Supplementary information for

The role of nitric acid in atmospheric new particle formation

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Section 1. Boundary conditions and concentration ranges

Section 2.

Figure S1. The most stable structures of binary clusters involving NA-SA-based, NA-A-based and SA-A-based clusters obtained at the M06-2X/6-311++G(3df,3pd) level of theory. The grey balls represent carbon atoms, red is for oxygen atoms, yellow is for sulfur atoms, blue is for nitrogen atoms and white is for hydrogen atoms. The hydrogen bonds are shown as dashed lines. The lengths of the hydrogen bonds are given in Å.

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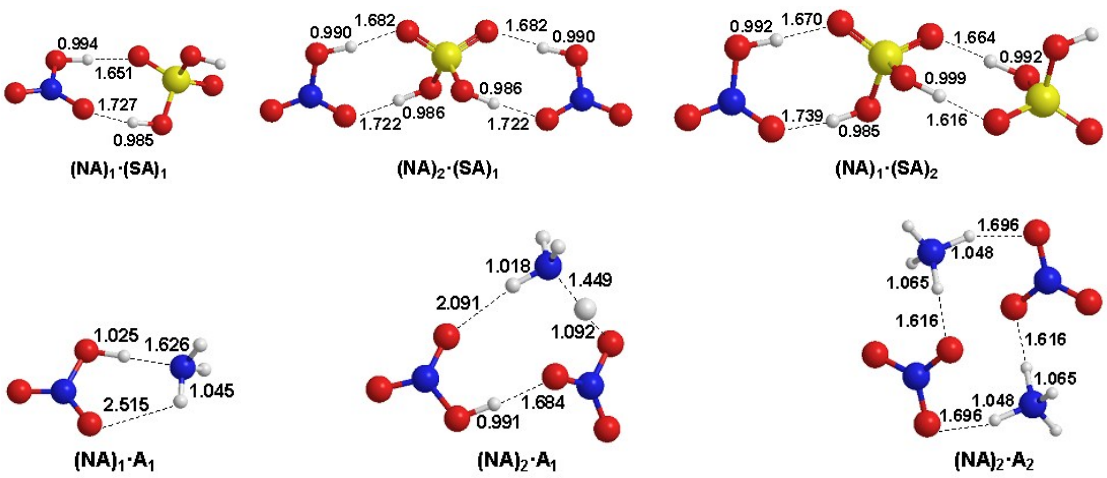
Tables S4-S15. Total contributions of the concentrations (w, %) of $\mathbf{a}_m\mathbf{b}_n$ clusters involving **NA** (**a**= acid ($(\mathbf{NA})_x(\mathbf{SA})_y$), **b**=base (**A**), $0 \le n \le m \le 3$, $0 \le x \le m$, $0 \le y \le m$, $x+y = m$ and x=1, 2, 3) to the total concentration (molecules cm^{-3}) of $\mathbf{a}_m\mathbf{b}_n$ clusters (x=0, 1, 2, 3). The contributions of a certain $(\mathbf{NA})_x(\mathbf{SA})_y\mathbf{A}_n$ cluster ($x \neq 0$) to the total concentrations of the corresponding $(\mathbf{NA})_x(\mathbf{SA})_y\mathbf{A}_n$ (x=1, 2, 3) clusters are shown in the pie chart. [**SA**] =10^5, 10^6, 10^7 molecules cm^{-3}. [**NA**] =10^9, 10^{10}, 10^{11} molecules cm^{-3}. [**A**] =10^8, 10^9, 10^{10} molecules cm^{-3}. The temperature is 220, 240, 260, 280 and 300 K.

Section 1. Boundary conditions and concentration range

The maximum number of acid or basic molecules in the studied system is three. Whether the cluster is allowed to leave the studied size range or not depends on the boundary conditions. The boundary conditions require the outgrowing clusters to have a favorable composition so that the clusters are stable enough not to evaporate back immediately. According to the ACDC simulations, the evaporation rate of **NA** molecule from the different clusters is relatively high (shown in Table S1). Whereas, $(\mathbf{SA})_4\mathbf{A}_3$ and $(\mathbf{SA})_4\mathbf{A}_4$ clusters are relatively stable enough to resist evaporation. Thus, boundary conditions were set to be $(\mathbf{SA})_4\mathbf{A}_3$ and $(\mathbf{SA})_4\mathbf{A}_4$ clusters.

The concentration of **SA** was set in a range of $10^5 \sim 10^8$ molecules cm^{-3} which is relevant to atmospheric particle formation.[1,2,3,4,5] The concentration of **A** varies widely in the atmosphere and was set approximately in the range of $10^8 \sim 10^{10}$ molecules cm^{-3}.[5] The common atmospheric concentration of **NA** is in the range of $10^9 \sim 10^{11}$ molecules cm^{-3}.[6,7]

Section 2.



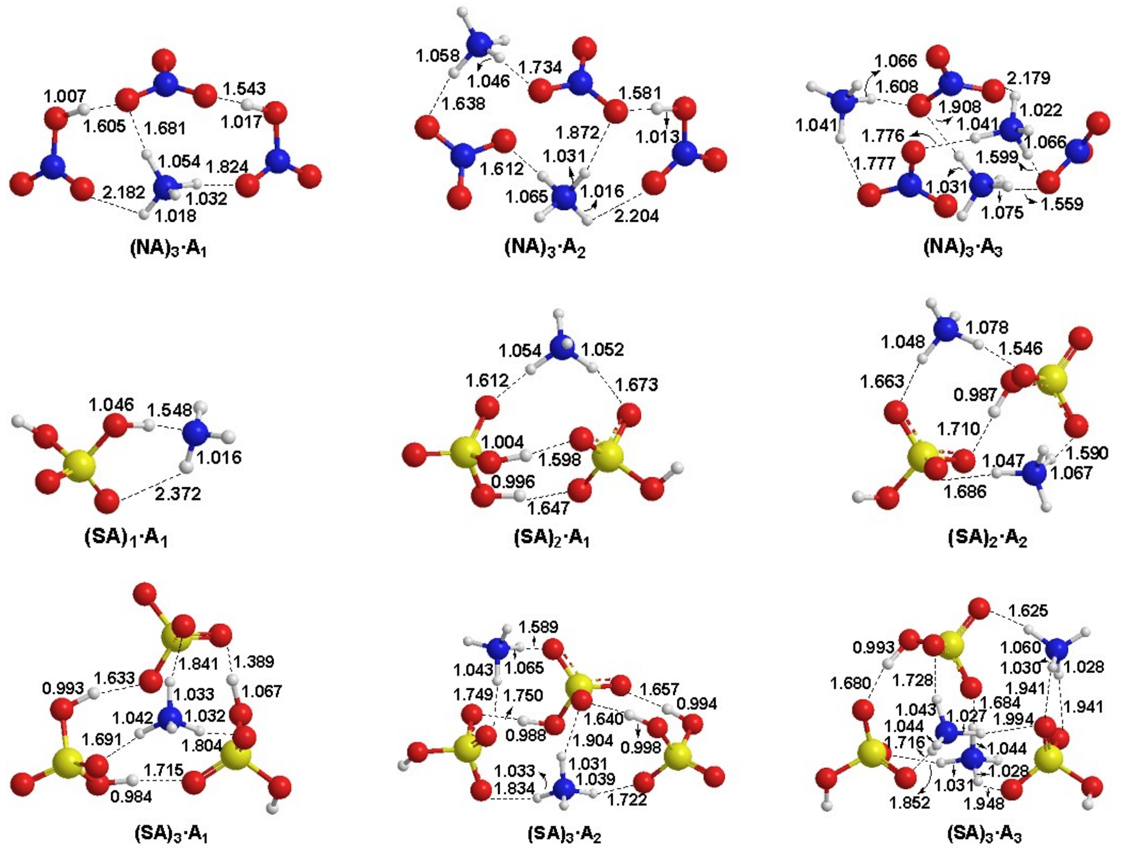


Figure S1. The most stable structures of binary clusters involving NA-SA-based, NA-A-based and SA-A-based clusters obtained at the M06-2X/6-311++G(3df,3pd) level of theory. The grey balls represent carbon atoms, red is for oxygen atoms, yellow is for sulfur atoms, blue is for nitrogen atoms and white is for hydrogen atoms. The hydrogen bonds are shown as dashed lines. The lengths of the hydrogen bonds are given in Å.

Table S1. Evaporation rates of the studied clusters at different temperatures of 220, 240, 260, 280 and 300 K.

Clusters	220K	240K	260 K	280 K	300 K
$(SA)_2$→SA+SA	5. 2E-02	1. 7E+00	3. 2E+01	4. 0E+02	3. 5E+03
$(NA)_2$→NA+NA	9. 3E+06	6. 5E+07	3. 3E+08	1. 4E+09	4. 5E+09
$(NA)_1(SA)_1$→NA+SA	3. 6E+03	4. 8E+04	4. 2E+05	2. 8E+06	1. 4E+07
$(SA)_3$→$(SA)_2$+SA	2. 2E+01	7. 3E+02	1. 4E+04	1. 7E+05	1. 5E+06
$(NA)_3$→$(NA)_2$+NA	9. 5E+11	3. 0E+12	7. 9E+12	1. 8E+13	3. 6E+13
$(NA)_1(SA)_2$→$(NA)_2$+NA	8. 5E+05	1. 2E+07	1. 1E+08	7. 2E+08	3. 7E+09
$(NA)_2(SA)_1$→$(NA)_1(SA)_1$+NA	6. 9E+04	8. 5E+05	6. 9E+06	4. 2E+07	2. 0E+08
$(SA)_1A_1$→SA+A	3. 0E+00	6. 6E+01	9. 0E+02	8. 2E+03	5. 7E+04
$(NA)_1A_1$→NA+A	8. 6E+02	1. 1E+04	1. 0E+05	6. 5E+05	3. 2E+06
$(SA)_2A_1$→$(SA)_2$+A	1. 7E-05	1. 8E-03	9. 7E-02	2. 9E+00	5. 4E+01

$(NA)_2A_1$→$(NA)_2$+A	8.2E+07	5.9E+08	3.0E+09	1.2E+10	4.2E+10
$(NA)_1(SA)_1A_1$→$(SA)_1A_1$+NA	2.8E+02	5.3E+03	6.3E+04	5.4E+05	3.4E+06
$(SA)_3A_1$→$(SA)_2A_1$+SA	2.2E-09	4.2E-07	3.6E-05	1.7E-03	4.6E-02
$(NA)_3A_1$→$(NA)_2A_1$+NA	2.2E+05	2.8E+06	2.3E+07	1.4E+08	6.9E+08
$(NA)_1(SA)_2A_1$→$(SA)_2A_1$+NA	5.3E+03	1.0E+05	1.2E+06	9.9E+06	6.1E+07
$(NA)_2(SA)_1A_1$→$(NA)_1(SA)_1A_1$+NA	3.2E+02	9.6E+03	1.7E+05	1.9E+06	1.5E+07
$(SA)_2A_2$→$(SA)_2A_1$+A	3.1E+01	6.8E+02	9.7E+03	9.3E+04	6.5E+05
$(NA)_2A_2$→$(NA)_2A_1$+A	3.0E+01	9.3E+02	1.6E+04	2.0E+05	1.7E+06
$(NA)_1(SA)_1A_2$→$(NA)_1(SA)_1A_1$+A	1.1E+01	3.8E+02	7.4E+03	9.3E+04	8.2E+05
$(SA)_3A_2$→$(SA)_3A_1$+A	1.1E-04	7.6E-03	2.8E-01	6.2E+00	9.0E+01
$(NA)_3A_2$→$(NA)_2A_2$+NA	9.2E+02	1.6E+04	1.8E+05	1.4E+06	8.0E+06
$(NA)_1(SA)_2A_2$→$(SA)_2A_2$+NA	7.0E+00	3.0E+02	7.0E+03	1.0E+05	1.1E+06
$(NA)_2(SA)_1A_2$→$(NA)_1(SA)_1A_2$+NA	2.4E+01	1.0E+03	2.4E+04	3.6E+05	3.7E+06
$(NA)_1(SA)_2A_3$→$(NA)_1(SA)_2A_2$+A	6.0E-05	4.2E-03	1.5E-01	3.2E+00	4.6E+01
$(NA)_2(SA)_1A_3$→$(NA)_2(SA)_1A_2$+A	2.7E-05	2.2E-03	8.9E-02	2.1E+00	3.4E+01
$(SA)_3A_3$→$(SA)_3A_2$+A	4.6E-04	3.2E-02	1.1E+00	2.4E+01	3.4E+02
$(NA)_3A_3$→$(NA)_3A_2$+A	2.4E+01	7.6E+02	1.5E+04	1.8E+05	1.6E+06

Table S2. AIM topological parameters for the stable clusters obtained at the M06-2X/6-311++G(3df,3pd) level.

Clusters	Bonds	r (Å)	ρ (a.u.)	∇²ρ(a.u.)
NA_2	N=O...H-O	1.716	0.0401	0.1148
$(NA)_1$·$(SA)_1$	S=O...H-O-N	1.651	0.0472	0.1188
	N=O...H-O-S	1.727	0.038	0.1176
$(NA)_1$·A_1	H-N...H-O-N	1.626	0.0662	0.0548
NA_3	N=O...H-O-N	1.772	0.033	0.1156
	N=O...H-O-N	1.843	0.0289	0.1044
	N=O...H-O-N	1.785	0.0353	0.11
$(NA)_1$·$(SA)_2$	S=O...H-O-N	1.67	0.0447	0.1188
	S-O-H...O=N	1.739	0.0366	0.1176
$(NA)_2$·$(SA)_1$	N-O-H...O=S	1.682	0.0431	0.1188
	N=O...H-O-S	1.722	0.0382	0.1184
	S=O...H-O-N	1.682	0.0431	0.1184
	N=O...H-O-S	1.722	0.0382	0.118
$(NA)_2$·A_1	N=O...H-N	2.091	0.0152	0.0672
	N=O...H-O-N	1.684	0.0435	0.1156
	N-O-H...N-H	1.449	0.1021	-0.0144
$(NA)_1$·$(SA)_1$·A_1	N=O...H-O-S	1.792	0.0316	0.1132
	S=O...H-O-N	1.597	0.0558	0.1128
	S-O-H...N-H	1.486	0.0926	0.0116
$(NA)_3$·A_1	N-O-H...O=N	1.605	0.0582	0.1036
	N=O...H-N	2.182	0.0146	0.07

	N=O...H-N	1.681	0.051	0.104
	N=O...H-N	1.824	0.0297	0.1092
	N=O...H-O-N	1.543	0.0683	0.0992
(NA)$_1$•**(SA)**$_2$•**A**$_1$	S=O...H-O-N	1.524	0.0718	0.1016
(NA)$_2$•**(SA)**$_1$•**A**$_1$	S=O...H-O-N	1.554	0.0638	0.1068
	S=O...H-O-N	1.565	0.0615	0.1068
	N=O...H-N	1.84	0.03	0.1084
(NA)$_2$•**A**$_2$	N=O...H-N	1.696	0.0493	0.1076
	N=O...H-N	1.616	0.061	0.0944
	N=O...H-N	1.696	0.0493	0.1076
	N=O...H-N	1.616	0.061	0.0944
(NA)$_1$•**(SA)**$_1$•**A**$_2$	N=O...H-N	1.598	0.0634	0.0956
	N=O...H-N	1.704	0.0484	0.1032
(NA)$_3$•**A**$_2$	N=O...H-N	1.734	0.0447	0.106
	N=O...H-N	1.638	0.0576	0.1008
	N=O...H-N	1.612	0.0617	0.094
	N=O...H-O-N	1.581	0.0626	0.0992
	N-H...O=N	2.204	0.014	0.0668
(NA)$_1$•**(SA)**$_2$•**A**$_2$	S=O...H-O-N	1.49	0.077	0.0972
	N=O...H-N	2.057	0.017	0.0684
	N=O...H-N	2.195	0.0141	0.0532
(NA)$_2$•**(SA)**$_1$•**A**$_2$	N=O...H-O-S	2.045	0.0174	0.0708
	N=O...H-O-N	1.578	0.0631	0.0992
	N=O...H-N	1.951	0.0223	0.0928
	N=O...H-N	1.866	0.0313	0.102
	N=O...H-N	1.878	0.0307	0.102
	N=O...H-N	2.239	0.016	0.064
(NA)$_3$•**A**$_3$	N=O...H-N	1.776	0.0397	0.1052
	N=O...H-N	1.599	0.063	0.0968
	N=O...H-N	2.179	0.0176	0.0716
	N=O...H-N	1.777	0.0406	0.116
	N=O...H-N	1.608	0.0623	0.096
	N=O...H-N	1.908	0.0279	0.0948
	N=O...H-N	1.559	0.0697	0.09
(NA)$_1$•**(SA)**$_2$•**A**$_3$	N=O...H-N	1.731	0.0448	0.1068
	N=O...H-N	2.26	0.0158	0.0624
	N=O...H-N	2.001	0.0226	0.0836
	N=O...H-N	1.952	0.0257	0.0988
(NA)$_2$•**(SA)**$_1$•**A**$_3$	N=O...H-N	1.699	0.0488	0.1028
	N=O...H-N	1.883	0.03	0.1076
	N=O...H-N	1.992	0.023	0.0852
	N=O...H-N	1.705	0.0474	0.1032
	N=O...H-N	1.948	0.027	0.1024
	N=O...H-O-S	1.795	0.0356	0.1132

Table S3. The Gibbs free energies (kcal/mol) of $(\mathbf{NA})_x(\mathbf{SA})_y\mathbf{A}_n$ ($0 \leq n \leq x+y \leq 3$) cluster formation at 220, 240, 260, 280 and 300 K.

Clusters	220 K	240 K	260 K	280 K	300 K
$(\mathbf{SA})_2$	-11.06	-10.38	-9.71	-9.03	-8.36
$(\mathbf{NA})_2$	-2.82	-2.13	-1.44	-0.75	-0.07
$(\mathbf{NA})_1(\mathbf{SA})_1$	-6.53	-5.87	-5.21	-4.55	-3.89
$(\mathbf{SA})_3$	-19.94	-18.39	-16.84	-15.30	-13.76
$(\mathbf{NA})_3$	-1.10	0.32	1.73	3.14	4.54
$(\mathbf{NA})_1(\mathbf{SA})_2$	-15.39	-13.83	-12.28	-10.72	-9.17
$(\mathbf{NA})_2(\mathbf{SA})_1$	-11.99	-10.61	-9.24	-7.87	-6.50
$(\mathbf{SA})_1\mathbf{A}_1$	-9.70	-9.09	-8.48	-7.88	-7.27
$(\mathbf{NA})_1\mathbf{A}_1$	-7.23	-6.64	-6.04	-5.45	-4.86
$(\mathbf{SA})_2\mathbf{A}_1$	-26.30	-24.75	-23.21	-21.66	-20.12
$(\mathbf{NA})_2\mathbf{A}_1$	-9.54	-8.20	-6.86	-5.53	-4.20
$(\mathbf{NA})_1(\mathbf{SA})_1\mathbf{A}_1$	-17.50	-16.17	-14.85	-13.52	-12.20
$(\mathbf{SA})_3\mathbf{A}_1$	-39.27	-36.94	-34.61	-32.29	-29.97
$(\mathbf{NA})_3\mathbf{A}_1$	-14.46	-12.34	-10.23	-8.13	-6.03
$(\mathbf{NA})_1(\mathbf{SA})_2\mathbf{A}_1$	-32.89	-30.52	-28.15	-25.79	-23.44
$(\mathbf{NA})_2(\mathbf{SA})_1\mathbf{A}_1$	-25.38	-23.13	-20.89	-18.66	-16.44
$(\mathbf{SA})_2\mathbf{A}_2$	-35.29	-33.06	-30.82	-28.58	-26.35
$(\mathbf{NA})_2\mathbf{A}_2$	-18.49	-16.30	-14.13	-11.95	-9.78
$(\mathbf{NA})_1(\mathbf{SA})_1\mathbf{A}_2$	-26.99	-24.83	-22.68	-20.52	-18.38
$(\mathbf{SA})_3\mathbf{A}_2$	-53.77	-50.70	-47.63	-44.57	-41.51
$(\mathbf{NA})_3\mathbf{A}_2$	-25.79	-22.89	-20.00	-17.11	-14.24
$(\mathbf{NA})_1(\mathbf{SA})_2\mathbf{A}_2$	-44.79	-41.61	-38.43	-35.26	-32.10
$(\mathbf{NA})_2(\mathbf{SA})_1\mathbf{A}_2$	-35.93	-32.77	-29.62	-26.47	-23.34
$(\mathbf{SA})_3\mathbf{A}_3$	-67.76	-63.92	-60.08	-56.26	-52.44
$(\mathbf{NA})_3\mathbf{A}_3$	-34.94	-31.20	-27.46	-23.73	-20.01
$(\mathbf{NA})_1(\mathbf{SA})_2\mathbf{A}_3$	-59.50	-55.61	-51.73	-47.86	-43.99
$(\mathbf{NA})_2(\mathbf{SA})_1\mathbf{A}_3$	-50.97	-47.06	-43.16	-39.26	-35.37

Table S4. Total contributions of the concentrations (w, %) of $\mathbf{a}_m\mathbf{b}_n$ clusters involving **NA** (**a**= acid ($(\mathbf{NA})_x(\mathbf{SA})_y$), **b**=base (**A**), $0 \le n \le m \le 3$, $0 \le x \le m$, $0 \le y \le m$, $x+y = m$ and x=1, 2, 3) to the total concentration (molecules cm^{-3}) of $\mathbf{a}_m\mathbf{b}_n$ clusters (x=0, 1, 2, 3). The contributions [a] of a certain $(\mathbf{NA})_x(\mathbf{SA})_y\mathbf{A}_n$ cluster ($x\neq0$) to the total concentrations of the corresponding $(\mathbf{NA})_x(\mathbf{SA})_y\mathbf{A}_n$ (x=1, 2, 3) clusters are shown in the pie chart. [**SA**] =10^5, 10^6, 10^7 molecules cm^{-3}. The temperature is 220 K.

Clusters	[**SA**]	w (%)	w_1 (%)	w_2 (%)	w_3 (%)
$\mathbf{a}_2$	10^5	99.90	4.62	95.38	--
	10^6	93.33	32.65	67.35	--
	10^7	35.64	82.90	17.10	--
$\mathbf{a}_3$	10^5	86.33	49.98	49.98	0.04
	10^6	38.70	50.00	50.00	0.00
	10^7	5.93	50.00	50.00	0.00
$\mathbf{a}_1\cdot\mathbf{b}_1$	10^5	99.72	--	--	--
	10^6	97.24	--	--	--
	10^7	77.92	--	--	--
$\mathbf{a}_2\cdot\mathbf{b}_1$	10^5	61.62	99.88	0.12	--
	10^6	14.39	99.99	0.01	--
	10^7	2.48	100.00	0.00	--
$\mathbf{a}_2\cdot\mathbf{b}_2$	10^5	98.58	8.51	91.49	--
	10^6	56.25	48.19	51.81	--
	10^7	9.40	90.27	9.73	--
$\mathbf{a}_3\cdot\mathbf{b}_1$	10^5	99.82	3.16	96.84	0.00
	10^6	87.95	23.73	76.27	0.00
	10^7	20.46	67.30	32.70	0.00
$\mathbf{a}_3\cdot\mathbf{b}_2$	10^5	99.73	31.50	54.40	14.09
	10^6	94.52	84.33	15.27	0.40
	10^7	75.51	97.32	2.67	0.01
$\mathbf{a}_3\cdot\mathbf{b}_3$	10^5	98.88	36.91	63.09	0.00

	10^6	81.04	84.42	15.58	0.00
	10^7	48.12	96.98	3.02	0.00

[a] w_1=[(**NA**)$_1$(**SA**)$_y$**A**$_n$]/∑[(**NA**)$_x$(**SA**)$_y$**A**$_n$],

w_2=[(**NA**)$_2$(**SA**)$_y$**A**$_n$]/∑[(**NA**)$_x$(**SA**)$_y$**A**$_n$],

w_3=[(**NA**)$_3$(**SA**)$_y$**A**$_n$]/∑[(**NA**)$_x$(**SA**)$_y$**A**$_n$].

Table S5. Total contributions of the concentrations (w, %) of **a**$_m$**b**$_n$ clusters involving **NA** (**a**= acid ((**NA**)$_x$(**SA**)$_y$), **b**=base (**A**), $0 \le n \le m \le 3$, $0 \le x \le m$, $0 \le y \le m$, $x+y = m$ and x=1, 2, 3) to the total concentration (molecules cm^{-3}) of **a**$_m$**b**$_n$ clusters (x=0, 1, 2, 3). The contributions [a] of a certain (**NA**)$_x$(**SA**)$_y$**A**$_n$ cluster ($x \neq 0$) to the total concentrations of the corresponding (**NA**)$_x$(**SA**)$_y$**A**$_n$ (x=1, 2, 3) clusters are shown in the pie chart. [**NA**] =10^9, 10^{10}, 10^{11} molecules cm^{-3}. The temperature is 220 K.

Clusters	[**NA**]	w (%)	w_1 (%)	w_2 (%)	w_3 (%)
a$_2$	10^9	35.40	82.90	17.10	--
	10^{10}	93.33	32.65	67.35	--
	10^{11}	99.90	4.62	95.38	--
a$_3$	10^9	5.94	50.00	50.00	0.00
	10^{10}	38.70	50.00	50.00	0.00
	10^{11}	86.21	49.98	49.98	0.04
a$_1$·**b**$_1$	10^9	77.88	--	--	--
	10^{10}	97.24	--	--	--
	10^{11}	99.72	--	--	--
a$_2$·**b**$_1$	10^9	0.35	100.00	0.00	--
	10^{10}	14.39	99.99	0.01	--
	10^{11}	92.36	99.88	0.12	--
a$_2$·**b**$_2$	10^9	1.42	90.39	9.61	--
	10^{10}	56.25	48.19	51.81	--
	10^{11}	99.83	7.80	92.20	--
a$_3$·**b**$_1$	10^9	15.62	93.66	6.34	0.00

	10^{10}	87.95	23.73	76.27	0.00
	10^{11}	99.97	0.43	99.57	0.00
$\mathbf{a}_3\cdot\mathbf{b}_2$	10^{9}	73.45	99.62	0.38	0.00
	10^{10}	94.52	84.33	15.27	0.40
	10^{11}	99.01	5.61	73.50	20.88
$\mathbf{a}_3\cdot\mathbf{b}_3$	10^{9}	61.55	99.54	0.46	0.00
	10^{10}	81.04	84.42	24.34	0.00
	10^{11}	91.91	24.34	75.66	0.00

[a] $w_1=[(\mathbf{NA})_1(\mathbf{SA})_y\mathbf{A}_n]/\sum[(\mathbf{NA})_x(\mathbf{SA})_y\mathbf{A}_n]$,

$w_2=[(\mathbf{NA})_2(\mathbf{SA})_y\mathbf{A}_n]/\sum[(\mathbf{NA})_x(\mathbf{SA})_y\mathbf{A}_n]$,

$w_3=[(\mathbf{NA})_3(\mathbf{SA})_y\mathbf{A}_n]/\sum[(\mathbf{NA})_x(\mathbf{SA})_y\mathbf{A}_n]$.

Table S6. Total contributions of the concentrations (w, %) of $\mathbf{a}_m\mathbf{b}_n$ clusters involving **NA** (**a**= acid $((\mathbf{NA})_x(\mathbf{SA})_y)$, **b**=base (**A**), $0 \le n \le m \le 3$, $0 \le x \le m$, $0 \le y \le m$, $x+y = m$ and x=1, 2, 3) to the total concentration (molecules cm^{-3}) of $\mathbf{a}_m\mathbf{b}_n$ clusters (x=0, 1, 2, 3). The contributions [a] of a certain $(\mathbf{NA})_x(\mathbf{SA})_y\mathbf{A}_n$ cluster ($x\neq0$) to the total concentrations of the corresponding $(\mathbf{NA})_x(\mathbf{SA})_y\mathbf{A}_n$ (x=1, 2, 3) clusters are shown in the pie chart. [**A**] =10^8, 10^9, 10^{10} molecules cm^{-3}. The temperature is 220 K.

Clusters	[**A**]	w (%)	w_1 (%)	w_2 (%)	w_3 (%)
$\mathbf{a}_2$	10^{8}	69.51	32.65	67.35	--
	10^{9}	93.33	32.65	67.35	--
	10^{10}	99.24	32.65	67.35	--
$\mathbf{a}_3$	10^{8}	37.72	50.00	50.00	0.00
	10^{9}	38.70	50.00	50.00	0.00
	10^{10}	46.92	50.00	50.00	0.00
$\mathbf{a}_1\cdot\mathbf{b}_1$	10^{8}	97.24	--	--	--
	10^{9}	97.24	--	--	--
	10^{10}	97.26	--	--	--
$\mathbf{a}_2\cdot\mathbf{b}_1$	10^{8}	0.49	99.99	0.01	--
	10^{9}	14.39	99.99	0.01	--

	10^{10}	93.04	99.99	0.01	--
$\mathbf{a}_2 \cdot \mathbf{b}_2$	10^8	3.59	48.47	51.53	--
	10^9	56.25	48.19	51.81	--
	10^{10}	99.03	45.84	54.16	--
$\mathbf{a}_3 \cdot \mathbf{b}_1$	10^8	16.46	91.42	8.58	0.00
	10^9	87.95	23.73	76.27	0.00
	10^{10}	99.98	0.39	99.61	0.00
$\mathbf{a}_3 \cdot \mathbf{b}_2$	10^8	28.70	99.49	0.49	0.01
	10^9	94.52	84.33	15.27	0.40
	10^{10}	98.93	4.73	92.00	3.28
$\mathbf{a}_3 \cdot \mathbf{b}_3$	10^8	23.58	99.34	0.66	0.00
	10^9	81.04	99.34	0.66	0.00
	10^{10}	85.75	27.59	72.41	0.00

[a] w_1=[(**NA**)$_1$(**SA**)$_y$**A**$_n$]/∑[(**NA**)$_x$(**SA**)$_y$**A**$_n$],

w_2=[(**NA**)$_2$(**SA**)$_y$**A**$_n$]/∑[(**NA**)$_x$(**SA**)$_y$**A**$_n$],

w_3=[(**NA**)$_3$(**SA**)$_y$**A**$_n$]/∑[(**NA**)$_x$(**SA**)$_y$**A**$_n$].

Table S7. Total contributions of the concentrations (w, %) of $\mathbf{a}_m\mathbf{b}_n$ clusters involving **NA** (**a**= acid ((**NA**)$_x$(**SA**)$_y$), **b**=base (**A**), $0 \le n \le m \le 3$, $0 \le x \le m$, $0 \le y \le m$, $x+y = m$ and x=1, 2, 3) to the total concentration (molecules cm^{-3}) of $\mathbf{a}_m\mathbf{b}_n$ clusters (x=0, 1, 2, 3). The contributions [a] of a certain (**NA**)$_x$(**SA**)$_y$**A**$_n$ cluster ($x \neq 0$) to the total concentrations of the corresponding (**NA**)$_x$(**SA**)$_y$**A**$_n$ (x=1, 2, 3) clusters are shown in the pie chart. [**SA**] =10^5, 10^6, 10^7 molecules cm^{-3}. The temperature is 240 K.

Clusters	[**SA**]	w (%)	w_1 (%)	w_2 (%)	w_3 (%)
$\mathbf{a}_2$	10^5	99.73	2.48	97.52	--
	10^6	82.18	20.29	79.71	--
	10^7	12.63	71.79	28.21	--
$\mathbf{a}_3$	10^5	93.38	49.96	49.96	0.08
	10^6	58.51	50.00	50.00	0.00
	10^7	12.35	50.00	50.00	0.00

$\mathbf{a}_1 \cdot \mathbf{b}_1$	10^5	99.83	--	--	--
	10^6	98.33	--	--	--
	10^7	85.46	--	--	--
$\mathbf{a}_2 \cdot \mathbf{b}_1$	10^5	0.30	99.45	0.55	--
	10^6	0.03	99.94	0.06	--
	10^7	0.01	99.99	0.01	--
$\mathbf{a}_2 \cdot \mathbf{b}_2$	10^5	17.35	3.73	96.27	--
	10^6	0.32	27.91	72.09	--
	10^7	0.03	79.46	20.54	--
$\mathbf{a}_3 \cdot \mathbf{b}_1$	10^5	51.25	96.49	3.51	0.00
	10^6	9.32	99.59	0.41	0.00
	10^7	1.06	99.90	0.10	0.00
$\mathbf{a}_3 \cdot \mathbf{b}_2$	10^5	3.96	99.47	0.21	0.32
	10^6	0.46	99.97	0.02	0.00
	10^7	0.12	99.99	0.01	0.00
$\mathbf{a}_3 \cdot \mathbf{b}_3$	10^5	14.40	99.64	0.36	0.00
	10^6	1.74	99.96	0.04	0.00
	10^7	0.27	99.99	0.01	0.00

[a] w_1=[$(\mathbf{NA})_1(\mathbf{SA})_y\mathbf{A}_n$]/∑[$(\mathbf{NA})_x(\mathbf{SA})_y\mathbf{A}_n$],

w_2=[$(\mathbf{NA})_2(\mathbf{SA})_y\mathbf{A}_n$]/∑[$(\mathbf{NA})_x(\mathbf{SA})_y\mathbf{A}_n$],

w_3=[$(\mathbf{NA})_3(\mathbf{SA})_y\mathbf{A}_n$]/∑[$(\mathbf{NA})_x(\mathbf{SA})_y\mathbf{A}_n$].

Table S8. Total contributions of the concentrations (w, %) of $\mathbf{a}_m\mathbf{b}_n$ clusters involving **NA** (**a**= acid ($(\mathbf{NA})_x(\mathbf{SA})_y$), **b**=base (**A**), $0 \le n \le m \le 3$, $0 \le x \le m$, $0 \le y \le m$, $x+y = m$ and x=1, 2, 3) to the total concentration (molecules cm^{-3}) of $\mathbf{a}_m\mathbf{b}_n$ clusters (x=0, 1, 2, 3). The contributions [a] of a certain $(\mathbf{NA})_x(\mathbf{SA})_y\mathbf{A}_n$ cluster ($x \neq 0$) to the total concentrations of the corresponding $(\mathbf{NA})_x(\mathbf{SA})_y\mathbf{A}_n$ (x=1, 2, 3) clusters are shown in the pie chart. [**NA**] =10^9, 10^{10}, 10^{11} molecules cm^{-3}. The temperature is 240 K.

Clusters	[**NA**]	w (%)	w_1 (%)	w_2 (%)	w_3 (%)
$\mathbf{a}_2$	10^9	11.53	71.79	28.21	--

	10^{10}	82.18	20.29	79.71	--
	10^{11}	99.74	2.48	97.52	--
$\mathbf{a}_3$	10^{9}	12.36	50.00	50.00	0.00
	10^{10}	58.51	50.00	50.00	0.00
	10^{11}	93.38	49.96	49.96	0.08
$\mathbf{a}_1\cdot\mathbf{b}_1$	10^{9}	85.46	--	--	--
	10^{10}	98.33	--	--	--
	10^{11}	99.83	--	--	--
$\mathbf{a}_2\cdot\mathbf{b}_1$	10^{9}	0.00	99.99	0.01	--
	10^{10}	0.03	99.94	0.06	--
	10^{11}	0.35	99.45	0.55	--
$\mathbf{a}_2\cdot\mathbf{b}_2$	10^{9}	0.01	79.44	20.56	--
	10^{10}	0.32	27.91	72.09	--
	10^{11}	19.44	3.73	96.27	--
$\mathbf{a}_3\cdot\mathbf{b}_1$	10^{9}	1.01	99.96	0.04	0.00
	10^{10}	9.32	99.59	0.41	0.00
	10^{11}	51.59	95.98	4.02	0.00
$\mathbf{a}_3\cdot\mathbf{b}_2$	10^{9}	0.05	100.00	0.00	0.00
	10^{10}	0.46	99.97	0.02	0.40
	10^{11}	4.33	99.39	0.24	20.88
$\mathbf{a}_3\cdot\mathbf{b}_3$	10^{9}	0.18	100.00	0.00	0.00
	10^{10}	1.74	99.96	0.04	0.00
	10^{11}	14.70	99.60	0.40	0.00

[a] $w_1=[(\mathbf{NA})_1(\mathbf{SA})_y\mathbf{A}_n]/\sum[(\mathbf{NA})_x(\mathbf{SA})_y\mathbf{A}_n]$,

$w_2=[(\mathbf{NA})_2(\mathbf{SA})_y\mathbf{A}_n]/\sum[(\mathbf{NA})_x(\mathbf{SA})_y\mathbf{A}_n]$,

$w_3=[(\mathbf{NA})_3(\mathbf{SA})_y\mathbf{A}_n]/\sum[(\mathbf{NA})_x(\mathbf{SA})_y\mathbf{A}_n]$.

Table S9. Total contributions of the concentrations (w, %) of $\mathbf{a}_m\mathbf{b}_n$ clusters involving **NA** (**a**= acid $((\mathbf{NA})_x(\mathbf{SA})_y)$, **b**=base (**A**), $0 \le n \le m \le 3$, $0 \le x \le m$, $0 \le y \le m$, $x+y = m$ and x=1, 2, 3) to the total concentration (molecules cm^{-3}) of $\mathbf{a}_m\mathbf{b}_n$ clusters (x=0, 1, 2, 3). The contributions [a] of a certain

$(\mathbf{NA})_x(\mathbf{SA})_y\mathbf{A}_n$ cluster ($x\neq0$) to the total concentrations of the corresponding $(\mathbf{NA})_x(\mathbf{SA})_y\mathbf{A}_n$ (x=1, 2, 3) clusters are shown in the pie chart. [**A**] =10^8, 10^9, 10^{10} molecules cm^{-3}. The temperature is 240 K.

Clusters	[**A**]	w (%)	w_1 (%)	w_2 (%)	w_3 (%)
$\mathbf{a}_2$	10^8	79.69	20.29	79.71	--
	10^9	82.18	20.29	79.71	--
	10^{10}	92.67	20.29	79.71	--
$\mathbf{a}_3$	10^8	58.47	50.00	50.00	0.00
	10^9	58.51	50.00	50.00	0.00
	10^{10}	58.83	50.00	50.00	0.00
$\mathbf{a}_1\cdot\mathbf{b}_1$	10^8	98.33	--	--	--
	10^9	98.33	--	--	--
	10^{10}	98.33	--	--	--
$\mathbf{a}_2\cdot\mathbf{b}_1$	10^8	0.03	99.94	0.06	--
	10^9	0.03	99.94	0.06	--
	10^{10}	0.11	99.94	0.06	--
$\mathbf{a}_2\cdot\mathbf{b}_2$	10^8	0.25	27.91	72.09	--
	10^9	0.32	27.91	72.09	--
	10^{10}	1.00	27.92	72.08	--
$\mathbf{a}_3\cdot\mathbf{b}_1$	10^8	1.93	99.68	0.32	0.00
	10^9	9.32	99.59	0.41	0.00
	10^{10}	49.41	98.71	1.29	0.00
$\mathbf{a}_3\cdot\mathbf{b}_2$	10^8	0.02	99.98	0.02	0.00
	10^9	0.46	99.97	0.02	0.00
	10^{10}	22.71	99.91	0.08	0.01
$\mathbf{a}_3\cdot\mathbf{b}_3$	10^8	0.06	99.97	0.03	0.00
	10^9	1.74	99.96	0.04	0.00
	10^{10}	51.82	99.87	0.13	0.00

[a] w_1=[$(\mathbf{NA})_1(\mathbf{SA})_y\mathbf{A}_n$]/∑[$(\mathbf{NA})_x(\mathbf{SA})_y\mathbf{A}_n$],

w_2=[$(\mathbf{NA})_2(\mathbf{SA})_y\mathbf{A}_n$]/∑[$(\mathbf{NA})_x(\mathbf{SA})_y\mathbf{A}_n$],

w_3=[$(\mathbf{NA})_3(\mathbf{SA})_y\mathbf{A}_n$]/∑[$(\mathbf{NA})_x(\mathbf{SA})_y\mathbf{A}_n$].

Table S10. Total contributions of the concentrations (w, %) of $\mathbf{a}_m\mathbf{b}_n$ clusters involving **NA** (**a**= acid ($(\mathbf{NA})_x(\mathbf{SA})_y$), **b**=base (**A**), $0 \le n \le m \le 3$, $0 \le x \le m$, $0 \le y \le m$, $x+y = m$ and x=1, 2, 3) to the total concentration (molecules cm^{-3}) of $\mathbf{a}_m\mathbf{b}_n$ clusters (x=0, 1, 2, 3). The contributions [a] of a certain $(\mathbf{NA})_x(\mathbf{SA})_y\mathbf{A}_n$ cluster ($x\neq0$) to the total concentrations of the corresponding $(\mathbf{NA})_x(\mathbf{SA})_y\mathbf{A}_n$ (x=1, 2, 3) clusters are shown in the pie chart. [**SA**] =10^5, 10^6, 10^7 molecules cm^{-3}. The temperature is 260 K.

Clusters	[**SA**]	w (%)	w_1 (%)	w_2 (%)	w_3 (%)
$\mathbf{a}_2$	10^5	99.91	1.45	98.55	--
	10^6	92.77	12.86	87.14	--
	10^7	21.69	59.60	40.40	--
$\mathbf{a}_3$	10^5	96.73	49.58	49.58	0.83
	10^6	74.61	50.00	50.00	0.00
	10^7	22.71	50.00	50.00	0.00
$\mathbf{a}_1\cdot\mathbf{b}_1$	10^5	99.89	--	--	--
	10^6	98.89	--	--	--
	10^7	89.89	--	--	--
$\mathbf{a}_2\cdot\mathbf{b}_1$	10^5	0.96	98.11	1.89	--
	10^6	0.09	99.81	0.19	--
	10^7	0.01	99.98	0.02	--
$\mathbf{a}_2\cdot\mathbf{b}_2$	10^5	51.33	1.84	98.16	--
	10^6	1.21	15.80	84.20	--
	10^7	0.03	65.23	34.77	--
$\mathbf{a}_3\cdot\mathbf{b}_1$	10^5	28.66	92.60	7.30	0.00
	10^6	3.62	99.21	0.79	0.00
	10^7	0.37	99.92	0.08	0.00
$\mathbf{a}_3\cdot\mathbf{b}_2$	10^5	0.20	96.25	0.50	3.25

	10^6	0.02	99.91	0.05	0.03
	10^7	0.00	99.99	0.01	0.00
$\mathbf{a}_3 \cdot \mathbf{b}_3$	10^5	1.05	99.10	0.90	0.00
	10^6	0.11	99.91	0.09	0.00
	10^7	0.01	99.99	0.01	0.00

[a] $w_1=[(\mathbf{NA})_1(\mathbf{SA})_y\mathbf{A}_n]/\sum[(\mathbf{NA})_x(\mathbf{SA})_y\mathbf{A}_n]$,

$w_2=[(\mathbf{NA})_2(\mathbf{SA})_y\mathbf{A}_n]/\sum[(\mathbf{NA})_x(\mathbf{SA})_y\mathbf{A}_n]$,

$w_3=[(\mathbf{NA})_3(\mathbf{SA})_y\mathbf{A}_n]/\sum[(\mathbf{NA})_x(\mathbf{SA})_y\mathbf{A}_n]$.

Table S11. Total contributions of the concentrations (w, %) of $\mathbf{a}_m\mathbf{b}_n$ clusters involving **NA** (**a**= acid ($(\mathbf{NA})_x(\mathbf{SA})_y$), **b**=base (**A**), $00 \leq n \leq m \leq 3$, $0 \leq x \leq m$, $0 \leq y \leq m$, $x+y = m$ and x=1, 2, 3) to the total concentration (molecules cm^{-3}) of $\mathbf{a}_m\mathbf{b}_n$ clusters (x=0, 1, 2, 3). The contributions [a] of a certain $(\mathbf{NA})_x(\mathbf{SA})_y\mathbf{A}_n$ cluster ($x\neq0$) to the total concentrations of the corresponding $(\mathbf{NA})_x(\mathbf{SA})_y\mathbf{A}_n$ (x=1, 2, 3) clusters are shown in the pie chart. [**NA**] =10^9, 10^{10}, 10^{11} molecules cm^{-3}. The temperature is 260 K.

Clusters	[**NA**]	w (%)	w_1 (%)	w_2 (%)	w_3 (%)
$\mathbf{a}_2$	10^9	21.69	59.60	40.40	--
	10^{10}	92.77	12.86	87.14	--
	10^{11}	99.91	1.45	98.55	--
$\mathbf{a}_3$	10^9	22.71	50.00	50.00	0.00
	10^{10}	74.61	50.00	50.00	0.00
	10^{11}	96.73	49.58	49.58	0.83
$\mathbf{a}_1 \cdot \mathbf{b}_1$	10^9	89.89	--	--	--
	10^{10}	98.89	--	--	--
	10^{11}	99.89	--	--	--
$\mathbf{a}_2 \cdot \mathbf{b}_1$	10^9	0.01	99.98	0.02	--
	10^{10}	0.09	99.81	0.19	--
	10^{11}	0.96	98.11	1.89	--
$\mathbf{a}_2 \cdot \mathbf{b}_2$	10^9	0.03	65.23	34.77	--
	10^{10}	1.21	15.80	84.20	--

	10^{11}	51.32	1.84	98.16	--
$\mathbf{a}_3 \cdot \mathbf{b}_1$	10^9	0.37	99.92	0.08	0.00
	10^{10}	3.62	99.21	0.79	0.00
	10^{11}	28.66	92.60	7.39	0.00
$\mathbf{a}_3 \cdot \mathbf{b}_2$	10^9	0.00	99.99	0.01	0.00
	10^{10}	0.02	99.91	0.05	0.03
	10^{11}	0.20	96.26	0.49	3.25
$\mathbf{a}_3 \cdot \mathbf{b}_3$	10^9	0.01	99.99	0.01	0.00
	10^{10}	0.11	99.91	0.09	0.00
	10^{11}	1.05	99.10	0.90	0.00

[a] $w_1=[(\mathbf{NA})_1(\mathbf{SA})_y\mathbf{A}_n]/\sum[(\mathbf{NA})_x(\mathbf{SA})_y\mathbf{A}_n]$,

$w_2=[(\mathbf{NA})_2(\mathbf{SA})_y\mathbf{A}_n]/\sum[(\mathbf{NA})_x(\mathbf{SA})_y\mathbf{A}_n]$,

$w_3=[(\mathbf{NA})_3(\mathbf{SA})_y\mathbf{A}_n]/\sum[(\mathbf{NA})_x(\mathbf{SA})_y\mathbf{A}_n]$.

Table S12. Total contributions of the concentrations (w, %) of $\mathbf{a}_m\mathbf{b}_n$ clusters involving **NA** (**a**= acid ($(\mathbf{NA})_x(\mathbf{SA})_y$), **b**=base (**A**), $0 \le n \le m \le 3$, $0 \le x \le m$, $0 \le y \le m$, $x+y = m$ and x=1, 2, 3) to the total concentration (molecules cm^{-3}) of $\mathbf{a}_m\mathbf{b}_n$ clusters (x=0, 1, 2, 3). The contributions [a] of a certain $(\mathbf{NA})_x(\mathbf{SA})_y\mathbf{A}_n$ cluster ($x\neq0$) to the total concentrations of the corresponding $(\mathbf{NA})_x(\mathbf{SA})_y\mathbf{A}_n$ (x=1, 2, 3) clusters are shown in the pie chart. [**A**] =10^8, 10^9, 10^{10} molecules cm^{-3}. The temperature is 260 K.

Clusters	[**A**]	w (%)	w_1 (%)	w_2 (%)	w_3 (%)
$\mathbf{a}_2$	10^8	92.77	12.86	87.14	--
	10^9	92.77	12.86	87.14	--
	10^{10}	92.79	12.86	87.14	--
$\mathbf{a}_3$	10^8	74.61	50.00	50.00	0.00
	10^9	74.61	50.00	50.00	0.00
	10^{10}	74.61	50.00	50.00	0.00
$\mathbf{a}_1 \cdot \mathbf{b}_1$	10^8	98.89	--	--	--
	10^9	98.89	--	--	--
	10^{10}	98.89	--	--	--

$\mathbf{a}_2\cdot\mathbf{b}_1$	10^8	0.09	99.81	0.19	--
	10^9	0.09	99.81	0.19	--
	10^{10}	0.10	99.81	0.19	--
$\mathbf{a}_2\cdot\mathbf{b}_2$	10^8	1.21	15.80	84.20	--
	10^9	1.21	15.80	84.20	--
	10^{10}	1.22	15.80	84.20	--
$\mathbf{a}_3\cdot\mathbf{b}_1$	10^8	3.61	99.21	0.79	0.00
	10^9	3.62	99.21	0.79	0.00
	10^{10}	4.05	99.21	0.79	0.00
$\mathbf{a}_3\cdot\mathbf{b}_2$	10^8	0.02	99.91	0.05	0.03
	10^9	0.02	99.91	0.05	0.03
	10^{10}	0.02	99.91	0.05	0.03
$\mathbf{a}_3\cdot\mathbf{b}_3$	10^8	0.10	99.91	0.09	0.00
	10^9	0.11	99.91	0.09	0.00
	10^{10}	0.12	99.91	0.09	0.00

[a] $w_1=[(\mathbf{NA})_1(\mathbf{SA})_y\mathbf{A}_n]/\sum[(\mathbf{NA})_x(\mathbf{SA})_y\mathbf{A}_n]$,

$w_2=[(\mathbf{NA})_2(\mathbf{SA})_y\mathbf{A}_n]/\sum[(\mathbf{NA})_x(\mathbf{SA})_y\mathbf{A}_n]$,

$w_3=[(\mathbf{NA})_3(\mathbf{SA})_y\mathbf{A}_n]/\sum[(\mathbf{NA})_x(\mathbf{SA})_y\mathbf{A}_n]$.

Table S13. Total contributions of the concentrations (w, %) of $\mathbf{a}_m\mathbf{b}_n$ clusters involving **NA** (**a**= acid ($(\mathbf{NA})_x(\mathbf{SA})_y$), **b**=base (**A**), $0 \le n \le m \le 3$, $0 \le x \le m$, $0 \le y \le m$, $x+y = m$ and x=1, 2, 3) to the total concentration (molecules cm^{-3}) of $\mathbf{a}_m\mathbf{b}_n$ clusters (x=0, 1, 2, 3). The contributions [a] of a certain $(\mathbf{NA})_x(\mathbf{SA})_y\mathbf{A}_n$ cluster ($x\neq0$) to the total concentrations of the corresponding $(\mathbf{NA})_x(\mathbf{SA})_y\mathbf{A}_n$ (x=1, 2, 3) clusters are shown in the pie chart. [**SA**] =10^5, 10^6, 10^7 molecules cm^{-3}. The temperature is 280 K.

Clusters	[**SA**]	w (%)	w_1 (%)	w_2 (%)	w_3 (%)
$\mathbf{a}_2$	10^5	99.7	0.92	99.08	--
	10^6	97.41	8.46	91.54	--
	10^7	39.88	48.04	51.96	--
$\mathbf{a}_3$	10^5	98.28	46.47	46.47	7.07

	10^6	84.20	49.96	49.96	0.08
	10^7	34.74	50.00	50.00	0.00
$\mathbf{a}_1 \cdot \mathbf{b}_1$	10^5	99.92	--	--	--
	10^6	99.22	--	--	--
	10^7	92.69	--	--	--
$\mathbf{a}_2 \cdot \mathbf{b}_1$	10^5	4.48	94.52	5.48	--
	10^6	0.44	99.42	0.58	--
	10^7	0.04	99.94	0.06	--
$\mathbf{a}_2 \cdot \mathbf{b}_2$	10^5	88.06	1.01	98.99	--
	10^6	7.45	9.25	90.75	--
	10^7	0.15	50.47	49.53	--
$\mathbf{a}_3 \cdot \mathbf{b}_1$	10^5	51.82	78.51	21.42	0.00
	10^6	7.98	97.34	2.66	0.00
	10^7	0.84	99.73	0.27	0.00
$\mathbf{a}_3 \cdot \mathbf{b}_2$	10^5	0.84	68.61	1.33	30.06
	10^6	0.06	99.37	0.19	0.44
	10^7	0.01	99.98	0.02	0.00
$\mathbf{a}_3 \cdot \mathbf{b}_3$	10^5	3.27	96.66	3.34	0.00
	10^6	0.33	99.65	0.35	0.00
	10^7	0.03	99.97	0.03	0.00

[a] w_1=[$(\mathbf{NA})_1(\mathbf{SA})_y\mathbf{A}_n$]/∑[$(\mathbf{NA})_x(\mathbf{SA})_y\mathbf{A}_n$],

w_2=[$(\mathbf{NA})_2(\mathbf{SA})_y\mathbf{A}_n$]/∑[$(\mathbf{NA})_x(\mathbf{SA})_y\mathbf{A}_n$],

w_3=[$(\mathbf{NA})_3(\mathbf{SA})_y\mathbf{A}_n$]/∑[$(\mathbf{NA})_x(\mathbf{SA})_y\mathbf{A}_n$].

Table S14. Total contributions of the concentrations (w, %) of $\mathbf{a}_m\mathbf{b}_n$ clusters involving **NA** (**a**= acid ($(\mathbf{NA})_x(\mathbf{SA})_y$), **b**=base (**A**), $0 \le n \le m \le 3$, $0 \le x \le m$, $0 \le y \le m$, $x+y = m$ and x=1, 2, 3) to the total concentration (molecules cm^{-3}) of $\mathbf{a}_m\mathbf{b}_n$ clusters (x=0, 1, 2, 3). The contributions [a] of a certain $(\mathbf{NA})_x(\mathbf{SA})_y\mathbf{A}_n$ cluster ($x \neq 0$) to the total concentrations of the corresponding $(\mathbf{NA})_x(\mathbf{SA})_y\mathbf{A}_n$ (x=1, 2, 3) clusters are shown in the pie chart. [**NA**] =10^9, 10^{10}, 10^{11} molecules cm^{-3}. The temperature is 280 K.

Clusters	[**NA**]	w (%)	w_1 (%)	w_2 (%)	w_3 (%)
$\mathbf{a}_2$	10^9	39.88	48.04	51.96	--
	10^{10}	97.41	8.46	91.54	--
	10^{11}	99.97	0.92	99.08	--
$\mathbf{a}_3$	10^9	34.74	50.00	50.00	0.00
	10^{10}	84.20	49.96	49.96	0.08
	10^{11}	98.28	46.47	46.47	7.07
$\mathbf{a}_1\cdot\mathbf{b}_1$	10^9	92.69	--	--	--
	10^{10}	99.22	--	--	--
	10^{11}	99.92	--	--	--
$\mathbf{a}_2\cdot\mathbf{b}_1$	10^9	0.04	99.94	0.06	--
	10^{10}	0.44	99.42	0.58	--
	10^{11}	4.48	94.52	5.48	--
$\mathbf{a}_2\cdot\mathbf{b}_2$	10^9	0.15	50.47	49.53	--
	10^{10}	7.45	9.25	90.75	--
	10^{11}	88.06	1.01	98.99	--
$\mathbf{a}_3\cdot\mathbf{b}_1$	10^9	0.84	99.73	0.27	0.00
	10^{10}	7.98	97.34	2.66	0.00
	10^{11}	51.82	78.51	21.42	0.00
$\mathbf{a}_3\cdot\mathbf{b}_2$	10^9	0.01	99.98	0.02	0.00
	10^{10}	0.06	99.37	0.19	0.44
	10^{11}	0.84	68.61	1.33	30.06
$\mathbf{a}_3\cdot\mathbf{b}_3$	10^9	0.03	99.97	0.03	0.00
	10^{10}	0.33	99.65	0.35	0.00
	10^{11}	3.27	96.66	3.34	0.00

[a] $w_1=[(\mathbf{NA})_1(\mathbf{SA})_y\mathbf{A}_n]/\sum[(\mathbf{NA})_x(\mathbf{SA})_y\mathbf{A}_n]$,

$w_2=[(\mathbf{NA})_2(\mathbf{SA})_y\mathbf{A}_n]/\sum[(\mathbf{NA})_x(\mathbf{SA})_y\mathbf{A}_n]$,

$w_3=[(\mathbf{NA})_3(\mathbf{SA})_y\mathbf{A}_n]/\sum[(\mathbf{NA})_x(\mathbf{SA})_y\mathbf{A}_n]$.

Table S15. Total contributions of the concentrations (w, %) of $\mathbf{a}_m\mathbf{b}_n$ clusters involving **NA** (**a**=

acid ((**NA**)$_x$(**SA**)$_y$), **b**=base (**A**), $0 \le n \le m \le 3$, $0 \le x \le m$, $0 \le y \le m$, $x+y = m$ and x=1, 2, 3) to the total concentration (molecules cm^{-3}) of $\mathbf{a}_m\mathbf{b}_n$ clusters (x=0, 1, 2, 3). The contributions [a] of a certain (**NA**)$_x$(**SA**)$_y$**A**$_n$ cluster ($x\neq0$) to the total concentrations of the corresponding (**NA**)$_x$(**SA**)$_y$**A**$_n$ (x=1, 2, 3) clusters are shown in the pie chart. [**A**] =10^8, 10^9, 10^{10} molecules cm^{-3}. The temperature is 280 K.

Clusters	[**A**]	w (%)	w_1 (%)	w_2 (%)	w_3 (%)
$\mathbf{a}_2$	10^8	97.41	8.46	91.54	--
	10^9	97.41	8.46	91.54	--
	10^{10}	97.41	8.46	91.54	--
$\mathbf{a}_3$	10^8	84.20	49.96	49.96	0.08
	10^9	84.20	49.96	49.96	0.08
	10^{10}	84.20	49.96	49.96	0.08
$\mathbf{a}_1\cdot\mathbf{b}_1$	10^8	99.22	--	--	--
	10^9	99.22	--	--	--
	10^{10}	99.22	--	--	--
$\mathbf{a}_2\cdot\mathbf{b}_1$	10^8	0.44	99.42	0.58	--
	10^9	0.44	99.42	0.58	--
	10^{10}	0.44	99.42	0.58	--
$\mathbf{a}_2\cdot\mathbf{b}_2$	10^8	7.45	9.25	90.75	--
	10^9	7.45	9.25	90.75	--
	10^{10}	7.45	9.25	90.75	--
$\mathbf{a}_3\cdot\mathbf{b}_1$	10^8	7.98	97.34	2.66	0.00
	10^9	7.98	97.34	2.66	0.00
	10^{10}	7.98	97.34	2.66	0.00
$\mathbf{a}_3\cdot\mathbf{b}_2$	10^8	0.06	99.37	0.19	0.44
	10^9	0.06	99.37	0.19	0.44
	10^{10}	0.06	99.37	0.19	0.44
$\mathbf{a}_3\cdot\mathbf{b}_3$	10^8	0.03	99.65	0.35	0.00
	10^9	0.03	99.65	0.35	0.00

	10^{10}	0.03	99.65	0.35	0.00

[a] $w_1=[(\mathbf{NA})_1(\mathbf{SA})_y\mathbf{A}_n]/\sum[(\mathbf{NA})_x(\mathbf{SA})_y\mathbf{A}_n]$,

$w_2=[(\mathbf{NA})_2(\mathbf{SA})_y\mathbf{A}_n]/\sum[(\mathbf{NA})_x(\mathbf{SA})_y\mathbf{A}_n]$,

$w_3=[(\mathbf{NA})_3(\mathbf{SA})_y\mathbf{A}_n]/\sum[(\mathbf{NA})_x(\mathbf{SA})_y\mathbf{A}_n]$.

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