Supplement of

Molecular-level evidence for marine aerosol nucleation of iodic acid and methanesulfonic acid

An Ning[1], Ling Liu[1], Lin Ji[2], and Xiuhui Zhang[1]

[1]Key Laboratory of Cluster Science, Ministry of Education of China, School of Chemistry and Chemical Engineering, Beijing Institute of Technology, Beijing 100081, China

[2]Department of Chemistry, Capital Normal University, Beijing 100048, China

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

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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 energy ΔG (kcal mol^{-1}) of the studied IA-MSA clusters at the RI-CC2/aug-cc-pV(T+d)Z(-PP)// ω B97X-D/6-311++G(3df,3pd) + aug-cc-pVTZ(-PP) with ECP28MDF (for I) level of theory, P = 1 atm and T = 218 ~ 298 K.

Table S3. The Gibbs formation free energy ΔG (kcal mol^{-1}) of the studied IA-MSA clusters at the RI-CC2/aug-cc-pV(T+d)Z(-PP)// ω B97X-D/6-311++G(3df,3pd) + aug-cc-pVTZ(-PP) with ECP28MDF (for I) level of theory, P = 1 atm and T = 253, 268, 270, 287, 290, and 300 K.

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

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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.

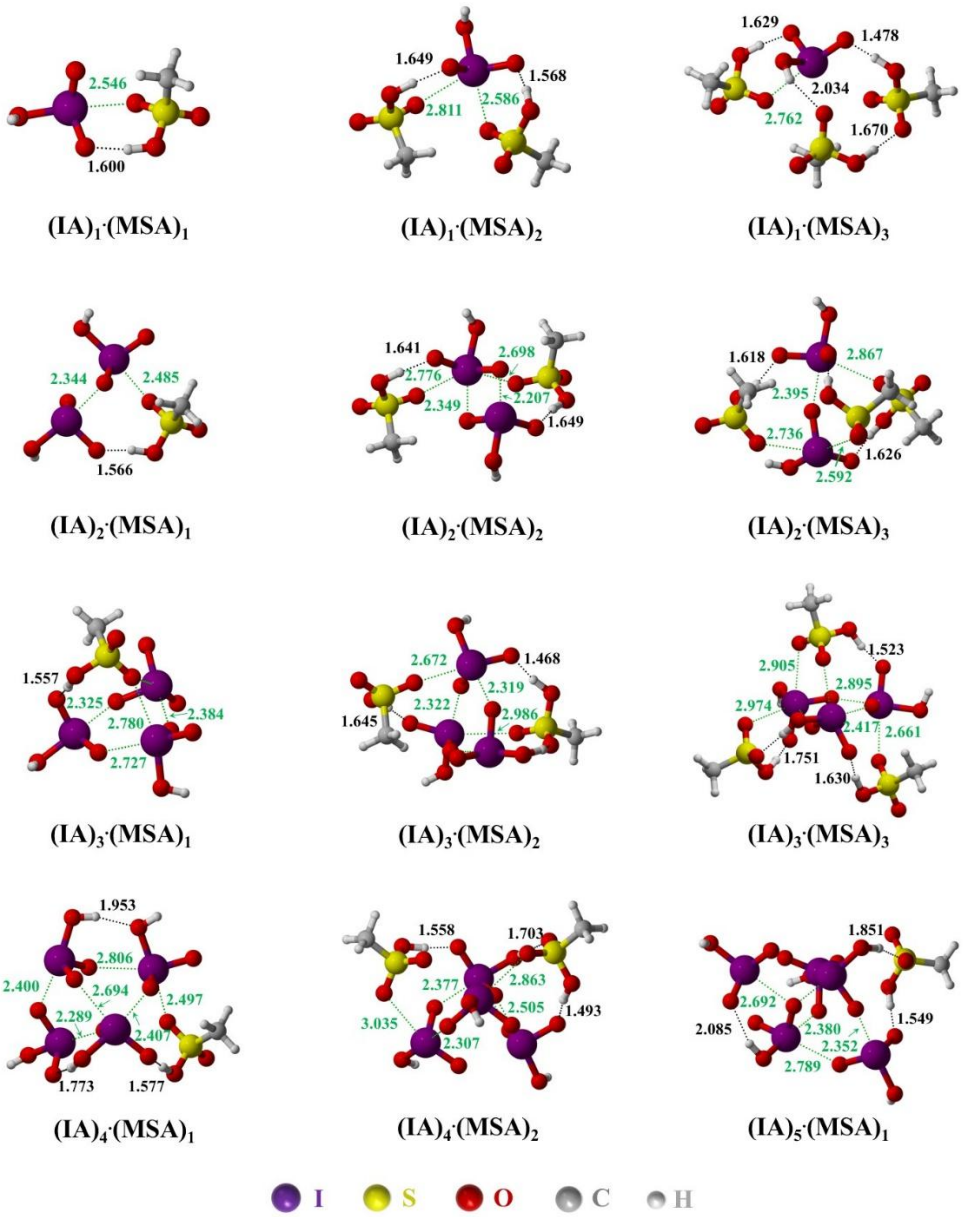


Figure S1. The identified stable configurations of the IA-MSA-based clusters at the ωB97X-D/6-311++G(3df,3pd) + aug-cc-pVTZ(-PP) with ECP28MDF (for I) level of theory. IA and MSA are the shorthand for iodic acid and methanesulfonic acid, respectively. The lengths of hydrogen and halogen bonds are given in Å.

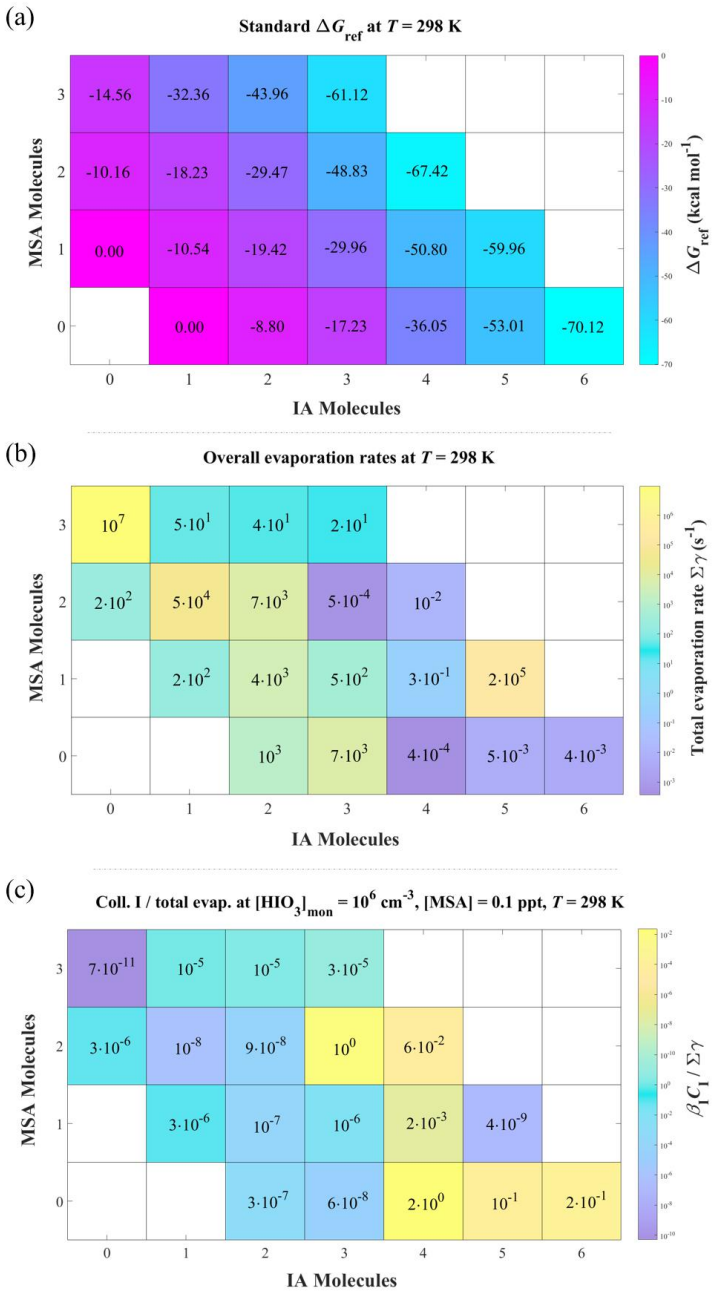


Figure S2. (a) Gibbs formation free energy (ΔG) of the $(IA)_x(MSA)_y$ ($0 \leq x \leq 6$, $0 \leq y \leq 3$, $x + y \leq 6$) clusters identified at the RI-CC2/aug-cc-pV(T+d)Z(-PP)// ω B97X-D/6-311++G(3df,3pd) + aug-cc-pVTZ(-PP) level of theory, T = 298 K, p = 1 atm. (b) the total evaporation rate coefficients ($\sum\gamma$ in s^{-1}) and (c) ratios of **IA** monomer collision frequencies versus total evaporation coefficient ($\beta C/\sum\gamma$) of the corresponding clusters.

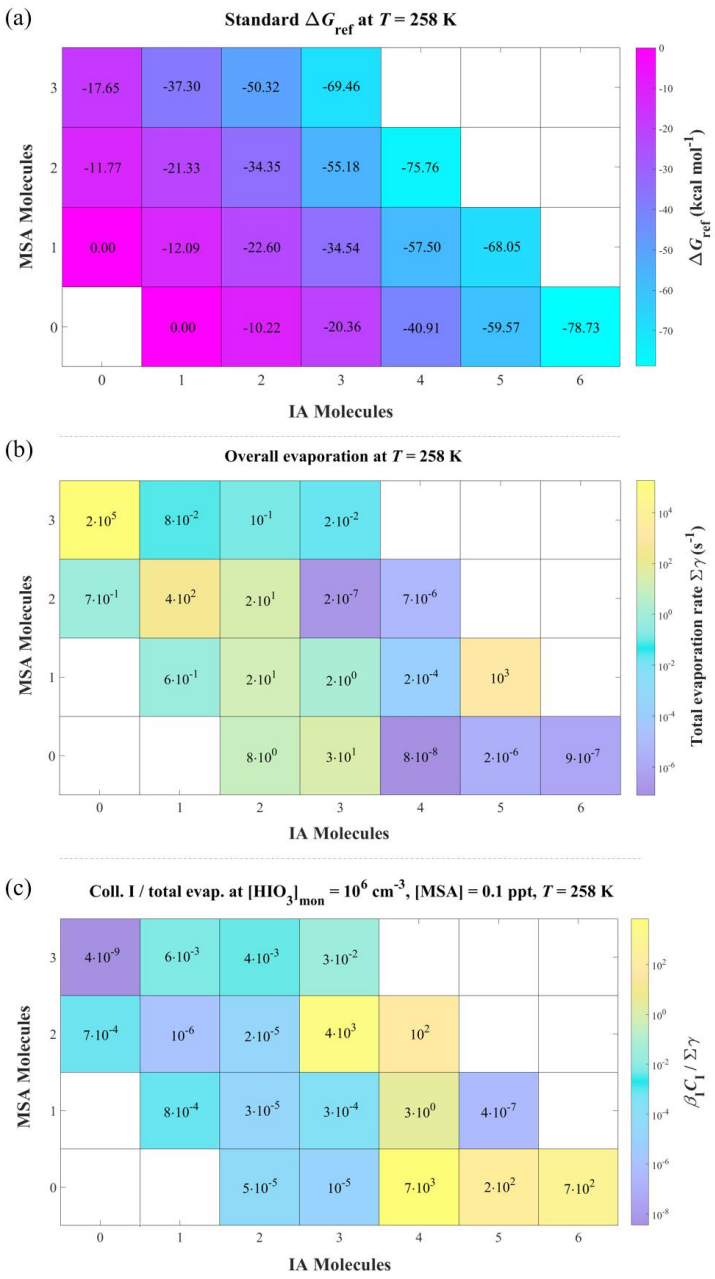


Figure S3. (a) Gibbs formation free energy (ΔG) of the $(IA)_x(MSA)_y$ ($0 \leq x \leq 6$, $0 \leq y \leq 3$, $x + y \leq 6$) clusters identified at the RI-CC2/aug-cc-pV(T+d)Z(-PP)// ω B97X-D/6-311++G(3df,3pd) + aug-cc-pVTZ(-PP) level of theory, T = 258 K, p = 1 atm. (b) the total evaporation rate coefficients ($\sum\gamma$ in s^{-1}) and (c) ratios of IA monomer collision frequencies versus total evaporation coefficient ($\beta C/\sum\gamma$) of the corresponding clusters.

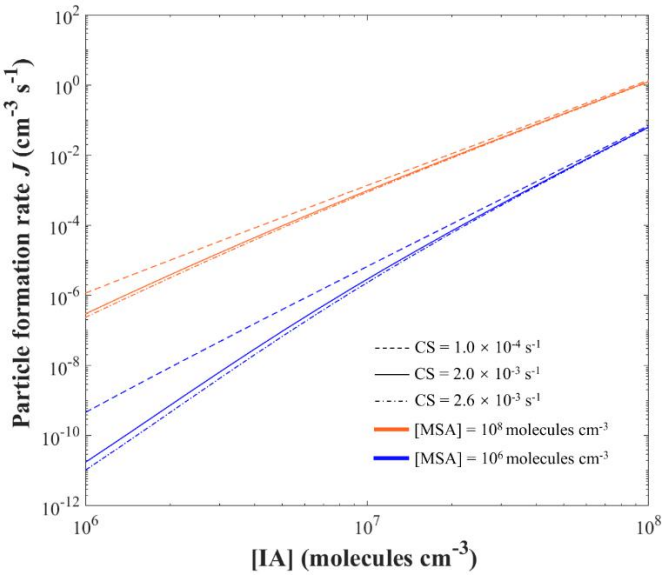


Figure S4. The simulated cluster formation rate J (cm^{-3} s^{-1}) of the IA-MSA system at different condensention sink (CS) coefficients (CS = $1.0 \times 10^{-4} \sim 2.6 \times 10^{-3}$ s^{-1}), T = 278 K, [IA] = $10^6 \sim 10^8$ molecules cm^{-3}, and [MSA] = 10^6, 10^8 molecules cm^{-3}.

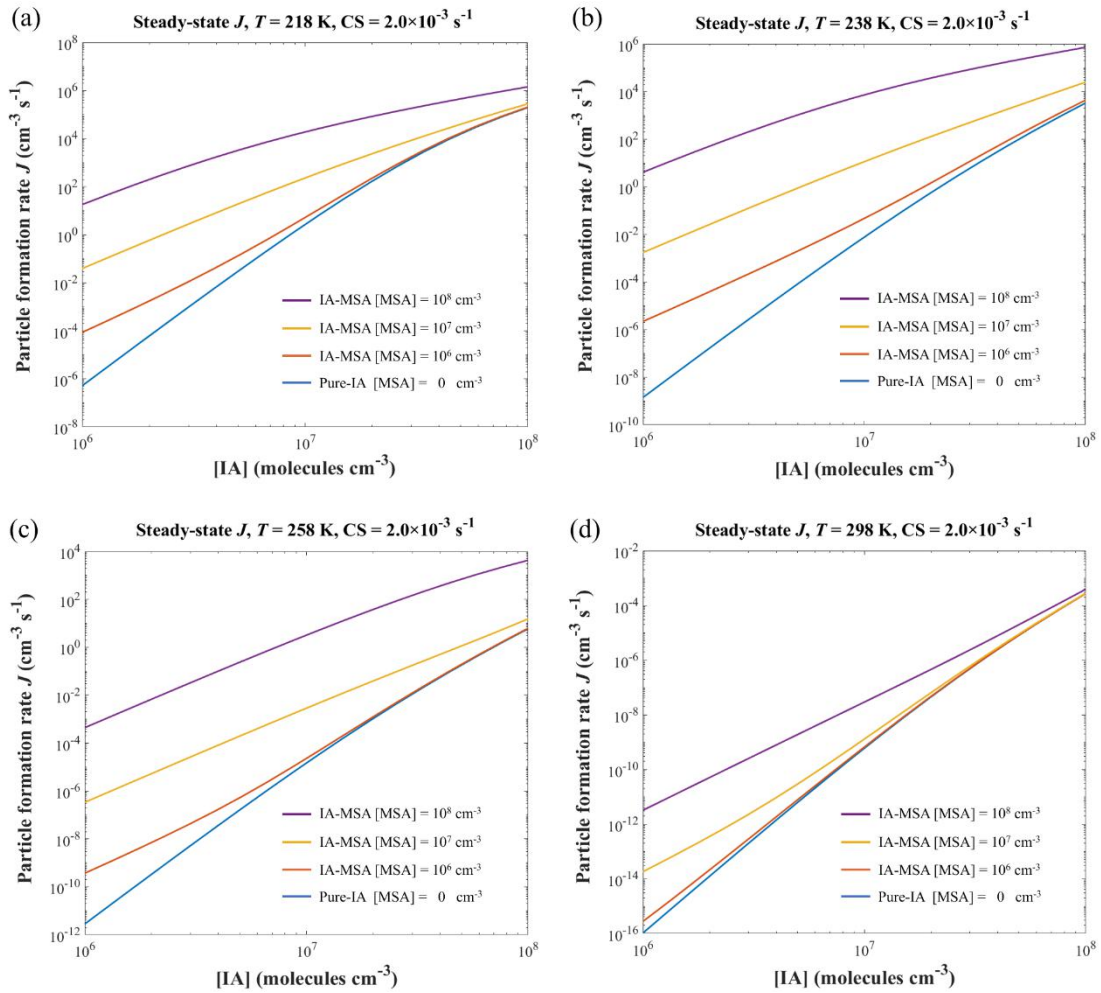


Figure S5. The simulated cluster formation rate J (cm^{-3} s^{-1}) of the IA-MSA system at different temperatures (T = 218 ~ 298 K), [IA] = 10^6 ~ 10^8 molecules cm^{-3}, and [MSA] = 0, 10^6, 10^7, 10^8 molecules cm^{-3}, CS = 2.0×10^{-3} s^{-1}.

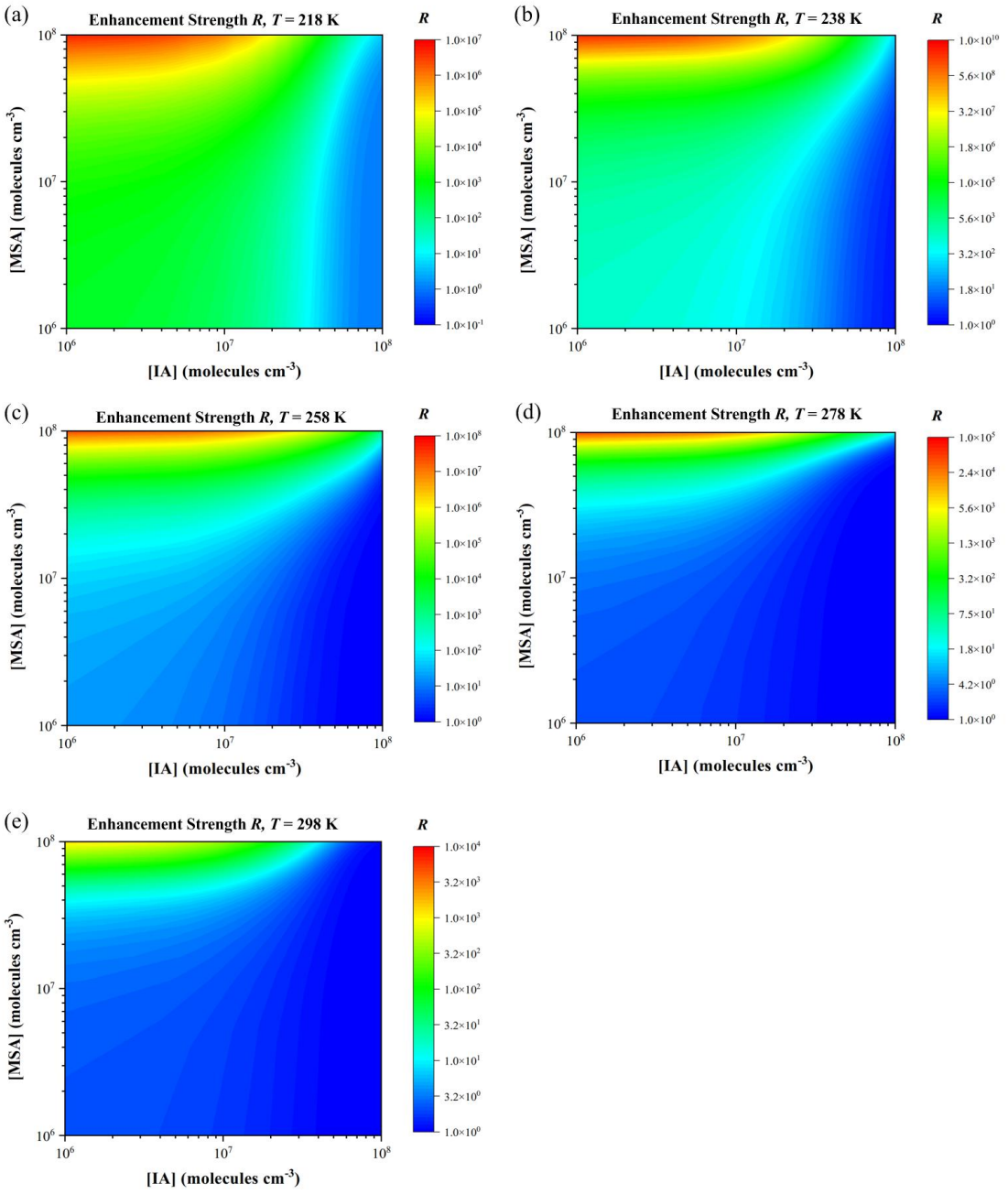
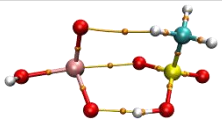
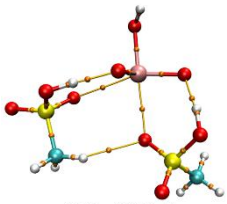
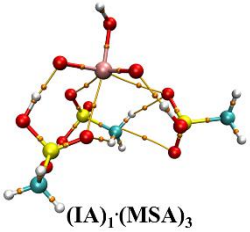
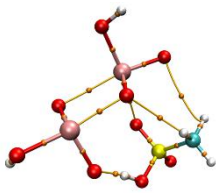
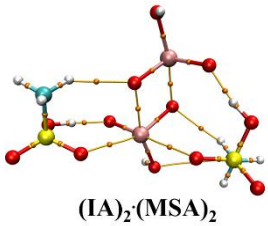
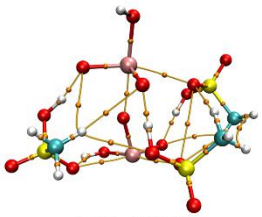
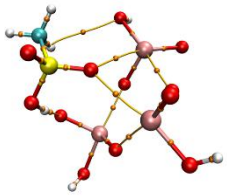
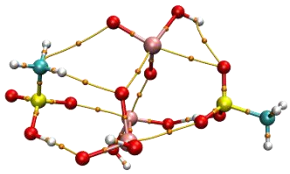
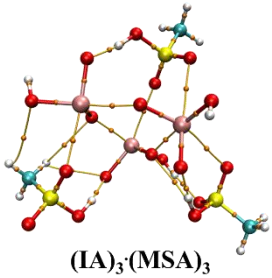
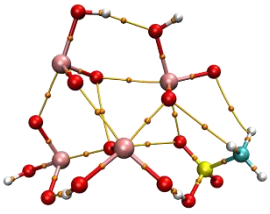
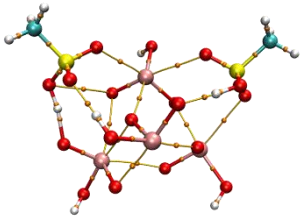


Figure S6. Contour plot of the enhancement strength R at different [IA] ($10^6 \sim 10^8$ molecules cm^{-3}) and [MSA] ($10^6 \sim 10^8$ molecules cm^{-3}) under the condition of T = (a) 218 K, (b) 238 K, (c) 258 K, (d) 278 K, (e) 298 K,CS = 2.0×10^{-3} s^{-1}.

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

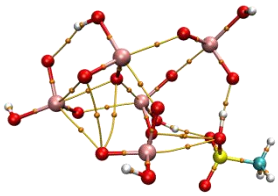
 $(IA)_5 \cdot (MSA)_1$	O-I···O	XB	0.0288	0.0810	-0.0003
	O-I···O	XB	0.0554	0.1361	-0.0074
	O-I···O	XB	0.0578	0.1463	-0.0081
	O-I···O	XB	0.0244	0.0802	0.0017
	O-I···O	XB	0.0558	0.1535	-0.0065

Table S2. The Gibbs formation free energy ΔG (kcal mol^{-1}) of the studied IA-MSA clusters at the RI-CC2/aug-cc-pV(T+d)Z(-PP)// ω B97X-D/6-311++G(3df,3pd) + aug-cc-pVTZ(-PP) with ECP28MDF (for I) level of theory, p = 1 atm and T = 218 ~ 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
$(IA)_1 \cdot (MSIA)_1$	-13.67	-12.88	-12.10	-11.32	-10.55
$(IA)_1 \cdot (MSIA)_2$	-24.47	-22.90	-21.34	-19.78	-18.23
$(IA)_1 \cdot (MSIA)_3$	-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
$(IA)_2$	-11.66	-10.94	-10.22	-9.51	-8.80
$(IA)_3$	-23.55	-21.95	-20.36	-18.79	-17.24
$(IA)_4$	-45.88	-43.39	-40.92	-38.48	-36.05
$(IA)_5$	-66.26	-62.91	-59.58	-56.28	-53.02
$(IA)_6$	-87.48	-83.09	-78.73	-74.41	-70.12

Table S3. The Gibbs formation free energy ΔG (kcal mol^{-1}) of the studied IA-MSA clusters at the RI-CC2/aug-cc-pV(T+d)Z(-PP)// ω B97X-D/6-311++G(3df,3pd) + aug-cc-pVTZ(-PP) with ECP28MDF (for I) level of theory, p = 1 atm and T = 253, 268, 287, 290 and 300 K.

Clusters	ΔG (kcal mol^{-1})				
	300 K	290 K	287 K	268 K	253 K
$(MSA)_2$	-10.08	-10.49	-10.61	-11.37	-11.98
$(MSA)_3$	-14.41	-15.18	-15.41	-16.88	-18.04
$(IA)_1 \cdot (MSIA)_1$	-10.47	-10.85	-10.97	-11.71	-12.29
$(IA)_1 \cdot (MSIA)_2$	-18.08	-18.85	-19.08	-20.56	-21.73
$(IA)_1 \cdot (MSIA)_3$	-32.12	-33.35	-33.72	-36.06	-37.92
$(IA)_2 \cdot (MSA)_1$	-19.27	-20.06	-20.30	-21.80	-23.01
$(IA)_2 \cdot (MSA)_2$	-29.24	-30.45	-30.81	-33.13	-34.97
$(IA)_2 \cdot (MSA)_3$	-43.66	-45.23	-45.71	-48.73	-51.13
$(IA)_3 \cdot (MSA)_1$	-29.74	-30.87	-31.21	-33.39	-35.13
$(IA)_3 \cdot (MSA)_2$	-48.52	-50.10	-50.57	-53.59	-55.99
$(IA)_3 \cdot (MSA)_3$	-60.71	-62.78	-63.41	-67.37	-70.52
$(IA)_4 \cdot (MSA)_1$	-50.48	-52.13	-52.64	-55.82	-58.36
$(IA)_4 \cdot (MSA)_2$	-67.02	-69.08	-69.71	-73.67	-76.82
$(IA)_5 \cdot (MSA)_1$	-59.57	-61.57	-62.18	-66.02	-69.08
$(IA)_2$	-8.74	-9.08	-9.19	-9.86	-10.40
$(IA)_3$	-17.09	-17.86	-18.09	-19.58	-20.76
$(IA)_4$	-35.82	-37.02	-37.38	-39.70	-41.54
$(IA)_5$	-52.70	-54.32	-54.81	-57.93	-60.41
$(IA)_6$	-69.71	-71.83	-72.48	-76.57	-79.82

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

Evaporation pathways	Evaporation coefficients (γ, s^{-1})
$(IA)_2 \rightarrow IA + IA$	1.23×10^{2}
$(IA)_3 \rightarrow (IA)_2 + IA$	5.64×10^{2}
$(IA)_4 \rightarrow (IA)_3 + IA$	3.67×10^{-6}
$(IA)_5 \rightarrow (IA)_4 + IA$	1.47×10^{-4}
$(IA)_6 \rightarrow (IA)_5 + IA$	7.97×10^{-5}
$(MSA)_2 \rightarrow MSA + MSA$	1.43×10^{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}
$(IA)_2\cdot(MSA)_1 \rightarrow (IA)_2 + MSA$	1.36×10^{-1}
$(IA)_2\cdot(MSA)_2 \rightarrow (IA)_2\cdot(MSA)_1 + MSA$	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}
$(IA)_3\cdot(MSA)_1 \rightarrow (IA)_3 + MSA$	4.04×10^{-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, respectively.

Temperature (K)	Boundary cluster
298 K	$(IA)_7$
	$(IA)_6 \cdot (MSA)_1$
	$(IA)_4 \cdot (MSA)_3$
258, 278 K	$(IA)_7$
	$(IA)_6 \cdot (MSA)_1$
	$(IA)_4 \cdot (MSA)_3$
	$(IA)_5 \cdot (MSA)_2$
218, 238 K	$(IA)_7$
	$(IA)_6 \cdot (MSA)_1$
	$(IA)_4 \cdot (MSA)_3$
	$(IA)_3 \cdot (MSA)_4$
	$(IA)_5 \cdot (MSA)_2$

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

[IA]	*R*	[MSA]	*R*	*T* (K)	*R*
1.0E+06	93.4	1.0E+06	1.0	218	25.7
1.8E+06	24.0	1.8E+06	1.1	228	471.6
3.2E+06	7.6	3.2E+06	1.1	238	1850.1
5.6E+06	3.2	5.6E+06	1.3	248	752.5
1.0E+07	1.8	1.0E+07	1.8	258	126.4
1.8E+07	1.4	1.8E+07	3.9	268	10.3
3.2E+07	1.2	3.2E+07	13.6	278	1.8
5.6E+07	1.1	5.6E+07	64.9	288	1.3
1.0E+08	1.0	1.0E+08	346.9	298	1.3

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	-0.0972210	0.0049300	-0.2430950
O	-0.8431630	-1.3456500	0.6284330
O	-0.5271120	1.5031140	0.6021730
O	1.7795500	-0.1822800	0.2317520
H	1.8785260	-0.0627760	1.1851670

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
C	3.1267240	1.3033180	1.5334940
H	2.2673230	-0.0820010	-0.1388570

H	3.5283760	-0.3795930	-0.7071300
H	1.1263090	0.0291050	-1.0384610
N	1.9247750	-1.1505350	0.9232180
C	0.9261270	-1.2411260	1.0163970
H	-1.2941080	-0.0006480	-0.2498380
H	-1.0464710	1.5856110	0.5005280
H	-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

$(IA)_5$-$(MSA)_1$:

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	2.2549570	-0.0178470	0.1703430
O	1.0444520	-1.1922840	0.7836320
O	2.3984610	-0.2943900	-1.5718140
O	1.3168040	1.6259870	0.3119740
H	0.4027420	1.5274470	-0.0812950
I	-2.2549520	0.0178440	-0.1703530
O	-2.3985330	0.2944080	1.5717940
O	-1.0444320	1.1922830	-0.7836050
O	-1.3167860	-1.6259860	-0.3119240
H	-0.4027230	-1.5274350	0.0813460

$(IA)_3$:

Atoms	X	Y	Z
I	2.0502760	-1.0029130	-0.1065160
O	3.2118700	-1.9599240	1.1228970
H	4.0825390	-1.5475730	1.1536720
O	0.5510230	0.4182740	-1.0709420
O	3.1917700	-0.8150810	-1.4395200
I	0.5179410	1.8407360	0.0856120
O	-0.9109420	2.6638930	-0.8913050
H	-1.5848740	1.9783540	-1.0872330
O	-0.4384840	1.3191470	1.5020620
O	2.2089230	0.5746000	0.8581940
I	-2.7728430	-0.9500980	-0.0681520
O	-2.6271120	-0.1362110	1.6403860
H	-1.8123930	0.4415940	1.6403940
O	-1.2674910	-1.8883370	-0.1858000
O	-2.6495640	0.4584130	-1.1593330

$(IA)_4$:

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	2.0142330	-1.9502430	0.1062340
O	3.5813460	-2.3077960	-0.6609640
O	1.2147740	-0.8403890	-1.0583760
O	1.0568390	-3.5830250	-0.4682790
H	1.3933920	-3.8971680	-1.3144030
I	4.0616510	1.1772010	0.5078450
O	3.6480600	1.4144440	-1.2121400
O	2.9102220	-0.0865740	1.1649480
O	5.4562590	-0.1115870	0.2184390
H	5.0709030	-0.9080240	-0.1938550
I	-1.9509040	-2.0075870	1.2785530
O	-0.3728890	-1.2094910	1.5384160
O	-2.2436270	-1.9045460	-0.4983290
O	-1.2923970	-3.8204880	1.2425070
H	-0.5887520	-3.9170540	0.5764410
I	-3.5541860	1.5105690	0.6518740
O	-4.9348430	2.0979990	1.5719390
O	-3.0518940	0.0320430	1.5940770
O	-4.5205320	0.6939320	-0.7634460
H	-3.9463030	0.3947540	-1.5156220
I	0.6743480	1.8105790	0.3807700
O	2.2811220	2.5127150	0.9739480
O	-0.4695840	3.0879240	0.7922740
O	1.0853560	2.2419120	-1.4546750
H	2.0513300	2.0382580	-1.5418810
I	-1.2858540	-0.3923390	-2.1824110
O	-1.2960600	0.8181160	-0.8255000
O	-2.9363330	-0.1593290	-2.8052690
O	-0.3635120	0.7547110	-3.4115000
H	0.1587040	1.3911450	-2.8870510