-6.88 (-8.54)
$(SA)_2$	-5.94	-6.35	-6.77 (-8.20)	-7.18	-7.59 (-9.77)
$(SA)_2$·A	-20.49	-21.26	-22.03 (-23.13)	-22.80	-23.57 (-24.65)
$(SA)_2$·$(A)_2$	-28.17	-29.32	-30.48 (-29.84)	-31.64	-32.80 (-32.07)
$(SA)_3$	-11.95	-12.76	-13.57 (-14.67)	-14.38	-15.20 (-16.41)
$(SA)_3$·A	-30.62	-31.76	-32.91 (-32.53)	-34.06	-35.21 (-34.91)
$(SA)_3$·$(A)_2$	-42.15	-46.80	-45.29 (-46.46)	-49.83	-48.43 (-49.50)
$(SA)_3$·$(A)_3$	-58.37	-60.26	-62.14	-64.03	-65.92
$(NSA)_2$	-4.03	-4.41	-4.80	-5.19	-5.58
A·NSA	-9.50	-9.87	-10.24	-10.61	-10.98
$(A)_2$·$(NSA)_2$	-38.14	-39.25	-40.35	-41.45	-42.56
A·$(NSA)_2$	-18.91	-19.69	-20.46	-21.24	-22.01
SA·NSA	-5.29	-5.68	-6.06	-6.46	-6.84
SA·A·NSA	-20.21	-20.94	-21.66	-22.39	-23.12
SA·$(A)_2$·NSA	-29.68	-30.81	-31.94	-33.06	-34.19
$(NSA)_3$	-3.92	-4.65	-5.39	-6.12	-6.86
SA_2·A·NSA	-29.19	-30.37	-31.56	-32.74	-33.93
$(SA)_2$·$(A)_2$·NSA	-39.94	-41.53	-43.11	-44.70	-46.28
$(SA)_2$·$(A)_3$·NSA	-52.70	-54.66	-56.63	-58.60	-60.57
SA·$(NSA)_2$	-7.31	-8.13	-8.94	-9.75	-10.57
A·$(NSA)_3$	-27.49	-28.59	-29.69	-30.80	-31.91
SA·$(A)_2$·$(NSA)_2$	-47.93	-49.47	-51.01	-52.55	-54.10
$(SA)_2$·NSA	-9.70	-10.45	-11.20	-11.95	-12.71
SA·A·$(NSA)_2$	-23.51	-24.73	-25.96	-27.19	-28.42
$(A)_2$·$(NSA)_3$	-39.30	-40.77	-42.26	-43.74	-45.22
SA·$(A)_3$·$(NSA)_2$	-61.03	-62.94	-64.85	-66.76	-68.68
$(A)_3$·$(NSA)_3$	-59.79	-61.68	-63.57	-65.46	-67.36

Table S8 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	288.15 K	278.15 K	268.15 K	258.15 K
SA + A	1.65×10^{-10}	1.59×10^{-10}	1.54×10^{-10}	1.48×10^{-10}	1.42×10^{-10}
SA + NSA	7.12×10^{-11}	6.88×10^{-11}	6.64×10^{-11}	6.40×10^{-11}	6.16×10^{-11}
A + NSA	2.03×10^{-10}	1.96×10^{-10}	1.89×10^{-10}	1.83×10^{-10}	1.83×10^{-10}
SA + SA	6.77×10^{-11}	6.55×10^{-11}	6.32×10^{-11}	6.09×10^{-11}	5.87×10^{-11}
NSA + NSA	7.06×10^{-11}	6.82×10^{-11}	6.58×10^{-11}	6.35×10^{-11}	6.11×10^{-11}
$(SA)_2$ + A	2.82×10^{-10}	2.73×10^{-10}	2.63×10^{-10}	2.54×10^{-10}	2.45×10^{-10}
SA·A + SA	8.95×10^{-11}	8.65×10^{-11}	8.35×10^{-11}	8.05×10^{-11}	7.75×10^{-11}
$(SA)_2$·A + A	2.95×10^{-10}	2.85×10^{-10}	2.75×10^{-10}	2.65×10^{-10}	2.55×10^{-10}
$(NSA)_2$ + A	3.04×10^{-10}	2.94×10^{-10}	2.84×10^{-10}	2.74×10^{-10}	2.63×10^{-10}
A·NSA + NSA	7.34×10^{-11}	7.01×10^{-11}	6.85×10^{-11}	6.60×10^{-11}	6.36×10^{-11}
A·$(NSA)_2$ + A	3.45×10^{-10}	3.33×10^{-10}	3.21×10^{-10}	3.10×10^{-10}	2.98×10^{-10}
$(SA)_2$ + NSA	8.13×10^{-11}	7.86×10^{-11}	7.59×10^{-11}	7.31×10^{-11}	7.04×10^{-11}
SA·NSA + SA	8.64×10^{-11}	8.35×10^{-11}	8.06×10^{-11}	7.77×10^{-11}	7.48×10^{-11}
$(NSA)_2$ + SA	8.48×10^{-11}	8.20×10^{-11}	7.91×10^{-11}	7.63×10^{-11}	7.34×10^{-11}
SA·NSA + NSA	7.92×10^{-11}	7.65×10^{-11}	7.39×10^{-11}	7.12×10^{-11}	6.86×10^{-11}
$(SA)_2$ + SA	8.67×10^{-11}	8.38×10^{-11}	8.09×10^{-11}	7.80×10^{-11}	7.51×10^{-11}
$(NSA)_2$ + NSA	7.65×10^{-11}	7.39×10^{-11}	7.14×10^{-11}	6.88×10^{-11}	6.62×10^{-11}
$(SA)_2$·A + SA	8.82×10^{-11}	8.52×10^{-11}	8.23×10^{-11}	7.93×10^{-11}	7.63×10^{-11}
$(SA)_3$ + A	4.00×10^{-10}	3.87×10^{-10}	3.73×10^{-10}	3.60×10^{-10}	3.46×10^{-10}
$(SA)_2$·$(A)_2$ + SA	9.40×10^{-11}	9.09×10^{-11}	8.77×10^{-11}	8.46×10^{-11}	8.14×10^{-11}
$(SA)_3$·A + A	3.16×10^{-10}	3.05×10^{-10}	2.95×10^{-10}	2.84×10^{-10}	2.73×10^{-10}
$(SA)_3$·$(A)_2$ + A	4.15×10^{-10}	4.01×10^{-10}	3.87×10^{-10}	3.73×10^{-10}	3.59×10^{-10}
A·$(NSA)_2$ + NSA	8.34×10^{-11}	8.06×10^{-11}	7.78×10^{-11}	7.50×10^{-11}	7.22×10^{-11}
$(NSA)_3$ + A	3.86×10^{-10}	3.73×10^{-10}	3.60×10^{-10}	3.47×10^{-10}	3.34×10^{-10}
$(A)_2$·$(NSA)_2$ + NSA	8.95×10^{-11}	8.65×10^{-11}	8.35×10^{-11}	8.05×10^{-11}	7.75×10^{-11}
A·$(NSA)_3$ + A	4.01×10^{-10}	3.88×10^{-10}	3.74×10^{-10}	3.61×10^{-10}	3.47×10^{-10}
$(A)_2$·$(NSA)_3$ + A	3.90×10^{-10}	3.77×10^{-10}	3.64×10^{-10}	3.51×10^{-10}	3.38×10^{-10}
A·NSA + SA	7.55×10^{-11}	7.30×10^{-11}	7.05×10^{-11}	6.79×10^{-11}	6.54×10^{-11}
SA·A + NSA	8.95×10^{-11}	8.65×10^{-11}	8.35×10^{-11}	8.05×10^{-11}	7.75×10^{-11}
SA·NSA + A	2.98×10^{-10}	2.88×10^{-10}	2.78×10^{-10}	2.68×10^{-10}	2.58×10^{-10}
SA·A·NSA + A	2.88×10^{-10}	2.79×10^{-10}	2.69×10^{-10}	2.59×10^{-10}	2.50×10^{-10}

Collisions	β ($cm^3 \cdot s^{-1}$)				
	298.15 K	288.15 K	278.15 K	268.15 K	258.15 K
SA·A·NSA + SA	8.27×10^{-11}	7.99×10^{-11}	7.71×10^{-11}	7.43×10^{-11}	7.16×10^{-11}
$(SA)_2$·A + NSA	8.18×10^{-11}	7.90×10^{-11}	7.63×10^{-11}	7.35×10^{-11}	7.08×10^{-11}
$(SA)_2$·NSA + A	4.53×10^{-10}	4.38×10^{-10}	4.22×10^{-10}	4.07×10^{-10}	3.92×10^{-10}
SA·$(A)_2$·NSA + SA	7.86×10^{-11}	7.60×10^{-11}	7.33×10^{-11}	7.07×10^{-11}	6.81×10^{-11}
$(SA)_2$·$(A)_2$ + NSA	8.60×10^{-11}	8.31×10^{-11}	8.03×10^{-11}	7.74×10^{-11}	7.45×10^{-11}
$(SA)_2$·A·NSA + A	4.36×10^{-10}	4.21×10^{-10}	4.06×10^{-10}	3.92×10^{-10}	3.77×10^{-10}
$(SA)_2$·$(A)_2$·NSA + A	3.66×10^{-10}	3.53×10^{-10}	3.41×10^{-10}	3.29×10^{-10}	3.17×10^{-10}
A·$(NSA)_2$ + SA	9.37×10^{-11}	9.06×10^{-11}	8.74×10^{-11}	8.43×10^{-11}	8.11×10^{-11}
SA·A·NSA + NSA	7.55×10^{-11}	7.29×10^{-11}	7.04×10^{-11}	6.79×10^{-11}	6.54×10^{-11}
SA·$(NSA)_2$ + A	4.94×10^{-10}	4.78×10^{-10}	4.61×10^{-10}	4.44×10^{-10}	4.28×10^{-10}
$(A)_2$·$(NSA)_2$ + SA	1.02×10^{-10}	9.83×10^{-11}	9.49×10^{-11}	9.15×10^{-11}	8.81×10^{-11}
SA·$(A)_2$·NSA + NSA	7.16×10^{-11}	6.92×10^{-11}	6.68×10^{-11}	6.44×10^{-11}	6.20×10^{-11}
SA·A·$(NSA)_2$ + A	4.18×10^{-10}	4.04×10^{-10}	3.90×10^{-10}	3.76×10^{-10}	3.62×10^{-10}
SA·$(A)_2$·$(NSA)_2$ + A	3.93×10^{-10}	3.80×10^{-10}	3.67×10^{-10}	3.54×10^{-10}	3.40×10^{-10}

Table S9 Evaporation rates γ (s^{-1}) for the studied clusters at different temperatures of 298.15, 288.15, 278.15, 268.15 and 258.15 K

Evaporation pathways	298.15 K	288.15 K	278.15 K	268.15 K	258.15 K
A·A → SA + A	3.11×10^{5}	1.29×10^{5}	4.98×10^{4}	3.27×10^{4}	2.08×10^{4}
SA·NSA → SA + NSA	2.31×10^{5}	8.56×10^{4}	3.00×10^{4}	1.99×10^{4}	1.28×10^{4}
A·NSA→ A + NSA	5.43×10^{2}	1.63×10^{2}	4.47×10^{1}	2.24×10^{1}	1.11×10^{1}
$(SA)_2$ → SA + SA	7.31×10^{4}	2.52×10^{4}	8.02×10^{3}	5.08×10^{3}	3.11×10^{3}
$(NSA)_2$ → NSA + NSA	1.94×10^{6}	7.81×10^{5}	2.93×10^{5}	2.12×10^{5}	1.50×10^{5}
$(SA)_2$·A → $(SA)_2$ + A	1.51×10^{-1}	3.43×10^{-2}	7.01×10^{-3}	2.50×10^{-3}	8.25×10^{-4}
$(SA)_2$·A → SA·A + SA	2.73×10^{-2}	5.17×10^{-3}	8.69×10^{-4}	2.99×10^{-4}	9.50×10^{-5}
$(SA)_2$·$(A)_2$ → $(SA)_2$·A + A	1.69×10^{4}	5.51×10^{3}	1.65×10^{3}	9.31×10^{2}	5.03×10^{2}
A·$(NSA)_2$ → $(NSA)_2$ + A	9.11×10^{-2}	1.93×10^{-2}	3.66×10^{-3}	1.27×10^{-3}	4.07×10^{-4}
A·$(NSA)_2$ → A·NSA + NSA	2.26×10^{2}	6.43×10^{1}	1.67×10^{1}	8.35×10^{0}	3.97×10^{0}
$(A)_2$·$(NSA)_2$ → A·$(NSA)_2$ + A	6.70×10^{-5}	1.23×10^{-5}	1.98×10^{-6}	5.18×10^{-7}	1.22×10^{-7}
$(SA)_2$·NSA → $(SA)_2$ + NSA	3.52×10^{6}	1.56×10^{6}	6.51×10^{5}	4.83×10^{5}	3.50×10^{5}
$(SA)_2$·NSA → SA·NSA + SA	1.24×10^{6}	5.12×10^{5}	1.95×10^{5}	1.38×10^{5}	9.46×10^{4}
SA·$(NSA)_2$ → $(NSA)_2$ + SA	8.12×10^{6}	3.19×10^{6}	1.17×10^{6}	8.81×10^{5}	6.52×10^{5}
SA·$(NSA)_2$ → SA·NSA + NSA	6.42×10^{7}	2.74×10^{7}	1.07×10^{7}	8.84×10^{6}	7.17×10^{6}
$(SA)_3$ → $(SA)_2$ + SA	8.48×10^{4}	2.96×10^{4}	9.57×10^{3}	6.05×10^{3}	3.69×10^{3}

Evaporation pathways	298.15 K	288.15 K	278.15 K	268.15 K	258.15 K
$(NSA)_3 \rightarrow (NSA)_2 + NSA$	2.25×10^{9}	1.23×10^{9}	6.48×10^{8}	6.23×10^{8}	5.97×10^{8}
$(SA)_3 \cdot A \rightarrow (SA)_2 \cdot A + SA$	8.09×10^{1}	2.32×10^{1}	6.06×10^{0}	2.91×10^{0}	1.32×10^{0}
$(SA)_3 \cdot A \rightarrow (SA)_3 + A$	2.01×10^{-4}	3.75×10^{-5}	6.19×10^{-6}	1.68×10^{-6}	4.11×10^{-7}
$(SA)_3 \cdot (A)_2 \rightarrow (SA)_2 \cdot (A)_2 + SA$	1.30×10^{-1}	1.28×10^{-4}	5.34×10^{-3}	1.97×10^{-3}	6.70×10^{-4}
$(SA)_3 \cdot (A)_2 \rightarrow (SA)_3 \cdot A + A$	2.74×10^{1}	3.06×10^{-2}	1.46×10^{0}	6.32×10^{-1}	2.57×10^{-1}
$(SA)_3 \cdot (A)_3 \rightarrow (SA)_3 \cdot (A)_2 + A$	1.29×10^{-2}	6.27×10^{-1}	5.78×10^{-4}	1.85×10^{-4}	5.44×10^{-5}
$A \cdot (NSA)_3 \rightarrow A \cdot (NSA)_2 + NSA$	1.06×10^{3}	3.61×10^{2}	1.14×10^{2}	6.12×10^{1}	3.13×10^{1}
$A \cdot (NSA)_3 \rightarrow (NSA)_3 + A$	5.00×10^{-8}	6.60×10^{-9}	7.51×10^{-10}	1.46×10^{-10}	2.49×10^{-11}
$(A)_2 \cdot (NSA)_3 \rightarrow (A)_2 \cdot (NSA)_2 + NSA$	3.15×10^{8}	1.53×10^{8}	7.00×10^{7}	6.16×10^{7}	5.36×10^{7}
$(A)_2 \cdot (NSA)_3 \rightarrow A \cdot (NSA)_3 + A$	2.16×10^{1}	5.61×10^{0}	1.32×10^{0}	5.65×10^{-1}	2.27×10^{-1}
$(A)_3 \cdot (NSA)_3 \rightarrow (A)_2 \cdot (NSA)_3 + A$	8.95×10^{-6}	1.32×10^{-6}	1.69×10^{-7}	4.00×10^{-8}	8.49×10^{-9}
$SA \cdot NSA \cdot A \rightarrow A \cdot NSA + SA$	2.59×10^{1}	7.44×10^{0}	1.95×10^{0}	9.02×10^{-1}	3.93×10^{-1}
$SA \cdot A \cdot NSA \rightarrow SA \cdot A + NSA$	4.34×10^{-2}	9.05×10^{-3}	1.68×10^{-3}	5.95×10^{-4}	1.94×10^{-4}
$SA \cdot A \cdot NSA \rightarrow SA \cdot NSA + A$	8.41×10^{-2}	1.96×10^{-2}	4.03×10^{-3}	1.41×10^{-3}	4.52×10^{-4}
$SA \cdot (A)_2 \cdot NSA \rightarrow SA \cdot A \cdot NSA + A$	8.03×10^{2}	2.30×10^{2}	5.99×10^{1}	3.00×10^{1}	1.42×10^{1}
$(SA)_2 \cdot A \cdot NSA \rightarrow SA \cdot A \cdot NSA + SA$	5.35×10^{2}	1.42×10^{2}	3.42×10^{1}	1.75×10^{1}	8.53×10^{0}
$(SA)_2 \cdot A \cdot NSA \rightarrow (SA)_2 \cdot A + NSA$	8.41×10^{2}	2.46×10^{2}	6.55×10^{1}	3.44×10^{1}	1.72×10^{1}

Evaporation pathways	298.15 K	288.15 K	278.15 K	268.15 K	258.15 K
$(SA)_2 \cdot A \cdot NSA \rightarrow (SA)_2 \cdot NSA + A$	5.76×10^{-5}	8.62×10^{-6}	1.12×10^{-6}	2.85×10^{-7}	6.48×10^{-8}
$(SA)_2 \cdot (A)_2 \cdot NSA \rightarrow SA \cdot (A)_2 \cdot NSA + SA$	5.80×10^{1}	1.43×10^{1}	3.17×10^{0}	1.49×10^{0}	6.61×10^{-1}
$(SA)_2 \cdot (A)_2 \cdot NSA \rightarrow (SA)_2 \cdot (A)_2 + NSA$	4.89×10^{0}	1.17×10^{0}	2.50×10^{-1}	1.07×10^{-1}	4.26×10^{-2}
$(SA)_2 \cdot (A)_2 \cdot NSA \rightarrow (SA)_2 \cdot A \cdot NSA + A$	1.38×10^{2}	3.67×10^{1}	8.83×10^{0}	4.05×10^{0}	1.75×10^{0}
$(SA)_2 \cdot (A)_3 \cdot NSA \rightarrow (SA)_2 \cdot (A)_2 \cdot NSA + A$	4.01×10^{0}	9.73×10^{-1}	2.13×10^{-1}	8.54×10^{-2}	3.20×10^{-2}
$SA \cdot A \cdot (NSA)_2 \rightarrow A \cdot (NSA)_2 + SA$	9.86×10^{5}	3.43×10^{5}	1.10×10^{5}	7.62×10^{4}	5.11×10^{4}
$SA \cdot A \cdot (NSA)_2 \rightarrow SA \cdot A \cdot NSA + NSA$	7.13×10^{6}	2.46×10^{6}	7.81×10^{5}	5.84×10^{5}	4.27×10^{5}
$SA \cdot A \cdot (NSA)_2 \rightarrow SA \cdot (NSA)_2 + A$	1.63×10^{-2}	3.06×10^{-3}	5.10×10^{-4}	1.62×10^{-4}	4.69×10^{-5}
$SA \cdot (A)_2 \cdot (NSA)_2 \rightarrow (A)_2 \cdot (NSA)_2 + SA$	1.67×10^{2}	4.39×10^{1}	1.05×10^{1}	5.10×10^{0}	2.35×10^{0}
$SA \cdot (A)_2 \cdot (NSA)_2 \rightarrow SA \cdot (A)_2 \cdot NSA + NSA$	7.38×10^{-5}	1.23×10^{-5}	1.79×10^{-6}	4.94×10^{-7}	1.24×10^{-7}
$SA \cdot (A)_2 \cdot (NSA)_2 \rightarrow SA \cdot A \cdot (NSA)_2 + A$	1.27×10^{-8}	1.76×10^{-9}	2.10×10^{-10}	3.88×10^{-11}	6.28×10^{-12}
$SA \cdot (A)_3 \cdot (NSA)_2 \rightarrow SA \cdot (A)_2 \cdot (NSA)_2 + A$	2.38×10^{0}	5.81×10^{-1}	1.28×10^{-1}	5.03×10^{-2}	1.84×10^{-2}

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

Clusters	$\sum\gamma$, (s^{-1})				
	298.15 K	288.15 K	278.15 K	268.15 K	258.15 K
SA·A	3.11×10^{5}	1.29×10^{5}	4.98×10^{4}	3.27×10^{4}	2.08×10^{4}
SA·NSA	2.31×10^{5}	8.56×10^{4}	3.00×10^{4}	1.99×10^{4}	1.28×10^{4}
A·NSA	5.43×10^{2}	1.63×10^{2}	4.47×10^{1}	2.24×10^{1}	1.11×10^{1}
$(SA)_2$	7.31×10^{4}	2.52×10^{4}	8.02×10^{3}	5.08×10^{3}	3.11×10^{3}
$(NSA)_2$	1.94×10^{6}	7.81×10^{5}	2.93×10^{5}	2.12×10^{5}	1.50×10^{5}
$(SA)_2$·A	1.78×10^{-1}	3.95×10^{-2}	7.88×10^{-3}	2.80×10^{-3}	9.20×10^{-4}
$(SA)_2$·$(A)_2$	1.69×10^{4}	5.51×10^{3}	1.65×10^{3}	9.31×10^{2}	5.03×10^{2}
A·$(NSA)_2$	2.26×10^{2}	6.43×10^{1}	1.67×10^{1}	8.36×10^{0}	3.97×10^{0}
$(A)_2$·$(NSA)_2$	6.70×10^{-5}	1.23×10^{-5}	1.98×10^{-6}	5.18×10^{-7}	1.22×10^{-7}
$(SA)_2$·NSA	4.76×10^{6}	2.07×10^{6}	8.46×10^{5}	6.20×10^{5}	4.44×10^{5}
SA·$(NSA)_2$	7.23×10^{7}	3.05×10^{7}	1.19×10^{7}	9.72×10^{6}	7.82×10^{6}
$(SA)_3$	8.48×10^{4}	2.96×10^{4}	9.57×10^{3}	6.05×10^{3}	3.69×10^{3}
$(NSA)_3$	2.25×10^{9}	1.23×10^{9}	6.48×10^{8}	6.23×10^{8}	5.97×10^{8}
$(SA)_3$·A	8.09×10^{1}	2.32×10^{1}	6.06×10^{0}	2.91×10^{0}	1.32×10^{0}
$(SA)_3$·$(A)_2$	2.75×10^{1}	3.07×10^{-2}	1.46×10^{0}	6.34×10^{-1}	2.58×10^{-1}
$(SA)_3$·$(A)_3$	1.29×10^{-2}	6.27×10^{-1}	5.78×10^{-4}	1.85×10^{-4}	5.44×10^{-5}
A·$(NSA)_3$	1.06×10^{3}	3.61×10^{2}	1.14×10^{2}	6.12×10^{1}	3.13×10^{1}
$(A)_2$·$(NSA)_3$	3.15×10^{8}	1.53×10^{8}	7.00×10^{7}	6.16×10^{7}	5.36×10^{7}
$(A)_3$·$(NSA)_3$	8.95×10^{-6}	1.32×10^{-6}	1.69×10^{-7}	4.00×10^{-8}	8.49×10^{-9}
SA·A·NSA	2.60×10^{1}	7.47×10^{0}	1.96×10^{0}	9.04×10^{-1}	3.94×10^{-1}
SA·$(A)_2$·NSA	8.03×10^{2}	2.30×10^{2}	5.99×10^{1}	3.00×10^{1}	1.42×10^{1}
SA_2·A·NSA	1.38×10^{3}	3.88×10^{2}	9.97×10^{1}	5.20×10^{1}	2.58×10^{1}
$(SA)_2$·$(A)_2$·NSA	2.01×10^{2}	5.21×10^{1}	1.23×10^{1}	5.65×10^{0}	2.45×10^{0}
$(SA)_2$·$(A)_3$·NSA	4.01×10^{0}	9.73×10^{-1}	2.13×10^{-1}	8.54×10^{-2}	3.20×10^{-2}
SA·A·$(NSA)_2$	8.12×10^{6}	2.80×10^{6}	8.91×10^{5}	6.60×10^{5}	4.79×10^{5}
SA·$(A)_2$·$(NSA)_2$	1.67×10^{2}	4.39×10^{1}	1.05×10^{1}	5.10×10^{0}	2.35×10^{0}
SA·$(A)_3$·$(NSA)_2$	2.38×10^{0}	5.81×10^{-1}	1.28×10^{-1}	5.03×10^{-2}	1.84×10^{-2}

Table S11 The formation rate J (s^{-1}) of NSA at the conditions of T = 258.15 K, [SA] = 10^4 - 10^8 molecules·cm^{-3}, [A] = 10^7 - 10^{11} molecules·cm^{-3} and [NSA] = 10^3 - 10^7 molecules·cm^{-3}. SA, A and NSA represent sulfuric acid, ammonia and nitrosulfonic acid, respectively

[SA]	[A]	[NSA] = 0	[NSA] = 10^3	[NSA] = 10^4	[NSA] = 10^5	[NSA] = 10^6	[NSA] = 10^7
[SA] = 10^4	[A] = 10^7	1.98×10^{-18}	2.18×10^{-18}	5.04×10^{-17}	9.39×10^{-14}	6.79×10^{-10}	4.87×10^{-6}
[SA] = 10^4	[A] = 10^8	1.26×10^{-15}	1.45×10^{-15}	4.87×10^{-14}	9.34×10^{-11}	6.79×10^{-7}	4.87×10^{-3}
[SA] = 10^4	[A] = 10^9	2.06×10^{-13}	3.55×10^{-13}	3.99×10^{-11}	8.96×10^{-8}	6.78×10^{-4}	4.80×10^{0}
[SA] = 10^4	[A] = 10^{10}	6.10×10^{-12}	4.54×10^{-11}	1.86×10^{-8}	7.91×10^{-5}	6.64×10^{-1}	3.48×10^{3}
[SA] = 10^4	[A] = 10^{11}	7.31×10^{-11}	8.34×10^{-9}	1.97×10^{-5}	1.54×10^{-1}	9.87×10^{2}	7.96×10^{5}
[SA] = 10^5	[A] = 10^7	1.98×10^{-14}	1.98×10^{-14}	2.18×10^{-14}	5.02×10^{-13}	9.07×10^{-10}	5.04×10^{-6}
[SA] = 10^5	[A] = 10^8	1.26×10^{-11}	1.26×10^{-11}	1.45×10^{-11}	4.85×10^{-10}	9.02×10^{-7}	5.03×10^{-3}
[SA] = 10^5	[A] = 10^9	2.05×10^{-9}	2.06×10^{-9}	3.54×10^{-9}	3.96×10^{-7}	8.62×10^{-4}	4.92×10^{0}
[SA] = 10^5	[A] = 10^{10}	6.07×10^{-8}	6.38×10^{-8}	4.52×10^{-7}	1.84×10^{-4}	7.35×10^{-1}	3.51×10^{3}
[SA] = 10^5	[A] = 10^{11}	7.27×10^{-7}	1.06×10^{-6}	8.26×10^{-5}	1.88×10^{-1}	1.00×10^{3}	7.97×10^{5}
[SA] = 10^6	[A] = 10^7	1.92×10^{-10}	1.92×10^{-10}	1.92×10^{-10}	2.15×10^{-10}	4.83×10^{-9}	6.77×10^{-6}
[SA] = 10^6	[A] = 10^8	1.22×10^{-7}	1.22×10^{-7}	1.22×10^{-7}	1.43×10^{-7}	4.65×10^{-6}	6.71×10^{-3}
[SA] = 10^6	[A] = 10^9	1.98×10^{-5}	1.98×10^{-5}	2.00×10^{-5}	3.46×10^{-5}	3.75×10^{-3}	6.20×10^{0}
[SA] = 10^6	[A] = 10^{10}	5.79×10^{-4}	5.79×10^{-4}	6.11×10^{-4}	4.31×10^{-3}	1.64×10^{0}	3.76×10^{3}
[SA] = 10^6	[A] = 10^{11}	6.91×10^{-3}	6.95×10^{-3}	1.02×10^{-2}	7.54×10^{-1}	1.18×10^{3}	8.08×10^{5}
[SA] = 10^7	[A] = 10^7	1.49×10^{-6}	1.49×10^{-6}	1.49×10^{-6}	1.52×10^{-6}	1.93×10^{-6}	3.64×10^{-5}
[SA] = 10^7	[A] = 10^8	9.44×10^{-4}	9.44×10^{-4}	9.46×10^{-4}	9.63×10^{-4}	1.28×10^{-3}	3.38×10^{-2}
[SA] = 10^7	[A] = 10^9	1.45×10^{-1}	1.45×10^{-1}	1.45×10^{-1}	1.49×10^{-1}	2.86×10^{-1}	2.37×10^{1}
[SA] = 10^7	[A] = 10^{10}	3.80×10^{0}	3.80×10^{0}	3.82×10^{0}	4.17×10^{0}	2.88×10^{1}	6.49×10^{3}
[SA] = 10^7	[A] = 10^{11}	4.39×10^{1}	4.40×10^{1}	4.51×10^{1}	7.42×10^{1}	3.61×10^{3}	9.17×10^{5}
[SA] = 10^8	[A] = 10^7	4.53×10^{-3}	4.53×10^{-3}	4.54×10^{-3}	4.61×10^{-3}	5.34×10^{-3}	1.27×10^{-2}
[SA] = 10^8	[A] = 10^8	2.75×10^{0}	2.75×10^{0}	2.76×10^{0}	2.80×10^{0}	3.25×10^{0}	7.92×10^{0}
[SA] = 10^8	[A] = 10^9	2.78×10^{2}	2.78×10^{2}	2.78×10^{2}	2.83×10^{2}	3.34×10^{2}	1.03×10^{3}
[SA] = 10^8	[A] = 10^{10}	4.58×10^{3}	4.59×10^{3}	4.60×10^{3}	4.76×10^{3}	6.53×10^{3}	4.60×10^{4}
[SA] = 10^8	[A] = 10^{11}	4.70×10^{4}	4.70×10^{4}	4.76×10^{4}	5.35×10^{4}	1.28×10^{5}	2.25×10^{6}

Table S12 The formation rate J (s^{-1}) of NSA at the conditions of T = 268.15 K, [SA] = 10^4 - 10^8 molecules·cm^{-3}, [A] = 10^7 - 10^{11} molecules·cm^{-3} and [NSA] = 10^3 - 10^7 molecules·cm^{-3}. SA, A and NSA represent sulfuric acid, ammonia and nitrosulfonic acid, respectively

[SA]	[A]	[NSA] = 0	[NSA] = 10^3	[NSA] = 10^4	[NSA] = 10^5	[NSA] = 10^6	[NSA] = 10^7
[SA] = 10^4	[A] = 10^7	1.58×10^{-19}	1.59×10^{-19}	4.55×10^{-19}	1.03×10^{-15}	8.58×10^{-12}	6.23×10^{-8}
[SA] = 10^4	[A] = 10^8	8.79×10^{-17}	8.87×10^{-17}	3.85×10^{-16}	1.03×10^{-12}	8.59×10^{-9}	6.23×10^{-5}
[SA] = 10^4	[A] = 10^9	1.51×10^{-14}	1.58×10^{-14}	3.06×10^{-13}	1.03×10^{-9}	8.61×10^{-6}	6.23×10^{-2}
[SA] = 10^4	[A] = 10^{10}	9.20×10^{-13}	1.48×10^{-12}	2.53×10^{-10}	1.02×10^{-6}	8.70×10^{-3}	5.97×10^{1}
[SA] = 10^4	[A] = 10^{11}	1.73×10^{-11}	1.90×10^{-10}	1.78×10^{-7}	1.13×10^{-3}	9.48×10^{0}	3.10×10^{4}
[SA] = 10^5	[A] = 10^7	1.58×10^{-15}	1.58×10^{-15}	1.58×10^{-15}	4.54×10^{-15}	9.91×10^{-12}	6.32×10^{-8}
[SA] = 10^5	[A] = 10^8	8.78×10^{-13}	8.78×10^{-13}	8.86×10^{-13}	3.83×10^{-12}	9.91×10^{-9}	6.32×10^{-5}
[SA] = 10^5	[A] = 10^9	1.50×10^{-10}	1.50×10^{-10}	1.58×10^{-10}	3.05×10^{-9}	9.90×10^{-6}	6.32×10^{-2}
[SA] = 10^5	[A] = 10^{10}	9.17×10^{-9}	9.21×10^{-9}	1.47×10^{-8}	2.51×10^{-6}	9.74×10^{-3}	6.04×10^{1}
[SA] = 10^5	[A] = 10^{11}	1.72×10^{-7}	1.83×10^{-7}	1.89×10^{-6}	1.75×10^{-3}	9.91×10^{0}	3.11×10^{4}
[SA] = 10^6	[A] = 10^7	1.56×10^{-11}	1.56×10^{-11}	1.56×10^{-11}	1.58×10^{-11}	4.43×10^{-11}	7.28×10^{-8}
[SA] = 10^6	[A] = 10^8	8.63×10^{-9}	8.63×10^{-9}	8.63×10^{-9}	8.73×10^{-9}	3.71×10^{-8}	7.28×10^{-5}
[SA] = 10^6	[A] = 10^9	1.46×10^{-6}	1.46×10^{-6}	1.46×10^{-6}	1.54×10^{-6}	2.92×10^{-5}	7.23×10^{-2}
[SA] = 10^6	[A] = 10^{10}	8.82×10^{-5}	8.82×10^{-5}	8.86×10^{-5}	1.43×10^{-4}	2.37×10^{-2}	6.68×10^{1}
[SA] = 10^6	[A] = 10^{11}	1.64×10^{-3}	1.64×10^{-3}	1.75×10^{-3}	1.80×10^{-2}	1.48×10^{1}	3.19×10^{4}
[SA] = 10^7	[A] = 10^7	1.46×10^{-7}	1.46×10^{-7}	1.46×10^{-7}	1.46×10^{-7}	1.50×10^{-7}	3.87×10^{-7}
[SA] = 10^7	[A] = 10^8	7.36×10^{-5}	7.36×10^{-5}	7.36×10^{-5}	7.38×10^{-5}	7.62×10^{-5}	2.96×10^{-4}
[SA] = 10^7	[A] = 10^9	7.36×10^{-5}	1.13×10^{-2}	1.13×10^{-2}	1.13×10^{-2}	1.23×10^{-2}	2.11×10^{-1}
[SA] = 10^7	[A] = 10^{10}	6.25×10^{-1}	6.25×10^{-1}	6.25×10^{-1}	6.30×10^{-1}	1.10×10^{0}	1.47×10^{2}
[SA] = 10^7	[A] = 10^{11}	1.08×10^{1}	1.08×10^{1}	1.08×10^{1}	1.17×10^{1}	1.14×10^{2}	4.00×10^{4}
[SA] = 10^8	[A] = 10^7	8.56×10^{-4}	8.56×10^{-4}	8.57×10^{-4}	8.59×10^{-4}	8.79×10^{-4}	1.08×10^{-3}
[SA] = 10^8	[A] = 10^8	2.93×10^{-1}	2.93×10^{-1}	2.93×10^{-1}	2.94×10^{-1}	3.01×10^{-1}	3.72×10^{-1}
[SA] = 10^8	[A] = 10^9	3.09×10^{1}	3.09×10^{1}	3.09×10^{1}	3.10×10^{1}	3.18×10^{1}	4.25×10^{1}
[SA] = 10^8	[A] = 10^{10}	1.03×10^{3}	1.03×10^{3}	1.03×10^{3}	1.03×10^{3}	1.08×10^{3}	2.57×10^{3}
[SA] = 10^8	[A] = 10^{11}	1.32×10^{4}	1.08×10^{1}	1.08×10^{1}	1.17×10^{1}	1.14×10^{2}	4.00×10^{4}

Table S13 The formation rate J (s^{-1}) of NSA at the conditions of T = 278.15 K, [SA] = 10^4 - 10^8 molecules·cm^{-3}, [A] = 10^7 - 10^{11} molecules·cm^{-3} and [NSA] = 10^3 - 10^7 molecules·cm^{-3}. SA, A and NSA represent sulfuric acid, ammonia and nitrosulfonic acid, respectively

[SA]	[A]	[NSA] = 0	[NSA] = 10^3	[NSA] = 10^4	[NSA] = 10^5	[NSA] = 10^6	[NSA] = 10^7
[SA] = 10^4	[A] = 10^7	1.84×10^{-22}	1.88×10^{-22}	3.63×10^{-21}	1.70×10^{-17}	1.49×10^{-13}	1.08×10^{-9}
[SA] = 10^4	[A] = 10^8	1.80×10^{-19}	1.84×10^{-19}	3.63×10^{-18}	1.70×10^{-14}	1.49×10^{-10}	1.08×10^{-6}
[SA] = 10^4	[A] = 10^9	1.48×10^{-16}	1.52×10^{-16}	3.59×10^{-15}	1.70×10^{-11}	1.49×10^{-7}	1.08×10^{-3}
[SA] = 10^4	[A] = 10^{10}	4.66×10^{-14}	5.04×10^{-14}	3.41×10^{-12}	1.71×10^{-8}	1.50×10^{-4}	1.08×10^{0}
[SA] = 10^4	[A] = 10^{11}	2.29×10^{-12}	4.88×10^{-12}	2.92×10^{-9}	1.75 × 10-5	1.56×10^{-1}	9.34×10^{2}
[SA] = 10^5	[A] = 10^7	1.83×10^{-18}	1.84×10^{-18}	1.87×10^{-18}	3.61×10^{-17}	1.63×10^{-13}	1.09×10^{-9}
[SA] = 10^5	[A] = 10^8	1.80×10^{-15}	1.80×10^{-15}	1.84×10^{-15}	3.60×10^{-14}	1.63×10^{-10}	1.09×10^{-6}
[SA] = 10^5	[A] = 10^9	1.48×10^{-12}	1.48×10^{-12}	1.52×10^{-12}	3.56×10^{-11}	1.63×10^{-7}	1.09×10^{-3}
[SA] = 10^5	[A] = 10^{10}	4.65×10^{-10}	4.65×10^{-10}	5.02×10^{-10}	3.38×10^{-8}	1.64×10^{-4}	1.09×10^{0}
[SA] = 10^5	[A] = 10^{11}	2.28×10^{-8}	2.30×10^{-8}	4.87×10^{-8}	2.89×10^{-5}	1.65×10^{-1}	9.38×10^{2}
[SA] = 10^6	[A] = 10^7	1.79×10^{-14}	1.79×10^{-14}	1.79×10^{-14}	1.83×10^{-14}	3.40×10^{-13}	1.17×10^{-9}
[SA] = 10^6	[A] = 10^8	1.75×10^{-11}	1.75×10^{-11}	1.75×10^{-11}	1.79×10^{-11}	3.39×10^{-10}	1.17×10^{-6}
[SA] = 10^6	[A] = 10^9	1.44×10^{-8}	1.44×10^{-8}	1.44×10^{-8}	1.48×10^{-8}	3.35×10^{-7}	1.17×10^{-3}
[SA] = 10^6	[A] = 10^{10}	4.50×10^{-6}	4.50×10^{-6}	4.51×10^{-6}	4.87×10^{-6}	3.17×10^{-4}	1.17×10^{0}
[SA] = 10^6	[A] = 10^{11}	2.20×10^{-4}	2.20×10^{-4}	2.21×10^{-4}	4.73×10^{-4}	2.66×10^{-1}	9.77×10^{2}
[SA] = 10^7	[A] = 10^7	1.41×10^{-10}	1.41×10^{-10}	1.41×10^{-10}	1.41×10^{-10}	1.44×10^{-10}	2.22×10^{-9}
[SA] = 10^7	[A] = 10^8	1.38×10^{-7}	1.38×10^{-7}	1.38×10^{-7}	1.38×10^{-7}	1.41 × 10-7	2.21×10^{-6}
[SA] = 10^7	[A] = 10^9	1.13×10^{-4}	1.13×10^{-4}	1.13×10^{-4}	1.13×10^{-4}	1.16×10^{-4}	2.18×10^{-3}
[SA] = 10^7	[A] = 10^{10}	3.44×10^{-2}	3.44×10^{-2}	3.44×10^{-2}	3.45×10^{-2}	3.77×10^{-2}	2.02×10^{0}
[SA] = 10^7	[A] = 10^{11}	1.58×10^{0}	1.58×10^{0}	1.58×10^{0}	1.60×10^{0}	3.67×10^{0}	1.38×10^{3}
[SA] = 10^8	[A] = 10^7	4.49×10^{-7}	4.49×10^{-7}	4.49×10^{-7}	4.49×10^{-7}	4.51×10^{-7}	4.84×10^{-7}
[SA] = 10^8	[A] = 10^8	4.39×10^{-4}	4.39×10^{-4}	4.39×10^{-4}	4.39×10^{-4}	4.40×10^{-4}	4.74×10^{-4}
[SA] = 10^8	[A] = 10^9	3.55×10^{-1}	3.55×10^{-1}	3.55×10^{-1}	3.55×10^{-1}	3.56×10^{-1}	3.87×10^{-1}
[SA] = 10^8	[A] = 10^{10}	9.24×10^{1}	9.24×10^{1}	9.24×10^{1}	9.24×10^{1}	9.28×10^{1}	1.14×10^{2}
[SA] = 10^8	[A] = 10^{11}	2.88×10^{3}	2.88×10^{3}	2.88×10^{3}	2.88×10^{3}	2.95×10^{3}	9.12×10^{3}

Table S14 The formation rate J (s^{-1}) of NSA at the conditions of T = 288.15 K, [SA] = 10^4 - 10^8 molecules·cm^{-3}, [A] = 10^7 - 10^{11} molecules·cm^{-3} and [NSA] = 10^3 - 10^7 molecules·cm^{-3}. SA, A and NSA represent sulfuric acid, ammonia and nitrosulfonic acid, respectively

[SA]	[A]	[NSA] = 0	[NSA] = 10^3	[NSA] = 10^4	[NSA] = 10^5	[NSA] = 10^6	[NSA] = 10^7
[SA] = 10^4	[A] = 10^7	2.35×10^{-24}	2.40×10^{-24}	7.53×10^{-23}	3.95×10^{-19}	3.49×10^{-15}	2.53×10^{-11}
[SA] = 10^4	[A] = 10^8	2.33×10^{-21}	2.38×10^{-21}	7.52×10^{-20}	3.95×10^{-16}	3.49×10^{-12}	2.53×10^{-8}
[SA] = 10^4	[A] = 10^9	2.13×10^{-18}	2.18×10^{-18}	7.50×10^{-17}	3.95×10^{-13}	3.49×10^{-9}	2.53×10^{-5}
[SA] = 10^4	[A] = 10^{10}	1.11×10^{-15}	1.16×10^{-15}	7.36×10^{-14}	3.96×10^{-10}	3.51×10^{-6}	2.53×10^{-2}
[SA] = 10^4	[A] = 10^{11}	1.30×10^{-13}	1.73×10^{-13}	6.92×10^{-11}	4.03×10^{-7}	3.60×10^{-3}	2.50×10^{1}
[SA] = 10^5	[A] = 10^7	2.35×10^{-20}	2.35×10^{-20}	2.40×10^{-20}	7.47×10^{-19}	3.79×10^{-15}	2.54×10^{-11}
[SA] = 10^5	[A] = 10^8	2.33×10^{-17}	2.33×10^{-17}	2.38×10^{-17}	7.47×10^{-16}	3.79×10^{-12}	2.54×10^{-8}
[SA] = 10^5	[A] = 10^9	2.13×10^{-14}	2.13×10^{-14}	2.18×10^{-14}	7.45×10^{-13}	3.79×10^{-9}	2.54×10^{-5}
[SA] = 10^5	[A] = 10^{10}	1.11×10^{-11}	1.11×10^{-11}	1.16×10^{-11}	7.30×10^{-10}	3.80×10^{-6}	2.54×10^{-2}
[SA] = 10^5	[A] = 10^{11}	1.29×10^{-9}	1.30×10^{-9}	1.72×10^{-9}	6.87×10^{-7}	3.85×10^{-3}	2.51×10^{1}
[SA] = 10^6	[A] = 10^7	2.35×10^{-16}	2.35×10^{-16}	2.35×10^{-16}	2.40×10^{-16}	6.98×10^{-15}	2.70×10^{-11}
[SA] = 10^6	[A] = 10^8	2.33×10^{-13}	2.33×10^{-13}	2.33×10^{-13}	2.38×10^{-13}	6.98×10^{-12}	2.70×10^{-8}
[SA] = 10^6	[A] = 10^9	2.12×10^{-10}	2.12×10^{-10}	2.12×10^{-10}	2.17×10^{-10}	6.95×10^{-9}	2.70×10^{-5}
[SA] = 10^6	[A] = 10^{10}	1.09×10^{-7}	1.09×10^{-7}	1.09×10^{-7}	1.14×10^{-7}	6.81×10^{-6}	2.70×10^{-2}
[SA] = 10^6	[A] = 10^{11}	1.26×10^{-5}	1.26×10^{-5}	1.26×10^{-5}	1.67×10^{-5}	6.37×10^{-3}	2.63×10^{1}
[SA] = 10^7	[A] = 10^7	2.35×10^{-12}	2.35×10^{-12}	2.35×10^{-12}	2.35×10^{-12}	2.38×10^{-12}	4.29×10^{-11}
[SA] = 10^7	[A] = 10^8	2.32×10^{-9}	2.32×10^{-9}	2.32×10^{-9}	2.32×10^{-9}	2.35×10^{-9}	4.28×10^{-8}
[SA] = 10^7	[A] = 10^9	2.06×10^{-6}	2.06×10^{-6}	2.06×10^{-6}	2.06×10^{-6}	2.09×10^{-6}	4.26×10^{-5}
[SA] = 10^7	[A] = 10^{10}	9.37×10^{-4}	9.37×10^{-4}	9.37×10^{-4}	9.37×10^{-4}	9.74×10^{-4}	4.11×10^{-2}
[SA] = 10^7	[A] = 10^{11}	9.67×10^{-2}	9.67×10^{-2}	9.67×10^{-2}	9.68×10^{-2}	1.29×10^{-1}	3.68×10^{1}
[SA] = 10^8	[A] = 10^7	2.27×10^{-8}	2.27×10^{-8}	2.27×10^{-8}	2.27×10^{-8}	2.27×10^{-8}	2.29×10^{-8}
[SA] = 10^8	[A] = 10^8	2.18×10^{-5}	2.18×10^{-5}	2.18×10^{-5}	2.18×10^{-5}	2.18×10^{-5}	2.20×10^{-5}
[SA] = 10^8	[A] = 10^9	1.57×10^{-2}	1.57×10^{-2}	1.57×10^{-2}	1.57×10^{-2}	1.57×10^{-2}	1.59×10^{-2}
[SA] = 10^8	[A] = 10^{10}	3.85×10^{0}	3.85×10^{0}	3.85×10^{0}	3.85×10^{0}	3.85×10^{0}	4.03×10^{0}
[SA] = 10^8	[A] = 10^{11}	2.69×10^{2}	2.69×10^{2}	2.69×10^{2}	2.69×10^{2}	2.70×10^{2}	4.05×10^{2}

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

[SA]	[A]	[NSA] = 0	[NSA] = 10^3	[NSA] = 10^4	[NSA] = 10^5	[NSA] = 10^6	[NSA] = 10^7
[SA] = 10^4	[A] = 10^7	3.13×10^{-27}	4.34×10^{-27}	2.13×10^{-24}	1.17×10^{-20}	1.04×10^{-16}	7.48×10^{-13}
[SA] = 10^4	[A] = 10^8	3.12×10^{-24}	4.34×10^{-24}	2.13×10^{-21}	1.17×10^{-17}	1.04×10^{-13}	7.48×10^{-10}
[SA] = 10^4	[A] = 10^9	3.11×10^{-21}	4.33×10^{-21}	2.13×10^{-18}	1.17×10^{-14}	1.04×10^{-10}	7.48×10^{-7}
[SA] = 10^4	[A] = 10^{10}	2.98×10^{-18}	4.19×10^{-18}	2.12×10^{-15}	1.17×10^{-11}	1.04×10^{-7}	7.49×10^{-4}
[SA] = 10^4	[A] = 10^{11}	1.99×10^{-15}	3.16×10^{-15}	2.09×10^{-12}	1.19×10^{-8}	1.05×10^{-4}	7.52×10^{-1}
[SA] = 10^5	[A] = 10^7	3.12×10^{-23}	3.12×10^{-23}	4.33×10^{-23}	2.11×10^{-20}	1.12×10^{-16}	7.53×10^{-13}
[SA] = 10^5	[A] = 10^8	3.12×10^{-20}	3.12×10^{-20}	4.33×10^{-20}	2.11×10^{-17}	1.12×10^{-13}	7.53×10^{-10}
[SA] = 10^5	[A] = 10^9	3.11×10^{-17}	3.11×10^{-17}	4.32×10^{-17}	2.11×10^{-14}	1.12×10^{-10}	7.53×10^{-7}
[SA] = 10^5	[A] = 10^{10}	2.98×10^{-14}	2.98×10^{-14}	4.18×10^{-14}	2.11×10^{-11}	1.13×10^{-7}	7.53×10^{-4}
[SA] = 10^5	[A] = 10^{11}	1.99×10^{-11}	1.99×10^{-11}	3.15×10^{-11}	2.08×10^{-8}	1.14×10^{-4}	7.55×10^{-1}
[SA] = 10^6	[A] = 10^7	3.09×10^{-19}	3.09×10^{-19}	3.09×10^{-19}	4.26×10^{-19}	1.96×10^{-16}	7.98×10^{-13}
[SA] = 10^6	[A] = 10^8	3.09×10^{-16}	3.09×10^{-16}	3.09×10^{-16}	4.26×10^{-16}	1.96×10^{-13}	7.98×10^{-10}
[SA] = 10^6	[A] = 10^9	3.08×10^{-13}	3.08×10^{-13}	3.08×10^{-13}	4.24×10^{-13}	1.96×10^{-10}	7.98×10^{-7}
[SA] = 10^6	[A] = 10^{10}	2.94×10^{-10}	2.94×10^{-10}	2.94×10^{-10}	4.11×10^{-10}	1.96×10^{-7}	7.98×10^{-4}
[SA] = 10^6	[A] = 10^{11}	1.95×10^{-7}	1.95×10^{-7}	1.95×10^{-7}	3.07×10^{-7}	1.93×10^{-4}	7.96×10^{-1}
[SA] = 10^7	[A] = 10^7	2.81×10^{-15}	2.81×10^{-15}	2.81×10^{-15}	2.81×10^{-15}	3.66×10^{-15}	1.15×10^{-12}
[SA] = 10^7	[A] = 10^8	2.81×10^{-12}	2.81×10^{-12}	2.81×10^{-12}	2.81×10^{-12}	3.66×10^{-12}	1.15×10^{-9}
[SA] = 10^7	[A] = 10^9	2.79×10^{-9}	2.79×10^{-9}	2.79×10^{-9}	2.79×10^{-9}	3.65×10^{-9}	1.15×10^{-6}
[SA] = 10^7	[A] = 10^{10}	2.65×10^{-6}	2.65×10^{-6}	2.65×10^{-6}	2.65×10^{-6}	3.50×10^{-6}	1.15×10^{-3}
[SA] = 10^7	[A] = 10^{11}	1.66×10^{-3}	1.66×10^{-3}	1.66×10^{-3}	1.66×10^{-3}	2.48×10^{-3}	1.12×10^{0}
[SA] = 10^8	[A] = 10^7	1.47×10^{-11}	1.47×10^{-11}	1.47×10^{-11}	1.47×10^{-11}	1.47×10^{-11}	1.74×10^{-11}
[SA] = 10^8	[A] = 10^8	1.47×10^{-8}	1.47×10^{-8}	1.47×10^{-8}	1.47×10^{-8}	1.47×10^{-8}	1.74×10^{-8}
[SA] = 10^8	[A] = 10^9	1.45×10^{-5}	1.45×10^{-5}	1.45×10^{-5}	1.45×10^{-5}	1.45×10^{-5}	1.73×10^{-5}
[SA] = 10^8	[A] = 10^{10}	2.34×10^{0}	1.33×10^{-2}	1.33×10^{-2}	1.33×10^{-2}	1.33×10^{-2}	1.33×10^{-2}
[SA] = 10^8	[A] = 10^{11}	6.58×10^{0}	6.58×10^{0}	6.58×10^{0}	6.58×10^{0}	6.59×10^{0}	9.19×10^{0}

Part S3 Enhancement factor R

To further evaluate the enhancement potential of NSA on the SA-A-driven NPF, $J_{\text{NSA-SA-A}}$ and $J_{\text{SA-A}}$ are compared by defining a ratio R_{NSA}, which stands for the ratio of the cluster formation rate with NSA to that without NSA,

$$R = \frac{J([\text{SA}]=x,[\text{A}]=y,[\text{NSA}]=z)}{J([\text{SA}]=x,[\text{A}]=y,[\text{NSA}]=0)} \tag{S4}$$

where [NSA], [SA] and [A] represent monomer concentrations of NSA, SA and A, respectively.

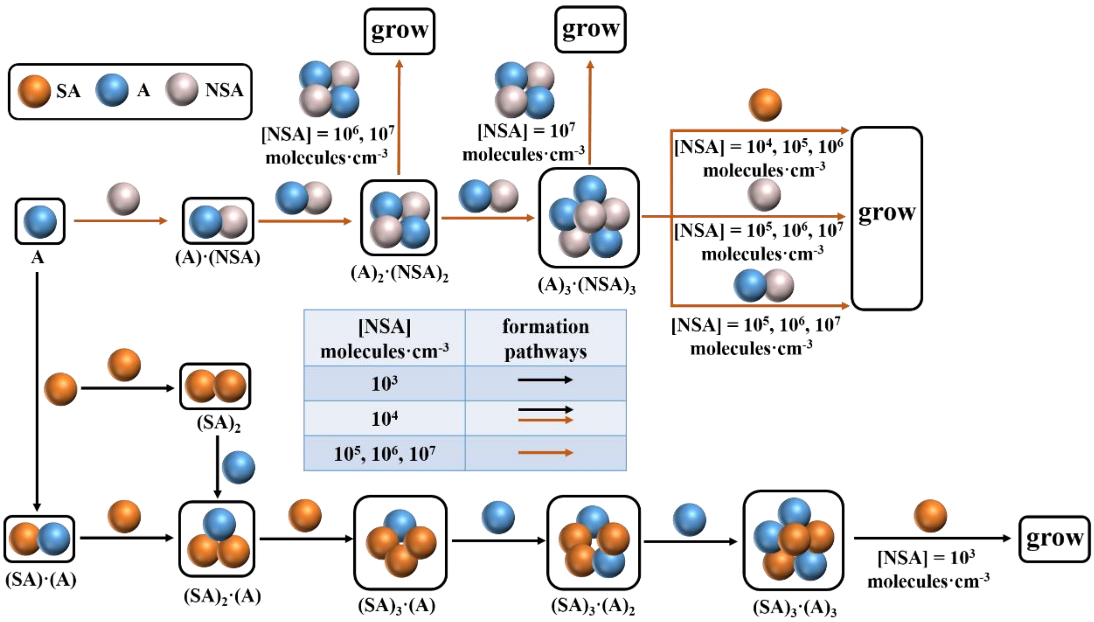

Fig. S10 Growth pathways of clusters under the conditions of T = 258.15 K, [SA] = 10^6 molecules·cm^{-3}, [A] = 10^9 molecules·cm^{-3} with varying concentrations of NSA. Arrows in different colors indicate the pathways at the corresponding conditions concentrations shown in the table on the middle

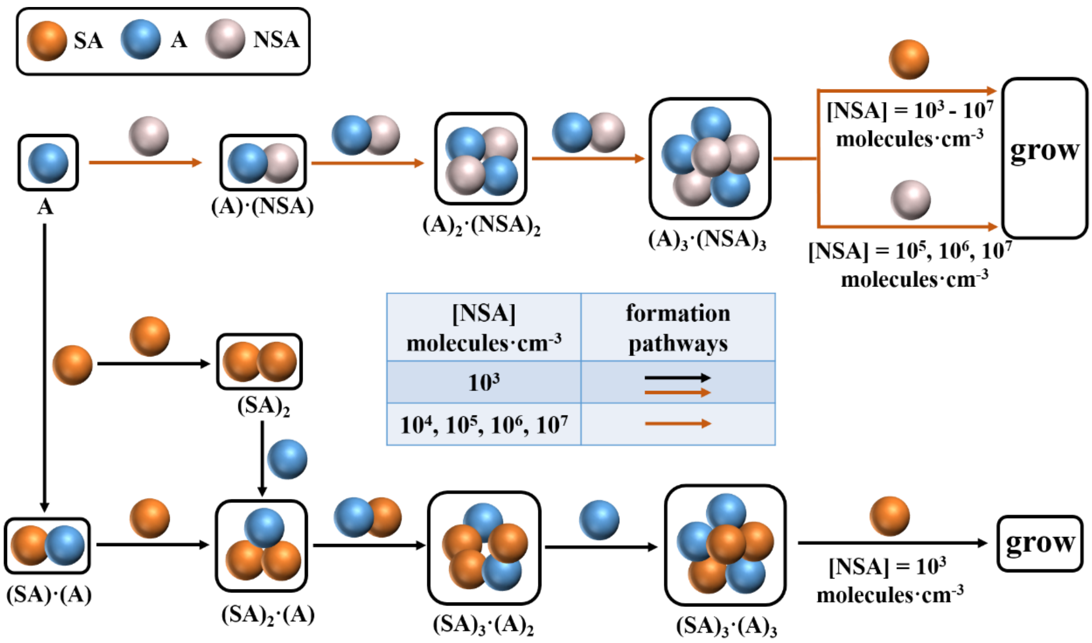

Fig. S11 Growth pathways of clusters under the conditions of T = 298.15 K, [SA] = 10^6 molecules·cm^{-3}, [A] = 10^9 molecules·cm^{-3} with varying concentrations of NSA. Arrows in different colors indicate the pathways at the corresponding conditions concentrations shown in the table on the middle

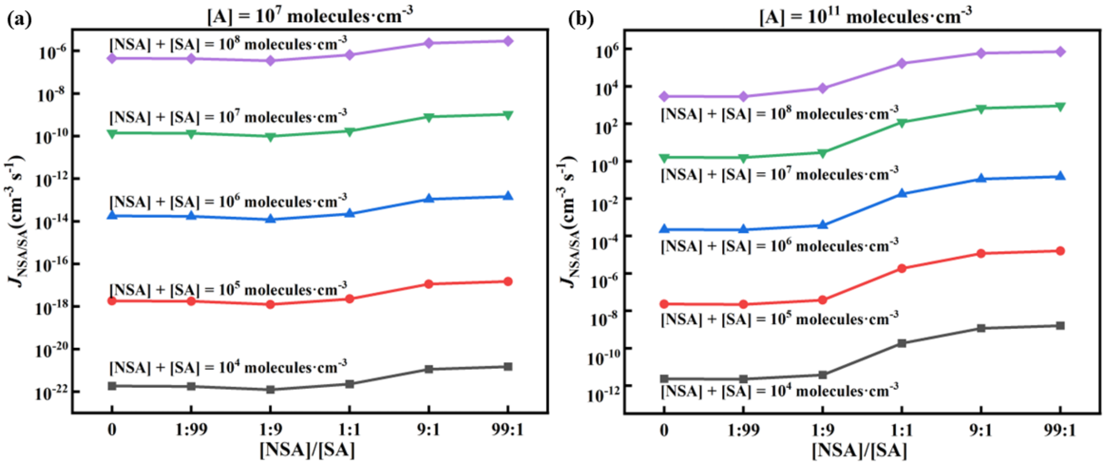

Fig. S12 The cluster formation rate as a function of the ratio [NSA]/[SA] at a simulated temperature of 278.15 K and A molecular concentrations of (a) 10^7 molecules·cm^{-3}, and (b) 10^{11} molecules·cm^{-3}. The concentrations of NSA and SA are collectively maintained constant (10^4-10^8 molecules·cm^{-3})

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

SA

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

A

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

NSA

Atom	X	Y	Z
S	1.00291300	-0.09490400	0.10200600
O	0.87276400	0.39285800	1.42424400
O	1.93042100	-1.07261400	-0.30406000
O	1.08766000	1.08766000	-0.91069500
N	-1.62875000	-0.05207800	-0.05767200
O	-2.57788000	-0.74339800	0.00921200
O	-1.51788400	1.13482500	0.01797900
O	-0.43988800	-0.79251600	-0.31367600
H	0.51309400	1.81297300	-0.61242500

SA·A

Atom	X	Y	Z
S	-0.59827600	-0.11336800	0.08617500
O	0.10893200	-0.09214100	1.32834700
O	-1.74906500	-0.92894600	-0.10565200
O	0.39576600	-0.37422800	-1.06128100
O	-1.03681100	1.39710200	-0.16132600
H	1.37463300	-0.19089300	-0.73462700
H	-1.78503200	1.40349300	-0.77106700
N	2.73855300	0.04357600	-0.05140800
H	3.20053200	0.91724700	-0.27070200
H	3.40981800	-0.70549900	-0.16620600
H	2.45200800	0.07021600	0.92295000

NSA·A

Atom	X	Y	Z
N	1.04820500	2.47297500	-0.02953000
H	0.96810900	2.03772800	0.89649700
H	0.20580500	3.00490600	-0.22570500
H	1.87816100	3.05135000	-0.09600500
S	0.84580100	-0.70042200	0.01922600
O	1.02265700	0.01104900	1.26205300
O	1.29714700	-2.03989000	-0.07790100

O	1.07934900	0.15069500	-1.15074200
N	-1.72968200	0.03901700	-0.00459800
O	-2.87115400	-0.28484600	-0.02307800
O	-1.28350400	1.16171200	0.04858000
O	-0.85735900	-1.00721400	-0.05533600
H	1.08834600	1.59677300	-0.67212200

$(SA)_2$

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

$(NSA)_2$

Atom	X	Y	Z
S	2.09213800	-0.95151400	-0.26598300
O	1.01884200	-0.63362400	-1.16426700
O	3.12954000	-1.83061300	-0.62690100
O	1.52517100	-1.33970300	1.10718500
N	2.13781300	1.60483500	0.43122200
O	2.74108200	2.59293000	0.23439500
O	1.07635800	1.39780800	0.91697200
O	2.89361400	0.43915800	0.01610100
H	0.58935300	-1.01729800	1.21765000
S	-2.09213900	-0.95151300	0.26598300
O	-1.01884200	-0.63362300	1.16426700
O	-3.12954100	-1.83061100	0.62690200
O	-1.52517200	-1.33970400	-1.10718400
N	-2.13781100	1.60483600	-0.43122300
O	-2.74107900	2.59293200	-0.23439300
O	-1.07635800	1.39780700	-0.91697400
O	-2.89361400	0.43915900	-0.01610200
H	-0.58935400	-1.01729900	-1.21764900

SA·NSA

Atom	X	Y	Z
S	2.39789600	-0.13003000	-0.03653100
O	1.50946700	-0.72393200	-1.00283100
O	3.73386200	-0.58333600	0.07591100
O	1.73307300	-0.18505100	1.35813300
O	2.40392500	1.40170400	-0.38641200
H	0.76865000	-0.40482100	1.29955800
H	3.20925100	1.81175400	-0.04198300
S	-1.72609700	-0.98457000	0.05251800
O	-0.79187000	-0.99117300	1.14063300

O	-2.84305600	-1.84027800	0.04350500
O	-0.99375600	-1.01369600	-1.28476300
N	-1.62766400	1.66220800	0.00296700
O	-2.26894000	2.64697400	0.06552100
O	-0.45072300	1.49557700	-0.08699500
O	-2.44898500	0.49733700	0.03338700
H	0.00299900	-0.84180100	-1.18284700

$(SA)_2\cdot A$

Atom	X	Y	Z
S	-1.77231300	-0.34077900	-0.04909000
O	-1.07131700	0.16352900	1.14296700
O	-0.99847000	-1.34675900	-0.75741300
O	-3.07876600	-1.07528900	0.45986500
H	-2.85067000	-1.96938800	0.74413600
O	-2.28848200	0.74869000	-0.85700500
H	-1.40689900	2.09302200	-0.44210900
O	1.42804700	1.08270500	-0.53209900
S	2.06372500	-0.11895200	-0.01742600
O	1.43416000	-0.42809800	1.36683400
O	3.47167000	-0.14405700	0.10310200
O	1.62893900	-1.30669600	-0.91181400
H	0.44446700	-0.24695300	1.34915800
H	0.63395000	-1.35519900	-0.95819300
N	-0.64527900	2.68400200	-0.01766800
H	0.24045900	2.13587500	-0.15608200
H	-0.82981700	2.75595300	0.97931500
H	-0.58337400	3.60217400	-0.44379900

SA·A·NSA

Atom	X	Y	Z
N	0.14544200	-1.22831200	1.85966600
H	1.05840900	-0.75212100	1.74627800
H	-0.06482900	-1.71395100	0.98715900
H	0.15843600	-1.87740200	2.63897700
S	-1.46187400	1.10877600	0.21144100
O	-0.25468900	0.47426100	-0.31709500
O	-1.71279100	2.44637400	-0.18077700
O	-1.70166900	0.73915600	1.59084200
N	-2.84774200	-1.03477300	-0.57471600
O	-3.75836800	-1.45440900	-1.20610700
O	-2.06486200	-1.65070700	0.10355300
O	-2.70966700	0.33110600	-0.66163100
H	-0.60811500	-0.50685500	1.96133200
S	2.89890500	-0.03427300	-0.20134700
O	2.52688600	0.05505400	1.18359900
O	4.25944700	0.00536300	-0.59120900
O	2.12441200	0.99733300	-1.03946700
O	2.25169800	-1.41949300	-0.64941100
H	1.14224000	0.96017200	-0.81057200
H	2.55430300	-1.65259700	-1.53769800

$(NSA)_2\cdot A$

Atom	X	Y	Z
N	-0.22572600	-1.22376300	2.16401100
H	-1.22245600	-1.22556200	1.83661700

H	0.22763800	-0.34847300	1.85355900
H	-0.16034400	-1.32215800	3.17227500
S	-2.22561700	-1.05440100	-0.45566700
O	-2.63598900	-1.33678800	0.90435000
O	-2.93182500	-1.66301400	-1.51889500
O	-0.75731600	-1.06602600	-0.56210900
N	-2.27042500	1.51496500	0.22874400
O	-2.82684800	2.54862000	0.09416500
O	-1.43479100	1.20049700	1.03341100
O	-2.64859100	0.56560900	-0.71564400
H	0.26114800	-1.98701700	1.69539500
S	1.81834900	1.18063400	-0.11001400
O	1.43452000	0.86229000	1.23202000
O	2.35700300	2.44061500	-0.43558700
O	0.78578800	0.75295100	-1.12579500
N	3.02064500	-1.18133000	-0.18955600
O	4.04845800	-1.74690500	-0.31039800
O	1.93890700	-1.60441700	0.11086800
O	3.12187100	0.18741500	-0.46482900
H	0.12935800	-0.03239400	-0.86178100

$(SA)_3$

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

$(NSA)_3$

Atom	X	Y	Z
S	1.67424400	-2.07525600	-1.25005100
O	1.36427000	-0.69261800	-1.45502800
O	2.50820100	-2.79372200	-2.12518700
O	0.36280300	-2.85012100	-1.01842800
N	1.84210700	-1.67786600	1.37629700
O	2.58907800	-1.71314200	2.27781000
O	0.71811300	-1.30996200	1.27933100
O	2.45433100	-2.21261300	0.17356500
H	-0.35622100	-2.24292600	-0.73622600
S	0.68418600	2.57170800	-0.75081000

O	-0.20330800	1.58798000	-0.21388400
O	0.23114600	3.80644800	-1.24793700
O	1.65245200	1.92758200	-1.75582200
N	2.32530000	2.02095400	1.24649800
O	2.70441800	2.43053400	2.27893900
O	2.42108400	0.94856300	0.73526000
O	1.66634500	3.03557700	0.47903500
H	1.70325000	0.94795700	-1.62828800
S	-2.37551300	-1.00442100	0.73669600
O	-2.15592700	-0.04499800	1.75125500
O	-2.37650500	-2.40248800	0.94611300
O	-1.43342700	-0.73798600	-0.48536900
N	-4.19221000	0.61013800	-0.29304300
O	-5.35642900	0.74186300	-0.38661600
O	-3.28574400	1.35179300	-0.47375200
O	-3.84814700	-0.74836300	0.08005200
H	-1.00211700	0.15527100	-0.43180700

$(SA)_2$·NSA

Atom	X	Y	Z
S	0.46655300	-0.82342000	-0.40446100
O	-0.66445400	-1.33075400	-1.13539200
O	1.64303000	-1.64183800	-0.36226700
O	0.05070500	-0.54349200	1.05461600
O	0.81442500	0.54942400	-0.99602600
H	-0.93518100	-0.52561600	1.16392600
H	1.77719500	0.78100400	-0.83078000
S	-3.66102100	-0.61319100	0.34658600
O	-2.58577200	-0.71218500	1.29102600
O	-4.92990800	-1.15368800	0.62515800
O	-3.18748600	-1.01065500	-1.04878400
N	-2.95554200	1.88932900	-0.16170400
O	-3.32856100	3.00455100	-0.17081200
O	-1.88574500	1.41419100	-0.38301700
O	-4.01302100	0.98448900	0.16723500
H	-2.17811300	-1.08424700	-1.10629500
S	4.28170300	0.36022600	0.29164200
O	3.33521700	0.97549900	-0.61474100
O	4.27259000	0.72032900	1.65669100
O	5.72159600	0.64320600	-0.24778800
O	4.20819600	-1.17787600	0.08924700
H	5.76550500	0.50146900	-1.20351200
H	3.26692500	-1.45190400	-0.06163600

SA·$(NSA)_2$

Atom	X	Y	Z
S	-0.32433100	2.42592600	0.09773100
O	0.45313700	1.60357300	0.97467300
O	-1.75721100	2.42144500	0.19889400
O	0.10337600	2.19577400	-1.35811200
O	0.14105600	3.89430600	0.35609800
H	0.62917400	1.34911100	-1.45009100
H	-0.58277600	4.51107000	0.17969300
S	1.64603900	-1.15296000	-0.64761500
O	1.60286900	0.05293700	-1.42389100
O	1.27305800	-2.39928500	-1.18302500
O	0.99559900	-0.93769200	0.72660200

N	3.96092800	-0.31702400	0.33596800
O	5.11273900	-0.55587100	0.35306200
O	3.33402000	0.61076500	0.72652300
O	3.21642800	-1.39966500	-0.26328100
H	0.78807700	0.02842600	0.88676500
S	-2.55035800	-0.78961500	-0.77063300
O	-1.21674900	-0.34432700	-1.00978500
O	-3.28785900	-1.54598100	-1.70136800
O	-3.40488400	0.38133100	-0.25015500
N	-1.83050600	-1.39021100	1.70328800
O	-1.60892000	-2.29181800	2.42622900
O	-1.60717800	-0.22406800	1.80906700
O	-2.50816100	-1.81273000	0.52132700
H	-2.81961900	1.13885100	0.01423300

$(SA)_2{\cdot}(A)_2$

Atom	X	Y	Z
S	-2.06184100	0.03024000	-0.13465200
O	-2.04117600	1.44224200	0.23783700
O	-3.44180400	-0.18999500	-0.89528300
O	-1.07447700	-0.35111100	-1.12711700
O	-2.07527000	-0.85956100	1.02215600
H	-0.62565200	2.17366500	0.71126100
H	-4.16339900	0.11236500	-0.33044200
S	2.14824600	-0.06917100	-0.20933500
O	1.98617900	-1.44915800	-0.67010100
O	1.31072900	0.84270300	-1.21025200
O	1.44496800	0.08726200	1.09667700
O	3.46837600	0.47040600	-0.23135200
H	0.82649800	-2.09927000	0.18550400
H	0.42274300	0.42956900	-1.33621000
N	0.16605000	-2.42220400	0.96179200
H	-0.03648600	-3.41297000	0.89015000
H	0.64646900	-2.21664600	1.83389300
H	-0.71778100	-1.86109400	0.94374900
N	0.35020200	2.43893700	0.98896700
H	0.35301500	3.05370700	1.79434900
H	0.86196200	1.50602200	1.17669400
H	0.81620300	2.87810800	0.19901900

$SA{\cdot}(A)_2{\cdot}NSA$

Atom	X	Y	Z
N	-0.50267400	-0.54491800	2.31272200
H	-1.36119900	-0.94117100	1.83103700
H	-0.54168000	0.45949100	2.14002300
H	-0.50413200	-0.74302400	3.30700600
S	1.82487400	-1.15028200	-0.40680800
O	0.57180200	-0.69635500	-0.98911300
O	2.67221800	-1.93162000	-1.23051300
O	1.72405900	-1.49671500	0.99198700
N	2.40271000	1.33575100	0.42694100
O	3.24196600	2.15547500	0.61325500
O	1.26078900	1.34374200	0.83368100
O	2.79253600	0.30746100	-0.37424600
H	0.35733800	-0.91908200	1.86294100
S	-2.81023300	-0.03031500	-0.00433800
O	-2.62184600	-1.18848600	0.86711600

O	-4.14591100	0.36439000	-0.29060200
O	-2.18617500	-0.43981800	-1.42161900
O	-1.92750500	1.07969700	0.46246100
H	-1.35486800	-0.92398800	-1.27932500
H	-1.11575100	1.64267600	-0.61822600
N	-0.46585000	1.86970700	-1.47794800
H	0.16012500	1.05588700	-1.53942000
H	0.06238400	2.72404700	-1.33699600
H	-1.03123800	1.92877200	-2.31996500

$(A)_2\cdot(NSA)_2$

Atom	X	Y	Z
N	1.10188900	-2.40592300	1.57815100
H	0.13609000	-2.50945000	1.20989300
H	1.14746000	-2.71763700	2.54262500
H	1.74897500	-2.93109900	0.99602800
S	2.58118700	0.76082800	0.45045700
O	3.81793000	0.05775000	0.47200500
O	2.58539100	2.20113700	0.46702700
O	1.51157900	0.20058700	1.27506600
N	1.72357000	-0.66673100	-1.65154600
O	1.39779900	-0.66653400	-2.78860500
O	1.86329800	-1.60113900	-0.90745400
O	1.96614200	0.59615400	-1.15171200
H	1.35137400	-1.37668200	1.49653000
S	-1.56784100	-0.69550600	0.39633800
O	-1.47239000	0.10443200	1.59359300
O	-1.48972200	-2.12162500	0.59952400
O	-0.84084200	-0.19204900	-0.74578600
N	-3.71280500	0.64946900	-0.35649400
O	-4.85883600	0.62403900	-0.65632000
O	-2.97592800	1.59672200	-0.28330100
O	-3.20360600	-0.60209400	-0.06061100
H	-0.34721900	1.63970700	-0.44061100
N	-0.25729300	2.30857800	0.33959100
H	-0.86817900	3.10432400	0.18559300
H	0.73256300	2.57719300	0.44985900
H	-0.57750400	1.76005600	1.15183500

$(SA)_3\cdot A$

Atom	X	Y	Z
N	-0.08306900	0.43034300	2.52884500
H	-0.96686500	0.21892000	2.01889600
H	0.62338000	-0.24748900	2.20270400
H	-0.22034100	0.36070000	3.53139300
S	1.14064300	1.97416100	-0.15831000
O	0.06648000	0.98458200	-0.29616000
O	1.25367800	2.50665600	1.17335800
H	0.26824900	1.36202900	2.25930200
O	2.38467600	1.45066900	-0.74121700
S	-2.89899900	-0.31614900	-0.11437500
O	-2.20892100	-1.35592600	-1.04413200
O	-2.49532900	1.05527200	-0.72151700
O	-4.29806300	-0.45733500	-0.25192500
O	-2.29521200	-0.43001100	1.19720400
H	-1.28439900	-1.55011900	-0.76684000
H	-1.51456700	1.18329100	-0.61120100

S	1.62500000	-1.74705900	-0.06495200
O	2.49474900	-3.05585900	-0.03919200
O	2.25892200	-0.95907300	-1.19405200
O	0.28429300	-2.14902000	-0.39499600
O	1.85113600	-1.10561700	1.19884400
H	2.13547100	-3.69945900	-0.66426200
H	2.33436100	0.08623200	-0.99483800
O	0.75413400	3.22380900	-1.04837100
H	0.93553700	3.03305100	-1.97763000

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

Atom	X	Y	Z
S	-0.65733800	2.01970400	-0.34506600
O	-1.66014000	1.93118900	0.71432700
O	-0.90289500	1.12200000	-1.45288500
O	-0.69739900	3.48851200	-0.92226400
H	-1.44816800	3.58455100	-1.52289400
O	0.68903500	1.94564600	0.23069800
H	0.89948000	0.09764000	2.00561700
O	-1.98709700	-1.19105400	1.17147600
S	-2.99481000	-1.15446000	0.13233400
O	-3.65528300	0.25604400	0.17018600
O	-4.01174400	-2.13427500	0.12980800
O	-2.28818900	-1.19911300	-1.25129200
H	-2.98083700	0.94341900	0.40902200
H	-1.67192000	-0.43598900	-1.35909900
N	-0.04058400	0.20078500	2.41756100
H	-0.73183900	-0.39210000	1.90177700
H	-0.34378200	1.16932000	2.29968000
H	-0.02375700	-0.05722100	3.39957900
S	3.27055700	-0.17166100	0.20820200
O	2.64602100	-0.12944800	1.49828100
O	4.67052200	-0.27517100	0.08382500
O	2.70116500	0.88436800	-0.71568000
N	1.40337200	-1.83074300	-0.68193300
O	1.19132200	-2.83690700	-1.25458500
O	0.65000800	-1.01722300	-0.23187800
O	2.78607500	-1.58466600	-0.52585500
H	1.81553400	1.32355000	-0.36388900

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

Atom	X	Y	Z
S	-0.10692100	2.21337700	-0.29618700
O	-0.51396200	1.22628900	-1.27414700
O	1.31923400	2.07638600	0.07828000
O	-0.90871700	2.33478000	0.89902000
O	-0.22715900	3.56385400	-1.10209700
H	0.04386000	1.31515300	2.14283600
H	-0.14030700	4.31352300	-0.49930800
S	-2.19610300	-1.53655900	0.06120500
O	-1.65476700	-0.81755100	1.17748700
O	-2.20564600	-2.94693900	0.03713200
O	-1.69709500	-0.97341000	-1.25649900
N	-4.21672900	0.17655400	0.00372200
O	-5.37745400	0.28071800	0.18985200
O	-3.37615800	0.98745000	-0.20565500
O	-3.80767200	-1.19557100	0.02806000

H	-1.25335900	-0.04695800	-1.18224200
S	3.69626300	-0.18737800	0.11255500
O	3.15094300	0.01362500	1.42424900
O	5.08534100	-0.35054000	-0.06767100
O	3.08614800	0.74725900	-0.89737200
N	1.76855900	-1.91294700	-0.47398600
O	1.50283800	-2.95293100	-0.95879300
O	1.04517500	-1.06308100	-0.02942900
O	3.14838800	-1.67740100	-0.42150500
H	2.25198800	1.32519400	-0.52024500
N	0.49819300	0.42775200	2.41530300
H	1.43530000	0.37215900	1.98397600
H	-0.10267100	-0.31313000	2.02711900
H	0.56770600	0.34000900	3.42412900

A·$(NSA)_3$

Atom	X	Y	Z
S	3.96954800	-0.47147600	0.60082500
O	3.07082700	-0.85300700	1.64982800
O	5.36053800	-0.64293700	0.73912100
O	3.63118600	0.89679700	0.04543400
N	2.34972400	-1.52350400	-1.22226500
O	2.28153600	-2.18903700	-2.18969700
O	1.49897400	-0.91928300	-0.63296600
O	3.65983800	-1.46484900	-0.70233600
H	2.67881800	1.23915700	0.28437300
S	-3.50668800	-0.93678700	0.65526100
O	-3.11969200	0.10465300	-0.38793800
O	-4.88825200	-0.89243500	0.92615200
O	-2.53228100	-1.02703800	1.69485600
N	-2.17659700	-2.78464200	-0.71650100
O	-2.25565400	-3.79924200	-1.31012500
O	-1.21846100	-2.10247400	-0.47858500
O	-3.42108600	-2.34866700	-0.23438900
H	-0.13095900	-1.04442800	2.83438700
S	0.24489300	1.82487500	-0.21535300
O	0.51217800	1.83590000	-1.60733700
O	1.37874200	1.70860900	0.69623900
O	-0.83146500	0.93560900	0.24343600
N	-1.40185200	3.86619500	-0.43139000
O	-1.53797400	5.01796200	-0.21459600
O	-2.05611900	3.10239000	-1.06439900
O	-0.24700600	3.34295800	0.22428200
H	-2.18155800	0.47829200	-0.24784900
N	0.23226600	-1.00111300	1.88647100
H	-0.21903400	-0.21367200	1.37990100
H	-0.03791900	-1.84391300	1.38072900
H	1.25651700	-0.88607800	1.86549300

$(SA)_3$·$(A)_2$

Atom	X	Y	Z
N	0.00518100	-2.07016200	0.13235300
H	-0.75853200	-2.16079900	-0.55462500
H	0.93474300	-1.88806300	-0.30515600
H	0.03719300	-2.89913000	0.71738900
N	-2.34720800	1.90536900	1.66490700
H	-3.28300000	2.15582800	1.35682500

H	-2.15626000	2.28748100	2.58494300
H	-2.28784300	0.86629500	1.66909200
S	-3.05154400	-0.82064200	-0.13076300
O	-2.54077100	-1.86675900	-0.99529000
O	-2.97918700	0.51386700	-0.72804800
O	-2.49768700	-0.83783600	1.22061400
H	-1.36657100	0.64835200	-1.39460500
S	0.28837400	1.51641400	-0.40036800
O	-0.38382400	0.61467600	-1.49818000
O	1.58674500	1.85904500	-0.92585500
O	-0.60465300	2.64712900	-0.17390700
O	0.36418400	0.67575900	0.81966400
H	-0.22309800	-1.24829000	0.70426700
H	-1.64624200	2.26948800	0.94588000
O	-4.59477800	-1.12522500	0.10609000
H	-5.01675300	-1.29530900	-0.74583900
S	3.45174800	-0.69237600	0.13959600
O	3.87133700	0.63659300	-0.53293900
O	2.71916700	-0.25160100	1.44404300
O	4.61983900	-1.39864900	0.50930300
O	2.47134100	-1.33631400	-0.71283100
H	3.05627700	1.14908100	-0.79026500
H	1.83331600	0.16880500	1.23453400

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

Atom	X	Y	Z
N	0.62151800	-3.05233600	1.24098200
H	-0.03749000	-3.22766200	0.46196400
H	0.25073800	-2.22294100	1.71160300
H	0.65292800	-3.84385600	1.87454400
S	2.30999200	-1.03301000	-0.80162800
O	0.88791500	-1.25149000	-0.93448500
O	3.03236000	-0.60693500	-1.94737500
O	2.93713400	-1.97846300	0.09421300
N	1.81962800	0.62041600	1.28356900
O	1.90291800	1.72842700	1.74293500
O	1.28304600	-0.32785700	1.77586300
O	2.42754000	0.49127200	0.08121700
H	1.56325500	-2.80700800	0.87742700
S	-2.23733800	-1.68951000	-0.14773100
O	-1.66089500	-2.99617800	-0.32746700
O	-3.64684200	-1.54127100	-0.11248600
O	-1.73940200	-0.73154000	-1.29121200
O	-1.54906900	-1.10447200	1.11084100
H	-0.75349100	-0.69877300	-1.30510100
H	-1.67922600	-0.06970200	1.17813100
S	-1.30581100	2.13998200	0.03522600
O	-1.84108000	1.36662300	1.15625600
O	-1.05848400	3.52978700	0.30584800
O	-2.41364800	2.13504400	-1.09077500
O	-0.13218900	1.45532200	-0.55102500
H	-2.59619200	1.21628800	-1.34843000
H	0.98691400	2.48189100	-0.73479800
N	1.63121600	3.34108200	-0.60686000
H	0.99677900	4.08315800	-0.30412000
H	2.12773100	3.59063900	-1.45501200
H	2.27760000	3.10830400	0.14727800

SA·(A)$_2$·(NSA)$_2$

Atom	X	Y	Z
N	-1.44161700	0.41137600	2.39778400
H	-0.47915800	0.18651200	2.66750500
H	-2.08343700	-0.34451900	2.62269900
H	-1.73382200	1.29410100	2.80836100
S	-1.60396700	1.97918900	-0.70528100
O	-2.54728100	2.64056600	0.13442800
O	-1.79273700	1.98693200	-2.13135200
O	-1.15418100	0.67530200	-0.20631200
N	0.46015000	3.11399600	0.53574500
O	1.42248200	3.79641000	0.44505200
O	-0.00621600	2.59066600	1.51103900
O	-0.18754400	2.92572400	-0.67382700
H	-1.41192200	0.52992400	1.34378600
S	1.73286500	-0.37640700	0.48637800
O	1.07686900	-1.54022100	-0.12701600
O	1.33655000	-0.13264100	1.84193500
O	1.82558900	0.74879600	-0.40533400
N	4.08474800	-1.21954800	-0.37942000
O	5.19831100	-1.48523300	-0.07796200
O	3.55833400	-1.20608300	-1.44867400
O	3.30310000	-0.88562300	0.74443300
H	0.79293900	0.19830100	-1.89527600
N	0.04387500	-0.16541000	-2.50744400
H	0.43685500	-0.56949100	-3.35130700
H	-0.60880800	0.60610300	-2.71552200
H	-0.47708500	-0.87379200	-1.96926400
S	-2.18182400	-2.26723000	0.18218300
O	-3.22305800	-1.50993400	0.80617800
O	-1.79168400	-2.03038300	-1.17301000
O	-2.60222300	-3.78675400	0.22498600
O	-0.95387300	-2.21462500	1.10757400
H	-3.21389000	-3.93342300	0.95774200
H	-0.07414100	-2.00092900	0.59049600

(A)$_2$·(NSA)$_3$

Atom	X	Y	Z
N	-0.51611800	1.86604900	-0.32762400
H	0.50886200	1.72594100	-0.20446100
H	-1.03646800	1.58061500	0.50827700
H	-0.71276200	2.83962600	-0.54031500
S	-0.01787500	-1.34100700	-1.53025700
O	0.88778300	-0.22384300	-1.50179000
O	0.27663000	-2.35761800	-2.49381600
O	-1.41499900	-0.95408400	-1.39184600
N	0.19541900	-1.64551000	1.12451900
O	0.50534900	-2.36087700	2.00955100
O	-0.22171500	-0.52247800	1.15356000
O	0.34038300	-2.24471400	-0.13201900
H	-0.83196500	1.26747600	-1.09224700
S	-3.67752100	0.04264000	1.19734500
O	-2.67418800	1.04187600	1.36985500
O	-4.47117300	-0.40914200	2.26890700
O	-3.18381500	-1.14558200	0.38434800
N	-4.43313800	1.33490100	-0.99039800
O	-5.31438000	1.91123000	-1.52042000
O	-3.28832400	1.20215600	-1.31675700

O	-4.84100400	0.70596400	0.19889500
H	-2.44579100	-0.98053500	-0.30340200
S	3.57975100	1.68979800	-0.23369500
O	2.18380200	1.94053600	0.03469400
O	4.46028800	2.80152500	-0.19384700
O	3.84279000	0.71022500	-1.27168200
N	3.45315700	-0.21360200	1.64247000
O	3.64913000	-0.50667700	2.77463600
O	2.77171300	-0.80572700	0.83335900
O	4.10364000	0.90704800	1.23031800
H	3.29517900	-0.74272800	-1.58769600
N	3.13640100	-1.77944100	-1.77679600
H	2.41038700	-1.91475700	-2.48388400
H	2.79993800	-2.18445300	-0.90189300
H	4.00452300	-2.22608000	-2.05610200

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

Atom	X	Y	Z
S	2.61550300	-1.21713100	0.07787100
O	1.50419700	-2.11956500	0.33153900
O	3.94552200	-2.09812300	0.14786300
O	2.66374100	-0.67863000	-1.27165400
H	3.94723000	-2.59642300	0.97400000
S	-2.80519300	-0.98920500	-0.06753700
O	-2.88751900	0.34179100	0.50484700
O	-4.14297800	-1.67881400	0.45755400
O	-2.85144000	-1.05270500	-1.52017700
H	-4.26188300	-2.51704700	-0.00442200
S	-0.33046500	2.24661500	0.03312700
O	0.21614600	0.92532100	-0.34071300
O	-0.53745000	2.32266200	1.47103800
O	-1.71152100	2.40034500	-0.67450000
O	0.49429700	3.31883300	-0.51434200
H	1.96174700	2.66009600	-0.62515700
O	2.74348300	-0.20042500	1.12633500
N	-0.09442900	-0.29203800	2.17408000
N	2.82992600	2.04774500	-0.59450900
N	-0.09600400	-1.28903300	-1.85188200
H	3.67861200	2.57105100	-0.77685000
H	2.87821600	1.57373000	0.31751000
H	2.72943200	1.26102800	-1.24862100
H	-2.31296100	1.69948700	-0.30930200
H	0.20493900	-1.93442300	-1.11044700
H	0.50390300	-1.39420000	-2.66253600
H	-1.09902400	-1.41255800	-2.04950500
H	0.02767100	-0.33907600	-1.43743600
H	0.89281000	-0.35062400	1.89832100
H	-0.65647300	-0.89341900	1.53205000
H	-0.39668000	0.69889100	2.05200600
H	-0.21685000	-0.59772400	3.13279700
O	-1.69080900	-1.77318400	0.47325800

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

Atom	X	Y	Z
N	0.35967200	-2.94456900	-1.17491000
H	0.91920100	-2.56751300	-0.35504900
H	0.58266900	-2.33038700	-1.95727400

H	0.64312000	-3.89629100	-1.38224400
S	-2.38575900	-1.67322300	0.54492100
O	-1.09001700	-1.53425100	1.16030800
O	-3.53196700	-1.53871500	1.37863000
O	-2.42741000	-2.64535600	-0.52166200
N	-1.76469300	0.18738500	-1.33239900
O	-2.01177900	1.25028000	-1.84151300
O	-0.89603100	-0.57279000	-1.63719800
O	-2.59647800	-0.12743100	-0.31239900
H	-0.65503500	-2.89083500	-0.98421400
S	2.90007500	-0.90996600	-0.06379800
O	2.00590900	-1.89102200	0.62927400
O	4.15494300	-1.47361300	-0.43449900
O	2.93511700	0.32458500	0.72262300
O	2.12564000	-0.57730700	-1.40006200
H	1.58257000	0.07809300	3.05143200
H	1.67497400	0.31316200	-1.35053800
S	0.50888900	2.33771300	-0.00515200
O	0.99718200	1.78734900	-1.25369400
O	-0.20858500	3.60427100	-0.13712400
O	1.75458200	2.67229800	0.88331300
O	-0.30971600	1.36789300	0.75166400
H	2.37915900	1.90759500	0.80019800
H	-2.43026300	2.03533300	0.90693300
N	-2.65662200	2.86295400	0.35015100
H	-1.70147000	3.32589600	0.14425400
H	-3.30495300	3.47324600	0.83421700
H	-3.03970600	2.52400100	-0.53346300
N	0.85239200	-0.37237800	2.50983600
H	1.28305600	-1.08512100	1.86349000
H	0.38504800	0.32004900	1.88054200
H	0.14966900	-0.81420400	3.09300600

SA·$(A)_3$·$(NSA)_2$

Atom	X	Y	Z
N	0.62761600	-1.44666200	2.02500900
H	0.45256200	-0.46894700	1.75830100
H	1.63270900	-1.65849100	1.92314400
H	0.28590200	-1.61609300	2.96494900
S	-2.05988900	-2.53613800	-0.51979200
O	-2.90976000	-3.39919700	0.22226100
O	-2.20873000	-2.45435000	-1.94941800
O	-0.66687900	-2.45702000	-0.10215400
N	-2.68212000	-0.46512800	1.10161600
O	-3.23332800	0.58187800	1.22846800
O	-2.15517100	-1.13627500	1.94785800
O	-2.64875700	-0.91566000	-0.19197300
H	0.07481500	-2.00494800	1.33902600
S	0.24115600	2.08758200	0.24570500
O	0.71043400	2.12904000	-1.12696200
O	1.12034300	2.70361300	1.20311000
O	-0.33599100	0.82057000	0.64440000
N	-2.17489200	2.86669800	-0.48288000
O	-3.06180200	3.62197400	-0.28896300
O	-2.10528700	1.94184500	-1.23797200
O	-1.04720100	3.15799700	0.30562400
H	-0.85030700	0.04834500	-1.24079200
N	-0.24773900	-0.36040900	-1.96502300

H	-0.07917300	0.35744000	-2.66356600
H	-0.72579600	-1.18838700	-2.34083000
H	0.63729800	-0.60808000	-1.49769000
S	3.42494700	-0.99824000	0.04170400
O	3.31521100	-1.78331700	1.25560100
O	2.17741200	-0.39008000	-0.40160600
O	3.76716700	-2.02236100	-1.12906100
O	4.51920300	-0.02688500	0.07385700
H	4.44059500	-2.64236700	-0.82223700
H	3.95654300	1.42933400	-0.18748900
N	3.45258000	2.35028400	-0.37291500
H	3.00678100	2.69100500	0.48530800
H	2.66520900	2.17290600	-1.01066700
H	4.08040500	3.04937800	-0.75453500

$(A)_3\cdot(NSA)_3$

Atom	X	Y	Z
N	0.08277300	-1.81457000	-0.75982300
H	-0.91384300	-2.10213300	-0.73907700
H	0.56143700	-1.99963600	0.12847500
H	0.59451600	-2.27310400	-1.51211700
S	0.50604100	2.28272900	-0.92311500
O	0.72951900	0.89306900	-0.60331600
O	-0.25594200	2.54435700	-2.11400700
O	1.60730700	3.15291600	-0.62674500
N	-0.60873700	2.47256700	1.52826600
O	-1.62685600	2.59681000	2.12960000
O	0.47592800	2.16612300	1.93020800
O	-0.74507600	2.75382500	0.18517600
H	0.14209900	-0.79391000	-0.88907600
S	3.35033500	-1.83182800	0.76684000
O	2.08963700	-1.18357700	1.11996700
O	3.42300300	-3.23357300	0.98167200
O	4.50698600	-1.02042200	1.01877500
N	2.96167600	-0.71384300	-1.65307200
O	2.24552900	-0.82738500	-2.60747900
O	3.49472600	0.28093000	-1.25290100
O	3.17423800	-1.88809100	-0.98741000
H	3.95855600	0.99992900	0.97786800
S	-3.83384400	-1.73749600	-0.44389600
O	-2.59269900	-2.42649700	-0.71207700
O	-4.98943300	-2.52400600	-0.21346800
O	-4.02398100	-0.52346200	-1.21750100
N	-2.49046500	-0.43210200	1.47225400
O	-2.24164400	-0.33499300	2.62697500
O	-1.86861200	0.05433700	0.54488600
O	-3.60301000	-1.15391200	1.18925800
H	-3.25012200	0.86789900	-1.35632200
N	-2.94942000	1.87831200	-1.43956300
H	-2.03923200	1.98295900	-1.91424900
H	-2.82352500	2.25731400	-0.50057700
H	-3.66294900	2.40448100	-1.93552200
N	3.06647700	1.45342600	1.19774900
H	2.36338200	0.69565300	1.17769300
H	2.79656400	2.15181000	0.49109200
H	3.07951900	1.87612500	2.12097600