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Rapid iodine oxoacid nucleation enhanced by dimethylamine in broad marine regions

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CCSD(T)/aug-cc-pVTZ (for H, C, N and O atoms) + aug-cc-pVTZ-PP with ECP28MDF (for I atom) [abbreviated as DLPNO-CCSD(T))] level of theory.

Table S3. The ratios of collision frequency between the clusters and monomer molecule at the concentration c to the total evaporation frequency of clusters in HIO_3-HIO_2-DMA system under field conditions of Zhejiang at $c(HIO_3) = 1.0 \times 10^7$ molecules cm^{-3}, $c(HIO_2) = 2.0 \times 10^5$ molecules cm^{-3}, c(DMA) = 4 pptv, T = 293 K, and CS = 1.0×10^{-2} s^{-1}. The clusters satisfying kinetically stable conditions ($\beta c/\Sigma\gamma > 1$, $n = 6$) in the simulated system and the corresponding $\beta c/\Sigma\gamma$ values are shown in red.

Table S4. The ratios of collision frequency between the clusters and monomer molecule at the concentration c to the total evaporation frequency of clusters in HIO_3-HIO_2-DMA system under field conditions of Mace Head at $c(HIO_3) = 1.0 \times 10^8$ molecules cm^{-3}, $c(HIO_2) = 2.0 \times 10^6$ molecules cm^{-3}, c(DMA) = 0.2 pptv, T = 287 K, and CS = 2.0×10^{-3} s^{-1}. The clusters satisfying kinetically stable conditions ($\beta c/\Sigma\gamma > 1$, $n = 6$) in the simulated system and the corresponding $\beta c/\Sigma\gamma$ values are shown in red.

Table S5. The ratios of collision frequency between the clusters and monomer molecule at the concentration c to the total evaporation frequency of clusters in HIO_3-HIO_2-DMA system under field conditions of Aboa at $c(HIO_3) = 1.0 \times 10^6$ molecules cm^{-3}, $c(HIO_2) = 2.0 \times 10^4$ molecules cm^{-3}, c(DMA) = 0.004 pptv, T = 268 K, and CS = 1.0×10^{-4} s^{-1}. The clusters satisfying kinetically stable conditions ($\beta c/\Sigma\gamma > 1$, $n = 6$) in the simulated system and the corresponding $\beta c/\Sigma\gamma$ values are shown in red.

Table S6. The ratios of collision frequency between the clusters and monomer molecule at the concentration c to the total evaporation frequency of clusters in HIO_3-HIO_2-DMA system under field conditions of Marambio at $c(HIO_3) = 1.0 \times 10^6$ molecules cm^{-3}, $c(HIO_2) = 2.0 \times 10^4$ molecules cm^{-3}, c(DMA) = 0.04 pptv, T = 273 K, and CS = 1.0×10^{-4} s^{-1}. The clusters satisfying kinetically stable conditions ($\beta c/\Sigma\gamma > 1$, $n = 6$) in the simulated system and the corresponding $\beta c/\Sigma\gamma$ values are shown in red.

Table S7. The cartesian coordinates of the most stable clusters in the $(HIO_3)_x \cdot (HIO_2)_y \cdot (DMA)_z$ ($1 \le x + y + z \le 5$; $x + y \ge z$) system at the ωB97X-D/6-311++G(3df,3pd) (for H, C, N, and O atoms) + aug-cc-pVTZ-PP with ECP28MDF (for I atom) level of theory.

Table S8. The total number of proton transfer (N) and the number of proton transfer between different precursors in ternary clusters (n_1, n_2, n_3 represent the number of proton transfer between HIO_3 and DMA, HIO_3 and HIO_2, and HIO_2 and DMA, respectively).

Section S7: References

Section S1: The detailed information on the parameters of ABCluster program.

The detailed information on the parameters of ABCluster program is given in Table S1. The number of initial isomer structures (120000) is obtained by multiplying the population size (SN = 300) by the maximal generations (g_{max} = 400).

Section S2: The details in the comparison of the single-point energy of clusters calculated by RI-CC2 and DLPNO-CCSD(T) methods.

The Gibbs free energies of formation (ΔG, kcal mol^{-1}) of HIO_3-HIO_2-DMA clusters calculated at RI-CC2/aug-cc-pVTZ (for H, C, N and O atoms) + aug-cc-pVTZ-PP with ECP28MDF (for I atom) and DLPNO-CCSD(T)/aug-cc-pVTZ (for H, C, N and O atoms) + aug-cc-pVTZ-PP with ECP28MDF (for I atom) level of theory are shown in Table S2. Based on the single-point energies obtained from two different methods, the ACDC simulations for cluster formation rates were conducted and compared with the CLOUD experiments results (He et al., 2021). As shown in Table S2 and Figure 1, without performing single-point energy correction, the cluster formation rates simulated at ωB97X-D/6-311++G(3df,3pd) level of theory (the diamond points) are significantly lower than the experimental results (the circular points). Therefore, we chose to perform the single-point correction to obtain simulated cluster formation rates that agree more with the experimental results. Compared to DLPNO-CCSD(T) results, the RI-CC2 results overestimate the ΔG of clusters to some extent, leading to higher cluster formation rates in ACDC simulations (Schmitz and Elm, 2020). The overestimation by the RI-CC2 method is more significant for larger clusters. However, it is worth noting that larger clusters typically possess stronger resistance to evaporation. For clusters that are stable enough (ΔG is low enough) to resist evaporation, further overestimation of the ΔG does not significantly enhance the cluster formation rates in ACDC simulations. Therefore, the difference in cluster formation rates simulated by the two methods is not substantial, especially under conditions of sufficient iodine oxoacid concentration. The comparison with CLOUD experiments indicates that, compared to the results of DLPNO-CCSD(T) method, the simulated cluster formation rates based on RI-CC2 method are more consistent with the experimental results at T = 263 K. Moreover, at T = 283 K, the RI-CC2 results exhibit a lower limit of cluster formation rates close to experimental results, and an upper limit of cluster formation rates overestimated by less than two orders of magnitude. The simulation results in Figure 1 demonstrate that ACDC simulations are highly sensitive to the quantum chemical methods and RI-CC2 method can effectively match the experimental results through a random cancellation of errors while saving computational resources. The random cancellation of errors is coming from the overestimation of binding energy obtained at RI-CC2 method compared with other methods (Schmitz and Elm, 2020) and the underestimation of cluster formation rates simulated by ACDC compared with the experimental results, possibly due to the lack of consideration of hydration, ionic effects, and inadequate sampling, etc. This is similar to the previous comparisons between field observation and theoretical simulation results (Lu et al., 2020), where the random cancellation of errors made the RI-CC2 results potentially more representative of field conditions. Considering that the RI-CC2 method can effectively match experimental results while saving computational resources, we finally chose the RI-CC2 method for single-point correction. It is important to note that this does not imply RI-CC2 results are inherently more accurate than those obtained using DLPNO-CCSD(T) method. We cautiously state that the choice of the RI-CC2 method in this study is due to its ability to effectively match the experimental results while saving computational resources.

Section S3: The boundary clusters in the simulated system and the influence of the size of the clusters.

The boundary clusters are the smallest clusters outside the simulated system. Once the boundary clusters are formed, they tend to keep growing rather than evaporating into fragmented clusters. The boundary clusters in this work were set to be the clusters formed by the combination of kinetically stable clusters ($\beta c/\Sigma\gamma > 1$) with five molecules (n = 6) and the corresponding monomers at the concentration c. In addition, for acid-base clusters such as HIO_3-DMA, "4×4" clusters were also set to be boundary clusters. The sizes of the kinetically stable clusters and boundary clusters are close to or have reached the size of critical nucleus (1.3 - 1.4 nm) Therefore, these settings of boundary clusters in the simulated system can, to some

extent, mitigate the issue of overestimating the system's formation rate due to the size of clusters being small, providing simulation results that align more closely with CLOUD experiment results (Figure S1). The clusters satisfying kinetically stable conditions ($\beta c/\Sigma\gamma > 1$, $n = 6$) in the simulated system and the corresponding $\beta c/\Sigma\gamma$ values can be seen from Tables S3-S6. The collision and total evaporation frequency of HIO_3-HIO_2/DMA clusters and pure-HIO_x ($x = 2, 3$) clusters presented in this work were adopted from the stable structures with the lowest Gibbs free energy of formation in previous studies (Rong et al., 2020; Zhang et al., 2022; Ning et al., 2022; Liu et al., 2023).

Limited by the computational resources, the maximum size of the HIO_3-HIO_2-DMA system is 6 molecules. On the one hand, the collision rates of six-molecule clusters exceed the evaporation rates, tending to grow to seven or eight-molecule clusters. On the other hand, the size of six-molecule clusters reaches 1.2-1.3 nm. The sizes of these clusters are close to or have reached the size of critical nucleus (Zhang, 2010). Moreover, as shown in Figure S1, the six-molecule system can, to some extent, mitigate the issue of overestimating the system's formation rate due to the size of clusters being small.

Section S4: The electrostatic potential (ESP) distribution on the molecular van der Waal (vdW) surfaces of monomer molecules.

In order to evaluate the interacting potential of HIO_3, HIO_2, and DMA, the electrostatic potential (ESP) distribution on the molecular van der Waal (vdW) surfaces of three monomer molecules was determined by the Visual Molecular Dynamics (VMD) (Humphrey, Dalke and Schulten, 1996) and the Multiwfn 3.7 program. In general, the sites with maximum ESP values, which possess electron-deficient properties, on the molecular surface tend to attract the electron-rich regions with minimum ESP values to form non-covalent interactions, such as hydrogen bonds (HBs) or halogen bonds (XBs). Figure S2 illustrates the presence of interaction regions on the surfaces of HIO_3, HIO_2, and DMA, characterized by positive or negative ESP values. DMA has a -NH group which can act as both donor and acceptor of non-covalent interactions, so that DMA can potentially form a spatial network structure with iodine oxoacids through HBs or XBs, providing possibility to form stable clusters.

Section S5: The proportion of nucleation pathways under a wide range of oceanic atmospheric conditions with different ratios of [HIO_3] and [HIO_2]

The ratio of [HIO_3] to [HIO_2] is about 20 to 100 depending on the concentration of iodine vapor (He et al., 2021). Three concentration ratios of [HIO_3] and [HIO_2] were adopted to evaluate the impact of the concentration of iodine vapor on the proportion of nucleation pathways. The results were shown in Figure S4 ([HIO_3] / [HIO_2] = 20), Figure 4 ([HIO_3] / [HIO_2] = 50), and Figure S5 ([HIO_3] / [HIO_2] = 100). Comparing the results under three conditions, when [DMA] is comparable to [HIO_2] (red dashed line in Figure S4, Figure 4, and Figure S5), the ternary nucleation pathways have significant contributions that cannot be ignored and the changes of [HIO_3] / [HIO_2] will not affect this result. In addition, when the [HIO_3] / [HIO_2] increases ([HIO_2] reducing without changing [HIO_3]), the contributions of HIO_3-HIO_2 binary pathways are also reduced correspondingly. Besides, except for ternary nucleation, the contributions of HIO_3-DMA are significantly higher than those of HIO_3-HIO_2 when [DMA] is equal to [HIO_2] as shown in Figure S4 marked by red dashed line. This indicates the important role of DMA in the nucleation of iodine oxoacids.

Section S6: Figures and Tables

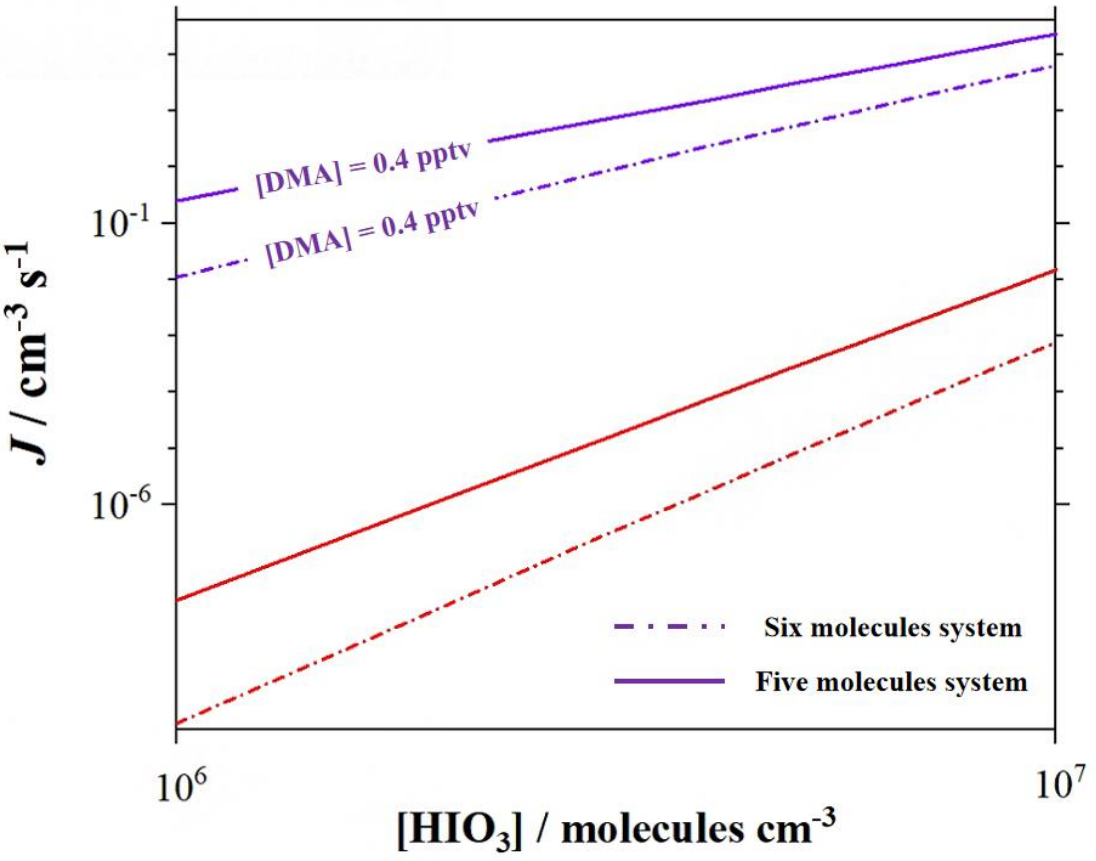

Figure S1. The simulated cluster formation rates (J, cm^{-3} s^{-1}) of HIO_3-HIO_2 (red) and HIO_3-HIO_2-DMA (purple) systems under the simulated conditions of [HIO_3] = 10^6 - 10^7, [HIO_2] = 2×10^4 - 2×10^5, [DMA] = 0.4 pptv, T = 293 K, and CS = 10^{-2} s^{-1}. The solid curves represent the simulated J for the five-molecule system, while the dashed curves represent the simulated J for the six-molecule system.

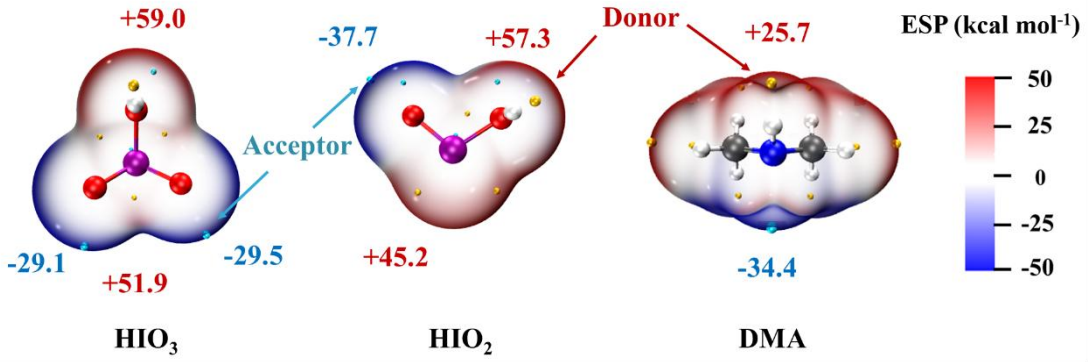

Figure S2. The ESP-mapped molecular van der Waals (vdW) surfaces of the HIO_3, HIO_2, and DMA monomer at the ωB97X-D/6-311++G(3df,3pd) (for H, C, N and O atoms) + aug-cc-pVTZ-PP with ECP28MDF (for I atom) level of theory. The yellow and cyan dots represent the maximum and minimum points of the ESP, respectively. The white, grey, blue, red, and purple spheres represent the H, C, N, O, and I atoms, respectively. The unit of ESP is kcal mol^{-1}.

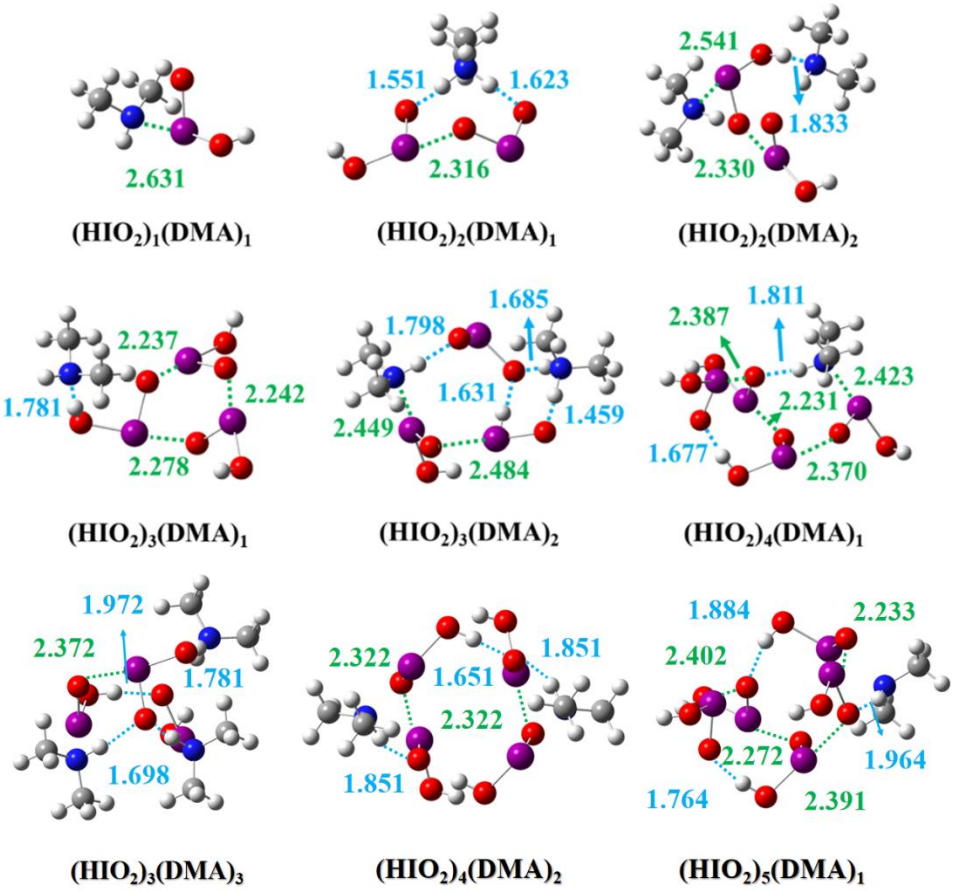

Figure S3. The most stable structures of HIO_2-DMA clusters identified at the ωB97X-D/6-311++G(3df,3pd) (for H, C, N, and O atoms) + aug-cc-pVTZ-PP with ECP28MDF (for I atom) level of theory. The white, grey, blue, red, and purple balls represent the H, C, N, O, and I atoms, respectively. The hydrogen bonds and halogen bonds are shown in blue and green dashed lines, respectively. The values of bond lengths are given in Å.

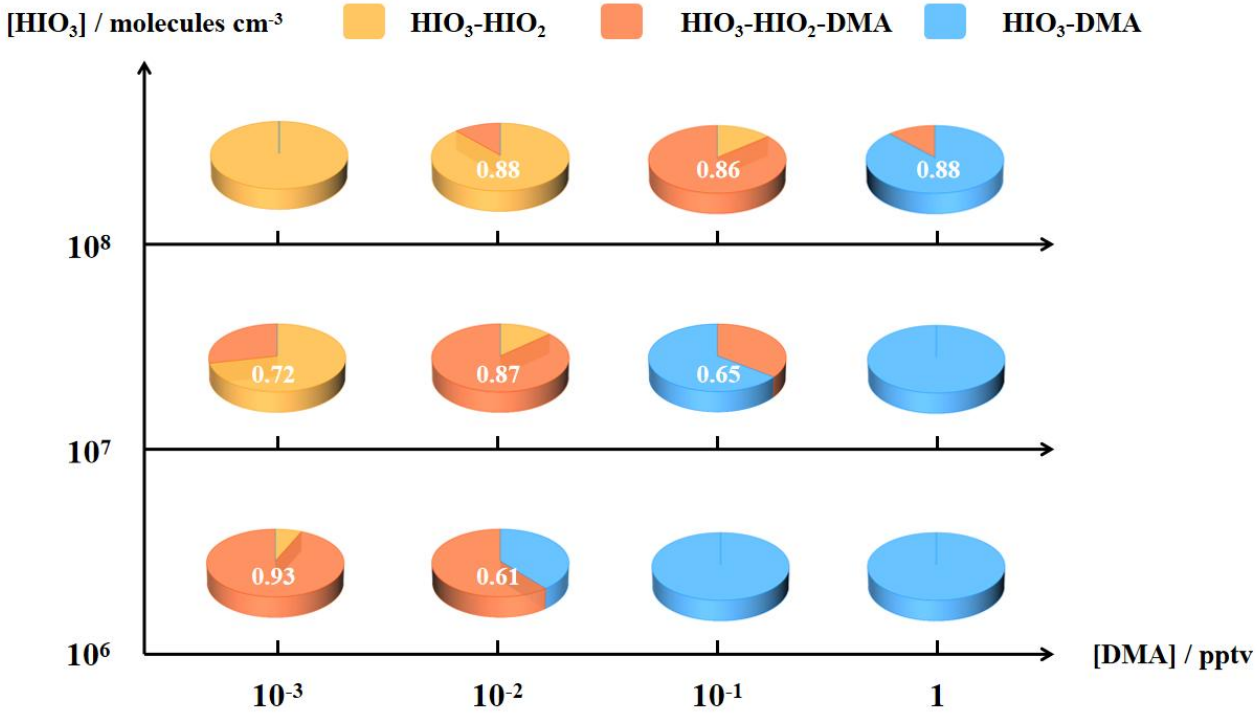

Figure S4. The contribution of main nucleation pathways at different concentrations of precursors. $[HIO_3] = 10^6 - 10^8$

molecules cm^{-3}, $[HIO_2]$ = 5.0 × 10^4 − 5.0 × 10^6 molecules cm^{-3} and [DMA] = 10^4 − 10^8 molecules cm^{-3}. The simulated temperature and condensation sink are 283K and 2.0 × 10^{-3} s^{-1} as typical values for oceanic atmosphere. The contribution of HIO_3-HIO_2, HIO_3-HIO_2-DMA, and HIO_3-DMA are shown in red, green, and blue, respectively. The red dashed line indicates the pie chart with significant contribution of ternary nucleation to the nucleation pathways.

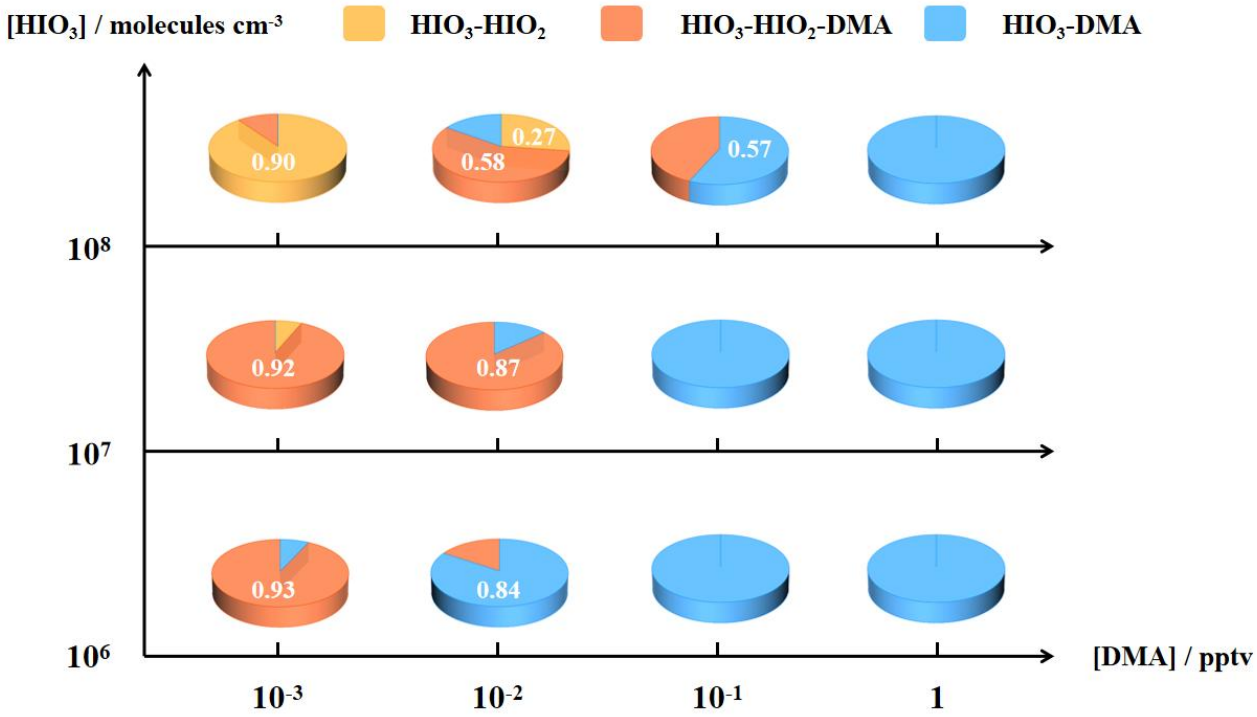

Figure S5. The contribution of main nucleation pathways at different concentrations of precursors. $[HIO_3]$ = 10^6 − 10^8 molecules cm^{-3}, $[HIO_2]$ = 10^4 − 10^6 molecules cm^{-3}, and [DMA] = 10^4 − 10^8 molecules cm^{-3}. The simulated temperature and condensation sink are 283K and 2.0 × 10^{-3} s^{-1} as typical values for oceanic atmosphere. The contribution of HIO_3-HIO_2, HIO_3-HIO_2-DMA, and HIO_3-DMA are shown in red, green, and blue, respectively. The red dashed line indicates the pie chart with significant contribution of ternary nucleation to the nucleation pathways.

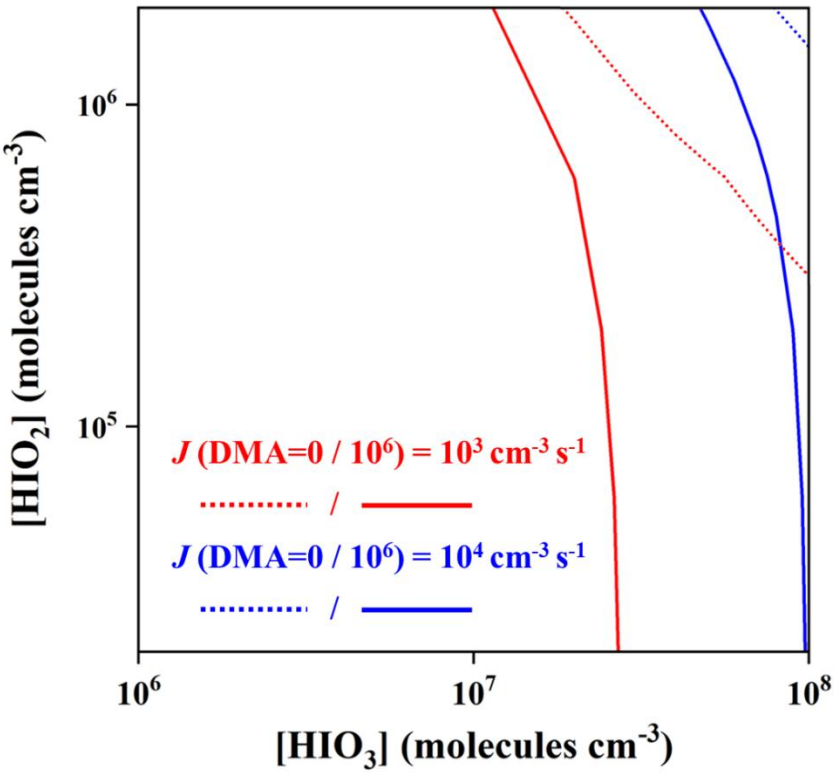

Figure S6. The isolines of formation rate (J, cm^{-3} s^{-1}) and the corresponding concentrations of precursors (molecules cm^{-3}) at T = 287 K and CS = 2.0×10^{-3} s^{-1}. The solid and dashed line indicates the formation rate with [DMA] = 10^6 molecules cm^{-3} and without DMA, respectively. The isoline of J = 10^3 and 10^4 cm^{-3} s^{-1} are shown in red and blue, respectively.

Table S1. The detailed parameters and corresponding information of ABCluster program. The number of initial isomer structures (120000) is obtained by multiplying the population size (SN = 300) by the maximal generations (g_{max} = 400).

Information	Parameters
Population size (SN)	300
Maximal cycle number (g_{max})	400
Scout limit (g_{limit})	3
Estimated cluster size (Å)	3 - 12
Number of local minima (LMs) to be saved	1000

Table S2. The Gibbs free energies of formation (ΔG, kcal mol^{-1}) of HIO_3-HIO_2-DMA clusters calculated at RI-CC2/aug-cc-pVTZ (for H, C, N and O atoms) + aug-cc-pVTZ-PP with ECP28MDF (for I atom) (abbreviated as RI-CC2) and DLPNO-CCSD(T)/aug-cc-pVTZ (for H, C, N and O atoms) + aug-cc-pVTZ-PP with ECP28MDF (for I atom) [abbreviated as DLPNO-CCSD(T))] level of theory.

Clusters	T = 283 K		T = 263 K	
	RI-CC2	DLPNO-CCSD(T)	RI-CC2	DLPNO-CCSD(T)
$(HIO_3)_2$	-7.89	-11.46	-8.63	-12.20

$(HIO_3)_3$	-18.08	-22.60	-19.65	-24.17
$(HIO_3)_4$	-37.87	-39.71	-40.31	-42.15
$(HIO_3)_5$	-55.47	-54.44	-58.76	-57.72
$(HIO_3)_6$	-73.34	-68.38	-77.65	-72.69
$(HIO_2)_2$	-17.43	-18.65	-18.26	-19.48
$(HIO_2)_3$	-38.65	-35.45	-40.35	-37.14
$(HIO_2)_4$	-58.08	-51.31	-60.62	-53.85
$(HIO_2)_5$	-75.10	-64.43	-78.47	-67.80
$(HIO_2)_6$	-98.38	-80.08	-102.71	-84.40
$(HIO_3)_1(DMA)_1$	-15.89	-10.47	-16.64	-11.22
$(HIO_3)_2(DMA)_1$	-34.65	-29.32	-36.17	-30.84
$(HIO_3)_2(DMA)_2$	-55.10	-40.94	-57.28	-43.13
$(HIO_3)_3(DMA)_1$	-47.24	-41.72	-49.52	-44.00
$(HIO_3)_3(DMA)_2$	-75.05	-59.02	-78.24	-62.21
$(HIO_3)_4(DMA)_1$	-66.00	-55.21	-69.13	-58.34
$(HIO_3)_3(DMA)_3$	-81.73	-60.57	-85.59	-64.43
$(HIO_3)_4(DMA)_2$	-92.94	-73.51	-96.97	-77.53
$(HIO_3)_5(DMA)_1$	-86.48	-71.29	-90.64	-75.45
$(HIO_2)_1(DMA)_1$	-9.21	-6.83	-9.89	-7.51
$(HIO_2)_2(DMA)_1$	-30.70	-22.43	-32.25	-23.97
$(HIO_2)_2(DMA)_2$	-36.47	-24.46	-38.83	-26.82
$(HIO_2)_3(DMA)_1$	-45.01	-37.26	-47.44	-39.69
$(HIO_2)_3(DMA)_2$	-59.35	-40.18	-62.60	-43.43
$(HIO_2)_4(DMA)_1$	-70.24	-56.24	-73.50	-59.51
$(HIO_2)_3(DMA)_3$	-68.19	-46.17	-72.19	-50.16
$(HIO_2)_4(DMA)_2$	-80.33	-61.54	-84.49	-65.70
$(HIO_2)_5(DMA)_1$	-91.32	-71.19	-95.54	-75.41
$(HIO_3)_1(HIO_2)_1$	-17.79	-17.50	-18.61	-18.32
$(HIO_3)_1(HIO_2)_2$	-39.36	-35.74	-41.04	-37.42
$(HIO_3)_2(HIO_2)_1$	-30.05	-32.74	-31.73	-34.42
$(HIO_3)_3(HIO_2)_1$	-51.07	-44.07	-53.54	-46.55
$(HIO_3)_1(HIO_2)_3$	-54.59	-50.72	-57.11	-53.24
$(HIO_3)_2(HIO_2)_2$	-54.58	-50.23	-57.04	-52.69
$(HIO_3)_3(HIO_2)_2$	-71.99	-67.84	-75.36	-71.22
$(HIO_3)_2(HIO_2)_3$	-77.70	-68.93	-81.08	-72.30
$(HIO_3)_4(HIO_2)_1$	-63.67	-60.95	-66.99	-64.27
$(HIO_3)_1(HIO_2)_4$	-79.91	-66.89	-83.38	-70.35
$(HIO_3)_5(HIO_2)_1$	-79.74	-75.66	-83.83	-79.75
$(HIO_3)_4(HIO_2)_2$	-90.25	-82.64	-94.52	-86.92
$(HIO_3)_3(HIO_2)_3$	-102.77	-90.97	-107.11	-95.31
$(HIO_3)_2(HIO_2)_4$	-100.94	-86.59	-105.22	-90.88
$(HIO_3)_1(HIO_2)_5$	-83.27	-68.28	-87.58	-72.59
$(HIO_3)_1(HIO_2)_1(DMA)_1$	-35.19	-27.95	-36.73	-29.49
$(HIO_3)_1(HIO_2)_1(DMA)_2$	-49.64	-36.00	-51.96	-38.32
$(HIO_3)_2(HIO_2)_1(DMA)_1$	-56.00	-40.76	-58.44	-43.20

$(HIO_3)_2(HIO_2)_1(DMA)_2$	-71.04	-52.63	-74.25	-55.84
$(HIO_3)_1(HIO_2)_2(DMA)_1$	-50.07	-45.57	-52.47	-47.97
$(HIO_3)_1(HIO_2)_2(DMA)_2$	-65.75	-47.40	-68.93	-50.57
$(HIO_3)_3(HIO_2)_1(DMA)_1$	-72.91	-58.76	-76.10	-61.94
$(HIO_3)_1(HIO_2)_3(DMA)_1$	-72.10	-56.91	-75.30	-60.11
$(HIO_3)_2(HIO_2)_2(DMA)_1$	-77.50	-61.93	-80.76	-65.19
$(HIO_3)_3(HIO_2)_1(DMA)_2$	-93.15	-82.93	-96.31	-86.19
$(HIO_3)_1(HIO_2)_3(DMA)_2$	-76.50	-59.80	-80.53	-63.83
$(HIO_3)_2(HIO_2)_2(DMA)_2$	-89.60	-66.80	-93.61	-70.81
$(HIO_3)_1(HIO_2)_2(DMA)_3$	-74.36	-51.52	-78.37	-55.54
$(HIO_3)_2(HIO_2)_1(DMA)_3$	-77.64	-54.47	-81.57	-58.39
$(HIO_3)_4(HIO_2)_1(DMA)_1$	-93.42	-76.74	-97.41	-80.73
$(HIO_3)_1(HIO_2)_4(DMA)_1$	-95.98	-75.22	-100.18	-79.42
$(HIO_3)_3(HIO_2)_2(DMA)_1$	-106.01	-88.24	-110.06	-92.29
$(HIO_3)_2(HIO_2)_3(DMA)_1$	-88.71	-68.26	-92.82	-72.37

Table S3. The ratios of collision frequency between the clusters and monomer molecule at the concentration c to the total evaporation frequency of clusters in HIO_3-HIO_2-DMA system under field conditions of Zhejiang at $c(HIO_3)$ = 1.0 × 10^7 molecules cm^{-3}, $c(HIO_2)$ = 2.0 × 10^5 molecules cm^{-3}, c(DMA) = 4 pptv, T = 293 K, and CS = 1.0 × 10^{-2} s^{-1}. The clusters satisfying kinetically stable conditions ($\beta c/\Sigma\gamma > 1$, n = 6) in the simulated system and the corresponding $\beta c/\Sigma\gamma$ values are shown in red.

Clusters	β	$\Sigma\gamma$	βc(DMA)/$\Sigma\gamma$	$\beta c(HIO_2)/\Sigma\gamma$	$\beta c(HIO_3)/\Sigma\gamma$
$(HIO_3)_2$	4.58×10^{-10}	7.88×10^{3}	5.81×10^{-6}	1.16×10^{-8}	5.81×10^{-7}
$(HIO_3)_3$	5.21×10^{-10}	3.55×10^{2}	1.47×10^{-4}	2.94×10^{-7}	1.47×10^{-5}
$(HIO_3)_4$	5.74×10^{-10}	2.70×10^{-5}	2.12×10^{3}	4.25×10^{0}	2.12×10^{2}
$(HIO_3)_5$	6.21×10^{-10}	1.27×10^{-3}	4.89×10^{1}	9.78×10^{-2}	4.89×10^{0}
$(HIO_3)_6$	3.61×10^{-10}	9.78×10^{-4}	3.70×10^{1}	7.39×10^{-2}	3.70×10^{0}
$(HIO_2)_2$	4.41×10^{-10}	6.35×10^{-4}	6.94×10^{1}	1.39×10^{-1}	6.94×10^{0}
$(HIO_2)_3$	4.99×10^{-10}	2.10×10^{-6}	2.38×10^{4}	4.76×10^{1}	2.38×10^{3}
$(HIO_2)_4$	5.51×10^{-10}	4.87×10^{-5}	1.13×10^{3}	2.26×10^{0}	1.13×10^{2}
$(HIO_2)_5$	5.97×10^{-10}	3.24×10^{-3}	1.84×10^{1}	3.69×10^{-2}	1.84×10^{0}
$(HIO_2)_6$	3.53×10^{-10}	8.41×10^{-8}	4.20×10^{5}	8.40×10^{2}	4.20×10^{4}
$(HIO_3)_1(DMA)_1$	2.95×10^{-10}	2.62×10^{-2}	1.13×10^{0}	2.25×10^{-3}	1.13×10^{-1}
$(HIO_3)_2(DMA)_1$	5.26×10^{-10}	1.50×10^{-4}	3.50×10^{2}	7.01×10^{-1}	3.50×10^{1}
$(HIO_3)_2(DMA)_2$	3.40×10^{-10}	1.32×10^{-5}	2.58×10^{3}	5.16×10^{0}	2.58×10^{2}
$(HIO_3)_3(DMA)_1$	5.76×10^{-10}	6.00×10^{0}	9.61×10^{-3}	1.92×10^{-5}	9.61×10^{-4}
$(HIO_3)_3(DMA)_2$	6.29×10^{-10}	2.68×10^{-5}	2.35×10^{3}	4.71×10^{0}	2.35×10^{2}

$(HIO_3)_4(DMA)_1$	6.26×10^{-10}	1.77×10^{-4}	3.54×10^{2}	7.07×10^{-1}	3.54×10^{1}
$(HIO_3)_3(DMA)_3$	3.83×10^{-10}	2.91×10^{5}	1.32×10^{-7}	2.63×10^{-10}	1.32×10^{-8}
$(HIO_3)_4(DMA)_2$	3.78×10^{-10}	8.25×10^{-4}	4.57×10^{1}	9.15×10^{-2}	4.57×10^{0}
$(HIO_3)_5(DMA)_1$	3.68×10^{-10}	1.15×10^{-5}	3.21×10^{3}	6.42×10^{0}	3.21×10^{2}
$(HIO_2)_1(DMA)_1$	2.97×10^{-10}	2.32×10^{3}	1.28×10^{-5}	2.57×10^{-8}	1.28×10^{-6}
$(HIO_2)_2(DMA)_1$	5.17×10^{-10}	2.62×10^{0}	1.97×10^{-2}	3.95×10^{-5}	1.97×10^{-3}
$(HIO_2)_2(DMA)_2$	3.36×10^{-10}	1.28×10^{6}	2.61×10^{-8}	5.23×10^{-11}	2.61×10^{-9}
$(HIO_2)_3(DMA)_1$	5.62×10^{-10}	4.21×10^{5}	1.34×10^{-7}	2.67×10^{-10}	1.34×10^{-8}
$(HIO_2)_3(DMA)_2$	3.50×10^{-10}	5.90×10^{-1}	5.94×10^{-2}	1.19×10^{-4}	5.94×10^{-3}
$(HIO_2)_4(DMA)_1$	6.07×10^{-10}	2.24×10^{1}	2.71×10^{-3}	5.42×10^{-6}	2.71×10^{-4}
$(HIO_2)_3(DMA)_3$	3.43×10^{-10}	7.36×10^{3}	4.65×10^{-6}	9.31×10^{-9}	4.65×10^{-7}
$(HIO_2)_4(DMA)_2$	2.94×10^{-10}	3.36×10^{2}	8.75×10^{-5}	1.75×10^{-7}	8.75×10^{-6}
$(HIO_2)_5(DMA)_1$	2.98×10^{-10}	5.36×10^{3}	5.55×10^{-6}	1.11×10^{-8}	5.55×10^{-7}
$(HIO_3)_1(HIO_2)_1$	4.48×10^{-10}	6.83×10^{-4}	6.57×10^{1}	1.31×10^{-1}	6.57×10^{0}
$(HIO_3)_1(HIO_2)_2$	5.05×10^{-10}	1.79×10^{-6}	2.83×10^{4}	5.66×10^{1}	2.83×10^{3}
$(HIO_3)_2(HIO_2)_1$	5.11×10^{-10}	1.03×10^{1}	4.98×10^{-3}	9.96×10^{-6}	4.98×10^{-4}
$(HIO_3)_3(HIO_2)_1$	5.68×10^{-10}	3.11×10^{-6}	1.83×10^{4}	3.65×10^{1}	1.83×10^{3}
$(HIO_3)_1(HIO_2)_3$	5.56×10^{-10}	8.59×10^{-2}	6.47×10^{-1}	1.29×10^{-3}	6.47×10^{-2}
$(HIO_3)_2(HIO_2)_2$	5.60×10^{-10}	6.43×10^{-2}	8.71×10^{-1}	1.74×10^{-3}	8.71×10^{-2}
$(HIO_3)_3(HIO_2)_2$	6.10×10^{-10}	1.87×10^{-3}	3.27×10^{1}	6.53×10^{-2}	3.27×10^{0}
$(HIO_3)_2(HIO_2)_3$	6.07×10^{-10}	1.99×10^{-7}	3.05×10^{5}	6.11×10^{2}	3.05×10^{4}
$(HIO_3)_4(HIO_2)_1$	6.16×10^{-10}	6.65×10^{0}	9.27×10^{-3}	1.85×10^{-5}	9.27×10^{-4}
$(HIO_3)_1(HIO_2)_4$	6.04×10^{-10}	9.11×10^{-7}	6.63×10^{4}	1.33×10^{2}	6.63×10^{3}
$(HIO_3)_5(HIO_2)_1$	3.67×10^{-10}	1.71×10^{-2}	2.15×10^{0}	4.30×10^{-3}	2.15×10^{-1}
$(HIO_3)_4(HIO_2)_2$	3.62×10^{-10}	4.39×10^{-4}	8.25×10^{1}	1.65×10^{-1}	8.25×10^{0}
$(HIO_3)_3(HIO_2)_3$	3.60×10^{-10}	3.91×10^{-9}	9.20×10^{6}	1.84×10^{4}	9.20×10^{5}
$(HIO_3)_2(HIO_2)_4$	3.59×10^{-10}	3.61×10^{-6}	9.95×10^{3}	1.99×10^{1}	9.95×10^{2}
$(HIO_3)_1(HIO_2)_5$	3.10×10^{-10}	8.70×10^{-8}	3.57×10^{5}	7.13×10^{2}	3.57×10^{4}
$(HIO_3)_1(HIO_2)_1(DMA)_1$	5.24×10^{-10}	2.34×10^{-3}	2.24×10^{1}	4.49×10^{-2}	2.24×10^{0}
$(HIO_3)_1(HIO_2)_1(DMA)_2$	3.39×10^{-10}	4.33×10^{-1}	7.83×10^{-2}	1.57×10^{-4}	7.83×10^{-3}
$(HIO_3)_2(HIO_2)_1(DMA)_1$	5.77×10^{-10}	7.20×10^{-6}	8.02×10^{3}	1.60×10^{1}	8.02×10^{2}
$(HIO_3)_2(HIO_2)_1(DMA)_2$	3.57×10^{-10}	1.96×10^{-1}	1.82×10^{-1}	3.65×10^{-4}	1.82×10^{-2}

$(HIO_3)_1(HIO_2)_2(DMA)_1$	5.66×10^{-10}	2.45×10^{2}	2.31×10^{-4}	4.63×10^{-7}	2.31×10^{-5}
$(HIO_3)_1(HIO_2)_2(DMA)_2$	6.20×10^{-10}	7.37×10^{-2}	8.41×10^{-1}	1.68×10^{-3}	8.41×10^{-2}
$(HIO_3)_3(HIO_2)_1(DMA)_1$	6.21×10^{-10}	3.75×10^{-3}	1.66×10^{1}	3.31×10^{-2}	1.66×10^{0}
$(HIO_3)_1(HIO_2)_3(DMA)_1$	6.15×10^{-10}	2.20×10^{-3}	2.79×10^{1}	5.58×10^{-2}	2.79×10^{0}
$(HIO_3)_2(HIO_2)_2(DMA)_1$	6.16×10^{-10}	1.76×10^{-6}	3.50×10^{4}	7.00×10^{1}	3.50×10^{3}
$(HIO_3)_3(HIO_2)_1(DMA)_2$	3.77×10^{-10}	9.01×10^{-4}	4.18×10^{1}	8.37×10^{-2}	4.18×10^{0}
$(HIO_3)_1(HIO_2)_3(DMA)_2$	3.71×10^{-10}	1.66×10^{7}	2.24×10^{-9}	4.48×10^{-12}	2.24×10^{-10}
$(HIO_3)_2(HIO_2)_2(DMA)_2$	3.75×10^{-10}	2.82×10^{1}	1.33×10^{-3}	2.65×10^{-6}	1.33×10^{-4}
$(HIO_3)_1(HIO_2)_2(DMA)_3$	3.80×10^{-10}	1.22×10^{4}	3.13×10^{-6}	6.25×10^{-9}	3.13×10^{-7}
$(HIO_3)_2(HIO_2)_1(DMA)_3$	3.83×10^{-10}	3.44×10^{5}	1.11×10^{-7}	2.23×10^{-10}	1.11×10^{-8}
$(HIO_3)_4(HIO_2)_1(DMA)_1$	3.71×10^{-10}	8.81×10^{-6}	4.21×10^{3}	8.42×10^{0}	4.21×10^{2}
$(HIO_3)_1(HIO_2)_4(DMA)_1$	3.63×10^{-10}	2.97×10^{-2}	1.22×10^{0}	2.45×10^{-3}	1.22×10^{-1}
$(HIO_3)_3(HIO_2)_2(DMA)_1$	3.71×10^{-10}	9.51×10^{-12}	3.90×10^{9}	7.81×10^{6}	3.90×10^{8}
$(HIO_3)_2(HIO_2)_3(DMA)_1$	3.68×10^{-10}	2.58×10^{2}	1.43×10^{-4}	2.85×10^{-7}	1.43×10^{-5}

Table S4. The ratios of collision frequency between the clusters and monomer molecule at the concentration c to the total evaporation frequency of clusters in HIO_3-HIO_2-DMA system under field conditions of Mace Head at $c(HIO_3)$ = 1.0 × 10^8 molecules cm^{-3}, $c(HIO_2)$ = 2.0 × 10^6 molecules cm^{-3}, c(DMA) = 0.2 pptv, T = 287 K, and CS = 2.0 × 10^{-3} s^{-1}. The clusters satisfying kinetically stable conditions ($\beta c/\Sigma\gamma > 1$, $n = 6$) in the simulated system and the corresponding $\beta c/\Sigma\gamma$ values are shown in red.

Clusters	β	$\Sigma\gamma$	βc(DMA)/$\Sigma\gamma$	βc(HIO_2)/$\Sigma\gamma$	βc(HIO_3)/$\Sigma\gamma$
$(HIO_3)_2$	4.53×10^{-10}	4.14×10^{3}	5.48×10^{-6}	2.19×10^{-7}	1.10×10^{-5}
$(HIO_3)_3$	5.16×10^{-10}	1.63×10^{2}	1.58×10^{-4}	6.33×10^{-6}	3.16×10^{-4}
$(HIO_3)_4$	5.68×10^{-10}	8.80×10^{-6}	3.23×10^{3}	1.29×10^{2}	6.46×10^{3}
$(HIO_3)_5$	6.15×10^{-10}	4.40×10^{-4}	6.99×10^{1}	2.80×10^{0}	1.40×10^{2}
$(HIO_3)_6$	3.61×10^{-10}	9.78×10^{-4}	3.70×10^{0}	7.39×10^{-1}	3.70×10^{1}
$(HIO_2)_2$	4.36×10^{-10}	2.29×10^{-4}	9.53×10^{1}	3.81×10^{0}	1.91×10^{2}
$(HIO_2)_3$	4.94×10^{-10}	6.27×10^{-7}	3.94×10^{4}	1.58×10^{3}	7.88×10^{4}
$(HIO_2)_4$	5.45×10^{-10}	1.63×10^{-5}	1.67×10^{3}	6.68×10^{1}	3.34×10^{3}
$(HIO_2)_5$	5.91×10^{-10}	1.14×10^{-3}	2.58×10^{1}	1.03×10^{0}	5.17×10^{1}
$(HIO_2)_6$	3.53×10^{-10}	8.41×10^{-8}	4.20×10^{4}	8.40×10^{3}	4.20×10^{5}
$(HIO_3)_1(DMA)_1$	2.92×10^{-10}	1.02×10^{-2}	1.44×10^{0}	5.76×10^{-2}	2.88×10^{0}
$(HIO_3)_2(DMA)_1$	5.21×10^{-10}	5.25×10^{-5}	4.96×10^{2}	1.98×10^{1}	9.92×10^{2}

$(HIO_3)_2(DMA)_2$	3.36×10^{-10}	4.64×10^{-6}	3.62×10^{3}	1.45×10^{2}	7.25×10^{3}
$(HIO_3)_3(DMA)_1$	5.70×10^{-10}	2.66×10^{0}	1.07×10^{-2}	4.29×10^{-4}	2.14×10^{-2}
$(HIO_3)_3(DMA)_2$	6.23×10^{-10}	7.95×10^{-6}	3.92×10^{3}	1.57×10^{2}	7.83×10^{3}
$(HIO_3)_4(DMA)_1$	6.19×10^{-10}	5.98×10^{-5}	5.18×10^{2}	2.07×10^{1}	1.04×10^{3}
$(HIO_3)_3(DMA)_3$	3.43×10^{-10}	7.36×10^{3}	4.65×10^{-7}	9.31×10^{-8}	4.65×10^{-6}
$(HIO_3)_4(DMA)_2$	3.83×10^{-10}	2.91×10^{5}	1.32×10^{-8}	2.63×10^{-9}	1.32×10^{-7}
$(HIO_3)_5(DMA)_1$	3.78×10^{-10}	8.25×10^{-4}	4.57×10^{0}	9.15×10^{-1}	4.57×10^{1}
$(HIO_2)_1(DMA)_1$	3.68×10^{-10}	1.15×10^{-5}	2.39×10^{-6}	1.44×10^{-7}	7.18×10^{-6}
$(HIO_2)_2(DMA)_1$	5.12×10^{-10}	1.13×10^{0}	2.26×10^{-2}	9.04×10^{-4}	4.52×10^{-2}
$(HIO_2)_2(DMA)_2$	3.32×10^{-10}	6.91×10^{5}	2.41×10^{-8}	9.62×10^{-10}	4.81×10^{-8}
$(HIO_2)_3(DMA)_1$	5.56×10^{-10}	2.37×10^{5}	1.17×10^{-7}	4.69×10^{-9}	2.34×10^{-7}
$(HIO_2)_3(DMA)_2$	3.46×10^{-10}	2.29×10^{-1}	7.55×10^{-2}	3.02×10^{-3}	1.51×10^{-1}
$(HIO_2)_4(DMA)_1$	6.00×10^{-10}	9.91×10^{0}	3.03×10^{-3}	1.21×10^{-4}	6.06×10^{-3}
$(HIO_2)_3(DMA)_3$	2.98×10^{-10}	5.36×10^{3}	5.55×10^{-7}	1.11×10^{-7}	5.55×10^{-6}
$(HIO_2)_4(DMA)_2$	2.94×10^{-10}	1.20×10^{3}	1.23×10^{-5}	4.91×10^{-7}	2.45×10^{-5}
$(HIO_2)_5(DMA)_1$	5.12×10^{-10}	1.13×10^{0}	2.26×10^{-2}	9.04×10^{-4}	4.52×10^{-2}
$(HIO_3)_1(HIO_2)_1$	4.44×10^{-10}	2.43×10^{-4}	9.14×10^{1}	3.66×10^{0}	1.83×10^{2}
$(HIO_3)_1(HIO_2)_2$	5.00×10^{-10}	5.33×10^{-7}	4.68×10^{4}	1.87×10^{3}	9.37×10^{4}
$(HIO_3)_2(HIO_2)_1$	5.05×10^{-10}	4.30×10^{0}	5.88×10^{-3}	2.35×10^{-4}	1.18×10^{-2}
$(HIO_3)_3(HIO_2)_1$	5.62×10^{-10}	9.84×10^{-7}	2.86×10^{4}	1.14×10^{3}	5.71×10^{4}
$(HIO_3)_1(HIO_2)_3$	5.50×10^{-10}	3.29×10^{-2}	8.37×10^{-1}	3.35×10^{-2}	1.67×10^{0}
$(HIO_3)_2(HIO_2)_2$	5.54×10^{-10}	2.55×10^{-2}	1.09×10^{0}	4.35×10^{-2}	2.17×10^{0}
$(HIO_3)_3(HIO_2)_2$	6.04×10^{-10}	6.29×10^{-4}	4.80×10^{1}	1.92×10^{0}	9.60×10^{1}
$(HIO_3)_2(HIO_2)_3$	6.01×10^{-10}	5.55×10^{-8}	5.41×10^{5}	2.17×10^{4}	1.08×10^{6}
$(HIO_3)_4(HIO_2)_1$	6.10×10^{-10}	2.80×10^{0}	1.09×10^{-2}	4.36×10^{-4}	2.18×10^{-2}
$(HIO_3)_1(HIO_2)_4$	5.97×10^{-10}	2.57×10^{-7}	1.16×10^{5}	4.65×10^{3}	2.32×10^{5}
$(HIO_3)_5(HIO_2)_1$	3.67×10^{-10}	1.71×10^{-2}	2.15×10^{-1}	4.30×10^{-2}	2.15×10^{0}
$(HIO_3)_4(HIO_2)_2$	3.62×10^{-10}	4.39×10^{-4}	8.25×10^{0}	1.65×10^{0}	8.25×10^{1}
$(HIO_3)_3(HIO_2)_3$	3.60×10^{-10}	3.91×10^{-9}	9.20×10^{5}	1.84×10^{5}	9.20×10^{6}
$(HIO_3)_2(HIO_2)_4$	3.59×10^{-10}	3.61×10^{-6}	9.95×10^{2}	1.99×10^{2}	9.95×10^{3}
$(HIO_3)_1(HIO_2)_5$	3.10×10^{-10}	8.70×10^{-8}	3.57×10^{4}	7.13×10^{3}	3.57×10^{5}
$(HIO_3)_1(HIO_2)_1(DMA)_1$	5.19×10^{-10}	8.55×10^{-4}	3.03×10^{1}	1.21×10^{0}	6.07×10^{1}

$(HIO_3)_1(HIO_2)_1(DMA)_2$	3.35×10^{-10}	1.76×10^{-1}	9.50×10^{-2}	3.80×10^{-3}	1.90×10^{-1}
$(HIO_3)_2(HIO_2)_1(DMA)_1$	5.71×10^{-10}	2.20×10^{-6}	1.30×10^{4}	5.20×10^{2}	2.60×10^{4}
$(HIO_3)_2(HIO_2)_1(DMA)_2$	3.50×10^{-10}	7.65×10^{-2}	2.29×10^{-1}	9.15×10^{-3}	4.57×10^{-1}
$(HIO_3)_1(HIO_2)_2(DMA)_1$	5.60×10^{-10}	1.18×10^{2}	2.37×10^{-4}	9.49×10^{-6}	4.74×10^{-4}
$(HIO_3)_1(HIO_2)_2(DMA)_2$	3.47×10^{-10}	2.81×10^{-2}	6.19×10^{-1}	2.48×10^{-2}	1.24×10^{0}
$(HIO_3)_3(HIO_2)_1(DMA)_1$	6.15×10^{-10}	1.42×10^{-3}	2.16×10^{1}	8.64×10^{-1}	4.32×10^{1}
$(HIO_3)_1(HIO_2)_3(DMA)_1$	6.08×10^{-10}	8.47×10^{-4}	3.59×10^{1}	1.44×10^{0}	7.18×10^{1}
$(HIO_3)_2(HIO_2)_2(DMA)_1$	6.10×10^{-10}	5.45×10^{-7}	5.60×10^{4}	2.24×10^{3}	1.12×10^{5}
$(HIO_3)_3(HIO_2)_1(DMA)_2$	3.77×10^{-10}	9.01×10^{-4}	4.18×10^{-1}	8.37×10^{-1}	4.18×10^{1}
$(HIO_3)_1(HIO_2)_3(DMA)_2$	3.71×10^{-10}	1.66×10^{7}	2.24×10^{-10}	4.48×10^{-11}	2.24×10^{-9}
$(HIO_3)_2(HIO_2)_2(DMA)_2$	3.75×10^{-10}	2.82×10^{1}	1.33×10^{-4}	2.65×10^{-5}	1.33×10^{-3}
$(HIO_3)_1(HIO_2)_2(DMA)_3$	3.80×10^{-10}	1.22×10^{4}	3.13×10^{-7}	6.25×10^{-8}	3.13×10^{-6}
$(HIO_3)_2(HIO_2)_1(DMA)_3$	3.83×10^{-10}	3.44×10^{5}	1.11×10^{-8}	2.23×10^{-9}	1.11×10^{-7}
$(HIO_3)_4(HIO_2)_1(DMA)_1$	3.71×10^{-10}	8.81×10^{-6}	4.21×10^{2}	8.42×10^{1}	4.21×10^{3}
$(HIO_3)_1(HIO_2)_4(DMA)_1$	3.63×10^{-10}	2.97×10^{-2}	1.22×10^{-1}	2.45×10^{-2}	1.22×10^{0}
$(HIO_3)_3(HIO_2)_2(DMA)_1$	3.71×10^{-10}	9.51×10^{-12}	3.90×10^{9}	7.81×10^{5}	3.90×10^{9}
$(HIO_3)_2(HIO_2)_3(DMA)_1$	3.68×10^{-10}	2.58×10^{2}	1.43×10^{-4}	2.85×10^{-6}	1.43×10^{-4}

Table S5. The ratios of collision frequency between the clusters and monomer molecule at the concentration c to the total evaporation frequency of clusters in HIO_3-HIO_2-DMA system under field conditions of Aboa at $c(HIO_3)$ = 1.0 × 10^6 molecules cm^{-3}, $c(HIO_2)$ = 2.0 × 10^4 molecules cm^{-3}, c(DMA) = 0.004 pptv, T = 268 K, and CS = 1.0 × 10^{-4} s^{-1}. The clusters satisfying kinetically stable conditions ($\beta c/\Sigma\gamma > 1$, n = 6) in the simulated system and the corresponding $\beta c/\Sigma\gamma$ values are shown in red.

Clusters	β	$\Sigma\gamma$	$\beta c(\mathrm{DMA})/\Sigma\gamma$	$\beta c(HIO_2)/\Sigma\gamma$	$\beta c(HIO_3)/\Sigma\gamma$
$(HIO_3)_2$	4.38×10^{-10}	4.32×10^{2}	1.01×10^{-6}	6.08×10^{-8}	3.04×10^{-6}
$(HIO_3)_3$	4.98×10^{-10}	1.10×10^{1}	4.51×10^{-5}	2.71×10^{-6}	1.35×10^{-4}
$(HIO_3)_4$	5.49×10^{-10}	1.71×10^{-7}	3.21×10^{3}	1.93×10^{2}	9.64×10^{3}
$(HIO_3)_5$	5.94×10^{-10}	1.16×10^{-5}	5.10×10^{1}	3.06×10^{0}	1.53×10^{2}
$(HIO_3)_6$	3.35×10^{-10}	3.82×10^{-2}	3.70×10^{-3}	7.39×10^{-4}	3.70×10^{-2}
$(HIO_2)_2$	4.22×10^{-10}	6.31×10^{-6}	6.68×10^{1}	4.01×10^{0}	2.01×10^{2}
$(HIO_2)_3$	4.78×10^{-10}	1.04×10^{-8}	4.60×10^{4}	2.76×10^{3}	1.38×10^{5}
$(HIO_2)_4$	5.27×10^{-10}	3.39×10^{-7}	1.56×10^{3}	9.34×10^{1}	4.67×10^{3}
$(HIO_2)_5$	5.71×10^{-10}	3.37×10^{-5}	1.69×10^{1}	1.02×10^{0}	5.08×10^{1}

$(HIO_2)_6$	3.23×10^{-10}	8.41×10^{-6}	3.51×10^{3}	8.40×10^{2}	3.51×10^{4}
$(HIO_3)_1(DMA)_1$	2.83×10^{-10}	3.99×10^{-4}	7.07×10^{-1}	4.24×10^{-2}	2.12×10^{0}
$(HIO_3)_2(DMA)_1$	5.03×10^{-10}	1.34×10^{-6}	3.74×10^{2}	2.25×10^{1}	1.12×10^{3}
$(HIO_3)_2(DMA)_2$	3.25×10^{-10}	1.16×10^{-7}	2.80×10^{3}	1.68×10^{2}	8.41×10^{3}
$(HIO_3)_3(DMA)_1$	5.51×10^{-10}	1.52×10^{-1}	3.63×10^{-3}	2.18×10^{-4}	1.09×10^{-2}
$(HIO_3)_3(DMA)_2$	6.02×10^{-10}	1.19×10^{-7}	5.05×10^{3}	3.03×10^{2}	1.52×10^{4}
$(HIO_3)_4(DMA)_1$	5.98×10^{-10}	1.35×10^{-6}	4.44×10^{2}	2.67×10^{1}	1.33×10^{3}
$(HIO_3)_3(DMA)_3$	3.13×10^{-10}	2.86×10^{2}	3.65×10^{-8}	9.31×10^{-9}	3.65×10^{-9}
$(HIO_3)_4(DMA)_2$	3.53×10^{-10}	3.91×10^{3}	2.87×10^{-9}	2.63×10^{-10}	2.87×10^{-8}
$(HIO_3)_5(DMA)_1$	3.48×10^{-10}	6.75×10^{-2}	4.57×10^{-2}	9.15×10^{-3}	4.57×10^{-1}
$(HIO_2)_1(DMA)_1$	2.84×10^{-10}	1.19×10^{2}	2.39×10^{-6}	1.44×10^{-7}	7.18×10^{-6}
$(HIO_2)_2(DMA)_1$	4.95×10^{-10}	6.41×10^{-2}	7.72×10^{-3}	4.63×10^{-4}	2.32×10^{-2}
$(HIO_2)_2(DMA)_2$	3.21×10^{-10}	8.55×10^{4}	3.76×10^{-9}	2.25×10^{-10}	1.13×10^{-8}
$(HIO_2)_3(DMA)_1$	5.37×10^{-10}	3.05×10^{4}	1.76×10^{-8}	1.06×10^{-9}	5.28×10^{-8}
$(HIO_2)_3(DMA)_2$	3.35×10^{-10}	9.44×10^{-3}	3.55×10^{-2}	2.13×10^{-3}	1.06×10^{-1}
$(HIO_2)_4(DMA)_1$	5.80×10^{-10}	6.32×10^{-1}	9.19×10^{-4}	5.51×10^{-5}	2.76×10^{-3}
$(HIO_2)_3(DMA)_3$	2.65×10^{-10}	7.26×10^{1}	3.14×10^{-8}	6.03×10^{-9}	3.14×10^{-7}
$(HIO_2)_4(DMA)_2$	2.71×10^{-10}	8.01×10^{1}	2.56×10^{-6}	4.11×10^{-8}	2.56×10^{-5}
$(HIO_2)_5(DMA)_1$	4.96×10^{-10}	3.23×10^{-2}	1.41×10^{-3}	2.82×10^{-5}	1.41×10^{-2}
$(HIO_3)_1(HIO_2)_1$	4.29×10^{-10}	6.63×10^{-6}	6.47×10^{1}	3.88×10^{0}	1.94×10^{2}
$(HIO_3)_1(HIO_2)_2$	4.83×10^{-10}	8.29×10^{-9}	5.83×10^{4}	3.50×10^{3}	1.75×10^{5}
$(HIO_3)_2(HIO_2)_1$	4.88×10^{-10}	2.13×10^{-1}	2.30×10^{-3}	1.38×10^{-4}	6.89×10^{-3}
$(HIO_3)_3(HIO_2)_1$	5.43×10^{-10}	1.87×10^{-8}	2.91×10^{4}	1.74×10^{3}	8.72×10^{4}
$(HIO_3)_1(HIO_2)_3$	5.31×10^{-10}	1.15×10^{-3}	4.62×10^{-1}	2.77×10^{-2}	1.39×10^{0}
$(HIO_3)_2(HIO_2)_2$	5.36×10^{-10}	9.95×10^{-4}	5.38×10^{-1}	3.23×10^{-2}	1.61×10^{0}
$(HIO_3)_3(HIO_2)_2$	5.83×10^{-10}	1.50×10^{-5}	3.90×10^{1}	2.34×10^{0}	1.17×10^{2}
$(HIO_3)_2(HIO_2)_3$	5.80×10^{-10}	6.94×10^{-10}	8.36×10^{5}	5.02×10^{4}	2.51×10^{6}
$(HIO_3)_4(HIO_2)_1$	5.90×10^{-10}	1.35×10^{-1}	4.36×10^{-3}	2.61×10^{-4}	1.31×10^{-2}
$(HIO_3)_1(HIO_2)_4$	5.77×10^{-10}	3.53×10^{-9}	1.64×10^{5}	9.82×10^{3}	4.91×10^{5}
$(HIO_3)_5(HIO_2)_1$	3.38×10^{-10}	3.72×10^{-4}	1.15×10^{-2}	2.03×10^{-2}	1.15×10^{-1}
$(HIO_3)_4(HIO_2)_2$	3.22×10^{-10}	2.93×10^{-6}	1.51×10^{-1}	5.10×10^{-2}	1.51×10^{0}
$(HIO_3)_3(HIO_2)_3$	3.24×10^{-10}	7.91×10^{-11}	4.92×10^{4}	9.84×10^{3}	4.92×10^{5}

$(HIO_3)_2(HIO_2)_4$	3.27×10^{-10}	4.65×10^{-8}	7.25×10^{1}	1.46×10^{0}	7.25×10^{2}
$(HIO_3)_1(HIO_2)_5$	2.88×10^{-10}	9.50×10^{-10}	3.17×10^{3}	6.04×10^{2}	3.17×10^{4}
$(HIO_3)_1(HIO_2)_1(DMA)_1$	5.01×10^{-10}	2.82×10^{-5}	1.78×10^{1}	1.07×10^{0}	5.33×10^{1}
$(HIO_3)_1(HIO_2)_1(DMA)_2$	3.26×10^{-10}	7.72×10^{-3}	4.22×10^{-2}	2.53×10^{-3}	1.27×10^{-1}
$(HIO_3)_2(HIO_2)_1(DMA)_1$	5.52×10^{-10}	3.40×10^{-8}	1.62×10^{4}	9.73×10^{2}	4.87×10^{4}
$(HIO_3)_2(HIO_2)_1(DMA)_2$	3.38×10^{-10}	3.01×10^{-3}	1.12×10^{-1}	6.75×10^{-3}	3.37×10^{-1}
$(HIO_3)_1(HIO_2)_2(DMA)_1$	5.41×10^{-10}	9.02×10^{0}	6.00×10^{-5}	3.60×10^{-6}	1.80×10^{-4}
$(HIO_3)_1(HIO_2)_2(DMA)_2$	5.93×10^{-10}	1.03×10^{-3}	5.77×10^{-1}	3.46×10^{-2}	1.73×10^{0}
$(HIO_3)_3(HIO_2)_1(DMA)_1$	5.94×10^{-10}	4.93×10^{-5}	1.20×10^{1}	7.22×10^{-1}	3.61×10^{1}
$(HIO_3)_1(HIO_2)_3(DMA)_1$	5.88×10^{-10}	2.99×10^{-5}	1.96×10^{1}	1.18×10^{0}	5.89×10^{1}
$(HIO_3)_2(HIO_2)_2(DMA)_1$	5.89×10^{-10}	9.06×10^{-9}	6.50×10^{4}	3.90×10^{3}	1.95×10^{5}
$(HIO_3)_3(HIO_2)_1(DMA)_2$	3.27×10^{-10}	7.63×10^{-5}	3.18×10^{-2}	8.37×10^{-3}	3.18×10^{-1}
$(HIO_3)_1(HIO_2)_3(DMA)_2$	3.60×10^{-10}	2.61×10^{5}	6.64×10^{-9}	4.48×10^{-13}	6.64×10^{-8}
$(HIO_3)_2(HIO_2)_2(DMA)_2$	3.67×10^{-10}	8.82×10^{-1}	7.33×10^{-5}	2.65×10^{-7}	7.33×10^{-4}
$(HIO_3)_1(HIO_2)_2(DMA)_3$	3.71×10^{-10}	3.51×10^{2}	3.13×10^{-8}	6.25×10^{-10}	3.13×10^{-7}
$(HIO_3)_2(HIO_2)_1(DMA)_3$	3.55×10^{-10}	7.14×10^{3}	2.22×10^{-9}	2.23×10^{-11}	2.22×10^{-8}
$(HIO_3)_4(HIO_2)_1(DMA)_1$	3.63×10^{-10}	7.15×10^{-6}	3.74×10^{1}	8.42×10^{-1}	3.74×10^{2}
$(HIO_3)_1(HIO_2)_4(DMA)_1$	3.50×10^{-10}	3.97×10^{-3}	3.82×10^{-1}	2.45×10^{-4}	3.82×10^{-0}
$(HIO_3)_3(HIO_2)_2(DMA)_1$	3.53×10^{-10}	2.91×10^{-13}	4.90×10^{8}	7.81×10^{3}	4.90×10^{9}
$(HIO_3)_2(HIO_2)_3(DMA)_1$	3.48×10^{-10}	2.58×10^{0}	1.43×10^{-5}	2.85×10^{-3}	1.43×10^{-4}

Table S6. The ratios of collision frequency between the clusters and monomer molecule at the concentration c to the total evaporation frequency of clusters in HIO_3-HIO_2-DMA system under field conditions of Marambio at $c(HIO_3)$ = 1.0 × 10^6 molecules cm^{-3}, $c(HIO_2)$ = 2.0 × 10^4 molecules cm^{-3}, c(DMA) = 0.04 pptv, T = 273 K, and CS = 1.0 × 10^{-4} s^{-1}. The clusters satisfying kinetically stable conditions ($\beta c/\Sigma\gamma > 1$, $n = 6$) in the simulated system and the corresponding $\beta c/\Sigma\gamma$ values are shown in red.

Clusters	β	$\Sigma\gamma$	βc(DMA)/$\Sigma\gamma$	$\beta c(HIO_2)/\Sigma\gamma$	$\beta c(HIO_3)/\Sigma\gamma$
$(HIO_3)_2$	4.50×10^{-10}	2.63×10^{3}	8.54×10^{-8}	3.42×10^{-7}	1.71×10^{-5}
$(HIO_3)_3$	5.12×10^{-10}	9.47×10^{1}	2.70×10^{-6}	1.08×10^{-5}	5.41×10^{-4}
$(HIO_3)_4$	5.64×10^{-10}	4.03×10^{-6}	7.00×10^{1}	2.80×10^{2}	1.40×10^{4}
$(HIO_3)_5$	6.11×10^{-10}	2.13×10^{-4}	1.44×10^{0}	5.74×10^{0}	2.87×10^{2}
$(HIO_3)_6$	3.35×10^{-10}	3.82×10^{-2}	3.70×10^{-2}	7.39×10^{-4}	3.70×10^{-2}
$(HIO_2)_2$	4.33×10^{-10}	1.11×10^{-4}	1.95×10^{0}	7.79×10^{0}	3.90×10^{2}
$(HIO_2)_3$	4.91×10^{-10}	2.82×10^{-7}	8.70×10^{2}	3.48×10^{3}	1.74×10^{5}

$(HIO_2)_4$	5.42×10^{-10}	7.42×10^{-6}	3.65×10^{1}	1.46×10^{2}	7.30×10^{3}
$(HIO_2)_5$	5.87×10^{-10}	5.81×10^{-4}	5.05×10^{-1}	2.02×10^{0}	1.01×10^{2}
$(HIO_2)_6$	3.23×10^{-10}	8.41×10^{-6}	3.51×10^{3}	8.40×10^{2}	3.51×10^{4}
$(HIO_3)_1(DMA)_1$	2.90×10^{-10}	5.40×10^{-3}	2.69×10^{-2}	1.08×10^{-1}	5.38×10^{0}
$(HIO_3)_2(DMA)_1$	5.17×10^{-10}	2.51×10^{-5}	1.03×10^{1}	4.12×10^{1}	2.06×10^{3}
$(HIO_3)_2(DMA)_2$	3.34×10^{-10}	2.20×10^{-6}	7.58×10^{1}	3.03×10^{2}	1.52×10^{4}
$(HIO_3)_3(DMA)_1$	5.67×10^{-10}	1.51×10^{0}	1.88×10^{-4}	7.51×10^{-4}	3.76×10^{-2}
$(HIO_3)_3(DMA)_2$	6.19×10^{-10}	3.44×10^{-6}	8.98×10^{1}	3.59×10^{2}	1.80×10^{4}
$(HIO_3)_4(DMA)_1$	6.15×10^{-10}	2.76×10^{-5}	1.11×10^{1}	4.46×10^{1}	2.23×10^{3}
$(HIO_3)_3(DMA)_3$	3.13×10^{-10}	2.86×10^{2}	3.65×10^{-7}	9.31×10^{-9}	3.65×10^{-9}
$(HIO_3)_4(DMA)_2$	3.53×10^{-10}	3.91×10^{3}	2.87×10^{-8}	2.63×10^{-10}	2.87×10^{-8}
$(HIO_3)_5(DMA)_1$	3.48×10^{-10}	6.75×10^{-2}	4.57×10^{-1}	9.15×10^{-3}	4.57×10^{-1}
$(HIO_2)_1(DMA)_1$	2.92×10^{-10}	7.52×10^{2}	1.94×10^{-7}	7.77×10^{-7}	3.89×10^{-5}
$(HIO_2)_2(DMA)_1$	5.08×10^{-10}	6.43×10^{-1}	3.95×10^{-4}	1.58×10^{-3}	7.91×10^{-2}
$(HIO_2)_2(DMA)_2$	3.30×10^{-10}	4.64×10^{5}	3.56×10^{-10}	1.42×10^{-9}	7.12×10^{-8}
$(HIO_2)_3(DMA)_1$	5.52×10^{-10}	1.57×10^{5}	1.76×10^{-9}	7.04×10^{-9}	3.52×10^{-7}
$(HIO_2)_3(DMA)_2$	3.44×10^{-10}	1.22×10^{-1}	1.41×10^{-3}	5.62×10^{-3}	2.81×10^{-1}
$(HIO_2)_4(DMA)_1$	5.96×10^{-10}	5.78×10^{0}	5.16×10^{-5}	2.06×10^{-4}	1.03×10^{-2}
$(HIO_2)_3(DMA)_3$	2.65×10^{-10}	7.26×10^{1}	3.14×10^{-7}	6.03×10^{-9}	3.14×10^{-7}
$(HIO_2)_4(DMA)_2$	2.71×10^{-10}	8.01×10^{1}	2.56×10^{-5}	4.11×10^{-8}	2.56×10^{-5}
$(HIO_2)_5(DMA)_1$	4.96×10^{-10}	3.23×10^{-2}	1.41×10^{-2}	2.82×10^{-5}	1.41×10^{-2}
$(HIO_3)_1(HIO_2)_1$	4.41×10^{-10}	1.19×10^{-4}	1.85×10^{0}	7.41×10^{0}	3.71×10^{2}
$(HIO_3)_1(HIO_2)_2$	4.96×10^{-10}	2.34×10^{-7}	1.06×10^{3}	4.23×10^{3}	2.12×10^{5}
$(HIO_3)_2(HIO_2)_1$	5.02×10^{-10}	2.37×10^{0}	1.06×10^{-4}	4.23×10^{-4}	2.12×10^{-2}
$(HIO_3)_3(HIO_2)_1$	5.58×10^{-10}	4.45×10^{-7}	6.27×10^{2}	2.51×10^{3}	1.25×10^{5}
$(HIO_3)_1(HIO_2)_3$	5.46×10^{-10}	1.68×10^{-2}	1.63×10^{-2}	6.51×10^{-2}	3.25×10^{0}
$(HIO_3)_2(HIO_2)_2$	5.50×10^{-10}	1.33×10^{-2}	2.07×10^{-2}	8.27×10^{-2}	4.14×10^{0}
$(HIO_3)_3(HIO_2)_2$	5.99×10^{-10}	2.95×10^{-4}	1.02×10^{0}	4.06×10^{0}	2.03×10^{2}
$(HIO_3)_2(HIO_2)_3$	5.96×10^{-10}	2.32×10^{-8}	1.29×10^{4}	5.14×10^{4}	2.57×10^{6}
$(HIO_3)_4(HIO_2)_1$	6.06×10^{-10}	1.53×10^{0}	1.98×10^{-4}	7.91×10^{-4}	3.95×10^{-2}
$(HIO_3)_1(HIO_2)_4$	5.93×10^{-10}	1.12×10^{-7}	2.65×10^{3}	1.06×10^{4}	5.30×10^{5}
$(HIO_3)_5(HIO_2)_1$	3.38×10^{-10}	3.72×10^{-4}	1.15×10^{-2}	2.03×10^{-2}	1.15×10^{-1}

$(HIO_3)_4(HIO_2)_2$	3.22×10^{-10}	2.93×10^{-6}	1.51×10^{-1}	5.10×10^{-2}	1.51×10^{0}
$(HIO_3)_3(HIO_2)_3$	3.24×10^{-10}	7.91×10^{-11}	4.92×10^{4}	9.84×10^{3}	4.92×10^{5}
$(HIO_3)_2(HIO_2)_4$	3.27×10^{-10}	4.65×10^{-8}	7.25×10^{1}	1.46×10^{0}	7.25×10^{2}
$(HIO_3)_1(HIO_2)_5$	2.88×10^{-10}	9.50×10^{-10}	3.17×10^{3}	6.04×10^{2}	3.17×10^{4}
$(HIO_3)_1(HIO_2)_1(DMA)_1$	5.15×10^{-10}	4.37×10^{-4}	5.90×10^{-1}	2.36×10^{0}	1.18×10^{2}
$(HIO_3)_1(HIO_2)_1(DMA)_2$	3.33×10^{-10}	9.38×10^{-2}	1.77×10^{-3}	7.10×10^{-3}	3.55×10^{-1}
$(HIO_3)_2(HIO_2)_1(DMA)_1$	5.67×10^{-10}	9.45×10^{-7}	3.00×10^{2}	1.20×10^{3}	6.00×10^{4}
$(HIO_3)_2(HIO_2)_1(DMA)_2$	3.51×10^{-10}	4.03×10^{-2}	4.35×10^{-3}	1.74×10^{-2}	8.70×10^{-1}
$(HIO_3)_1(HIO_2)_2(DMA)_1$	5.56×10^{-10}	7.01×10^{1}	3.97×10^{-6}	1.59×10^{-5}	7.93×10^{-4}
$(HIO_3)_1(HIO_2)_2(DMA)_2$	3.45×10^{-10}	1.46×10^{-2}	1.18×10^{-2}	4.73×10^{-2}	2.36×10^{0}
$(HIO_3)_3(HIO_2)_1(DMA)_1$	6.10×10^{-10}	7.37×10^{-4}	4.14×10^{-1}	1.65×10^{0}	8.27×10^{1}
$(HIO_3)_1(HIO_2)_3(DMA)_1$	6.04×10^{-10}	4.33×10^{-4}	6.98×10^{-1}	2.79×10^{0}	1.40×10^{2}
$(HIO_3)_2(HIO_2)_2(DMA)_1$	6.06×10^{-10}	2.42×10^{-7}	1.25×10^{3}	5.00×10^{3}	2.50×10^{5}
$(HIO_3)_3(HIO_2)_1(DMA)_2$	3.27×10^{-10}	7.63×10^{-5}	3.18×10^{-1}	8.37×10^{-3}	3.18×10^{-1}
$(HIO_3)_1(HIO_2)_3(DMA)_2$	3.60×10^{-10}	2.61×10^{5}	6.64×10^{-8}	4.48×10^{-13}	6.64×10^{-8}
$(HIO_3)_2(HIO_2)_2(DMA)_2$	3.67×10^{-10}	8.82×10^{-1}	7.33×10^{-4}	2.65×10^{-7}	7.33×10^{-4}
$(HIO_3)_1(HIO_2)_2(DMA)_3$	3.71×10^{-10}	3.51×10^{2}	3.13×10^{-7}	6.25×10^{-10}	3.13×10^{-7}
$(HIO_3)_2(HIO_2)_1(DMA)_3$	3.55×10^{-10}	7.14×10^{3}	2.22×10^{-8}	2.23×10^{-11}	2.22×10^{-8}
$(HIO_3)_4(HIO_2)_1(DMA)_1$	3.63×10^{-10}	7.15×10^{-6}	3.74×10^{2}	8.42×10^{-1}	3.74×10^{2}
$(HIO_3)_1(HIO_2)_4(DMA)_1$	3.50×10^{-10}	3.97×10^{-3}	3.82×10^{0}	2.45×10^{-4}	3.82×10^{-0}
$(HIO_3)_3(HIO_2)_2(DMA)_1$	3.53×10^{-10}	2.91×10^{-13}	4.90×10^{9}	7.81×10^{3}	4.90×10^{9}
$(HIO_3)_2(HIO_2)_3(DMA)_1$	3.48×10^{-10}	2.58×10^{0}	1.43×10^{-4}	2.85×10^{-3}	1.43×10^{-4}

Table S7. The cartesian coordinates of the most stable clusters in the $(HIO_3)_x\cdot(HIO_2)_y\cdot(DMA)_z$ ($1 \le x + y + z \le 5$; $x + y \ge z$) system at the ωB97X-D/6-311++G(3df,3pd) (for H, C, N, and O atoms) + aug-cc-pVTZ-PP with ECP28MDF (for I atom) level of theory.

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$(HIO_2)_1(DMA)_1$	X	Y	Z
I	0.658571	-0.020269	-0.190744
O	0.187400	0.169519	1.564530
O	2.645047	-0.099895	-0.022326
H	2.965606	0.766330	0.240732
N	-1.948511	-0.053029	-0.540662
H	-2.207771	-0.152829	-1.513594
C	-2.449431	1.217424	-0.021533
H	-2.028979	1.370161	0.972172
H	-2.121540	2.031231	-0.666460
H	-3.542177	1.232301	0.043851
C	-2.439451	-1.198138	0.222855
H	-2.105616	-2.122357	-0.245965

H	-2.018438	-1.145113	1.226754
H	-3.532070	-1.206991	0.290983

$(HIO_2)_2(DMA)_1$	X	Y	Z
I	1.734427	-1.241216	-0.097416
O	0.273177	-0.658953	0.957135
O	2.607205	0.339725	-0.515932
H	1.647693	1.626316	-0.270023
I	-1.853283	-0.347197	0.093926
O	-1.434824	1.400392	-0.349535
O	-3.725856	-0.272920	-0.604296
H	-4.255105	0.283394	-0.028400
N	0.964943	2.389075	-0.018593
H	0.002429	1.953974	-0.164307
C	1.129874	3.541499	-0.910760
H	2.121769	3.970674	-0.782479
H	1.007399	3.208216	-1.937633
H	0.374069	4.290226	-0.683111
C	1.112484	2.690935	1.411597
H	0.969604	1.765149	1.963293
H	2.107226	3.088017	1.604058
H	0.357916	3.415884	1.709721

$(HIO_2)_2(DMA)_2$	X	Y	Z
I	-1.658755	0.460005	-0.467585
O	-0.314217	-0.489985	-1.344284
O	-1.277141	2.196062	-1.274214
H	-0.542544	2.531125	-0.695740
I	1.718889	-0.942050	-0.299461
O	0.903723	-0.398470	1.269363
O	3.464459	-1.515882	0.497269
H	3.966036	-0.738487	0.751943
N	-1.792827	-1.694265	0.873085
H	-0.854216	-1.540427	1.248524
C	-1.847742	-2.941638	0.122425
H	-2.831838	-3.046756	-0.335402
H	-1.100638	-2.914435	-0.667617
H	-1.666918	-3.812247	0.760758
C	-2.774948	-1.607961	1.942704
H	-2.666056	-0.655321	2.461378
H	-3.779753	-1.665620	1.521612
H	-2.663915	-2.412799	2.675797
N	0.739315	2.644537	0.609266
H	0.855898	1.692045	0.957495
C	0.272453	3.487898	1.698538
H	0.033711	4.482070	1.317388
H	-0.634017	3.061985	2.127386
H	1.015274	3.598599	2.498619
C	1.995945	3.108408	0.041421
H	2.319336	2.419626	-0.737957
H	1.854118	4.090210	-0.412997
H	2.794145	3.192886	0.790181

$(HIO_2)_3(DMA)_1$	X	Y	Z
I	-1.288793	-0.614419	-1.150838
O	-0.912311	0.679673	0.183622
O	-3.156270	-0.055064	-1.309194
H	-3.592690	-0.193879	-0.427498
I	1.838934	-1.439461	0.517583
O	0.947791	-1.044224	-1.087961
O	1.936499	-3.400347	0.149404
H	1.099429	-3.814144	0.370319
I	0.864578	2.024041	-0.019902

O	1.814685	0.753979	0.982315
O	2.458268	3.205825	-0.228735
H	2.690215	3.592930	0.618639
N	-4.155644	-0.177217	1.262100
H	-5.117068	-0.482339	1.328407
C	-4.065103	1.240158	1.596674
H	-3.045823	1.575056	1.405321
H	-4.735806	1.811815	0.957515
H	-4.311017	1.443129	2.645863
C	-3.320454	-1.002677	2.126185
H	-3.447213	-2.053378	1.868517
H	-2.275363	-0.729647	1.972391
H	-3.551189	-0.871174	3.190396

$(HIO_2)_3(DMA)_2$	X	Y	Z
I	0.718367	-2.101422	0.405252
O	2.558331	-2.411959	0.315507
O	0.479007	-1.393225	-1.390836
H	0.864683	-0.469335	-1.390017
I	0.831779	2.429419	-0.488019
O	0.436562	1.838567	1.225399
O	1.669167	0.945507	-1.288459
H	3.031043	0.381488	-0.471691
I	-2.468416	-0.336251	-0.532182
O	-1.720609	-1.652224	0.537839
O	-2.576665	-1.470118	-2.160190
H	-1.664950	-1.647590	-2.419862
N	-2.269814	1.079736	1.455589
H	-1.252993	1.268640	1.454065
C	-2.658427	0.416303	2.694456
H	-3.731619	0.220797	2.684987
H	-2.136423	-0.534392	2.764723
H	-2.421547	1.032578	3.566605
C	-2.967930	2.338428	1.231894
H	-2.625908	2.784965	0.297140
H	-4.042619	2.162535	1.161743
H	-2.783504	3.053586	2.038041
N	3.692322	-0.118706	0.168140
H	3.243477	-1.124303	0.270678
C	3.676826	0.556637	1.473589
H	4.177681	1.521490	1.400426
H	2.640527	0.716254	1.770510
H	4.185809	-0.063670	2.208664
C	5.019289	-0.244440	-0.440521
H	4.918238	-0.748573	-1.397984
H	5.462443	0.739011	-0.590528
H	5.661506	-0.837180	0.208086

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$(HIO_2)_3(DMA)_3$	X	Y	Z
I	-1.944305	-0.954095	-1.039031
O	-2.269256	0.879863	-1.138033
O	-0.643645	-1.05149	-2.494351
H	0.222646	-0.845417	-2.073777
I	-0.722932	2.220303	0.066484
O	-0.952688	0.984429	1.439417
O	0.654791	3.32821	0.941824
H	1.500847	3.005255	0.550318
I	2.053613	-1.886054	0.112889
O	1.551329	-0.45356	-0.947569
O	2.73998	-3.024276	-1.388144
H	3.519316	-2.616341	-1.772685

N	1.149318	-0.65436	1.987102
H	0.324442	-0.124114	1.635001
C	0.706926	-1.590288	3.013338
H	1.555766	-2.161791	3.395695
H	-0.015615	-2.287331	2.589999
H	0.240944	-1.067845	3.852669
C	2.08564	0.340298	2.507326
H	2.29843	1.067362	1.727975
H	3.013345	-0.141333	2.82101
H	1.653222	0.875463	3.355691
N	2.816496	2.237891	-0.545512
H	2.520796	1.268347	-0.659556
C	2.658681	2.916011	-1.823689
H	2.801711	3.989923	-1.692487
H	1.652439	2.748297	-2.205335
H	3.372684	2.56491	-2.579636
C	4.184748	2.296722	-0.061668
H	4.28022	1.735135	0.867394
H	4.455363	3.333462	0.145814
H	4.910913	1.897449	-0.782525
N	-3.367295	-0.613496	1.019368
H	-2.704763	0.08275	1.373041
C	-4.667722	-0.003451	0.779581
H	-5.33711	-0.735819	0.326251
H	-4.542022	0.829488	0.091131
H	-5.126548	0.358208	1.705339
C	-3.410674	-1.761021	1.909368
H	-2.400863	-2.142553	2.06152
H	-4.015993	-2.55271	1.464777
H	-3.837391	-1.514247	2.886766

$(HIO_2)_4(DMA)_1$	**X**	**Y**	**Z**
I	-0.775912	1.312470	-1.642183
O	-1.002013	1.141753	0.215034
O	-1.976055	2.903948	-1.765655
H	-2.886062	2.602173	-1.822264
I	0.394235	-1.941535	-0.550373
O	0.711552	-0.344403	-1.501518
O	-1.194610	-2.476698	-1.530316
H	-1.950227	-1.959687	-1.144707
I	3.226659	0.292934	0.452531
O	2.287316	-1.290244	0.717225
O	4.669929	-0.536051	-0.641935
H	5.196001	-1.122115	-0.092325
I	-2.861345	-0.043979	1.128917
O	-3.036581	-0.844767	-0.520275
O	-4.258183	-1.081694	2.100344
H	-5.124293	-0.817468	1.780864
N	1.410289	1.310798	1.692552
H	0.573417	1.164400	1.111121
C	1.641033	2.748482	1.800094
H	2.556730	2.937117	2.363101
H	1.741770	3.179270	0.804294
H	0.811727	3.247701	2.305982
C	1.196018	0.664006	2.985346
H	1.042183	-0.400607	2.826951
H	2.074263	0.803247	3.616434
H	0.326519	1.086599	3.495564

$(HIO_2)_4(DMA)_2$	X	Y	Z
I	-1.983975	1.542278	0.947511
O	-2.366153	0.844639	-0.747207
O	-0.732843	2.924712	0.353766
H	0.186554	2.545995	0.402062
I	-1.684781	-1.239918	-1.520132
O	-1.651634	-1.799022	0.256718
O	-1.240200	-3.022056	-2.274427
H	-0.336412	-3.233477	-2.016242
I	1.983681	-1.542833	0.946878
O	2.365955	-0.844323	-0.747454
O	0.732616	-2.924993	0.352342
H	-0.186791	-2.546318	0.400786
I	1.685185	1.240838	-1.519343
O	1.651441	1.798844	0.257828
O	1.241218	3.023479	-2.272828
H	0.337310	3.234866	-2.015059
N	3.54559	0.256838	1.669295
H	3.016117	1.022048	1.235998
C	4.869256	0.149457	1.068809
H	5.385378	-0.721931	1.474029
H	4.761051	0.021239	-0.006309
H	5.47627	1.037676	1.267152
C	3.568695	0.406954	3.115606
H	2.552074	0.535854	3.486427
H	3.999336	-0.485138	3.574705
H	4.161685	1.271274	3.428909
N	-3.545916	-0.257814	1.66876
H	-3.016322	-1.02275	1.235116
C	-4.869484	-0.150203	1.068098
H	-5.385736	0.720943	1.473672
H	-4.761087	-0.021432	-0.006935
H	-5.47647	-1.038567	1.265877
C	-3.569265	-0.408718	3.114983
H	-2.552698	-0.537717	3.485921
H	-4.000074	0.483087	3.574482
H	-4.162226	-1.273267	3.427713

$(HIO_2)_5(DMA)_1$	X	Y	Z
I	1.134629	2.340843	0.349016
O	1.058342	0.993106	-0.955054
O	2.086924	3.630876	-0.830451
H	3.027316	3.436285	-0.805794
I	2.854495	-0.597007	-1.116619
O	3.433109	0.062559	0.501314
O	4.155782	-2.093254	-1.299905
H	5.026176	-1.737855	-1.495515
I	-2.387459	1.136233	-1.068135
O	-2.688655	-0.683597	-1.448603
O	-1.190944	1.449723	-2.591175
H	-0.293393	1.312455	-2.230076
I	0.456088	-0.759959	2.094644
O	-0.089471	0.998182	1.706297
O	2.172339	-0.290301	2.887349
H	2.778788	-0.207705	2.114354

I	-1.327092	-2.270644	-0.66115
O	-1.561224	-1.502154	1.039856
O	-0.199773	-3.773072	0.027256
H	0.726861	-3.528307	-0.044258
N	-3.689462	0.507926	0.910119
H	-3.122272	-0.311907	1.135688
C	-5.06806	0.115396	0.640868
H	-5.636285	0.984697	0.309015
H	-5.075606	-0.633303	-0.148399
H	-5.549509	-0.29617	1.532128
C	-3.544566	1.510365	1.960196
H	-2.484076	1.67724	2.147491
H	-4.009205	2.445621	1.642611
H	-4.023312	1.190663	2.889465

$(HIO_3)_1(HIO_2)_1(DMA)_1$	X	Y	Z
I	2.316688	-0.503442	-0.206126
O	1.554964	-1.284788	1.371024
O	2.056555	1.305175	0.022866
H	0.567314	1.928605	0.052495
N	-0.329147	2.475749	0.165587
H	-1.064453	1.791422	0.473196
C	-0.724339	3.019663	-1.143411
H	0.050378	3.692654	-1.504422
H	-0.848141	2.183503	-1.826794
H	-1.664721	3.557538	-1.040815
C	-0.134557	3.489150	1.212355
H	0.172394	2.990503	2.127328
H	0.639710	4.187367	0.902679
H	-1.068271	4.021299	1.380638
I	-2.037764	-0.796127	-0.112645
O	-2.269014	0.715891	0.861029
O	-0.992352	-0.216395	-1.454518
O	-0.936709	-1.818050	0.895461
H	0.582676	-1.473509	1.190872

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$(HIO_3)_1(HIO_2)_1(DMA)_2$	X	Y	Z
I	-2.237208	-0.193672	-0.270067
O	-1.599683	0.722399	1.212037
O	-3.312564	1.374459	-0.953898
H	-4.047101	1.536146	-0.357827
N	0.249304	2.468104	0.509521
H	-0.451917	1.720292	0.809376
C	-0.028847	2.814372	-0.896180
H	0.584982	3.663491	-1.191092
H	0.223718	1.949412	-1.507101
H	-1.085315	3.052619	-1.006478
C	0.153496	3.599210	1.439785
H	0.345442	3.242908	2.448246
H	0.889042	4.355792	1.174300
H	-0.846456	4.024892	1.389297
N	-0.884171	-1.975303	0.521170
H	0.042282	-1.560366	0.695305
C	-0.725104	-2.987014	-0.519658
H	-1.698304	-3.402389	-0.789346
H	-0.268415	-2.523459	-1.393047
H	-0.082298	-3.800582	-0.176486
C	-1.381332	-2.509318	1.787294
H	-1.481377	-1.691033	2.497194
H	-2.355161	-2.976193	1.635501
H	-0.688811	-3.251664	2.190482

I	2.595470	-0.364202	-0.249910
O	1.840992	-1.398348	1.020775
O	1.274629	-0.204560	-1.464410
O	2.679538	1.286177	0.497475
H	1.203311	2.033364	0.562316

$(HIO_3)_2(HIO_2)_1(DMA)_1$	X	Y	Z
N	0.284414	2.278090	0.392016
H	-0.733907	2.117166	0.587880
C	0.392173	2.435112	-1.077689
H	1.437420	2.558928	-1.344379
H	-0.021210	1.546152	-1.547184
H	-0.196808	3.304029	-1.362721
C	0.798228	3.436594	1.150002
H	0.664680	3.247940	2.211645
H	1.854815	3.554692	0.923008
H	0.242773	4.324328	0.857117
I	3.208060	0.068202	-0.045293
O	1.938410	-0.567373	-1.191455
O	3.458041	1.768710	-0.532297
O	2.183240	0.210282	1.451831
H	0.811349	1.452675	0.712039
I	-3.243375	0.558139	-0.143597
O	-2.384788	2.047421	0.411286
O	-2.074171	-0.193428	-1.312883
O	-3.155319	-0.547321	1.277211
H	-2.191403	-1.897047	0.999753
O	-1.589641	-2.568892	0.584998
I	-0.126109	-1.603976	-0.200890
O	1.135231	-2.391962	1.046974
H	1.466445	-1.630529	1.557886

$(HIO_3)_2(HIO_2)_1(DMA)_2$	X	Y	Z
I	3.280965	0.691446	-0.497634
O	3.117687	-1.068087	0.076504
O	2.072102	1.634054	0.600972
H	1.450785	0.529791	1.754418
N	1.108589	-0.149032	2.473223
H	0.608183	-0.897917	1.936657
C	0.154890	0.517935	3.374666
H	0.639678	1.372225	3.843097
H	-0.711795	0.828958	2.794939
H	-0.164495	-0.187212	4.138857
C	2.273099	-0.745646	3.148710
H	2.911148	-1.189923	2.388317
H	2.813194	0.032049	3.685418
H	1.930071	-1.505669	3.846938
N	-0.207652	2.466714	-0.611746
H	0.594381	1.970775	-0.147557
C	-0.689235	3.538763	0.271398
H	-1.486991	4.082445	-0.229264
H	-1.085253	3.079988	1.173659
H	0.135902	4.205958	0.510390
C	0.242148	2.924661	-1.934854
H	0.578694	2.055701	-2.493723
H	-0.590877	3.395062	-2.452067
H	1.057865	3.634596	-1.814091
I	-0.285846	-1.939108	-0.647979
O	-0.175966	-2.112279	1.136539
O	0.066701	-0.217427	-0.971896
O	1.431354	-2.620322	-1.107527
H	2.135321	-2.022225	-0.682084
I	-3.331281	0.339395	0.070510

O	-2.638433	-1.283993	-0.386276
O	-2.414133	0.869146	1.520448
O	-2.735448	1.463491	-1.206035
H	-0.982106	1.798840	-0.765099

$(HIO_3)_1(HIO_2)_2(DMA)_1$	X	Y	Z
I	2.427309	-0.247135	-0.556539
O	1.762962	1.046571	0.611066
O	2.966225	1.066267	-1.952035
H	2.186205	1.330196	-2.447773
I	-0.344297	1.979106	0.482502
O	-0.669179	0.702779	-0.868938
O	-2.123879	2.789484	0.332162
H	-2.741931	2.078173	0.572016
N	1.736738	-1.757810	1.167199
H	0.716877	-1.649841	1.099037
C	2.207284	-1.398037	2.502026
H	3.291294	-1.505914	2.549677
H	1.948393	-0.361865	2.702157
H	1.756495	-2.041951	3.260825
C	2.070644	-3.124875	0.778617
H	1.609986	-3.347101	-0.182963
H	3.153234	-3.237429	0.698270
H	1.698940	-3.846313	1.509033
I	-2.144800	-0.942144	-0.476218
O	-2.983318	0.138951	0.679473
O	-0.953977	-1.843297	0.515219
O	-3.533649	-2.330247	-0.430875
H	-3.890900	-2.400696	0.460386

$(HIO_3)_1(HIO_2)_2(DMA)_2$	X	Y	Z
I	2.373448	1.100392	0.225742
O	0.699414	0.192903	0.430804
O	1.357040	2.795669	0.359926
H	0.745498	2.786285	-0.430274
I	1.278152	-1.932200	-0.091764
O	2.939794	-1.008930	0.205477
O	2.235361	-3.644192	-0.391237
H	2.633333	-3.642809	-1.264695
N	-1.203121	1.544661	1.842851
H	-0.515466	1.203615	1.141771
C	-0.499663	1.645645	3.130005
H	-1.206116	1.921399	3.909383
H	-0.056346	0.680173	3.357288
H	0.280423	2.399242	3.046587
C	-1.826910	2.798069	1.392865
H	-2.362917	2.591558	0.469990
H	-2.522490	3.144660	2.154303
H	-1.049138	3.539477	1.226131
N	-0.386012	2.460116	-1.758226
H	-1.089764	1.825560	-1.382022
C	0.267176	1.765580	-2.860639
H	1.126281	2.341628	-3.209196
H	0.617302	0.793219	-2.516566
H	-0.407484	1.603917	-3.709891
C	-1.037153	3.686812	-2.191555
H	-1.548342	4.151001	-1.348435
H	-0.288978	4.391151	-2.558868
H	-1.770533	3.518084	-2.989218
I	-2.951638	-0.937131	-0.167158
O	-2.600037	0.649565	-0.949305
O	-1.476024	-1.934404	-0.429133
O	-2.912769	-0.510528	1.596131

H	-1.922235	0.774867	1.864539

$(HIO_3)_1(HIO_2)_3(DMA)_1$	X	Y	Z
I	-0.460929	-2.091419	-0.868175
O	-1.144462	-0.780118	-2.048324
O	1.027738	-2.574785	-2.004876
H	1.770430	-1.966456	-1.773982
I	-1.830808	1.196469	-1.509716
O	-0.919027	1.036372	0.137942
O	-2.367465	3.092268	-1.059574
H	-3.154168	3.087060	-0.510673
I	-1.799370	-0.230667	1.875917
O	-2.280762	-1.437507	0.537074
O	-2.359382	-1.384544	3.386965
H	-3.317479	-1.447572	3.404450
N	1.304111	2.633475	0.368844
H	0.625995	1.864823	0.207564
C	1.002312	3.736106	-0.559193
H	1.647891	4.582055	-0.335280
H	1.192785	3.396615	-1.574074
H	-0.044619	4.016987	-0.459427
C	1.208038	2.989789	1.793701
H	1.425727	2.094375	2.371056
H	1.935421	3.765435	2.021172
H	0.202913	3.348194	2.006955
I	3.489001	-0.220361	0.339687
O	2.036306	-0.223022	1.401115
O	2.904359	-0.838608	-1.249260
O	3.723246	1.555101	0.032483
H	2.271436	2.244384	0.186135

$(HIO_3)_3(HIO_2)_1(DMA)_1$	X	Y	Z
I	2.685796	0.056689	0.838679
O	0.798717	-0.054666	0.498709
O	2.344151	1.201103	2.390284
H	1.975802	2.023245	2.013715
N	-0.747757	-1.347963	2.439159
H	-0.135390	-0.981997	1.690805
C	-0.151742	-2.565751	3.011840
H	-0.837290	-2.984799	3.744504
H	0.020438	-3.272353	2.205487
H	0.790475	-2.314324	3.494549
C	-0.981171	-0.257010	3.405231
H	-1.514404	0.539883	2.890679
H	-1.587008	-0.632154	4.226535
H	-0.024372	0.106259	3.774409
I	0.756176	-1.555458	-1.329889
O	0.262125	-2.811950	-0.178887
O	2.548717	-1.351463	-0.928638
O	1.116249	-2.746289	-2.818023
H	1.447745	-3.585497	-2.478151
I	-3.217178	-0.292159	-0.061801
O	-2.810373	1.145473	0.937312
O	-1.744852	-0.429891	-1.115129
O	-3.061754	-1.668212	1.100404
H	-1.653799	-1.576276	1.953302
I	-0.072887	2.199549	-0.490783
O	0.875218	1.616003	-1.885053
O	1.133340	2.948513	0.600677
O	-0.760280	3.811653	-1.326219
H	-0.111550	4.111278	-1.974796

$(HIO_3)_2(HIO_2)_2(DMA)_1$	X	Y	Z

I	2.605369	-1.264764	0.260061
O	1.212760	-0.075171	0.744079
O	3.945182	-0.163505	1.191982
H	3.901435	0.713056	0.771251
I	-0.726983	-1.882105	-1.050222
O	0.967684	-2.577354	-0.625093
O	-0.295622	-0.927192	-2.642126
H	0.088935	-0.051045	-2.363824
N	-0.661456	-0.404327	2.639736
H	0.020691	-0.333937	1.846005
C	-0.344392	-1.607310	3.424972
H	-1.076643	-1.727035	4.219797
H	-0.373835	-2.473644	2.768827
H	0.652095	-1.509243	3.849980
C	-0.595790	0.855351	3.400783
H	-0.881491	1.662545	2.730809
H	-1.290005	0.810191	4.236637
H	0.418677	1.006771	3.762830
I	1.137208	2.059389	-0.312679
O	0.892526	1.268264	-1.900228
O	2.917654	2.108077	-0.158940
O	0.924365	3.888097	-0.953090
H	1.548051	4.045522	-1.670827
I	-3.251686	0.593137	0.118394
O	-1.695830	1.498335	0.230203
O	-3.025921	-0.612035	-1.210207
O	-3.167745	-0.422847	1.619448
H	-1.624195	-0.478335	2.223226

$(HIO_3)_3(HIO_2)_1(DMA)_2$	X	Y	Z
H	2.304359	0.437012	-1.982676
O	1.415155	0.355016	-2.428748
I	0.414117	-1.011004	-1.514092
O	1.379297	-2.504808	-2.313856
H	2.13066	-2.650413	-1.717233
H	-2.352246	2.593771	-0.861115
N	-3.244265	2.085976	-0.64155
H	-3.085521	1.067659	-0.77926
C	-3.545112	2.29896	0.786693
H	-3.707952	3.359566	0.961461
H	-2.695741	1.958274	1.371824
H	-4.428297	1.724561	1.055259
C	-4.311909	2.526252	-1.551829
H	-4.0032	2.335407	-2.575748
H	-4.484907	3.590863	-1.413931
H	-5.2207	1.969402	-1.336589
H	0.368309	-0.175467	1.65745
N	-0.0935	-0.62509	2.456671
H	-1.106089	-0.720357	2.229521
C	0.489344	-1.969726	2.623556
H	1.554818	-1.867702	2.805766
H	0.321186	-2.53337	1.710562
H	0.004179	-2.461923	3.463409
C	0.068823	0.251539	3.632561
H	-0.372705	1.216372	3.401574
H	1.130863	0.384451	3.81676
H	-0.418103	-0.211129	4.487837
I	3.679158	-0.288949	0.494203
O	2.245616	0.459545	1.31587

O	3.672121	0.542859	-1.109871
O	3.152951	-1.97184	0.133799
I	-3.060669	-1.861875	0.330435
O	-2.780458	-0.904555	1.837266
O	-1.392072	-2.413133	-0.095496
O	-3.485696	-0.623149	-0.908154
I	0.286939	2.438343	-0.016977
O	-0.520036	0.795997	-0.234586
O	-0.126601	2.764414	1.690608
O	-0.899939	3.432069	-0.950054

$(HIO_3)_1(HIO_2)_3(DMA)_2$	X	Y	Z
I	-1.405107	2.410516	0.561568
O	-1.207978	0.97107	1.685088
O	-2.669642	1.778962	-0.753137
H	-2.165945	1.057171	-1.274112
I	2.506005	0.524507	-1.421592
O	1.992726	0.958731	0.339534
O	0.917213	1.274747	-2.263848
H	0.154874	0.660658	-2.140139
I	-1.677056	-1.674117	-0.879128
O	-1.339137	-0.099725	-1.823453
O	-3.430622	-2.043165	-1.614379
H	-4.047789	-1.447635	-1.09575
N	-4.889423	-0.271561	-0.127107
H	-4.481991	0.60887	-0.422621
C	-4.645196	-0.437792	1.301308
H	-4.880327	-1.462052	1.594903
H	-3.594028	-0.249383	1.51781
H	-5.254836	0.239695	1.911589
C	-6.303138	-0.308961	-0.469702
H	-6.428997	-0.132104	-1.536704
H	-6.706235	-1.29651	-0.241462
H	-6.892387	0.432924	0.083034
N	4.457933	-0.337268	-0.186426
H	3.966512	-0.771898	0.60359
C	5.307513	0.741502	0.305502
H	5.750735	1.275236	-0.536337
H	4.698944	1.433804	0.883495
H	6.112385	0.36083	0.940461
C	5.178061	-1.346847	-0.950274
H	4.497886	-2.154657	-1.215319
H	5.577698	-0.906366	-1.866196
H	6.013534	-1.765181	-0.382424
I	1.138586	-0.620315	1.683949
O	2.767581	-1.347783	1.882529
O	0.571519	-1.448372	0.176202
O	0.262465	-1.887668	2.908077
H	0.755226	-2.714754	2.882786

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$(HIO_3)_2(HIO_2)_2(DMA)_2$	X	Y	Z
I	0.594415	-2.613648	-0.050729
O	-1.031755	-3.116988	0.676955
O	0.909036	-0.986838	0.951635
H	0.424209	-0.290402	0.440196

I	-3.096891	-1.714305	0.070213
O	-4.530787	-0.645863	-0.438671
O	-2.347342	-0.462301	1.356025
H	-1.698226	0.064683	0.840258
H	-3.135067	2.227271	-0.490965
N	-4.111262	1.934892	-0.277919
H	-4.213079	0.873341	-0.408528
C	-5.006892	2.626465	-1.216019
H	-4.891621	3.702286	-1.102789
H	-4.744491	2.338298	-2.230081
H	-6.035292	2.337111	-1.012116
C	-4.37689	2.247223	1.136202
H	-3.718336	1.638231	1.749102
H	-4.188577	3.303383	1.316251
H	-5.411316	2.002389	1.366522
H	2.817689	0.686395	1.783377
N	2.286002	1.369533	2.370502
H	1.568893	1.818046	1.754069
C	3.228614	2.423233	2.780923
H	4.011453	1.987828	3.397283
H	3.667349	2.856613	1.887173
H	2.692995	3.189854	3.335809
C	1.617441	0.689766	3.492849
H	0.951973	-0.068346	3.091158
H	2.367561	0.221828	4.126496
H	1.051688	1.420636	4.066344
I	-0.103189	2.357223	-0.668378
O	-0.640722	0.64164	-0.38265
O	-1.713236	3.162763	-0.787626
O	0.479787	2.827613	0.972913
I	3.652876	-0.077307	-0.919398
O	4.041992	-0.033351	0.84526
O	2.84683	-1.66655	-1.198952
O	2.359094	1.178052	-1.070124

$(HIO_3)_1(HIO_2)_2(DMA)_3$	X	Y	Z
I	-0.624953	0.646498	1.889145
O	-0.384566	1.972069	0.605875
O	1.184498	0.798823	2.647976
H	1.768227	0.330507	2.009699
I	-2.910012	-0.725402	-0.547119
O	-2.798177	0.361901	0.969232
O	-3.888525	-2.205896	0.384652
H	-3.277311	-2.694304	0.940607
N	-1.846911	1.11321	-1.654066
H	-1.034767	1.269633	-1.046088
C	-2.690431	2.304348	-1.603099
H	-3.622049	2.121063	-2.139958
H	-2.90791	2.531196	-0.562691
H	-2.187039	3.160827	-2.059774
C	-1.439778	0.733302	-3.002171
H	-0.721871	-0.080744	-2.934091
H	-2.315451	0.423044	-3.577234
H	-0.970673	1.572813	-3.521681
N	2.048781	-3.285	0.133893

H	1.741425	-3.942261	-0.570052
C	0.99727	-3.102864	1.122693
H	1.319824	-2.343631	1.835327
H	0.101875	-2.731842	0.62628
H	0.766738	-4.024137	1.672783
C	3.306062	-3.722467	0.717267
H	4.047672	-3.872474	-0.06777
H	3.67026	-2.939954	1.383856
H	3.215353	-4.653138	1.29183
H	1.124607	2.453602	0.303077
N	2.008972	2.85362	-0.11383
H	2.323923	2.115193	-0.808066
C	3.033066	3.028086	0.924528
H	2.655577	3.687208	1.70324
H	3.256911	2.052763	1.346058
H	3.930046	3.453437	0.477948
C	1.653501	4.082434	-0.831866
H	0.896901	3.843473	-1.574643
H	1.25525	4.814114	-0.131904
H	2.533371	4.487097	-1.327841
I	2.356662	-0.700208	-1.046124
O	0.567353	-0.849002	-1.164797
O	2.656735	0.924036	-1.820325
O	2.693325	-0.308224	0.692659

$(HIO_3)_2(HIO_2)_1(DMA)_3$	X	Y	Z
I	0.729755	-2.359462	-0.143759
O	2.493793	-2.886542	0.091553
O	0.431743	-1.532646	1.570108
H	0.598376	-0.571998	1.385074
H	-0.048119	3.200762	0.510945
N	-0.829087	3.150179	1.208879
H	-1.292634	2.21639	1.091815
C	-0.260668	3.231547	2.562246
H	0.216891	4.199666	2.697342
H	0.476111	2.439097	2.656544
H	-1.052467	3.100213	3.296581
C	-1.818756	4.188391	0.892181
H	-2.153043	4.037755	-0.130777
H	-1.35961	5.170004	0.986126
H	-2.663162	4.103923	1.572517
H	3.853821	-0.033546	0.023053
N	4.135941	-0.888242	0.564564
H	3.448258	-1.675289	0.313049
C	5.486886	-1.302419	0.165606
H	6.20148	-0.519807	0.412137
H	5.497754	-1.478514	-0.906558
H	5.751171	-2.221133	0.685136
C	3.991095	-0.60433	2.001015
H	2.984558	-0.232105	2.170637
H	4.715537	0.150914	2.299415
H	4.148103	-1.521338	2.564524
I	-2.444846	0.230825	-0.642397
O	-1.681008	-1.410696	-0.562065
O	-1.154618	1.245927	-1.414876

O	-2.395442	0.924239	1.032419
I	1.544707	1.478247	-0.848467
O	3.349886	1.305209	-0.823507
O	1.247086	3.238693	-0.578659
O	1.146687	0.861742	0.817014
N	-4.487395	-1.30894	0.570451
H	-5.280638	-0.732504	0.816412
C	-4.894481	-2.353255	-0.355296
H	-4.002729	-2.879533	-0.697207
H	-5.382858	-1.910433	-1.224002
H	-5.579172	-3.084451	0.092655
C	-3.871945	-1.833251	1.782647
H	-3.598908	-1.00543	2.433258
H	-2.953707	-2.3532	1.511232
H	-4.528705	-2.527277	2.321616

$(HIO_3)_4(HIO_2)_1(DMA)_1$	X	Y	Z
H	-3.928635	-3.275411	0.714916
O	-4.310365	-2.454047	0.391835
I	-2.880729	-1.141302	0.108392
O	-2.434144	-1.772535	-1.650634
H	-1.664036	-2.39906	-1.503148
H	-1.408277	3.270002	-1.37339
N	-1.203989	3.901645	-0.568329
H	-0.934623	3.29303	0.241824
C	-2.420831	4.639662	-0.192524
H	-2.733511	5.273499	-1.018969
H	-3.202423	3.922214	0.040673
H	-2.213019	5.245554	0.685881
C	-0.046146	4.750834	-0.904637
H	0.768251	4.095827	-1.201844
H	-0.312398	5.416709	-1.722355
H	0.236964	5.327219	-0.027277
I	-0.450012	0.760648	-2.072819
O	-1.19377	0.483498	-0.386512
O	-1.570269	2.061104	-2.618165
O	1.012212	1.709751	-1.662819
I	1.011082	-2.613586	-0.109043
O	0.289397	-1.975629	1.398474
O	-0.403423	-3.285541	-1.015549
O	1.283884	-1.072523	-1.093706
I	3.202415	0.189967	-0.198026
O	3.537546	-1.444367	0.462191
O	2.305638	1.005278	1.10849
O	4.960709	0.941565	0.17626
H	5.228623	0.693871	1.068574
I	-0.378949	0.891441	2.012403
O	-2.079239	0.377754	2.286128
O	-0.560081	2.65045	1.718025
O	0.089599	0.993121	3.887003
H	-0.730384	1.119149	4.380148

$(HIO_3)_1(HIO_2)_4(DMA)_1$	X	Y	Z
I	1.224613	1.015606	-2.175508
O	1.289225	2.105249	-0.617843

O	-0.377934	1.879965	-2.892867
H	-1.11507	1.305036	-2.613824
I	-1.044264	2.451657	0.616065
O	-0.141174	1.900000	2.136575
O	-2.858486	2.519975	1.306912
H	-3.239496	1.644596	1.083476
I	2.466136	0.633475	0.844304
O	2.927032	0.027194	-0.898013
O	3.338775	-0.840518	1.781826
H	2.67828	-1.561452	1.764232
I	0.636719	-2.614309	-0.332292
O	0.936757	-2.327292	1.476812
O	2.501481	-2.815483	-0.877569
H	2.855978	-1.909132	-0.957785
H	-0.095602	-1.26745	2.324554
N	-0.449577	-0.586869	3.033334
H	-0.365805	0.382318	2.607328
C	0.451047	-0.655262	4.19709
H	0.369167	-1.635496	4.660844
H	1.474841	-0.503133	3.863896
H	0.1767	0.118775	4.909597
C	-1.861725	-0.84923	3.361014
H	-2.458598	-0.744304	2.459345
H	-1.959507	-1.857528	3.757155
H	-2.191164	-0.124545	4.102482
I	-3.02603	-1.130032	-0.761226
O	-3.523572	-0.015843	0.563125
O	-2.020023	-0.151278	-1.884158
O	-1.840689	-2.232189	0.069642

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$(HIO_3)_3(HIO_2)_2(DMA)_1$	X	Y	Z
H	1.520157	1.041073	1.540589
O	2.473979	0.897668	1.810377
I	3.459486	1.031887	0.182616
O	3.572635	2.955373	0.20087
H	2.66933	3.295897	-0.019146
H	-2.813914	0.582628	-2.006013
O	-2.391956	0.125611	-2.765826
I	-0.865575	-0.786039	-2.028457
O	-1.774435	-2.50053	-1.968739
H	-2.346606	-2.431468	-1.183013
H	-1.613809	-0.252993	2.477796
N	-0.829168	-0.880449	2.751557
H	-0.222194	-1.021489	1.933831
C	-1.401536	-2.188336	3.122413
H	-2.075533	-2.048297	3.964094
H	-1.953965	-2.567176	2.267029
H	-0.595432	-2.868558	3.381472
C	-0.038423	-0.244692	3.82031
H	0.223746	0.760096	3.504846
H	-0.637818	-0.201456	4.72644
H	0.863224	-0.827473	3.989259
I	-0.369353	2.452704	-0.297668
O	0.030218	1.512753	-1.80252
O	0.017566	1.246197	1.005214

O	1.011591	3.598583	-0.211519
I	2.200093	-2.58047	0.014762
O	3.530679	-1.359956	0.276253
O	1.032468	-2.276131	1.339504
O	1.37886	-1.976831	-1.468692
I	-3.927189	0.045498	0.723969
O	-3.176395	0.446104	2.312092
O	-3.13066	1.208875	-0.419713
O	-3.191895	-1.548866	0.312553

$(HIO_3)_2(HIO_2)_3(DMA)_1$	X	Y	Z
H	2.894537	-2.149356	-0.635638
N	3.811531	-1.71833	-0.816974
H	3.671055	-0.68491	-0.828189
C	4.276554	-2.14101	-2.148456
H	4.414311	-3.219635	-2.156797
H	3.523484	-1.857838	-2.878121
H	5.215847	-1.641828	-2.37219
C	4.721655	-2.05171	0.294423
H	4.264688	-1.690737	1.212275
H	4.855716	-3.130073	0.337828
H	5.677689	-1.561626	0.128182
I	-0.128249	-2.344117	-0.687009
O	1.519263	-3.268047	-0.021495
O	0.980405	-1.225397	-1.801413
H	0.946306	-0.288608	-1.491607
I	-2.335797	2.519667	-0.187891
O	-3.524988	1.306251	-0.884364
O	-1.108489	2.900879	-1.631171
H	-0.345979	2.28065	-1.540163
I	2.593111	2.167493	-0.577739
O	1.065067	1.387892	-1.188516
O	2.44911	2.037243	1.211522
O	3.85465	0.973202	-1.047446
I	-3.143054	-1.113125	-0.228975
O	-2.549525	-0.353235	1.295701
O	-1.706294	-0.895254	-1.401804
O	-2.799839	-2.858857	0.074499
H	1.693288	-2.762703	0.799208
O	1.998328	-1.121693	1.505648
I	0.872841	0.12663	2.266568
O	-0.517118	-1.015668	2.998768
H	-1.284642	-0.944254	2.386225

Table S8. The total number of proton transfer (*N*) and the number of proton transfer between different precursors in ternary clusters (n_1, n_2, n_3 represent the number of proton transfer between HIO_3 and DMA, HIO_3 and HIO_2, and HIO_2 and DMA, respectively).

Clusters	*N*	n_1	n_2	n_3
$(HIO_3)_1(HIO_2)_1(DMA)_1$	1	1	0	0
$(HIO_3)_1(HIO_2)_1(DMA)_2$	1	1	0	0
$(HIO_3)_2(HIO_2)_1(DMA)_1$	2	1	1	0

$(HIO_3)_2(HIO_2)_1(DMA)_2$	2	1	0	1
$(HIO_3)_1(HIO_2)_2(DMA)_1$	0	0	0	0
$(HIO_3)_1(HIO_2)_2(DMA)_2$	1	1	0	0
$(HIO_3)_3(HIO_2)_1(DMA)_1$	1	1	0	0
$(HIO_3)_1(HIO_2)_3(DMA)_1$	1	1	0	0
$(HIO_3)_2(HIO_2)_2(DMA)_1$	1	1	0	0
$(HIO_3)_3(HIO_2)_1(DMA)_2$	3	2	1	0
$(HIO_3)_1(HIO_2)_3(DMA)_2$	0	0	0	0
$(HIO_3)_2(HIO_2)_2(DMA)_2$	2	2	0	0
$(HIO_3)_1(HIO_2)_2(DMA)_3$	1	1	0	0
$(HIO_3)_2(HIO_2)_1(DMA)_3$	2	2	0	0
$(HIO_3)_4(HIO_2)_1(DMA)_1$	2	1	1	0
$(HIO_3)_1(HIO_2)_4(DMA)_1$	1	1	0	0
$(HIO_3)_3(HIO_2)_2(DMA)_1$	3	1	2	0
$(HIO_3)_2(HIO_2)_3(DMA)_1$	2	1	1	0

Section S7: References

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