Supplement of

Mechanistic insights into marine boundary layer nucleation: synergistic interactions of typical sulfur, iodine, and nitrogen precursors

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Totally, 35 pages, 4 figures and 4 tables

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atom) level of theory.

Supplementary Methods

Multi-Step Cluster Conformational Searching Method

Initially, the artificial bee colony algorithm combined with UFF force field (Rappé et al., 1992) was utilized via ABCluster (Zhang and Dolg, 2015) to generate over 5000 configurations for each cluster. Subsequently, up to 1000 relatively low-energy structures were selected and subjected to optimize at the PM7 semi-empirical method (Stewart, 2013) using MOPAC 2016 (Stewart, 2016). Following this step, approximately 100 of the lowest-energy configurations were re-optimized at the ωB97X-D/6-31+G* (for C, H, O, N, and S atoms) + Lanl2DZ (for I atom) level of theory (Elm and Kristensen, 2017), based on the proven accuracy of the ωB97X-D functional in studying atmospheric clusters. Finally, the 10 most stable isomers were further optimized at a higher level of theory: ωB97X-D/6-311++G(3df,3pd) (for C, H, O, N, and S atoms) + aug-cc-pVTZ-PP with ECP28MDF (for I atom) (Francl et al., 1982; Peterson et al., 2003), to identify the global minimum structure.

The Equations in Atmospheric Cluster Dynamics Code (ACDC)

The birth-death equation (Eq. (S1)) of IA–MSA–DMA system as following:

$$\frac{d_{C_i}}{dt} = \frac{1}{2}\sum_{j<i}\beta_{j,(i-j)}C_jC_{(i-j)} + \sum_j \gamma_{(i+j)\to i}C_{i+j} - \sum_j \beta_{i,j}C_iC_j - \frac{1}{2}\sum_{j<i}\gamma_{i\to j}C_i + Q_i - S_i \quad \text{(S1)}$$

where C_i refers to the concentration of cluster i (where i denotes the cluster index). $\beta_{i,j}$ represents the collision rate coefficient between clusters i and j, while $\gamma_{(i+j)\to i}$ describes evaporation rate constant for the decomposition of cluster $(i + j)$ into smaller clusters i and j. Q_i and S_i denote the external source and possible loss term of cluster i, respectively.

The collision rate coefficient between clusters i and j ($\beta_{i,j}$) is obtained based on the kinetic gas theory, which is given as:

$$\beta_{i,j} = \left(\frac{3}{4\pi}\right)^{1/6}\left(\frac{6k_BT}{m_i} + \frac{6k_BT}{m_j}\right)^{1/2}\left(V_i^{1/3} + V_j^{1/3}\right)^2 \quad \text{(S2)}$$

where m_i and V_i are the mass and volume of cluster i, respectively. Equation (S2) is derived from the hard-sphere collision theory where the volume of molecule clusters $V_i = 3/4 \times \pi \times (d_i/2)^3$. The diameter d_i of cluster i is derived from the cluster volume V_i calculated by Multiwfn 3.7 (Lu and Chen, 2012). Evaporation rate coefficient $\gamma_{(i+j)\to i}$ is derived from the collision coefficients based on the detailed balance assumption:

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

where P_{ref} is the reference pressure (1 atm) and ΔG_i is the Gibbs free energy of the formation of cluster i.

Surface Electrostatic Potential (ESP) Analysis

The molecular electrostatic potential (ESP) analysis can provide insights into the reactive sites of the nucleation precursors. As shown in Fig.1, the MSA molecule exhibits a pronounced ESP maximum (+63.95 kcal mol^{-1}) at the hydrogen atom of the –OH group, indicating strong electrophilic character and suggesting its potential as a hydrogen bond (HB) donor. Further analysis reveals two ESP minima (-29.46 and -32.10 kcal mol^{-1}) located at the terminal O atoms of the –SO_3H group, indicating nucleophilic regions capable of acting as HB or halogen bond (XB) acceptors. Similarly, the DMA molecule displays an ESP minimum (-34.38 kcal mol^{-1}) at the N atom of the –NH group, making it a potential acceptor site for HB or XB interactions. In addition, the H atom within the –NH group presents an ESP maximum (+25.79 kcal mol^{-1}), indicating its potential as a HB donor. For the IA molecule, a significant ESP maximum (+59.09 kcal mol^{-1}) is located at the H atom of the –OH group, allowing it to serve as an HB donor. Moreover, an ESP maximum (+51.90 kcal mol^{-1}) is identified along the O–I direction, highlighting its capacity to function as a HB donor. The terminal O atoms of the IA molecule exhibit two ESP minima (-29.10 and -29.47 kcal mol^{-1}), suggesting that these sites can act as HB or XB acceptors. These ESP-based observations collectively indicate that IA, MSA, and DMA molecules possess complementary electrostatic features that facilitate the formation of stable molecular clusters via hydrogen and/or halogen bonding. For instance, Fig. 1(d) illustrates the optimized structure of $(IA)_2(MSA)_1(DMA)_1$ cluster, where blue dashed lines denote HBs and red dashed lines represent XBs, further confirming the critical role of intermolecular interactions in stabilizing cluster formation.

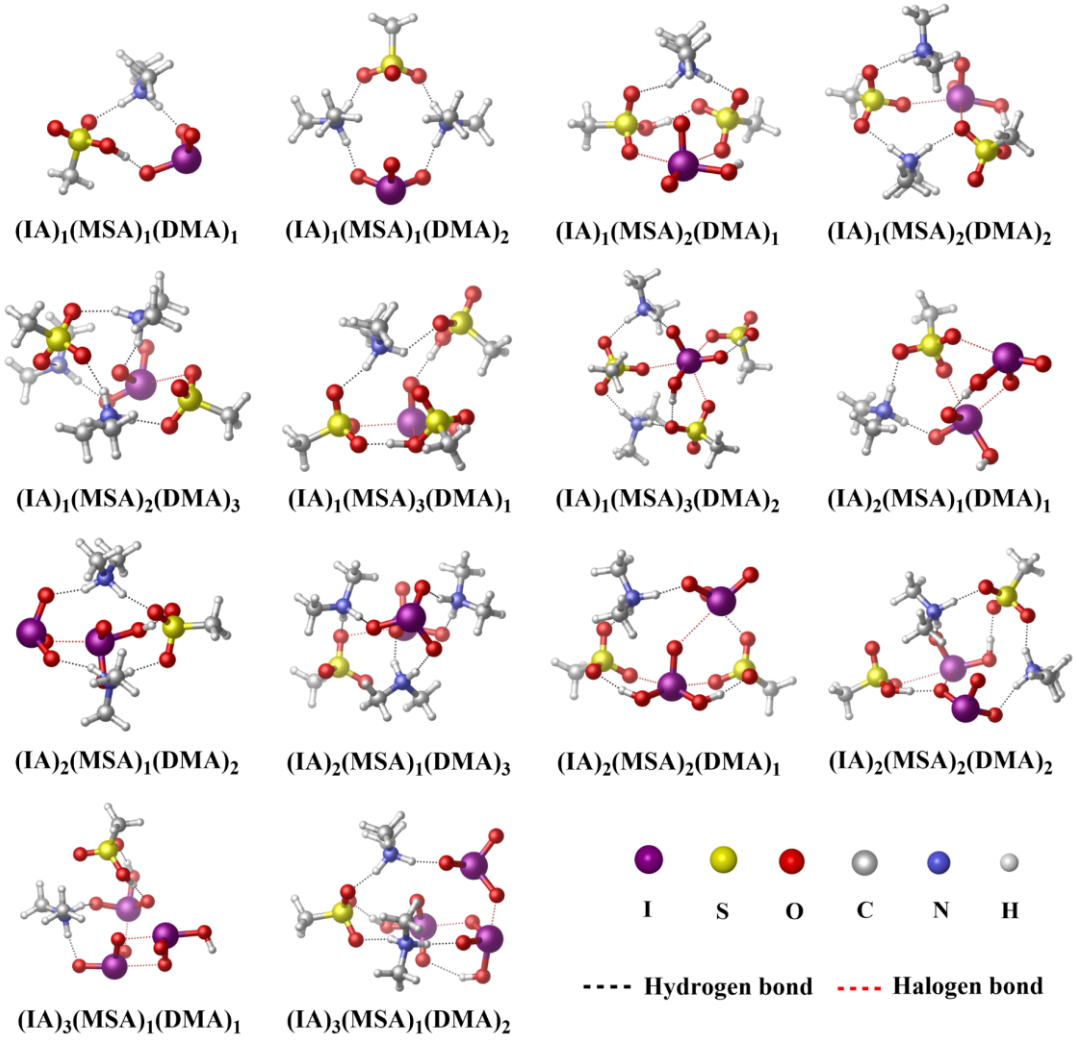

Figure S1. Lowest Gibbs free energy conformations of $(IA)_x(MSA)_y(DMA)_z$ ($x + y + z \leq 6$, $z \leq x + y$) cluster optimized at the ωB97X-D/6-311++G(3df, 3pd) (for C, H, O, N, and S atoms) + aug-cc-pVTZ-PP (for I atom) level of theory.

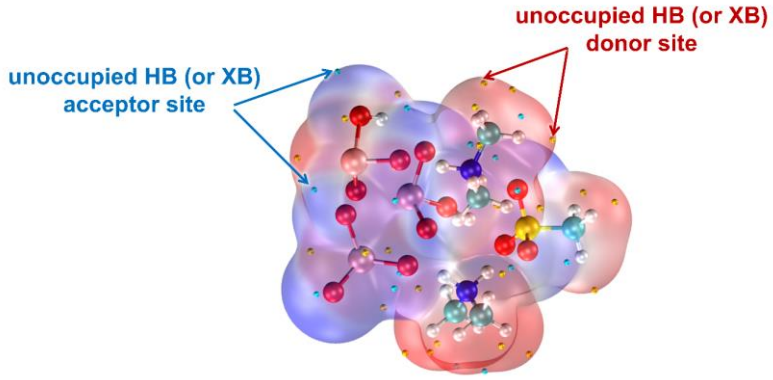

Figure S2. ESP-mapped van der Waals (vdW) surface of the $(IA)_3(MSA)_1(DMA)_2$ cluster. The red region is the electron-deficient region, and the blue region is the electron-rich region.

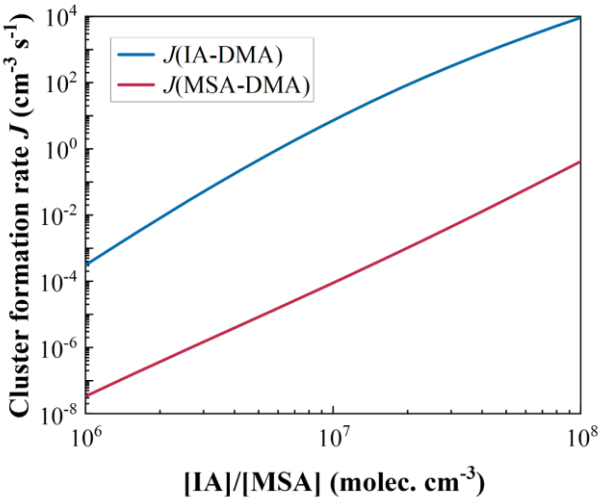

Figure S3. Cluster formation rates J of IA–DMA and MSA–DMA nucleation. The ACDC simulations were performed at the conditions of T = 278 K, CS = 2.0×10^{-3} s^{-1}, [IA] (or [MSA]) = 10^6 – 10^8 molec. cm^{-3}, and [DMA] = 0.25 pptv.

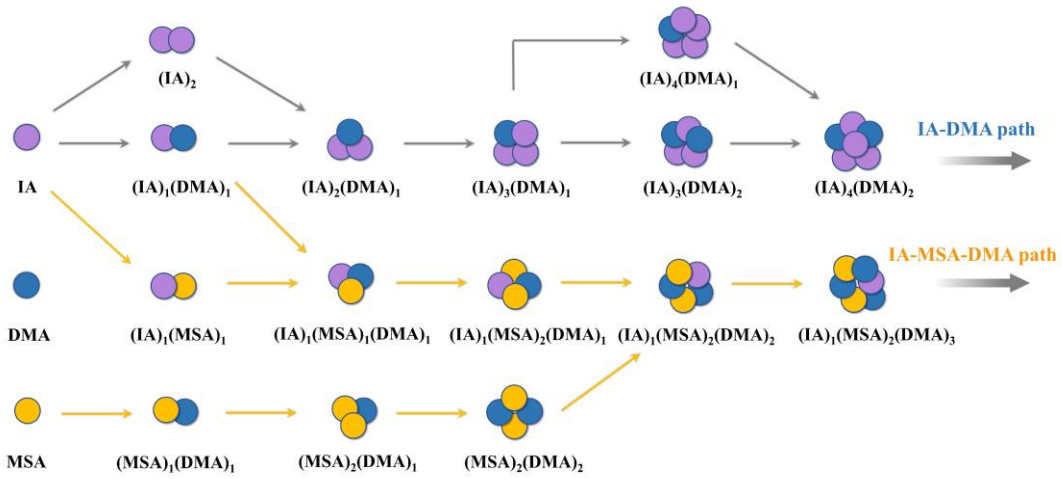

Figure S4. The simulated primary cluster growth pathways of IA–MSA–DMA system at the simulation conditions of T = 288 – 298 K, CS = 2.0 × 10^{-3} s^{-1}, [IA] = 10^7 molec. cm^{-3}, [MSA] = 10^7 molec. cm^{-3}, and [DMA] = 0.25 pptv.

Table S1. The Gibbs formation free energies ΔG_{ref} (kcal mol^{-1}) of the studied IA–MSA–DMA clusters at the DLPNO-CCSD(T)/aug-cc-pVTZ(-PP)//ωB97X-D/6-311++G(3df,3pd) (for C, H, O, N, and S atoms) + aug-cc-pVTZ-PP with ECP28MDF (for I atom) level of theory, P = 1 atm, and T = 258, 268, 278, 288, and 298 K.

Clusters	ΔG (kcal mol^{-1})				
	258 K	**268 K**	**278 K**	**288 K**	**298 K**
$(IA)_1(MSA)_1$	-12.85	-12.46	-12.07	-11.69	-11.30
$(IA)_1(MSA)_2$	-20.43	-19.65	-18.87	-18.10	-17.33
$(IA)_1(MSA)_3$	-32.12	-30.88	-29.64	-28.41	-27.18
$(IA)_2(MSA)_1$	-24.43	-23.63	-22.83	-22.04	-21.25
$(IA)_2(MSA)_2$	-33.93	-32.70	-31.48	-30.26	-29.04
$(IA)_2(MSA)_3$	-45.25	-43.65	-42.06	-40.47	-38.89
$(IA)_3(MSA)_1$	-34.10	-32.95	-31.80	-30.65	-29.51
$(IA)_3(MSA)_2$	-53.40	-51.80	-50.21	-48.62	-47.04
$(IA)_3(MSA)_3$	-64.94	-62.84	-60.75	-58.67	-56.59
$(IA)_4(MSA)_1$	-57.37	-55.69	-54.01	-52.33	-50.67
$(IA)_4(MSA)_2$	-72.45	-70.36	-68.27	-66.18	-64.11
$(IA)_5(MSA)_1$	-67.40	-65.36	-63.34	-61.31	-59.30
$(MSA)_2$	-9.22	-8.81	-8.41	-8.01	-7.60
$(MSA)_3$	-14.68	-13.89	-13.10	-12.43	-11.66
$(IA)_2$	-12.96	-12.59	-12.22	-11.85	-11.48
$(IA)_3$	-25.35	-24.55	-23.77	-22.98	-22.20
$(IA)_4$	-44.75	-43.52	-42.30	-41.09	-39.88
$(IA)_5$	-61.35	-59.70	-58.06	-56.42	-54.79
$(IA)_6$	-77.14	-75.06	-72.97	-70.90	-68.84
$(IA)_1(DMA)_1$	-11.79	-11.42	-11.04	-10.67	-10.30
$(IA)_1(DMA)_2$	-18.85	-18.12	-17.38	-16.65	-15.92
$(IA)_1(DMA)_3$	-18.91	-17.82	-16.74	-15.67	-14.60
$(IA)_2(DMA)_1$	-32.35	-31.59	-30.83	-30.07	-29.31
$(IA)_2(DMA)_2$	-45.39	-44.29	-43.20	-42.11	-41.02
$(IA)_2(DMA)_3$	-38.85	-37.33	-35.82	-34.32	-32.82
$(IA)_3(DMA)_1$	-46.39	-45.25	-44.11	-42.98	-41.85
$(IA)_3(DMA)_2$	-65.15	-63.56	-61.96	-60.37	-58.79
$(IA)_3(DMA)_3$	-60.92	-58.99	-57.05	-55.13	-53.21

$(IA)_4(DMA)_1$	-61.86	-60.29	-58.72	-57.16	-55.61
$(IA)_4(DMA)_2$	-81.61	-79.60	-77.58	-75.58	-73.58
$(IA)_5(DMA)_1$	-80.97	-78.89	-76.81	-74.73	-72.66
$(DMA)_2$	4.03	4.37	4.71	5.05	5.39
$(DMA)_3$	6.07	6.78	7.49	8.19	8.89
$(MSA)_1(DMA)_1$	-10.37	-9.98	-9.58	-9.19	-8.80
$(MSA)_2(DMA)_1$	-28.16	-27.38	-26.60	-25.82	-25.04
$(MSA)_2(DMA)_2$	-44.56	-43.39	-42.22	-41.05	-39.89
$(MSA)_3(DMA)_1$	-40.01	-38.81	-37.62	-36.43	-35.24
$(MSA)_3(DMA)_2$	-55.65	-54.07	-52.49	-50.91	-49.35
$(MSA)_3(DMA)_3$	-75.22	-73.28	-71.34	-69.41	-67.49
$(IA)_1(MSA)_1(DMA)_1$	-28.28	-27.54	-26.79	-26.05	-25.31
$(IA)_1(MSA)_1(DMA)_2$	-46.29	-45.19	-44.10	-43.01	-41.92
$(IA)_2(MSA)_1(DMA)_1$	-46.49	-45.33	-44.17	-43.01	-41.86
$(IA)_2(MSA)_1(DMA)_2$	-66.27	-64.66	-63.06	-61.45	-59.86
$(IA)_2(MSA)_1(DMA)_3$	-79.76	-77.77	-75.79	-73.81	-71.84
$(IA)_3(MSA)_1(DMA)_1$	-59.06	-57.45	-55.85	-54.25	-52.66
$(IA)_3(MSA)_1(DMA)_2$	-81.40	-79.37	-77.33	-75.31	-73.29
$(IA)_1(MSA)_2(DMA)_1$	-44.03	-42.86	-41.70	-40.54	-39.39
$(IA)_1(MSA)_2(DMA)_2$	-62.26	-60.74	-59.23	-57.73	-56.22
$(IA)_1(MSA)_2(DMA)_3$	-78.95	-76.97	-74.99	-73.01	-71.04
$(IA)_2(MSA)_2(DMA)_1$	-63.22	-61.61	-60.00	-58.40	-56.80
$(IA)_2(MSA)_2(DMA)_2$	-83.35	-81.40	-79.45	-77.50	-75.57
$(IA)_1(MSA)_3(DMA)_1$	-56.10	-54.54	-52.98	-51.42	-49.87
$(IA)_1(MSA)_3(DMA)_2$	-75.92	-73.89	-71.86	-69.84	-67.82

Table S2. The total evaporation rate coefficients ($\Sigma\gamma$, s^{-1}) of IA–MSA–DMA clusters calculated at 268 – 288 K.

Clusters	$\Sigma\gamma$ (s^{-1})		
	268 K	**278 K**	**288 K**
$(IA)_2$	1.80×10^{-1}	8.09×10^{-1}	3.27×10^{0}
$(IA)_3$	1.26×10^{0}	5.83×10^{0}	2.47×10^{1}
$(IA)_4$	2.64×10^{-6}	2.07×10^{-5}	1.36×10^{-4}
$(IA)_5$	5.37×10^{-4}	3.36×10^{-3}	1.88×10^{-2}
$(IA)_6$	2.67×10^{-3}	1.67×10^{-2}	8.87×10^{-2}
$(MSA)_2$	3.44×10^{2}	1.26×10^{3}	4.23×10^{3}
$(MSA)_3$	8.18×10^{5}	2.29×10^{6}	4.85×10^{6}
$(DMA)_2$	2.30×10^{13}	3.12×10^{13}	4.12×10^{13}
$(DMA)_3$	1.28×10^{12}	2.09×10^{12}	3.23×10^{12}
$(IA)_1(MSA)_1$	1.18×10^{0}	5.46×10^{0}	2.22×10^{11}
$(IA)_1(MSA)_2$	1.43×10^{4}	4.63×10^{4}	1.38×10^{5}
$(IA)_1(MSA)_3$	8.23×10^{0}	3.97×10^{1}	1.71×10^{2}
$(IA)_2(MSA)_1$	1.57×10^{1}	6.99×10^{1}	2.78×10^{2}
$(IA)_2(MSA)_2$	4.53×10^{2}	1.76×10^{3}	6.31×10^{3}
$(IA)_2(MSA)_3$	1.51×10^{1}	6.08×10^{1}	2.22×10^{2}
$(IA)_3(MSA)_1$	1.71×10^{3}	5.80×10^{3}	1.78×10^{4}
$(IA)_3(MSA)_2$	7.65×10^{-6}	5.76×10^{-5}	3.77×10^{-4}
$(IA)_3(MSA)_3$	1.32×10^{1}	6.76×10^{1}	3.03×10^{2}
$(IA)_4(MSA)_1$	1.37×10^{0}	7.05×10^{0}	3.28×10^{1}
$(IA)_4(MSA)_2$	1.41×10^{-2}	7.82×10^{-2}	3.85×10^{-1}
$(IA)_5(MSA)_1$	2.99×10^{5}	8.57×10^{5}	2.32×10^{6}
$(IA)_1(DMA)_1$	9.93×10^{0}	4.19×10^{1}	1.57×10^{2}
$(IA)_1(DMA)_2$	4.24×10^{4}	1.26×10^{5}	3.45×10^{5}
$(IA)_1(DMA)_3$	2.48×10^{10}	4.41×10^{10}	7.55×10^{10}
$(IA)_2(DMA)_1$	4.12×10^{-6}	2.97×10^{-5}	1.87×10^{-4}
$(IA)_2(DMA)_2$	6.08×10^{-1}	2.56×10^{0}	9.74×10^{0}
$(IA)_2(DMA)_3$	7.33×10^{15}	9.62×10^{15}	1.22×10^{16}
$(IA)_3(DMA)_1$	5.88×10^{-2}	2.89×10^{-1}	1.25×10^{3}

$(IA)_3(DMA)_2$	1.95×10^{-5}	1.54×10^{-4}	1.05×10^{-3}
$(IA)_3(DMA)_3$	8.78×10^{13}	1.17×10^{14}	1.51×10^{14}
$(IA)_4(DMA)_1$	4.98×10^{-3}	2.94×10^{-2}	1.53×10^{-1}
$(IA)_4(DMA)_2$	7.75×10^{-4}	4.81×10^{-3}	2.59×10^{-2}
$(IA)_5(DMA)_1$	9.85×10^{-6}	8.29×10^{-5}	6.09×10^{-4}
$(MSA)_1(DMA)_1$	1.74×10^{2}	6.90×10^{2}	2.45×10^{3}
$(MSA)_2(DMA)_1$	7.67×10^{-5}	4.90×10^{-4}	2.80×10^{-3}
$(MSA)_2(DMA)_2$	1.15×10^{-3}	6.73×10^{-3}	3.49×10^{-2}
$(MSA)_3(DMA)_1$	5.06×10^{0}	2.26×10^{1}	9.08×10^{1}
$(MSA)_3(DMA)_2$	2.29×10^{1}	9.72×10^{1}	3.73×10^{2}
$(MSA)_3(DMA)_3$	3.34×10^{-6}	2.31×10^{-5}	1.37×10^{-4}
$(IA)_1(MSA)_1(DMA)_1$	7.30×10^{-3}	3.84×10^{-2}	1.81×10^{-1}
$(IA)_1(MSA)_1(DMA)_2$	5.78×10^{-5}	3.46×10^{-4}	1.86×10^{-3}
$(IA)_2(MSA)_1(DMA)_1$	6.79×10^{-2}	3.48×10^{-1}	1.59×10^{0}
$(IA)_2(MSA)_1(DMA)_2$	4.21×10^{-6}	3.58×10^{-5}	2.68×10^{-4}
$(IA)_2(MSA)_1(DMA)_3$	3.42×10^{-1}	1.62×10^{0}	6.77×10^{0}
$(IA)_3(MSA)_1(DMA)_1$	2.48×10^{0}	1.25×10^{1}	5.70×10^{1}
$(IA)_3(MSA)_1(DMA)_2$	1.13×10^{-2}	6.71×10^{-2}	3.36×10^{-1}
$(IA)_1(MSA)_2(DMA)_1$	5.59×10^{-3}	3.20×10^{-2}	1.64×10^{-1}
$(IA)_1(MSA)_2(DMA)_2$	2.70×10^{-3}	1.62×10^{-2}	8.43×10^{-2}
$(IA)_1(MSA)_2(DMA)_3$	9.98×10^{-4}	6.86×10^{-3}	4.20×10^{-2}
$(IA)_2(MSA)_2(DMA)_1$	6.41×10^{-4}	4.27×10^{-3}	2.45×10^{-2}
$(IA)_2(MSA)_2(DMA)_2$	2.90×10^{-4}	1.67×10^{-3}	8.32×10^{-3}
$(IA)_1(MSA)_3(DMA)_1$	3.71×10^{0}	1.65×10^{1}	6.64×10^{1}
$(IA)_1(MSA)_3(DMA)_2$	2.51×10^{-1}	1.54×10^{0}	8.28×10^{0}

Table S3. Boundary conditions of the ACDC simulations at 258 – 298 K, respectively.

Temperature (K)	Boundary cluster
258 K	$(IA)_7$
	$(IA)_6(MSA)_1$
	$(IA)_6(DMA)_1$
	$(IA)_5(MSA)_2$
	$(IA)_5(DMA)_2$
	$(IA)_4(MSA)_3$
	$(IA)_4(DMA)_3$
	$(MSA)_4(DMA)_3$
	$(IA)_4(MSA)_1(DMA)_2$
	$(IA)_5(MSA)_1(DMA)_1$
	$(IA)_1(MSA)_3(DMA)_3$
	$(IA)_2(MSA)_2(DMA)_3$
	$(IA)_3(MSA)_2(DMA)_2$
	$(IA)_2(MSA)_3(DMA)_2$
268 K	$(IA)_7$
	$(IA)_6(DMA)_1$
	$(IA)_5(DMA)_2$
	$(MSA)_4(DMA)_3$
	$(IA)_4(MSA)_1(DMA)_2$
	$(IA)_5(MSA)_1(DMA)_1$
	$(IA)_1(MSA)_3(DMA)_3$
	$(IA)_2(MSA)_2(DMA)_3$
	$(IA)_3(MSA)_2(DMA)_2$
	$(IA)_2(MSA)_3(DMA)_2$
278 K	$(IA)_6(DMA)_1$
	$(IA)_5(DMA)_2$
	$(MSA)_4(DMA)_3$
	$(IA)_5(MSA)_1(DMA)_1$

	$(IA)_1(MSA)_3(DMA)_3$
	$(IA)_3(MSA)_2(DMA)_2$
	$(IA)_2(MSA)_3(DMA)_2$
288 K	$(IA)_6(DMA)_1$
	$(IA)_5(DMA)_2$
	$(MSA)_4(DMA)_3$
	$(IA)_5(MSA)_1(DMA)_1$
	$(IA)_1(MSA)_3(DMA)_3$
298 K	$(IA)_6(DMA)_1$
	$(MSA)_4(DMA)_3$
	$(IA)_5(MSA)_1(DMA)_1$
	$(IA)_1(MSA)_3(DMA)_3$

Table S4. Cartesian coordinates of all IA–MSA–DMA clusters in the present study at the ωB97X-D/6-311++G(3df,3pd) (for C, H, O, N, and S atoms) + aug-cc-pVTZ-PP with ECP28MDF (for I atom) level of theory.

$(IA)_1(MSA)_1(DMA)_1$:

Atoms	X	Y	Z
I	-2.045639	-0.663977	0.097891
O	-1.984089	-0.165251	-1.640758
O	-0.404451	-1.464759	0.394057
O	-1.898779	0.915942	1.026222
H	-0.615576	1.762805	0.511423
N	0.250909	2.249925	0.151151
H	1.045400	1.624169	0.380376
C	0.429770	3.529977	0.854085
H	-0.422702	4.173195	0.649465
H	0.496140	3.339536	1.921556
H	1.344348	4.007563	0.510438
C	0.156781	2.373430	-1.316752
H	-0.020901	1.388806	-1.741471
H	-0.679990	3.021397	-1.565340
H	1.084721	2.789834	-1.701883
C	2.940222	-1.862277	1.047131
H	1.990308	-1.996256	1.559384
H	3.727081	-1.604665	1.750885
H	3.205784	-2.748438	0.477916
S	2.775392	-0.514882	-0.075307
O	3.940248	-0.406072	-0.881841
O	2.401529	0.640833	0.714897
O	1.598302	-0.921800	-0.970786
H	0.718889	-1.116430	-0.435237

$(IA)_1(MSA)_1(DMA)_2$:

Atoms	X	Y	Z
C	4.784265	-0.000222	0.110274
H	5.053507	-0.893429	0.667368
H	5.053734	0.892676	0.667756
H	5.262118	-0.000069	-0.865559
S	3.030786	0.000049	-0.125507
O	2.737714	1.216677	-0.884503
O	2.411760	-0.000111	1.185884
O	2.737386	-1.216234	-0.884931
H	1.289813	-1.896092	-0.364859
N	0.463975	-2.462837	-0.068571
H	-0.405417	-1.989185	-0.417299
C	0.411211	-2.509348	1.403996
H	1.351412	-2.902385	1.782790
H	-0.418235	-3.144137	1.708571
H	0.255343	-1.501434	1.774857
C	0.570817	-3.782878	-0.708338
H	1.466962	-4.284668	-0.350802
H	0.636232	-3.645797	-1.783961
H	-0.309959	-4.373066	-0.466140
N	0.463942	2.462887	-0.068574
H	1.289893	1.896292	-0.364830
C	0.411155	2.509365	1.403993
H	-0.418422	3.143979	1.708576
H	1.351276	2.902586	1.782797
H	0.255483	1.501414	1.774837
C	0.570564	3.782956	-0.708322
H	-0.310320	4.372986	-0.466128
H	0.636012	3.645900	-1.783945
H	1.466619	4.284895	-0.350769
I	-2.594348	-0.000025	-0.061083
O	-1.879450	-1.429732	-0.912654
O	-1.762617	0.000020	1.528978
O	-1.879330	1.429551	-0.912777
H	-0.405367	1.989099	-0.417325

$(IA)_1(MSA)_2(DMA)_1$:

Atoms	X	Y	Z
C	1.450018	-3.413371	-2.049811
H	0.686349	-4.192685	-2.039295
H	2.408893	-3.810552	-1.713246
H	1.539446	-2.974941	-3.045017
S	0.948197	-2.131404	-0.919158
O	2.031497	-1.097932	-0.962853
O	0.858269	-2.752258	0.420795
O	-0.344979	-1.608909	-1.425120
H	-2.102234	-2.048506	-0.548022
C	2.102046	3.816397	-0.925397
H	3.183520	3.730522	-0.816103
H	1.694031	4.539816	-0.217063
H	1.827304	4.081146	-1.947330
S	1.369651	2.247391	-0.538937
O	-0.072905	2.344645	-0.737188
O	1.843702	1.800338	0.770656
O	2.019888	1.368353	-1.674105
H	1.972200	0.374809	-1.441647
N	1.449694	-0.668997	2.209631
H	1.070962	-1.465583	1.658700
C	0.831970	-0.647246	3.554612
H	1.218291	0.212069	4.106075
H	1.085008	-1.572534	4.075780
H	-0.246208	-0.556829	3.422861
C	2.926075	-0.747955	2.205113
H	3.331668	0.139589	2.693100
H	3.255681	-0.790020	1.166816
H	3.233810	-1.650740	2.736498
I	-2.058884	0.310801	-0.065816
O	-2.803040	-1.486529	-0.157863
O	-3.503937	1.117078	0.569188
O	-0.938607	0.080634	1.304417
H	1.148935	0.168888	1.687682

$(IA)_1(MSA)_2(DMA)_2$:

Atoms	X	Y	Z
I	-0.321538	-1.711869	-0.857758
O	-2.080449	-2.455792	-0.765508
O	0.281871	-2.302742	0.731801
O	0.398439	-2.817604	-2.036708
N	1.786793	-0.851436	2.348196
H	2.424702	-0.258401	1.777244
C	2.588575	-1.753775	3.187696
H	1.926498	-2.398318	3.760904
H	3.210893	-1.168195	3.860944
H	3.217927	-2.362390	2.544746
C	0.866739	0.020776	3.097169
H	0.220674	-0.594644	3.719249
H	0.252746	0.566761	2.385199
H	1.440177	0.705632	3.718038
N	-0.218073	2.776825	-0.549695
H	-0.596453	1.981526	0.003063
C	-0.658637	2.587169	-1.944907
H	-0.289366	3.410670	-2.551515
H	-1.744911	2.551741	-1.966112
H	-0.241089	1.651565	-2.306695
C	-0.662212	4.049366	0.047675
H	-0.281067	4.874155	-0.549946
H	-0.260768	4.119394	1.055126
H	-1.747804	4.058100	0.078330
C	3.990940	0.755100	-1.659230
H	3.558292	1.030299	-2.616995
H	4.204002	-0.310077	-1.631152
H	4.889752	1.332917	-1.462468
S	2.813012	1.113512	-0.394828
O	3.440668	0.738557	0.867273
O	1.626127	0.308365	-0.679960
O	2.522281	2.540064	-0.489265
H	0.819284	2.712101	-0.511732
C	-3.655493	0.505973	2.078859
H	-4.728772	0.632617	1.965822
H	-3.263948	1.217796	2.800519
H	-3.422139	-0.514048	2.373168
S	-2.906029	0.821466	0.508585
O	-1.454039	0.621156	0.717219
O	-3.210869	2.187737	0.152871
O	-3.445851	-0.172140	-0.407799
H	-2.700751	-1.699877	-0.619288
I	1.215952	-1.416093	1.662139

$(IA)_1(MSA)_2(DMA)_3$:

Atoms	X	Y	Z
N	-2.667806	1.915634	-0.497422
H	-2.602864	0.886727	-0.593359
C	-3.757793	2.388381	-1.360994
H	-3.856239	3.466633	-1.260254
H	-4.685631	1.900388	-1.071651
H	-3.525230	2.139911	-2.392956
C	-2.855846	2.225930	0.931787
H	-2.981958	3.299502	1.049781
H	-1.966589	1.909294	1.468351
H	-3.726517	1.690748	1.302490
N	0.064638	-1.015223	2.268811
H	-0.966865	-1.040213	2.224535
C	0.529266	-0.080924	3.310770
H	1.615659	-0.064681	3.292021
H	0.165045	-0.415565	4.279942
H	0.164627	0.916488	3.076815
C	0.588511	-2.384164	2.414938
H	1.668208	-2.358607	2.308783
H	0.164662	-2.997086	1.625781
H	0.299892	-2.770161	3.390991
I	0.879404	1.985822	-0.081099
O	-0.018700	0.401938	-0.023671
O	-0.260712	2.862867	-1.199889
O	0.501457	2.671756	1.531018
N	0.296231	-1.573319	-2.001856
H	-0.243944	-1.662403	-1.127633
C	0.643635	-2.925249	-2.468784
H	1.174731	-2.851131	-3.415000
H	-0.270014	-3.501341	-2.592370
H	1.284921	-3.380861	-1.719784
C	-0.506763	-0.784045	-2.950310
H	0.028330	-0.704128	-3.893791
H	-0.660237	0.201477	-2.521030
H	-1.467219	-1.272209	-3.095181
C	-4.031766	-2.930195	0.361375
H	-4.951291	-2.424630	0.643354
H	-3.752575	-3.661224	1.115072
H	-4.140768	-3.406034	-0.609382
S	-2.741709	-1.723846	0.255701
O	-1.533290	-2.462689	-0.097728
O	-2.660717	-1.106893	1.574805
O	-3.154234	-0.788716	-0.786964

H	-1.741130	2.321410	-0.817376
C	4.888209	-0.989146	-0.243124
H	5.254771	-1.405224	0.691581
H	5.289900	0.008427	-0.398301
H	5.145400	-1.639334	-1.074918
S	3.124420	-0.877875	-0.143352
O	2.837203	0.011242	0.975555
O	2.625371	-2.228144	0.040873
O	2.693443	-0.305887	-1.428945
H	1.168046	-1.055486	-1.766119
H	0.308359	-0.608709	1.339129

$(IA)_1(MSA)_3(DMA)_1$:

Atoms	X	Y	Z
I	-0.439023	-2.022909	-0.362748
O	-0.030309	-3.182537	-1.627210
O	0.484720	-0.526190	-0.753054
O	0.749991	-2.684820	1.004612
H	0.838166	-1.991143	1.688201
N	0.250629	2.348767	-1.104139
H	0.813620	1.734426	-0.510215
C	0.586245	2.084855	-2.516848
H	-0.034523	2.716242	-3.147143
H	1.639826	2.297222	-2.673843
H	0.382108	1.038759	-2.722016
C	0.479082	3.743127	-0.684592
H	-0.146068	4.397173	-1.287292
H	0.215795	3.831844	0.364524
H	1.529966	3.979301	-0.825536
C	3.858985	-0.293945	0.988109
H	2.861802	-0.461469	1.387164
H	4.382936	-1.228644	0.811633
H	4.427966	0.346400	1.657478
S	3.713979	0.563898	-0.541114
O	2.846393	1.691934	-0.324638
O	5.003331	0.788177	-1.092311
O	2.991680	-0.456810	-1.463122
H	2.026949	-0.553929	-1.217398
C	-0.799102	0.967495	4.135827
H	0.007301	1.536948	4.590758
H	-1.692223	1.579088	4.039011
H	-1.001012	0.064580	4.704519
S	-0.266734	0.505317	2.523771
O	-0.086195	1.692580	1.748847
O	0.847669	-0.394209	2.668458
O	-1.428650	-0.334713	1.977680
H	-2.211084	0.196269	1.454605
C	-4.812301	0.871154	-1.264898
H	-4.800223	0.901970	-2.350935
H	-5.351001	-0.002957	-0.910760
H	-5.242674	1.782477	-0.859668
S	-3.143021	0.753616	-0.716104
O	-3.237796	0.739627	0.762144
O	-2.607298	-0.492749	-1.233916
O	-2.460339	1.938326	-1.201714
H	-0.745121	2.104485	-0.962685

$(IA)_1(MSA)_3(DMA)_2$:

Atoms	X	Y	Z
I	-0.752924	0.016707	-1.004936
O	0.628388	-0.319461	-2.273488
O	-1.129393	1.688856	-1.540338
O	-2.046621	-0.931075	-1.812624
N	-0.931910	3.599522	0.350141
H	0.091855	3.777829	0.418798
C	-1.408261	3.054033	1.635469
H	-0.773297	2.213620	1.900574
H	-2.432635	2.708511	1.526270
H	-1.341682	3.824600	2.400025
C	-1.645432	4.804349	-0.099010
H	-2.697989	4.568668	-0.235947
H	-1.221194	5.133760	-1.043358
H	-1.537560	5.590106	0.645190
N	3.424126	-0.614839	1.356789
H	2.934361	-1.003639	0.529178
C	2.543513	-0.736287	2.536716
H	3.044243	-0.295813	3.395743
H	2.332446	-1.788361	2.705805
H	1.625840	-0.196806	2.324513
C	4.707636	-1.324639	1.495763
H	4.503365	-2.383980	1.629439
H	5.246783	-0.928336	2.352740
H	5.290278	-1.173149	0.591454
C	2.516531	2.350351	-1.641769
H	1.554116	2.514681	-2.120709
H	2.901119	1.374422	-1.924759
H	3.224500	3.133378	-1.898934
S	2.279158	2.374744	0.108474
O	3.566061	2.054251	0.711961
O	1.276725	1.342753	0.399690
O	1.799083	3.710178	0.439783
H	-1.019222	2.850608	-0.383229
C	1.206204	-4.204288	-1.412062
H	2.184632	-4.591166	-1.682716
H	0.712964	-3.758362	-2.272149
H	0.588696	-4.990419	-0.985982
S	1.416176	-2.953109	-0.184444
O	2.100707	-3.534187	0.942523
O	0.083925	-2.437577	0.107661
O	2.239126	-1.900364	-0.836123
H	1.298316	-0.897607	-1.826494

C	-3.000644	-2.358527	1.651315
H	-3.758599	-3.133967	1.587951
H	-2.708068	-2.194696	2.685376
H	-2.128998	-2.601037	1.044971
S	-3.707353	-0.855125	1.068620
O	-4.137388	-1.183223	-0.373277
O	-2.643109	0.128777	1.018743
O	-4.864087	-0.544529	1.831118
H	3.575544	0.394398	1.151404
H	-3.342655	-1.094764	-1.008035

$(IA)_2(MSA)_1(DMA)_1$:

Atoms	X	Y	Z
I	2.761771	0.368019	0.237782
O	4.324157	-0.421807	0.496584
O	1.833889	-0.691394	-0.881078
O	1.895409	-0.088276	1.878847
H	0.972199	-0.364256	1.647373
I	-0.739574	-1.447543	-0.651879
O	-2.522805	-1.658818	-0.658947
O	-0.519855	-0.923721	1.053180
O	-0.242794	-3.296341	-0.360885
H	-0.338229	-3.500459	0.576488
N	-3.478191	0.297249	0.996313
H	-3.154196	-0.475850	0.368795
C	-4.785580	0.783638	0.528755
H	-5.097860	1.627392	1.139498
H	-5.518506	-0.016596	0.598221
H	-4.684407	1.098078	-0.506139
C	-3.454585	-0.172491	2.392038
H	-3.710954	0.650528	3.054958
H	-2.450976	-0.528810	2.605692
H	-4.171215	-0.982030	2.510855
C	-0.947596	3.449415	-1.625338
H	-1.959193	3.456136	-2.021029
H	-0.225875	3.278116	-2.419078
H	-0.732594	4.379867	-1.106639
S	-0.805584	2.133619	-0.457054
O	0.565476	2.128144	0.001634
O	-1.167639	0.920301	-1.219728
O	-1.785818	2.399982	0.588279
H	-2.781537	1.066119	0.880972

$(IA)_2(MSA)_1(DMA)_2$:

Atoms	X	Y	Z
N	0.548707	-0.147391	2.484557
H	1.338937	-0.419477	1.869758
C	0.197042	-1.261115	3.382245
H	-0.639572	-0.957753	4.007190
H	1.059210	-1.504867	3.998763
H	-0.078038	-2.112627	2.766186
C	0.931233	1.092794	3.180259
H	0.065365	1.483019	3.709026
H	1.280434	1.805510	2.438164
H	1.738102	0.875470	3.875863
N	0.558663	2.378289	-1.251472
H	-0.356290	1.931532	-1.043385
C	0.995131	1.984479	-2.602309
H	1.933333	2.484032	-2.831294
H	0.230516	2.264337	-3.323073
H	1.156002	0.911329	-2.603184
C	0.422704	3.829765	-1.063113
H	1.390526	4.304309	-1.205696
H	0.063839	4.017145	-0.055162
H	-0.298354	4.218371	-1.778063
I	-2.906558	0.647551	0.211062
O	-2.118663	1.831714	-0.898689
O	-2.554349	-0.992833	-0.493503
O	-1.951194	0.726956	1.735761
H	1.262066	2.006082	-0.580349
I	-0.219839	-1.823693	-0.903737
O	0.178224	-0.150108	-0.408314
O	1.486343	-2.201934	-1.705345
O	-0.136834	-2.768991	0.599243
C	5.077523	0.721294	0.411171
H	5.406161	1.398346	-0.372524
H	5.603418	-0.226915	0.341735
H	5.223459	1.170049	1.389856
S	3.351520	0.405496	0.190653
O	2.695337	1.712378	0.313630
O	2.974748	-0.506955	1.261047
O	3.216278	-0.169769	-1.139828
H	2.151060	-1.527068	-1.421624
H	-0.267958	0.063492	1.886010

$(IA)_2(MSA)_1(DMA)_3$:

Atoms	X	Y	Z
N	-2.143149	2.470538	0.055856
H	-1.205410	2.638053	0.513216
C	-3.208167	2.543603	1.067110
H	-4.172809	2.409319	0.582777
H	-3.168983	3.512810	1.558929
H	-3.055986	1.744381	1.788197
C	-2.288571	3.426916	-1.056180
H	-3.188963	3.187118	-1.617348
H	-1.405628	3.343750	-1.686667
H	-2.355452	4.434098	-0.650824
N	0.044268	-0.946387	2.249003
H	0.378864	-0.557745	1.335744
C	0.490199	-2.336595	2.433466
H	0.088069	-2.719578	3.369891
H	1.575397	-2.360205	2.434686
H	0.122357	-2.922723	1.596004
C	0.470797	-0.019434	3.310293
H	0.026985	-0.321735	4.256595
H	0.143930	0.984425	3.045636
H	1.555441	-0.041841	3.370052
I	-2.925572	-1.431857	-0.067825
O	-1.383131	-2.284881	-0.454558
O	-2.669968	-0.819004	1.616464
O	-2.905094	0.060848	-1.080133
I	1.322278	1.928194	-0.085169
O	0.303389	0.422598	-0.017330
O	0.876521	2.554641	-1.706286
O	0.325344	2.953561	1.043552
N	0.718240	-1.422020	-2.077247
H	1.569373	-0.983118	-1.676939
C	0.144212	-0.534031	-3.104320
H	-0.800036	-0.952110	-3.445274
H	0.843556	-0.455295	-3.933486
H	-0.014729	0.445503	-2.662079
C	1.044541	-2.777440	-2.549001
H	0.129847	-3.271157	-2.867591
H	1.503754	-3.315424	-1.724918
H	1.744612	-2.708349	-3.378532
C	5.101623	-1.291447	0.244790
H	5.356359	-1.844761	1.144851
H	5.571148	-0.311624	0.254695
H	5.396659	-1.847282	-0.641078

S	3.344768	-1.073528	0.209820
O	3.073202	-0.315623	-1.024766
O	3.005293	-0.310802	1.402986
O	2.755202	-2.397852	0.171732
H	-2.142967	1.510344	-0.336403
H	-0.986457	-0.918108	2.139948
H	0.040002	-1.500400	-1.301994

$(IA)_2(MSA)_2(DMA)_1$:

Atoms	X	Y	Z
I	0.843747	-1.600292	-0.537454
O	2.159299	-1.360282	-1.879691
O	0.281397	0.071619	-0.353667
O	-0.268386	-2.167803	-1.960057
H	-1.212546	-2.143538	-1.651519
I	-2.277751	1.603808	-0.146995
O	-1.675641	1.555022	1.684090
O	-3.839027	2.419587	-0.006925
O	-1.130784	2.888072	-0.654459
H	0.474713	2.690815	-0.287816
N	1.511144	2.779700	-0.184622
H	1.860135	2.034701	0.433945
C	1.816880	4.077191	0.442392
H	1.456230	4.875104	-0.201630
H	2.891129	4.160530	0.585647
H	1.311492	4.127789	1.402336
C	2.126762	2.593006	-1.512540
H	1.804906	3.399292	-2.166848
H	1.794007	1.638644	-1.909349
H	3.208164	2.586006	-1.406751
C	-3.375837	-3.433562	1.173283
H	-3.200487	-3.549155	2.239124
H	-3.043219	-4.312225	0.628116
H	-4.425619	-3.232810	0.977234
S	-2.453115	-2.045846	0.605953
O	-2.673201	-1.930754	-0.830966
O	-1.037197	-2.365223	0.886586
O	-2.919618	-0.894973	1.354201
H	-1.943750	0.682478	2.019163
C	5.114981	-0.528203	1.698213
H	5.455327	-1.482312	1.306165
H	4.838065	-0.615099	2.745061
H	5.877382	0.234729	1.565479
S	3.691553	-0.029028	0.788629
O	3.272063	1.247290	1.327350
O	2.692031	-1.096336	1.011850
O	4.066395	0.021858	-0.620767
H	2.947903	-0.896397	-1.491989

$(IA)_2(MSA)_2(DMA)_2$:

Atoms	X	Y	Z
I	-0.773365	-0.667522	1.890054
O	-0.835212	-1.582277	3.404347
O	-0.926314	-1.889141	0.592273
O	1.113844	-0.334717	1.702172
H	1.537970	-1.102066	1.226764
I	-0.143623	2.762668	-0.660699
O	0.832237	2.919227	0.845824
O	-1.139039	1.273810	-0.305938
O	1.031872	2.186572	-1.880390
N	-0.106957	-1.994292	-1.950983
H	0.925194	-2.094808	-2.004809
C	-0.757373	-3.286307	-2.237404
H	-1.829706	-3.169917	-2.101896
H	-0.528021	-3.587128	-3.257165
H	-0.378821	-4.022918	-1.534687
C	-0.537603	-0.895825	-2.834657
H	-1.604283	-0.734752	-2.698542
H	0.014672	0.003240	-2.573199
H	-0.328925	-1.168120	-3.867074
N	3.232479	1.556519	0.667757
H	2.256246	1.895666	0.770618
C	3.833084	1.378539	2.001056
H	4.826068	0.951193	1.885316
H	3.895295	2.343924	2.497727
H	3.201824	0.705773	2.573752
C	3.961495	2.494929	-0.204989
H	4.961137	2.105686	-0.380555
H	3.419622	2.570532	-1.143942
H	4.010827	3.467722	0.278459
C	4.501735	-3.232416	-0.608887
H	4.026339	-4.204334	-0.706380
H	5.229227	-3.080929	-1.401728
H	4.969901	-3.132579	0.366342
S	3.254339	-1.990468	-0.754636
O	2.649542	-2.170869	-2.067619
O	2.306341	-2.241543	0.328376
O	3.941137	-0.711949	-0.607363
H	-2.508483	0.972437	-0.832796
C	-5.717546	-0.217000	-0.551449
H	-5.941919	0.708805	-0.030744
H	-5.985886	-0.153944	-1.602128
H	-6.219407	-1.057664	-0.079422

S	-3.990181	-0.530737	-0.433674
O	-3.430110	0.703227	-1.186963
O	-3.605192	-0.454237	0.947972
O	-3.695945	-1.720071	-1.167061
H	3.233261	0.635810	0.187547
H	-0.335026	-1.766446	-0.958764

$(IA)_3(MSA)_1(DMA)_1$:

Atoms	X	Y	Z
I	0.070600	2.011541	-1.137997
O	-0.492361	3.675426	-0.916514
O	0.595723	1.483091	0.496667
O	1.843504	2.328897	-1.811639
H	2.488649	2.010719	-1.149815
I	0.267876	-2.199968	-0.663756
O	0.468064	-0.801901	-1.745805
O	0.557663	-1.546661	0.993643
O	1.975831	-3.034185	-0.922321
H	2.696611	-2.383574	-0.786444
I	-3.246531	-0.448279	0.026224
O	-3.166219	-0.515651	1.822170
O	-2.122160	-1.778790	-0.502948
O	-2.371533	1.074426	-0.367792
H	-0.336080	0.914113	1.695409
N	-0.893623	0.853999	2.582728
H	-1.721281	0.262691	2.373972
C	-0.077686	0.240713	3.641100
H	0.850000	0.798328	3.743944
H	-0.627734	0.254355	4.579572
H	0.143745	-0.783152	3.353924
C	-1.350414	2.226101	2.868475
H	-0.483105	2.862496	3.023838
H	-1.904290	2.584098	2.004601
H	-1.985422	2.223677	3.751498
C	5.215201	-0.099532	1.626489
H	5.287047	-1.090931	2.063180
H	6.061310	0.099976	0.974046
H	5.139168	0.665733	2.393484
S	3.776858	-0.024057	0.621562
O	3.681702	1.302637	0.097718
O	3.811125	-1.101785	-0.329898
O	2.689982	-0.300839	1.678236
H	1.850751	-0.747192	1.309212

$(IA)_3(MSA)_1(DMA)_2$:

Atoms	X	Y	Z
I	2.003008	2.038126	-0.335798
O	3.074740	0.852855	0.637451
O	3.056171	3.464230	-0.420174
O	0.722168	2.484559	0.855630
H	-0.918858	2.444852	0.383330
I	2.728792	-1.307285	0.545713
O	1.943541	-0.938242	-1.057503
O	2.431711	-3.219329	0.330699
O	1.503254	-1.111842	1.829109
H	-0.224684	-1.222779	1.696293
I	-0.429251	-1.321140	-1.605300
O	-0.694633	0.202329	-0.696744
O	-2.178811	-1.510807	-2.339079
O	-0.428713	-2.611569	-0.364143
N	-1.896408	2.766986	0.213640
H	-2.563740	2.029186	0.523261
C	-2.114098	3.971779	1.031910
H	-1.405601	4.739446	0.731380
H	-3.134850	4.320257	0.895365
H	-1.947261	3.721044	2.075561
C	-2.093698	2.981634	-1.230910
H	-1.377715	3.721844	-1.582851
H	-1.946708	2.030574	-1.731944
H	-3.108184	3.332262	-1.403129
N	-1.158975	-1.088951	2.116007
H	-1.872702	-1.065613	1.370741
C	-1.466816	-2.250281	2.966093
H	-0.699370	-2.344192	3.730233
H	-2.444509	-2.109141	3.419117
H	-1.478607	-3.135246	2.336306
C	-1.148987	0.207026	2.818702
H	-0.559355	0.113946	3.727030
H	-0.674061	0.938426	2.168820
H	-2.173137	0.492531	3.046231
C	-5.947100	-0.326219	0.453885
H	-6.213316	-1.230145	-0.087111
H	-6.170913	-0.433713	1.511569
H	-6.461665	0.534896	0.036879
S	-4.208483	-0.075344	0.274824
O	-3.900004	1.139550	1.033446
O	-3.563152	-1.254444	0.830813
O	-3.959831	0.087785	-1.153338

H	-2.854251	-0.973036	-1.845030
H	1.490436	-3.344475	0.121245

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