Supplement of Atmos. Chem. Phys., 22, 6103–6114, 2022
https://doi.org/10.5194/acp-22-6103-2022-supplement

Atmospheric Chemistry and Physics Open Access

Supplement of

Molecular-level nucleation mechanism of iodic acid and methanesulfonic acid

An Ning et al.

Correspondence to: Xiuhui Zhang (zhangxiuhui@bit.edu.cn)

Table of Contents

Table S1. The bond type, electron density $\rho(r)$ (a.u), Laplacian electron density $\nabla^2\rho(r)$ (a.u.), energy density $H(r)$ at corresponding BCPs in the studied IA-MSA-based clusters. The orange balls represent bond critical points (BCPs) in the AIM theory analysis. IA and MSA represent iodic acid (HIO_3) and methanesulfinic acid ($CH_3S(O)_2OH$), respectively. HB (hydrogen bond), XB (halogen bond).

Table S2. The Gibbs formation free energies ΔG_{278K} of the studied IA clusters in Rong et al. 2020 (RI-CC2/aug-cc-pVTZ(-PP)//ωB97X-D/6-311++G(3df,3pd) + aug-cc-pVDZ-PP (for I)) and in this study (RI-CC2/aug-cc-pV(T+d)Z(-PP)//ωB97X-D/6-311++G(3df,3pd) + aug-cc-pVTZ-PP (for I)).

Table S3. The Gibbs formation free energies ΔG (kcal mol^{-1}) of the studied IA-MSA clusters at the RI-CC2/aug-cc-pV(T+d)Z(-PP)//ωB97X-D/6-311++G(3df,3pd) + aug-cc-pVTZ-PP with ECP28MDF (for I) level of theory, p = 1 atm and T = 218, 238, 258, 278, and 298 K.

Table S4. The evaporation rate coefficients (γ, s^{-1}) for all evaporation pathways of clusters at 278 K.

Table S5. Boundary conditions in ACDC simulations at T = 218 ~ 298 K, [IA] =10^6 ~ 10^8, and [MSA] = 10^6 ~ 10^8 molecules cm^{-3}.

Table S6. Enhancement strength R of MSA on cluster formation rates under different atmospheric conditions: T = 218 ~ 298 K ([IA] = 10^7 and [MSA] = 10^7 molecules cm^{-3}), [MSA] = 10^6 ~ 10^8 molecules cm^{-3} (T = 278 K and [IA] = 10^7 molecules cm^{-3}), [IA] = 10^6 ~ 10^8 molecules cm^{-3} (T = 278 K and [MSA] = 10^7 molecules cm^{-3}), and CS = 2.0 × 10^{-3} s^{-1}.

Table S7. Cartesian coordinates of all molecules and clusters in the present study at the ωB97X-D/6-311++G(3df,3pd) + aug-cc-pVTZ-PP with ECP28MDF (for I) level of theory.

Section S1: Determination of the boundary conditions in ACDC simulations.

In ACDC simulations, "nucleation" generally refers to the formation of relatively stable clusters for which collisions with molecules can be assumed to dominate over cluster evaporation. Once these stable clusters on the boundary form and grow further out of the simulated system, these formed clusters out of system are unlikely evaporate back into the system (Oona and Tinja, 2020; McGrath et al., 2012). Thus, finding stable clusters with growth potential on the boundary of the simulation box is a key step in determining boundary conditions of ACDC simulations. Take the $(IA)_4(MSA)_2$ cluster in this study as an example. Specifically, it is to calculate the ratio of the rate at which the studied $(IA)_4(MSA)_2$ cluster collides with the IA (or MSA) monomer to its total evaporation rate.

$$\frac{\beta_{IA} C_{IA} C_{(IA)_4(MSA)_2}}{\sum \gamma_{(IA)_4(MSA)_2} C_{(IA)_4(MSA)_2}} = \frac{\beta_{IA} C_{IA}}{\sum \gamma} \quad \text{(S1)}$$

where β_{IA} is the rate coefficient of cluster collision with IA monomer, C_{IA} is the concentration of IA monomer, and $\sum \gamma$ is the total evaporation rate coefficient of the studied cluster. If $\beta_{IA} C_{IA} / \sum \gamma > 1$, the corresponding cluster is more likely to collide with molecules for further growth, and vice versa, the cluster is more inclined to decompose.

According to Eq. S1, the IA monomer concentrations (C_I) can affect the values of $\beta_{IA} C_{IA} / \sum \gamma$. It is worth noting that all presented values of $\beta_{IA} C_{IA} / \sum \gamma$ in this study (Fig. 2C, Fig. S2C and Fig. S3C) are the minimum values at the lowest C_{IA} (10^6 molecules cm^{-3}). Take the $(IA)_6$ cluster in Fig. S2 as an example, the $\beta C / \sum \gamma$ of the $(IA)_6$ cluster is in the range of 5 ~ 20 under the studied range of IA or MSA concentration (10^6 ~ 10^8 molecules cm^{-3}).

In addition to the monomer concentration, the temperature also affects the setting of the boundary conditions. Herein, the boundary conditions at different temperatures (218 K ~ 298 K), IA and MSA concentrations are summarized in Table S5.

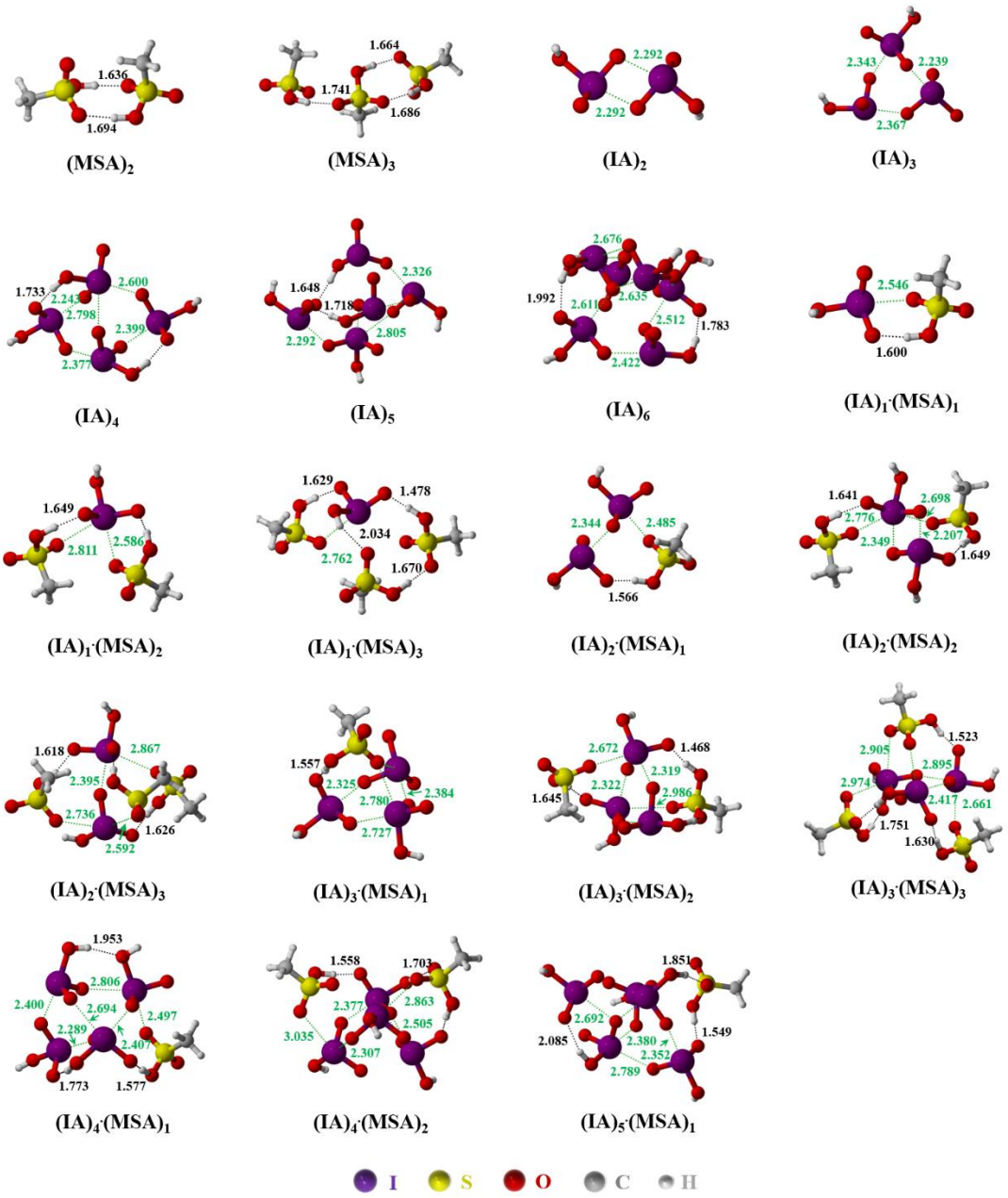


Figure S1. The identified configurations of the studied clusters with lowest free energy (298.15 K) at the ωB97X-D/6-311++G(3df,3pd) + aug-cc-pVTZ-PP with ECP28MDF (for I) level of theory. IA and MSA are the shorthand for iodic acid and methanesulfonic acid, respectively. The black and green dashed lines indicate hydrogen and halogen bonds, respectively. The lengths of hydrogen and halogen bonds are given in Å.

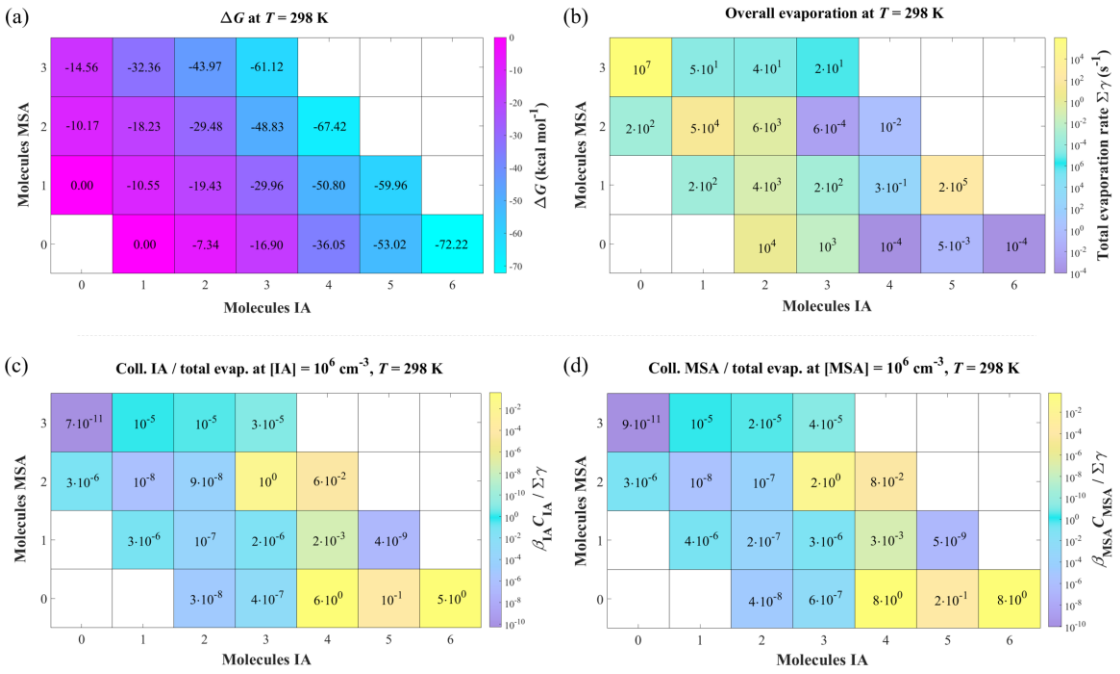


Figure S2. (a) Gibbs formation free energies (ΔG) of the $(IA)_x(MSA)_y$ ($0 \le x \le 6$, $0 \le y \le 3$, $x+y \le 6$) clusters identified at the RI-CC2/aug-cc-pV(T+d)Z(-PP)// ωB97X-D/6-311++G(3df,3pd) + aug-cc-pVTZ-PP (for I) level of theory, T = 298 K, p = 1 atm. (b) the total evaporation rate coefficients ($\sum\gamma$ in s^{-1}) and and the ratios of collision frequencies with (c) IA monomer or (d) MSA monomer versus total evaporation rate coefficients ($\beta_{IA}C_{IA}/\sum\gamma$ or $\beta_{MSA}C_{MSA}/\sum\gamma$) of the corresponding clusters.

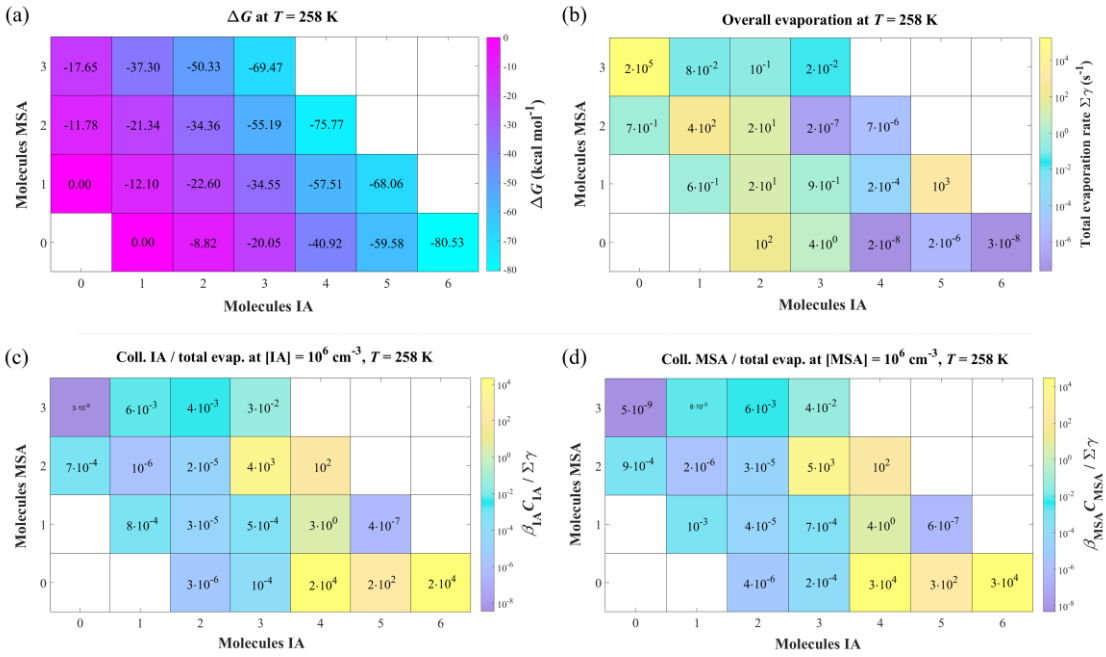


Figure S3. (a) Gibbs formation free energies (ΔG) of the $(IA)_x(MSA)_y$ ($0 \le x \le 6, 0 \le y \le 3, x+y \le 6$) clusters identified at the RI-CC2/aug-cc-pV(T+d)Z(-PP)// ωB97X-D/6-311++G(3df,3pd) + aug-cc-pVTZ-PP (for I) level of theory, T = 258 K, p = 1 atm. (b) the total evaporation rate coefficients ($\sum\gamma$ in s^{-1}) and and the ratios of collision frequencies with (c) IA monomer or (d) MSA monomer versus total evaporation rate coefficients ($\beta_{IA}C_{IA}/\sum\gamma$ or $\beta_{MSA}C_{MSA}/\sum\gamma$) of the corresponding clusters.

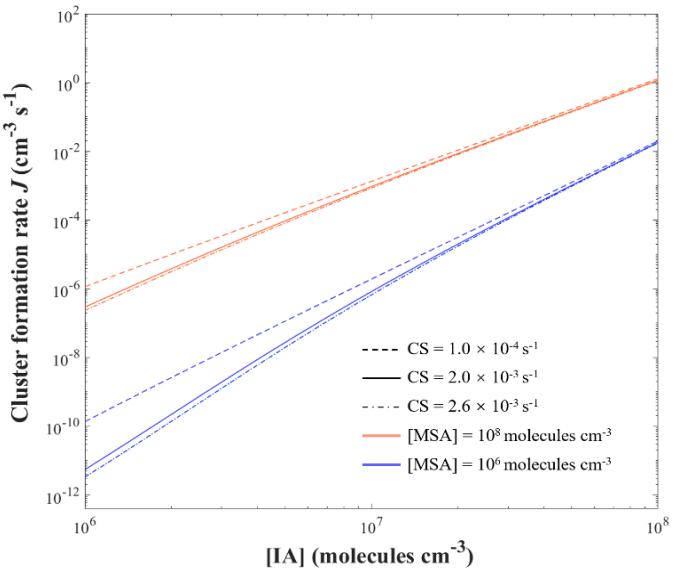


Figure S4. The simulated cluster formation rate J (cm^{-3} s^{-1}) of the IA-MSA system at different condensention sink (CS) coefficients (CS = $1.0 \times 10^{-4} \sim 2.6 \times 10^{-3}$ s^{-1}), T = 278 K, [IA] = $10^6 \sim 10^8$ molecules cm^{-3}, and [MSA] = 10^6 (blue lines), 10^8 (orange lines) molecules cm^{-3}.

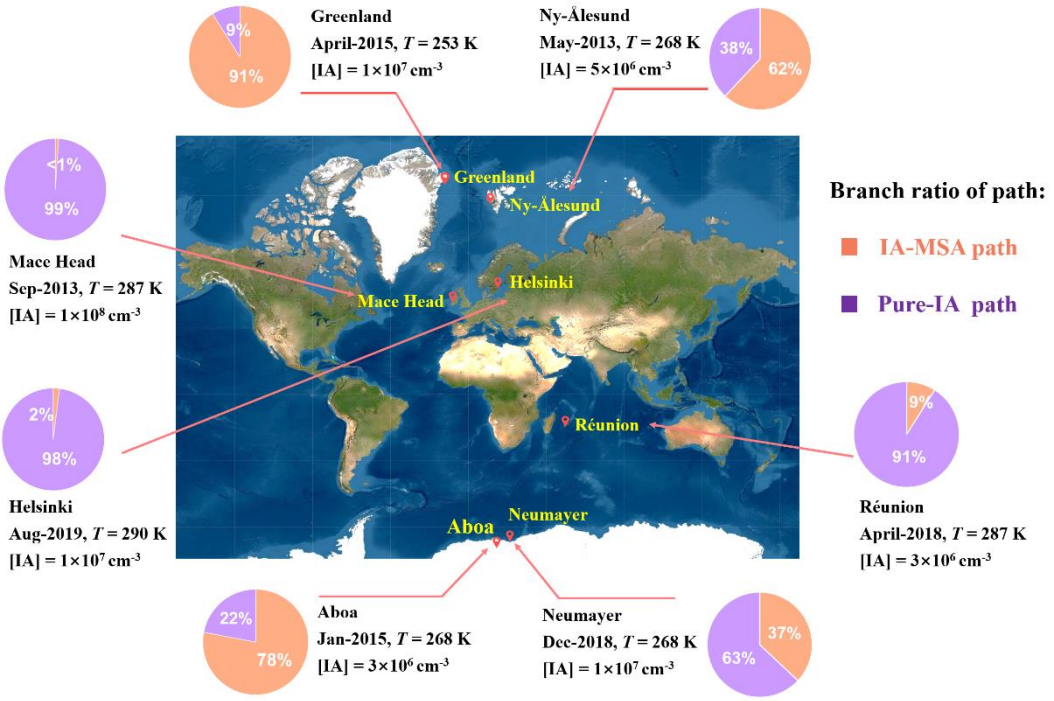


Figure S5. Branch ratio of IA-MSA (orange pie) and pure-IA (purple pie) growth pathway in different regions with different [IA] and [MSA] = 2.5 × 10^6 molecules cm^{-3}. The employed [IA] and temperatures (*T*, K) in the simulation are referenced to data from the study (He et al., 2021). The map is from © Google Maps (https://www.google.com/maps).

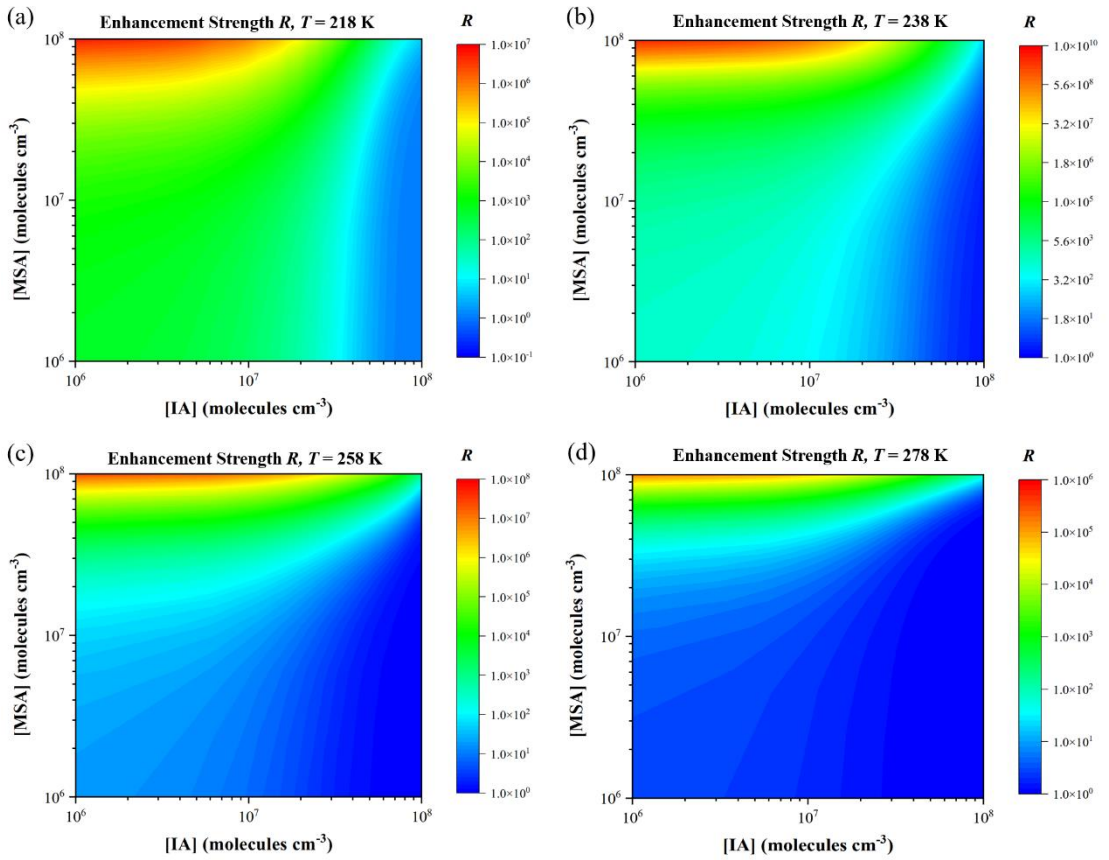
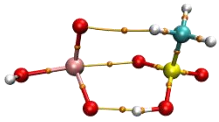
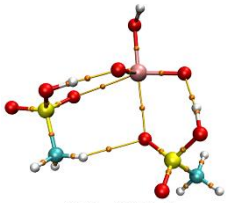
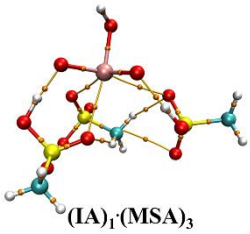
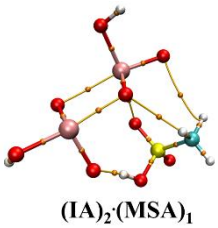
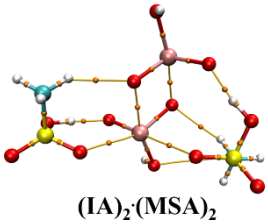
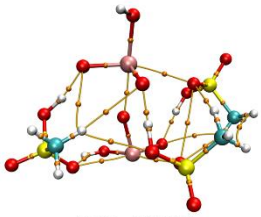
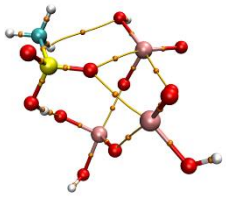
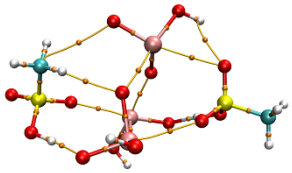
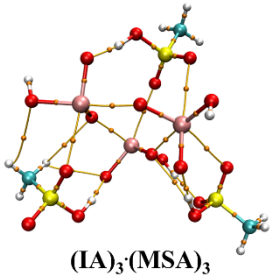
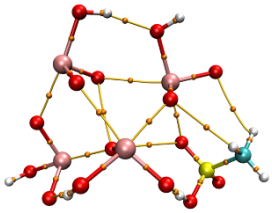
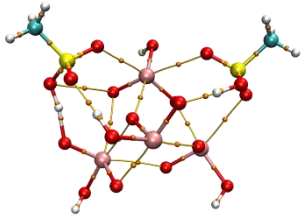


Figure S6. Contour plot of the enhancement strength R at different [IA] (10^6 ~ 10^8 molecules cm^{-3}) and [MSA] (10^6 ~ 10^8 molecules cm^{-3}) under the condition of T = (a) 218 K, (b) 238 K, (c) 258 K, (d) 278 K, and CS = 2.0×10^{-3} s^{-1}.

Table S1. The bond type, electron density $\rho(r)$ (a.u), Laplacian electron density $\nabla^2\rho(r)$ (a.u.), energy density $H(r)$ at corresponding BCPs in the studied IA-MSA-based clusters. The orange balls represent bond critical points (BCPs) in the AIM theory analysis. IA and MSA represent iodic acid (HIO_3) and methanesulfinic acid ($CH_3S(O)_2OH$), respectively. HB (hydrogen bond), XB (halogen bond).

Cluster	Bond	Bond type	$\rho(r)$ (a.u.)	$\nabla^2\rho(r)$ (a.u.)	$H(r)$ (a.u.)
 $(IA)_1 \cdot (MSA)_1$	O···H-O	HB	0.0581	0.1104	-0.0166
	O-I···O	XB	0.0385	0.1079	-0.0015
 $(IA)_1 \cdot (MSA)_2$	O···H-O	HB	0.0505	0.1113	-0.0119
	O···H-O	HB	0.0634	0.1085	-0.0202
	O-I···O	XB	0.0349	0.1021	-0.0005
	O-I···O	XB	0.0233	0.0740	0.0012
 $(IA)_1 \cdot (MSA)_3$	O···H-O	HB	0.0562	0.1105	-0.0156
	O···H-O	HB	0.0357	0.1066	-0.0032
	O-I···O	XB	0.0722	0.1073	-0.0265
	O-I···O	XB	0.0283	0.0865	0.0005
	O-I···O	XB	0.0167	0.0537	0.0012
	O-I···O	XB	0.0311	0.0992	0.0007
 $(IA)_2 \cdot (MSA)_1$	O···H-O	HB	0.0598	0.1117	-0.0186
	O-I···O	XB	0.0620	0.1370	-0.0116
	O-I···O	XB	0.0428	0.1243	-0.0021
	O-I···O	XB	0.0266	0.0772	-0.0002
 $(IA)_2 \cdot (MSA)_2$	O···H-O	HB	0.0516	0.1110	-0.0126
	O···H-O	HB	0.0482	0.1093	-0.0112
	O-I···O	XB	0.0250	0.0786	0.0011
	O-I···O	XB	0.0287	0.0928	0.0010
	O-I···O	XB	0.0634	0.1319	-0.0129
	O-I···O	XB	0.0849	0.1560	-0.0265
	O···H-O	HB	0.0203	0.0794	0.0022

 $(IA)_2 \cdot (MSA)_3$	O···H-O	HB	0.0528	0.1106	-0.0136
	O···H-O	HB	0.0704	0.1122	-0.0255
	O···H-O	HB	0.0531	0.1084	-0.0142
	O-I···O	XB	0.0342	0.1035	0.0000
	O-I···O	XB	0.0252	0.0832	0.0011
	O-I···O	XB	0.0492	0.1445	-0.0039
	O-I···O	XB	0.0202	0.0658	0.0016
 $(IA)_3 \cdot (MSA)_1$	O···H-O	HB	0.0655	0.1105	-0.0219
	O-I···O	XB	0.0255	0.0829	0.0014
	O-I···O	XB	0.0244	0.0768	0.0013
	O-I···O	XB	0.0608	0.1583	-0.0088
	O-I···O	XB	0.0171	0.0562	0.0015
	O-I···O	XB	0.0549	0.1380	-0.0067
 $(IA)_3 \cdot (MSA)_2$	O···H-O	HB	0.0493	0.1094	-0.0117
	O···H-O	HB	0.0796	0.0929	-0.0332
	O-I···O	XB	0.0426	0.1200	-0.0020
	O-I···O	XB	0.0153	0.0531	0.0018
	O-I···O	XB	0.0180	0.0564	0.0009
	O-I···O	XB	0.0610	0.1562	-0.0091
	O-I···O	XB	0.0288	0.1006	0.0017
	O-I···O	XB	0.0610	0.1576	-0.0091
 $(IA)_3 \cdot (MSA)_3$	O···H-O	HB	0.0373	0.1035	-0.0046
	O···H-O	HB	0.0517	0.1117	-0.0128
	O···H-O	HB	0.0660	0.1040	-0.0226
	O···H-O	HB	0.0688	0.1014	-0.0249
	O-I···O	XB	0.0498	0.1365	-0.0044
	O-I···O	XB	0.0167	0.0529	0.0012
	O-I···O	XB	0.0546	0.1414	-0.0067
	O-I···O	XB	0.0302	0.0993	0.0011

	O-I···O	XB	0.0183	0.0638	0.0019
	O-I···O	XB	0.0535	0.1440	-0.0056
	O-I···O	XB	0.0197	0.0594	0.0009
	O···H-O	HB	0.0373	0.1030	-0.0043
	O···H-O	HB	0.0601	0.1090	-0.0185
 $(IA)_4 \cdot (MSA)_1$	O···H-O	HB	0.0232	0.0814	0.0013
	O-I···O	XB	0.0667	0.1589	-0.0127
	O-I···O	XB	0.0296	0.0899	0.0006
	O-I···O	XB	0.0526	0.1329	-0.0060
	O-I···O	XB	0.0529	0.1339	-0.0063
	O-I···O	XB	0.0415	0.1205	-0.0017
	O-I···O	XB	0.0244	0.0730	0.0009
	O···H-O	HB	0.0738	0.1020	-0.0285
	O···H-O	HB	0.0411	0.1096	-0.0068
	O···H-O	HB	0.0621	0.1095	-0.0199
	O-I···O	XB	0.0192	0.0587	0.0012
	O-I···O	XB	0.0291	0.0815	-0.0005
	O-I···O	XB	0.0435	0.1118	-0.0038
 $(IA)_4 \cdot (MSA)_2$	O-I···O	XB	0.0547	0.1416	-0.0067
	O-I···O	XB	0.0143	0.0409	0.0007
	O-I···O	XB	0.0636	0.1576	-0.0106
	O-I···O	XB	0.0146	0.0471	0.0013
	O-I···O	XB	0.0425	0.1186	-0.0023
	O-I···O	XB	0.0202	0.0661	0.0016
	O-I···O	XB	0.0190	0.0632	0.0016
	O···H-O	HB	0.0744	0.1063	-0.0288
	O···H-O	HB	0.0421	0.1076	-0.0073
	O···H-O	HB	0.0375	0.1082	-0.0043
	O-I···O	XB	0.0557	0.1463	-0.0069

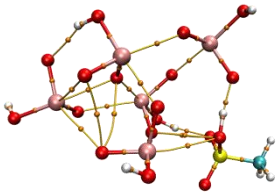
 $(IA)_5 \cdot (MSA)_1$	O-I···O	XB	0.0288	0.0810	-0.0003
	O-I···O	XB	0.0554	0.1361	-0.0074
	O-I···O	XB	0.0578	0.1463	-0.0081
	O-I···O	XB	0.0244	0.0802	0.0017
	O-I···O	XB	0.0558	0.1535	-0.0065

Table S2. The Gibbs formation free energies ΔG_{278K} of the studied IA clusters in Rong et al. 2020 (RI-CC2/aug-cc-pVTZ(-PP)//ωB97X-D/6-311++G(3df,3pd) + aug-cc-pVDZ-PP (for I)) and in this study (RI-CC2/aug-cc-pV(T+d)Z(-PP)//ωB97X-D/6-311++G(3df,3pd) + aug-cc-pVTZ-PP (for I)).

Cluster	ΔG_{278K} (Rong et al. 2020)	ΔG_{278K} (This study)
$(IA)_2$	-5.92	-8.07
$(IA)_3$	-15.73	-18.47
$(IA)_4$	-34.41	-38.48
$(IA)_5$	-52.37	-56.28
$(IA)_6$	-70.67	-76.36

Table S3. The Gibbs formation free energies ΔG (kcal mol^{-1}) of the studied IA-MSA clusters at the RI-CC2/aug-cc-pV(T+d)Z(-PP)//ωB97X-D/6-311++G(3df,3pd) + aug-cc-pVTZ-PP with ECP28MDF (for I) level of theory, p = 1 atm and T = 218, 238, 258, 278, and 298 K.

Clusters	ΔG (kcal mol^{-1})				
	218 K	238 K	258 K	278 K	298 K
$(MSA)_2$	-13.40	-12.59	-11.78	-10.97	-10.17
$(MSA)_3$	-20.76	-19.21	-17.65	-16.10	-14.56
$(IA)_1 \cdot (MSA)_1$	-13.67	-12.88	-12.10	-11.32	-10.55
$(IA)_1 \cdot (MSA)_2$	-24.47	-22.90	-21.34	-19.78	-18.23
$(IA)_1 \cdot (MSA)_3$	-42.27	-39.78	-37.30	-34.83	-32.36
$(IA)_2 \cdot (MSA)_1$	-25.83	-24.21	-22.60	-21.01	-19.43
$(IA)_2 \cdot (MSA)_2$	-39.30	-36.83	-34.36	-31.91	-29.48
$(IA)_2 \cdot (MSA)_3$	-56.76	-53.54	-50.33	-47.14	-43.97
$(IA)_3 \cdot (MSA)_1$	-39.22	-36.87	-34.55	-32.24	-29.96
$(IA)_3 \cdot (MSA)_2$	-61.64	-58.41	-55.19	-52.00	-48.83
$(IA)_3 \cdot (MSA)_3$	-77.91	-73.68	-69.47	-65.28	-61.12
$(IA)_4 \cdot (MSA)_1$	-64.32	-60.90	-57.51	-54.14	-50.80
$(IA)_4 \cdot (MSA)_2$	-84.23	-79.99	-75.77	-71.58	-67.42
$(IA)_5 \cdot (MSA)_1$	-76.29	-72.16	-68.06	-63.99	-59.96
$(IA)_2$	-10.34	-9.57	-8.82	-8.07	-7.34
$(IA)_3$	-23.27	-21.65	-20.05	-18.47	-16.90
$(IA)_4$	-45.88	-43.39	-40.92	-38.48	-36.05
$(IA)_5$	-66.26	-62.91	-59.58	-56.28	-53.02
$(IA)_6$	-88.99	-84.75	-80.53	-76.36	-72.22

Table S4. The evaporation rate coefficients (γ, s^{-1}) for all evaporation pathways of clusters at 278 K.

Evaporation pathways	Evaporation rate coefficients (γ, s^{-1})
$(IA)_2 \rightarrow IA + IA$	1.67×10^{3}
$(IA)_3 \rightarrow (IA)_2 + IA$	7.43×10^{1}
$(IA)_4 \rightarrow (IA)_3 + IA$	2.05×10^{-6}
$(IA)_5 \rightarrow (IA)_4 + IA$	1.47×10^{-4}
$(IA)_6 \rightarrow (IA)_5 + IA$	2.33×10^{-6}
$(MSA)_2 \rightarrow MSA + MSA$	1.44×10^{1}
$(MSA)_3 \rightarrow (MSA)_2 + MSA$	1.57×10^{6}
$(IA)_1\cdot(MSA)_1 \rightarrow IA + MSA$	1.22×10^{1}
$(IA)_1\cdot(MSA)_2 \rightarrow IA + (MSA)_2$	1.56×10^{3}
$(IA)_1\cdot(MSA)_2 \rightarrow MSA + (IA)_1\cdot(MSA)_1$	3.54×10^{3}
$(IA)_1\cdot(MSA)_3 \rightarrow IA + (MSA)_3$	3.38×10^{-5}
$(IA)_1\cdot(MSA)_3 \rightarrow MSA + (IA)_1\cdot(MSA)_2$	2.71×10^{-2}
$(IA)_2\cdot(MSA)_1 \rightarrow (IA)_1\cdot(MSA)_1 + IA$	2.89×10^{2}
$(IA)_2\cdot(MSA)_1 \rightarrow (IA)_2 + MSA$	1.01×10^{0}
$(IA)_2\cdot(MSA)_2 \rightarrow (IA)_2\cdot(MSA)_1 + MSA$	4.15×10^{1}
$(IA)_2\cdot(MSA)_2 \rightarrow (IA)_1\cdot(MSA)_2 + IA$	4.00×10^{0}
$(IA)_2\cdot(MSA)_3 \rightarrow (IA)_2\cdot(MSA)_2 + MSA$	2.15×10^{-2}
$(IA)_2\cdot(MSA)_3 \rightarrow (IA)_1\cdot(MSA)_3 + IA$	2.96×10^{0}
$(IA)_3\cdot(MSA)_1 \rightarrow (IA)_2\cdot(MSA)_1 + IA$	1.68×10^{1}
$(IA)_3\cdot(MSA)_1 \rightarrow (IA)_3 + MSA$	2.27×10^{-1}
$(IA)_3\cdot(MSA)_2 \rightarrow (IA)_2\cdot(MSA)_2 + IA$	2.39×10^{-6}
$(IA)_3\cdot(MSA)_2 \rightarrow (IA)_3\cdot(MSA)_1 + MSA$	4.91×10^{-6}
$(IA)_3\cdot(MSA)_3 \rightarrow (IA)_2\cdot(MSA)_3 + IA$	8.38×10^{-5}
$(IA)_3\cdot(MSA)_3 \rightarrow (IA)_3\cdot(MSA)_2 + MSA$	8.10×10^{-1}
$(IA)_4\cdot(MSA)_1 \rightarrow (IA)_3\cdot(MSA)_1 + IA$	7.41×10^{-8}
$(IA)_4\cdot(MSA)_1 \rightarrow (IA)_4 + MSA$	9.73×10^{-3}
$(IA)_4\cdot(MSA)_2 \rightarrow (IA)_3\cdot(MSA)_2 + IA$	6.59×10^{-6}
$(IA)_4\cdot(MSA)_2 \rightarrow (IA)_4\cdot(MSA)_1 + MSA$	3.69×10^{-4}
$(IA)_5\cdot(MSA)_1 \rightarrow (IA)_4\cdot(MSA)_1 + IA$	2.47×10^{2}
$(IA)_5\cdot(MSA)_1 \rightarrow (IA)_5 + MSA$	1.72×10^{4}

Table S5. Boundary conditions in ACDC simulations at T = 218 ~ 298 K, [IA] =10^6 ~ 10^8, and [MSA] = 10^6 ~ 10^8 molecules cm^{-3}.

Temperature (K)	Boundary cluster	
298 K		[IA] = 10^6 ~ 10^8 molecules cm^{-3}
	[MSA] = 10^6 ~ 10^7 molecules cm^{-3}	$(IA)_7$, $(IA)_6 \cdot (MSA)_1$
	[MSA] = 10^8 molecules cm^{-3}	$(IA)_7$, $(IA)_6 \cdot (MSA)_1$, $(IA)_4 \cdot (MSA)_3$
258 & 278 K		[IA] = 10^6 ~ 10^8 molecules cm^{-3}
	[MSA] = 10^6 ~ 10^8 molecules cm^{-3}	$(IA)_7$
		$(IA)_6 \cdot (MSA)_1$
		$(IA)_4 \cdot (MSA)_3$
		$(IA)_5 \cdot (MSA)_2$
218 & 238 K		[IA] = 10^6 ~ 10^8 molecules cm^{-3}
	[MSA] = 10^6 ~ 10^8 molecules cm^{-3}	$(IA)_7$
		$(IA)_6 \cdot (MSA)_1$
		$(IA)_4 \cdot (MSA)_3$
		$(IA)_3 \cdot (MSA)_4$
		$(IA)_5 \cdot (MSA)_2$

Table S6. Enhancement strength R of MSA on cluster formation rates under different atmospheric conditions: T = 218 ~ 298 K ([IA] = 10^7 and [MSA] = 10^7 molecules cm^{-3}), [MSA] = 10^6 ~ 10^8 molecules cm^{-3} (T = 278 K and [IA] = 10^7 molecules cm^{-3}), [IA] = 10^6 ~ 10^8 molecules cm^{-3} (T = 278 K and [MSA] = 10^7 molecules cm^{-3}), and CS = 2.0×10^{-3} s^{-1}.

[IA]	R	[MSA]	R	T (K)	R
1.0E+06	210.9	1.0E+06	1.0	218	184.2
1.8E+06	52.4	1.8E+06	1.1	228	1717.1
3.2E+06	15.6	3.2E+06	1.2	238	5651.6
5.6E+06	5.9	5.6E+06	1.5	248	2276.2
1.0E+07	2.9	1.0E+07	2.9	258	400.6
1.8E+07	1.8	1.8E+07	9.1	268	30.3
3.2E+07	1.4	3.2E+07	41.3	278	2.9
5.6E+07	1.2	5.6E+07	215.5	288	1.4
1.0E+08	1.1	1.0E+08	1180.4	298	1.2

Table S7. Cartesian coordinates of all molecules and clusters in the present study at the ωB97X-D/6-311++G(3df,3pd) + aug-cc-pVTZ-PP with ECP28MDF (for I) level of theory.

IA:

Atoms	X	Y	Z
I	-0.097221	0.004930	-0.243095
O	-0.843163	-1.345650	0.628433
O	-0.527112	1.503114	0.602173
O	1.779550	-0.182280	0.231752
H	1.878526	-0.062776	1.185167

MSA:

Atoms	X	Y	Z
C	1.6002660	-0.3584400	-0.0280610
H	1.7053540	-1.3498820	0.4023310
H	2.1691410	0.3683770	0.5465350
H	1.9071020	-0.3432120	-1.0698640
S	-0.0884700	0.1352070	0.0652370
O	-0.2299430	1.3852010	-0.5885960
O	-0.5695130	-0.0688710	1.3923850
O	-0.7848540	-0.9581670	-0.8605600
H	-1.2931960	-1.5532640	-0.3002540

$(MSA)_2$:

Atoms	X	Y	Z
S	-1.8655950	0.0944030	0.0515410
O	-1.7145970	1.5028880	-0.1091770
O	-1.1965300	-0.5078530	1.1812570
O	-1.4477700	-0.6580090	-1.2394410
S	2.0382990	-0.1223980	-0.0694780
O	1.4791460	-0.6020900	1.3003370
H	0.4902990	-0.6039330	1.3098130
O	1.1722560	-0.6075090	-1.1193350
O	3.4103790	-0.4661750	-0.1158210
H	-0.4527540	-0.6891120	-1.2922900
C	-3.5649490	-0.3308100	0.1101160
H	-3.6544980	-1.4096200	0.1919040
H	-3.9767470	0.1597460	0.9882970
H	-4.0395940	0.0409130	-0.7933260
C	1.8582430	1.6265820	0.0024120

H	2.4366140	1.9917240	0.8460990
H	2.2478990	2.0245460	-0.9311990
H	0.8026770	1.8690200	0.1099650

$(MSA)_3$:

Atoms	X	Y	Z
S	0.0564930	1.1175030	-0.1377890
O	1.2765290	1.8091120	-0.4633360
O	-1.1634920	1.7430090	-0.5381060
H	-2.8341590	1.2692020	-0.4159030
C	0.0299390	0.7899000	1.5818620
O	0.0694330	-0.2847490	-0.8023270
O	-3.7572320	0.9391720	-0.3934740
S	-3.8058890	-0.5213070	0.1698510
C	-3.3590140	-1.4913230	-1.2333690
O	-5.1591800	-0.7835340	0.5059120
O	3.7635710	0.8703400	-0.5354730
H	2.8949610	1.3473270	-0.5573380
O	-2.7777110	-0.6705970	1.1556430
O	3.3346740	-0.4147440	1.5109760
H	0.9730140	-0.6960240	-0.7721770
O	2.5416270	-1.2384710	-0.6494100
S	3.5486390	-0.5289340	0.1069390
C	5.1103730	-1.2519930	-0.2179590
H	-2.3492560	-1.2233980	-1.5343830
H	-4.0755220	-1.2987220	-2.0263640
H	-3.3997350	-2.5332860	-0.9257330
H	5.2625120	-1.2941460	-1.2920820
H	5.0803460	-2.2505310	0.2104630
H	5.8715550	-0.6495920	0.2694270
H	0.9419650	0.2552260	1.8414230
H	-0.8649540	0.2072280	1.7897580
H	-0.0021500	1.7547310	2.0824740

$(IA)_1 \cdot (MSA)_1$:

Atoms	X	Y	Z
C	2.3555390	1.4150570	0.7767370
H	1.3798610	1.6097900	1.2173730
H	2.6170500	2.2012050	0.0730370
H	3.1267240	1.3033180	1.5334940
S	2.2673230	-0.0820010	-0.1388570

O	3.5283760	-0.3795930	-0.7071300
O	1.1263090	0.0291050	-1.0384610
O	1.9247750	-1.1505350	0.9232180
H	0.9261270	-1.2411260	1.0163970
I	-1.2941080	-0.0006480	-0.2498380
O	-1.0464710	1.5856110	0.5005280
O	-0.6713610	-1.1829160	0.9523370
O	-3.1769260	-0.2594150	0.1083110
H	-3.3500450	-0.1552010	1.0519590

$(IA)_1 \cdot (MSA)_2$:

Atoms	X	Y	Z
I	0.0965070	1.4223980	-0.2022120
O	1.7993570	1.8524080	0.1782290
O	-0.5094530	0.8792200	1.3872710
O	-0.6367360	3.2022210	-0.1880090
H	-0.5599360	3.5772990	0.6985750
C	-1.8486310	-2.5930040	-0.1304480
H	-0.8175510	-2.3590480	0.1219300
H	-1.9104810	-3.0085150	-1.1330950
H	-2.2888610	-3.2738950	0.5922830
S	-2.7893770	-1.1057280	-0.1286540
O	-4.1486050	-1.4052610	-0.3960590
O	-2.1042000	-0.1494140	-0.9673270
O	-2.6809590	-0.6177760	1.3434360
H	-1.8738310	-0.0446300	1.4477500
C	3.5723970	-1.5836000	-1.1814690
H	3.6885360	-0.6264470	-1.6826900
H	3.2130500	-2.3413180	-1.8728130
H	4.5039660	-1.8973040	-0.7188590
S	2.3681390	-1.4135490	0.0886020
O	2.2809760	-2.6235150	0.8197140
O	1.1521870	-0.9140390	-0.5360320
O	2.9426110	-0.3047230	0.9891800
H	2.5660400	0.6018720	0.7332320

$(IA)_1 \cdot (MSA)_3$:

Atoms	X	Y	Z
I	-0.4480450	-1.1263200	-0.4233170
O	-1.7824640	-2.3005740	-0.2621890
O	0.8362600	-2.1057790	-1.2066770

O	-1.1673120	-0.2695050	-1.9839290
H	-0.6183050	0.5160580	-2.1394310
C	4.4591370	-1.7206060	1.5005960
H	4.0252040	-2.7102460	1.6107990
H	4.6232830	-1.2587330	2.4705140
H	5.3835860	-1.7586300	0.9312750
S	3.3139930	-0.7143730	0.6316030
O	3.9260230	0.5777610	0.4606570
O	2.0443680	-0.7447810	1.3069440
O	3.2022020	-1.4062960	-0.7263040
H	2.2337260	-1.7044880	-0.9390210
C	0.5729280	2.3791980	1.2786270
H	1.1028130	1.5470560	1.7376550
H	-0.4973260	2.1808950	1.2537650
H	0.7816260	3.3148760	1.7890020
S	1.1140770	2.5351340	-0.3861320
O	0.5290030	3.6775970	-0.9860200
O	0.9212880	1.2515960	-1.0324200
O	2.6371220	2.7880280	-0.2662700
H	3.1345970	1.9590390	-0.0448520
C	-4.2734690	0.8548190	-0.7705280
H	-3.6946650	0.3569400	-1.5448370
H	-4.1209330	1.9304750	-0.8124280
H	-5.3298370	0.6142280	-0.8473280
S	-3.6947140	0.3093420	0.7986310
O	-4.4920010	0.8750170	1.8237710
O	-2.2633650	0.5320260	0.8340020
O	-3.9422080	-1.2192910	0.7676190
H	-3.1539760	-1.7010310	0.3794200

$(IA)_2{\cdot}(MSA)_1$:

Atoms	X	Y	Z
I	-2.0664560	-0.4865060	0.2507680
O	-1.1566250	-2.0285160	0.2432210
O	-1.6098320	0.3846870	-1.2465170
O	-3.7341770	-1.2061510	-0.4237360
H	-3.6182770	-1.5339380	-1.3231110
I	0.6921080	1.5835940	-0.2265200
O	2.1523570	2.0900450	0.6333680
O	-0.1636970	0.6127430	1.0657050
O	-0.3272140	3.2115260	0.0137720
H	0.0344910	3.6788900	0.7775100
C	2.6722520	-1.2118790	1.4622710

H	1.7440220	-0.8521480	1.8999020
H	3.4079870	-0.4120050	1.4343860
H	3.0547060	-2.0800500	1.9910340
S	2.3631490	-1.6907520	-0.1998750
O	3.5241700	-2.2740990	-0.7612650
O	1.7915150	-0.5431900	-0.8910310
O	1.2770510	-2.7742480	-0.0899170
H	0.3452040	-2.4055010	0.0107030

$(IA)_2 \cdot (MSA)_2$:

Atoms	X	Y	Z
I	0.8005820	2.1871330	-0.2929970
O	2.2358830	1.8455890	0.7075060
O	-0.5688460	1.2404140	0.4728810
O	0.3168600	3.8249190	0.6243920
H	0.3744710	3.7171770	1.5806100
I	-0.3591180	-0.8308600	-0.6148410
O	1.0018670	0.2347220	-1.3029550
O	-1.6536680	-0.3706900	-1.7582540
O	0.2222900	-2.3588440	-1.6455800
H	-0.1453460	-2.2677600	-2.5337380
C	-3.8137380	0.8834760	1.4930300
H	-2.9520660	1.4074770	1.0863970
H	-3.6908430	0.7209810	2.5608400
H	-4.7397260	1.4135760	1.2899160
S	-3.9107400	-0.7050230	0.7415710
O	-5.0743660	-1.3724110	1.1972790
O	-2.6241670	-1.3421320	0.9055360
O	-4.0923630	-0.3764000	-0.7674560
H	-3.2019580	-0.3526790	-1.2153880
C	3.5096590	-2.0284650	-0.8089970
H	3.0505610	-1.2643700	-1.4307790
H	3.0952500	-3.0054910	-1.0434800
H	4.5911700	-2.0303060	-0.9089720
S	3.1146530	-1.6950080	0.8726560
O	3.7970450	-2.6140230	1.7073220
O	1.6768820	-1.5974190	0.9800770
O	3.7239480	-0.2890990	1.1138380
H	3.0918530	0.4523380	0.9215350

$(IA)_2 \cdot (MSA)_3$:

Atoms	X	Y	Z
I	0.2165770	2.2546010	-0.0049540
O	0.2199900	1.6788360	1.6945110
O	-1.5069750	2.6624920	-0.2600130
O	0.8280600	4.0362710	0.3902550
H	0.2937890	4.4214250	1.0956100
I	-0.5095520	-1.6897400	-1.0156040
O	1.0260920	-2.0057870	-1.8582820
O	-0.4799210	0.0798470	-0.7260630
O	-1.5507200	-1.6833940	-2.6202860
H	-2.4633270	-1.4853670	-2.3558800
C	4.1180310	-1.3948400	-0.3167060
H	3.2407130	-2.0146150	-0.1427060
H	4.6489300	-1.2058800	0.6130650
H	4.7831080	-1.8400350	-1.0508630
S	3.5827000	0.1668480	-0.9293600
O	4.6992720	0.9778970	-1.2562230
O	2.6137220	0.6814060	0.0083600
O	2.8699100	-0.1901740	-2.2598950
H	2.1113030	-0.8249580	-2.1256990
C	-3.4553150	0.4652150	1.5883870
H	-2.3929980	0.6938410	1.5924110
H	-3.6678140	-0.3690340	2.2516020
H	-4.0407450	1.3385360	1.8609460
S	-3.9305380	-0.0245060	-0.0313950
O	-5.3357550	-0.1861140	-0.1180140
O	-3.1243620	-1.1773030	-0.3923930
O	-3.5387550	1.1757780	-0.9199100
H	-2.6724220	1.6263350	-0.6923060
C	2.2822820	-0.8188460	2.9836130
H	2.4522120	-0.0093290	2.2761050
H	3.0843830	-1.5513370	2.9365860
H	2.1602770	-0.4513500	3.9984190
S	0.8063000	-1.6531430	2.5212200
O	0.5205500	-2.7136840	3.4170610
O	0.9378390	-1.9862140	1.1137860
O	-0.2954240	-0.5859000	2.6787480
H	-0.0832750	0.2861240	2.1999540

$(IA)_3 \cdot (MSA)_1$:

Atoms	X	Y	Z
I	-2.3099380	-0.7282310	-0.6512250
O	-2.6190820	-0.2400040	1.0477060
O	-0.8909390	-1.8029610	-0.5287830
O	-3.6371200	-2.1414220	-0.7379360
H	-3.4408350	-2.8353170	-0.0981490
I	0.6134140	1.9773010	-0.9278990
O	-1.0274070	1.1867040	-0.9540300
O	0.8908160	2.3678380	-2.6243080
O	-0.0841250	3.7079990	-0.3508090
H	-0.5578750	4.1254680	-1.0796330
I	1.7894290	-1.5430070	-0.0965000
O	3.4914190	-1.4946520	0.3784450
O	1.6495920	-0.1457520	-1.2407360
O	1.8864070	-2.9342000	-1.4270080
H	2.7884520	-2.9402910	-1.7745750
C	-0.7690580	2.0337070	2.8786800
H	-1.4666370	2.0164980	2.0436900
H	-0.0479670	2.8391240	2.7631530
H	-1.2923190	2.1214330	3.8264270
S	0.1273080	0.5197010	2.8890760
O	0.9408000	0.4213770	4.0438860
O	0.7763240	0.4180620	1.5931350
O	-0.9678060	-0.5615440	2.9800990
H	-1.6003960	-0.5172570	2.1925900

$(IA)_3 \cdot (MSA)_2$:

Atoms	X	Y	Z
I	-0.4043110	-1.8012940	-1.3619690
O	-2.1615210	-1.9049260	-1.6523470
O	-0.3339150	-1.6576460	0.4325000
O	-0.0827700	-3.7147400	-1.4254580
H	-0.8102580	-4.1849870	-1.0018350
I	1.0832020	-0.3989200	2.0580890
O	-0.2587600	-0.4617580	3.1968120
O	0.7926610	1.0736200	1.0327940
O	2.3169470	0.4836050	3.2508230
H	3.1124080	0.6841240	2.7376910
I	-0.4381850	2.0458870	-0.6750690
O	-0.5050630	0.5041390	-1.6173260
O	1.1463950	2.6768820	-1.2398730
O	-1.4636470	3.0708930	-1.9448290

H	-0.9932420	3.1064490	-2.7863420
C	-3.2943200	-0.8799550	1.9760990
H	-4.1242340	-1.5432180	2.2020230
H	-3.0070850	-0.2971510	2.8473280
H	-2.4284980	-1.4220920	1.6040710
S	-3.8171650	0.2516440	0.7393830
O	-2.6793580	1.0770270	0.4094590
O	-5.0194890	0.8914390	1.1333880
O	-4.1550080	-0.6500040	-0.4764570
H	-3.3508950	-1.0458270	-0.9088190
C	4.9690490	-0.4324250	-1.4740570
H	4.8210560	-0.3590570	-2.5472320
H	5.1863460	-1.4561460	-1.1810810
H	5.7544440	0.2394290	-1.1403400
S	3.4732730	0.0215140	-0.6765570
O	3.6931620	-0.0228600	0.7476720
O	2.4055180	-0.8124290	-1.1592930
O	3.3247470	1.4565380	-1.1657710
H	2.3772430	1.8832940	-1.1353880

$(IA)_3 \cdot (MSA)_3$:

Atoms	X	Y	Z
I	-0.0395200	-0.6454130	1.9428920
O	0.9211290	-2.1482000	2.0008380
O	-0.7448340	-0.7381860	0.2831540
O	-1.6066370	-1.2309220	2.8500370
H	-2.1593180	-1.8087290	2.2739360
I	2.3619750	1.0464780	-0.7033110
O	1.8462970	0.4702690	0.9235030
O	2.3153210	2.8237640	-0.4495780
O	4.2665050	0.9322440	-0.3551960
H	4.5157200	1.7301100	0.1275860
I	-1.5446850	0.7287120	-1.4005840
O	-1.5251950	-0.7798160	-2.3704540
O	0.1541080	1.3222740	-1.5590710
O	-2.2506890	1.7915320	-2.8459240
H	-2.0664780	1.3220250	-3.6689360
C	-1.5774850	4.5836300	2.1354880
H	-0.9096420	4.6634440	2.9879270
H	-2.5519980	4.2104470	2.4394140
H	-1.6741440	5.5347100	1.6201860
S	-0.9155930	3.4061280	1.0156290
O	-1.7604670	3.3377430	-0.1424270

O	-0.7125050	2.1608430	1.7106490
O	0.4249920	4.0738940	0.6962330
H	1.1210790	3.4963080	0.2148460
C	4.1436450	-2.3163580	0.7966670
H	3.5363640	-1.7123690	1.4667820
H	4.9755540	-1.7337410	0.4098190
H	4.4904420	-3.2233050	1.2828690
S	3.1494780	-2.7745920	-0.5819130
O	3.8487620	-3.6830690	-1.4163400
O	2.6526710	-1.5551780	-1.1779480
O	1.9715850	-3.5465670	0.0580870
H	1.4687830	-2.9918090	0.7176370
C	-5.0161810	-3.1821560	-0.5666030
H	-5.2935270	-2.9141950	-1.5817920
H	-5.7930260	-2.8973100	0.1380080
H	-4.7975480	-4.2432620	-0.4867220
S	-3.5696660	-2.2865470	-0.1300960
O	-3.1845630	-2.7187590	1.1841650
O	-3.8017100	-0.8813430	-0.3252840
O	-2.5536050	-2.7950110	-1.1649740
H	-2.1007870	-2.0251590	-1.6554260

$(IA)_4{\cdot}(MSA)_1$:

Atoms	X	Y	Z
I	-2.2423260	1.8691210	0.0199620
O	-0.9661490	1.5637320	-1.2034900
O	-1.6033190	1.2228940	1.5619660
O	-1.7972180	3.7223600	0.2983320
H	-0.8317660	3.8111090	0.2017610
I	1.7766550	1.6534800	-0.6180490
O	3.4565190	2.2107590	-0.6458920
O	1.6131350	0.9945350	1.0596060
O	1.0378800	3.4260710	-0.2108520
H	1.7707200	3.9434430	0.1469180
I	-2.0232090	-1.7322390	-1.0551330
O	-3.0352730	-0.3367480	-0.4959490
O	-2.2693470	-2.9559750	0.2195740
O	-3.3570510	-2.4539880	-2.2575850
H	-4.0788120	-2.8456280	-1.7516090
I	0.1880970	-0.7633210	1.8794400
O	1.6335420	-1.8106580	1.9939940
O	-0.2007430	-0.9859150	0.1106010
O	-1.1309760	-1.9845440	2.5147950
H	-1.5491470	-2.4681590	1.7646310
C	4.5857330	-0.7570610	0.3066070

H	3.9588400	-0.4342600	1.1354040
H	5.0272200	0.1050980	-0.1867230
H	5.3431930	-1.4631040	0.6338620
S	3.5680080	-1.5710020	-0.8718970
O	4.3486810	-2.1630350	-1.8945960
O	2.5434540	-0.6253380	-1.2932180
O	2.8967570	-2.7036040	-0.0724720
H	2.3396000	-2.3676670	0.6982360

$(IA)_4 \cdot (MSA)_2$:

Atoms	X	Y	Z
I	-1.8602190	-2.0437490	-0.4521340
O	-3.4319860	-1.2076210	-0.2207840
O	-1.4112860	-2.5133780	1.2199060
O	-2.5765110	-3.7634630	-0.9565370
H	-2.9916400	-4.1642850	-0.1831210
I	0.0382960	1.3035270	-1.5668790
O	-1.3145680	0.3986930	-2.2789010
O	1.3846850	0.0957680	-1.7424580
O	0.4748640	2.3219510	-3.1456340
H	0.1057180	1.8530900	-3.9049170
I	2.3416970	-1.6339110	-0.5540040
O	0.9448180	-2.6533870	-0.9790130
O	1.8659020	-0.9457080	1.0535400
O	3.4176490	-3.0722430	0.1869990
H	2.8445160	-3.7132030	0.6231640
I	-0.1453540	-0.2695430	2.1253970
O	-0.7539880	0.0274770	0.4196150
O	0.7142610	1.2650620	2.4488200
O	-1.7746530	0.1661430	2.9780710
H	-2.2836980	0.8463200	2.4752760
C	-4.5518000	3.5834190	0.0619740
H	-4.7079240	3.7872440	-0.9932620
H	-4.1573580	4.4600060	0.5688670
H	-5.4657530	3.2384840	0.5357750
S	-3.3382180	2.3235610	0.2058500
O	-3.2201740	1.9633370	1.5945660
O	-2.1402890	2.7807200	-0.4408790
O	-4.0136890	1.2092450	-0.5914120
H	-3.6772530	0.2497140	-0.4321220
C	4.6791270	3.2780090	0.4890500
H	4.2477690	4.1606440	0.9511730
H	4.9869350	3.4850270	-0.5325340

H	5.5136240	2.8959350	1.0699710
S	3.4447910	2.0317020	0.4046540
O	4.0324760	0.8561710	-0.1658170
O	2.2767890	2.5711580	-0.2371040
O	3.1594490	1.8259600	1.9049420
H	2.2016620	1.5560210	2.0880230

$(IA)_5{\cdot}(MSA)_1$:

Atoms	X	Y	Z
I	0.1505380	-0.2791510	-1.9128560
O	0.3866870	-1.5359970	-0.6482260
O	1.4642930	0.9261960	-1.6135090
O	1.1220070	-1.2685180	-3.2179940
H	1.9262050	-1.6239890	-2.7823710
I	-0.1893680	-1.9540780	1.6035950
O	-1.8867400	-2.0539580	1.0945930
O	0.1198750	-0.2065320	1.9905360
O	-0.4661900	-2.5060050	3.4381150
H	-1.2923090	-2.1283090	3.7641400
I	2.7997530	2.2906770	-0.2397440
O	3.5869790	0.8813780	0.5356580
O	1.3888220	2.6644360	0.7826660
O	3.9961130	3.6207190	0.5056390
H	3.9878110	3.5759420	1.4688480
I	-3.6207100	-0.2288560	-0.7025630
O	-2.6806470	-0.7599100	-2.1294410
O	-3.9635880	1.5017220	-0.9724000
O	-5.3504200	-0.9325490	-1.2165610
H	-5.6506920	-0.4763120	-2.0121540
I	-1.1659060	1.6789780	1.3135330
O	-2.6074320	0.9621020	2.0557530
O	-1.1700620	0.8117290	-0.3056410
O	-2.0123220	3.2212060	0.5460990
H	-2.7615450	2.8939200	0.0094400
C	5.0952230	-2.8333570	0.0217680
H	5.6212790	-1.8847670	-0.0458800
H	5.4549670	-3.5262110	-0.7345390
H	5.1888410	-3.2654130	1.0137470
S	3.3886640	-2.5487330	-0.3027530
O	2.6591970	-3.7513930	-0.0910430
O	3.3056180	-1.8839860	-1.5752360
O	2.9744290	-1.5758120	0.8343600
H	3.1642890	-0.6048190	0.6411780

$(IA)_2$:

Atoms	X	Y	Z
I	1.6050510	0.1089320	0.2598180
O	1.9965970	1.4714830	-0.7927990
O	0.4738030	-0.9431450	-0.7457170
O	3.1405690	-1.0172580	-0.1236880
H	3.2598540	-1.1157400	-1.0751180
I	-1.6050500	-0.1089310	-0.2598170
O	-0.4738030	0.9431390	0.7457250
O	-1.9966050	-1.4714830	0.7927960
O	-3.1405660	1.0172630	0.1236830
H	-3.2598560	1.1157440	1.0751130

$(IA)_3$:

Atoms	X	Y	Z
I	1.5511910	-1.4445600	0.2414280
O	2.0279340	-0.5409040	-1.2208860
O	-0.1840680	-1.9011750	-0.0585960
O	2.2553500	-3.1531740	-0.3622160
H	2.1828020	-3.2199290	-1.3208450
I	0.6615010	1.8896760	-0.2072040
O	0.9115570	0.5509110	1.0314770
O	-0.2932740	3.0724790	0.6892890
O	2.3948310	2.7109990	0.0991610
H	2.3539690	3.2139620	0.9215730
I	-2.1902120	-0.6462100	-0.1039850
O	-1.2583870	0.7196240	-0.8673280
O	-2.1356540	-0.3853530	1.6405650
O	-3.9302950	0.1409120	-0.4479620
H	-4.0321980	0.9493840	0.0685690

$(IA)_4$:

Atoms	X	Y	Z
I	2.9241890	0.0435110	-0.8635460
O	3.4950440	-0.6745010	0.6711170
O	1.9713920	1.4750800	-0.3687730
O	4.5693860	0.9748140	-1.2764300
H	4.9240130	1.3900130	-0.4811820
I	0.2317490	-2.0071310	0.7956480
O	-0.0713050	-0.5315140	1.7446800

O	1.0258200	-1.4171480	-0.7295220
O	1.8394770	-2.5933650	1.6451140
H	2.5536030	-1.9454660	1.4363170
I	-0.3259520	2.0528480	0.7034780
O	-1.0643480	1.0904900	-0.6857680
O	-0.2420710	3.6804340	0.0405260
O	-1.9324550	2.2147620	1.7238760
H	-2.6001000	1.5685270	1.3920640
I	-2.8044640	-0.3056100	-0.9144760
O	-3.5466570	0.3829290	0.5550570
O	-1.8552880	-1.7279890	-0.3078030
O	-4.3636280	-1.3633030	-1.3845380
H	-4.8331290	-1.6303950	-0.5859930

$(IA)_5$:

Atoms	X	Y	Z
I	-3.5344100	0.1308410	-0.2864200
O	-2.3106830	0.4860440	-1.5573360
O	-2.8863020	0.8466670	1.2197090
O	-4.7264700	1.6024060	-0.7214750
H	-4.2652980	2.4482090	-0.7101150
I	0.5419420	-0.3031000	2.1338430
O	-0.0741840	-0.0385660	0.4181770
O	0.9630280	1.3736900	2.5290590
O	-1.1922830	-0.4342310	2.8969190
H	-1.8540270	0.0348080	2.3268070
I	-0.6603030	-1.9860300	-0.6874280
O	-2.3422030	-1.8028680	0.0183110
O	0.1904330	-2.7400970	0.6892570
O	-1.0382730	-3.6578070	-1.5878760
H	-1.1153910	-4.3629530	-0.9345750
I	3.1946460	-0.4312220	-0.6996330
O	1.8776140	-1.2203240	-1.6029460
O	2.7205390	-0.5548800	1.0381290
O	4.4015030	-1.9487530	-0.6485380
H	3.9425020	-2.7354500	-0.3313170
I	0.7506300	2.6262840	-0.3288090
O	2.2075810	1.6687680	-0.8598400
O	1.2180120	4.2713930	-0.7484960
O	-0.3987350	2.2831850	-1.7974870
H	-1.0871970	1.5894170	-1.6076160

$(IA)_6$:

Atoms	X	Y	Z
I	2.2808360	-0.2753710	-2.1881650
O	2.9719550	-0.8720370	-0.6598240
O	0.7608060	0.5949180	-1.7316370
O	3.3326370	1.3014170	-2.4413400
H	2.9510610	2.0411620	-1.9103970
I	0.6413140	2.4184810	-0.0083520
O	-0.8608180	3.0004440	-0.8644300
O	1.9683430	3.1662190	-0.9376500
O	0.6243090	3.7769460	1.3626620
H	1.1942090	4.4944990	1.0581850
I	-2.7890380	1.8068790	-0.2953190
O	-1.7709380	1.3170510	1.1505700
O	-2.4200660	0.6546250	-1.5917610
O	-4.3947320	0.9695600	0.3615050
H	-4.1653500	0.0378670	0.5465660
I	-1.4589660	-1.0321300	1.8638060
O	-0.1031870	-0.9421340	0.6382260
O	-2.8761320	-1.3267160	0.8107060
O	-1.1795240	-2.8714060	2.2946450
H	-1.2063490	-3.3478930	1.4394730
I	-0.9196570	-2.0764910	-1.5666630
O	-1.0281490	-3.5252090	-0.5362830
O	0.7784970	-2.1746890	-2.1884340
O	-1.7723570	-2.8490540	-3.1160810
H	-1.6671070	-3.8081140	-3.0746010
I	2.1173610	-0.7524830	2.0447950
O	0.8024440	-0.7625620	3.2681640
O	2.3028120	0.9848650	1.6935780
O	3.6177060	-0.9370970	3.2444890
H	3.6566860	-0.1695010	3.8285950

Reference

He, X.-C., Tham, Y. J., Dada, L., Wang, M., Finkenzeller, H., Stolzenburg, D., Iyer, S., Simon, M., Kürten, A., Shen, J., Rörup, B., Rissanen, M., Schobesberger, S., Baalbaki, R., Wang, D. S., Koenig, T. K., Jokinen, T., Sarnela, N., Beck, L. J., Almeida, J., Amanatidis, S., Amorim, A., Ataei, F., Baccarini, A., Bertozzi, B., Bianchi, F., Brilke, S., Caudillo, L., Chen, D., Chiu, R., Chu, B., Dias, A., Ding, A., Dommen, J., Duplissy, J., El Haddad, I., Gonzalez Carracedo, L., Granzin, M., Hansel, A., Heinritzi, M., Hofbauer, V., Junninen, H., Kangasluoma, J., Kemppainen, D., Kim, C., Kong, W., Krechmer, J. E., Kvashin, A., Laitinen, T., Lamkaddam, H., Lee, C. P., Lehtipalo, K., Leiminger, M., Li, Z., Makhmutov, V., Manninen, H. E., Marie, G., Marten, R., Mathot, S., Mauldin, R. L., Mentler, B., Möhler, O., Müller, T., Nie, W., Onnela, A., Petäjä, T., Pfeifer, J., Philippov, M., Ranjithkumar, A., Saiz-Lopez, A., Salma, I., Scholz, W., Schuchmann, S., Schulze, B., Steiner, G., Stozhkov, Y., Tauber, C., Tomé, A., Thakur, R. C., Väisänen, O., Vazquez-Pufleau, M., Wagner, A. C., Wang, Y., Weber, S. K., Winkler, P. M., Wu, Y., Xiao, M., Yan, C., Ye, Q., Ylisirniö, A., Zauner-Wieczorek, M., Zha, Q., Zhou, P., Flagan, R. C., Curtius, J., Baltensperger, U., Kulmala, M., Kerminen, V.-M., Kurtén, T., et al.: Role of iodine oxoacids in atmospheric aerosol nucleation, Science, 371, 589–595, https://doi.org/10.1126/science.abe0298, 2021.

McGrath, M. J., Olenius, T., Ortega, I. K., Loukonen, V., Paasonen, P., Kurtén, T., Kulmala, M., and Vehkamäki, H.: Atmospheric Cluster Dynamics Code: a flexible method for solution of the birth-death equations, Atmos. Chem. Phys., 12, 2345–2355, https://doi.org/10.5194/acp-12-2345-2012, 2012.

Oona, K.-M. and Tinja, O.: Atmospheric Cluster Dynamics Code Technical manual, https://github.com/tolenius/ACDC/blob/main/ACDC_Manual_2020_11_25.pdf, 2020.