

1 *Supplement of*

2 **Enhancement Mechanism of Ethylenediamine on Iodine**

3 **Oxoacid-Driven New Particle Formation in Marine Areas**

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Section S1 Selection of boundary clusters

Figure S1 Identified global minimum configurations of $(\text{HIO}_2)_{0-3}(\text{EDA})_{0-3}$ clusters at the DLPNO-CCSD(T)/aug-cc-pVTZ(-pp)// $\omega\text{B97X-D/aug-cc-pVDZ(-pp)}$ level of theory. The dashed red and purple lines indicate HBs and XBs, respectively.

Figure S2 The ratio of the collision frequency between the cluster and monomer molecule at the concentration C to the total evaporation frequency of the cluster $(\beta C/\sum \gamma)$ for $(\text{HIO}_3)_x(\text{HIO}_2)_y(\text{EDA})_z$ ($x = 1-3$, $y + z = 2-3$) clusters at (a) $C_{[\text{HIO}_3]} = 10^6 \text{ cm}^{-3}$, (b) $C_{[\text{HIO}_2]} = 2 \times 10^4 \text{ cm}^{-3}$, and (c) $C_{[\text{EDA}]} = 0.1 \text{ ppt}$ and $T = 258.15 \text{ K}$.

Figure S3 The ratio of the collision frequency between the cluster and monomer molecule at the concentration C to the total evaporation frequency of the cluster $(\beta C/\sum \gamma)$ for $(\text{HIO}_3)_x(\text{HIO}_2)_y(\text{EDA})_z$ ($x = 1-3$, $y + z = 2-3$) clusters at (a) $C_{[\text{HIO}_3]} = 10^6 \text{ cm}^{-3}$, (b) $C_{[\text{HIO}_2]} = 2 \times 10^4 \text{ cm}^{-3}$, and (c) $C_{[\text{EDA}]} = 0.1 \text{ ppt}$ and $T = 268.15 \text{ K}$.

Figure S4 The ratio of the collision frequency between the cluster and monomer molecule at the concentration C to the total evaporation frequency of the cluster $(\beta C/\sum \gamma)$ for $(\text{HIO}_3)_x(\text{HIO}_2)_y(\text{EDA})_z$ ($x = 1-3$, $y + z = 2-3$) clusters at (a) $C_{[\text{HIO}_3]} = 10^6 \text{ cm}^{-3}$, (b) $C_{[\text{HIO}_2]} = 2 \times 10^4 \text{ cm}^{-3}$, and (c) $C_{[\text{EDA}]} = 0.1 \text{ ppt}$ and $T = 288.15 \text{ K}$.

Figure S5 The ratio of the collision frequency between the cluster and monomer molecule at the concentration C to the total evaporation frequency of the cluster $(\beta C/\sum \gamma)$ for $(\text{HIO}_3)_x(\text{HIO}_2)_y(\text{EDA})_z$ ($x = 1-3$, $y + z = 2-3$) clusters at (a) $C_{[\text{HIO}_3]} = 10^6 \text{ cm}^{-3}$, (b) $C_{[\text{HIO}_2]} = 2 \times 10^4 \text{ cm}^{-3}$, and (c) $C_{[\text{EDA}]} = 0.1 \text{ ppt}$ and $T = 298.15 \text{ K}$.

Figure S6 (a) Aerosol formation rates J ($\text{cm}^{-3} \text{ s}^{-1}$) of HIO_3 - HIO_2 system and HIO_3 - HIO_2 -EDA system and (b) corresponding enhancement factor of EDA (R_{EDA}) for HIO_3 - HIO_2 -EDA system compared with HIO_3 - HIO_2 system at $T = 258.15 \text{ K}$, 1 atm , $\text{CS} = 0.002 \text{ s}^{-1}$, $[\text{HIO}_3] = 10^6 - 10^8 \text{ cm}^{-3}$, $[\text{HIO}_2] = 2 \times 10^4 - 2 \times 10^6 \text{ cm}^{-3}$, $[\text{EDA}] = 0.01, 0.1, 1, 5, 10 \text{ ppt}$, and $\text{CS} = 0.002 \text{ s}^{-1}$.

Figure S7 (a) Aerosol formation rates J ($\text{cm}^{-3} \text{ s}^{-1}$) of HIO_3 - HIO_2 system and HIO_3 - HIO_2 -EDA system and (b) corresponding enhancement factor of EDA (R_{EDA}) for HIO_3 - HIO_2 -EDA system compared with HIO_3 - HIO_2 system at $T = 268.15 \text{ K}$, 1 atm , $\text{CS} = 0.002 \text{ s}^{-1}$, $[\text{HIO}_3] = 10^6 - 10^8 \text{ cm}^{-3}$, $[\text{HIO}_2] = 2 \times 10^4 - 2 \times 10^6 \text{ cm}^{-3}$, $[\text{EDA}] = 0.01, 0.1, 1, 5, 10 \text{ ppt}$, and $\text{CS} = 0.002 \text{ s}^{-1}$.

Figure S8 (a) Aerosol formation rates J ($\text{cm}^{-3} \text{ s}^{-1}$) of HIO_3 - HIO_2 system and HIO_3 - HIO_2 -EDA system and (b) corresponding enhancement factor of EDA (R_{EDA}) for HIO_3 - HIO_2 -EDA system

compared with HIO₃-HIO₂ system at T = 288.15 K, 1atm, CS = 0.002 s⁻¹, [HIO₃] = 10⁶ - 10⁸ cm⁻³, [HIO₂] = 2 × 10⁴ - 2 × 10⁶ cm⁻³, [EDA] = 0.01, 0.1, 1, 5, 10 ppt, and CS = 0.002 s⁻¹.

Figure S9 (a) Aerosol formation rates J (cm⁻³ s⁻¹) of HIO₃-HIO₂ system and HIO₃-HIO₂-EDA system and (b) corresponding enhancement factor of EDA (R_{EDA}) for HIO₃-HIO₂-EDA system compared with HIO₃-HIO₂ system at T = 298.15 K, 1atm, CS = 0.002 s⁻¹, [HIO₃] = 10⁶ - 10⁸ cm⁻³, [HIO₂] = 2 × 10⁴ - 2 × 10⁶ cm⁻³, [EDA] = 0.01, 0.1, 1, 5, 10 ppt, and CS = 0.002 s⁻¹.

Figure S10 Variation of the aerosol formation rate J (cm⁻³ s⁻¹) for (a) HIO₃-HIO₂ system and (b) HIO₃-HIO₂-EDA system and (c) the corresponding enhancement factor of EDA (R_{EDA}) as a function of [HIO₃] at T = 278.15 K, [HIO₃] = 10⁶ - 10⁸ cm⁻³, [HIO₂] = 2 × 10⁴ - 2 × 10⁶ cm⁻³, [EDA] = 1 ppt, and CS = 0.01 s⁻¹, 0.002 s⁻¹, 0.0004 s⁻¹, 0.0002 s⁻¹ and 0.0001 s⁻¹.

Figure S11 (a) Aerosol formation rate (J , cm⁻³ s⁻¹) of HIO₃-HIO₂ system and HIO₃-HIO₂-EDA system and (b) corresponding enhancement factor of EDA (R_{EDA}) for HIO₃-HIO₂-EDA system compared with HIO₃-HIO₂ system at T = 278.15 K, 1atm, CS = 0.002 s⁻¹, [HIO₃] = 10⁶ - 10⁸ cm⁻³, [HIO₂] = 5 × 10⁴ - 5 × 10⁶ cm⁻³, [EDA] = 0.01, 0.1, 1, 5, 10 ppt. (c) Aerosol formation rate (J , cm⁻³ s⁻¹) of HIO₃-HIO₂ system and HIO₃-HIO₂-EDA system and (d) corresponding enhancement factor of EDA (R_{EDA}) for HIO₃-HIO₂-EDA system compared with HIO₃-HIO₂ system at T = 258.15, 268.15, 288.15, 298.15 K, 1atm, CS = 0.002 s⁻¹, [HIO₃] = 10⁶ - 10⁸ cm⁻³, [HIO₂] = 5 × 10⁴ - 5 × 10⁶ cm⁻³, [EDA] = 1 ppt.

Figure S12 (a) Aerosol formation rate (J , cm⁻³ s⁻¹) of HIO₃-HIO₂ system and HIO₃-HIO₂-EDA system and (b) corresponding enhancement factor of EDA (R_{EDA}) for HIO₃-HIO₂-EDA system compared with HIO₃-HIO₂ system at T = 278.15 K, 1atm, CS = 0.002 s⁻¹, [HIO₃] = 10⁶ - 10⁸ cm⁻³, [HIO₂] = 10⁴ - 10⁶ cm⁻³, [EDA] = 0.01, 0.1, 1, 5, 10 ppt. (c) Aerosol formation rate (J , cm⁻³ s⁻¹) of HIO₃-HIO₂ system and HIO₃-HIO₂-EDA system and (d) corresponding enhancement factor of EDA (R_{EDA}) for HIO₃-HIO₂-EDA system compared with HIO₃-HIO₂ system at T = 258.15, 268.15, 288.15, 298.15 K, 1atm, CS = 0.002 s⁻¹, [HIO₃] = 10⁶ - 10⁸ cm⁻³, [HIO₂] = 10⁴ - 10⁶ cm⁻³, [EDA] = 1 ppt.

Figure S13 The influence of (a) T (258.15, 268.15, 278.15, 288.15, 298.15 K) and (b) CS (0.01, 0.002, 0.0004, 0.0002, 0.0001 s⁻¹) at [HIO₃] = 10⁷, [HIO₂] = 2 × 10⁵ cm⁻³, [EDA] = 0.1 ppt at CS = 0.002 s⁻¹ and T = 278.15 K, respectively, on the relative contribution of the HIO₃-HIO₂, HIO₃-EDA, and the HIO₃-HIO₂-EDA clustering route to the system flux. Others indicate that the

route contribution of the cluster growing out of the studied system is less than 5%.

Figure S14 The influence of [EDA] (0.01-10 ppt), [HIO₃] and [HIO₂] ((a) [HIO₃] = 10⁶, [HIO₂] = 5 × 10⁴ cm⁻³, (b) [HIO₃] = 10⁷, [HIO₂] = 5 × 10⁵ cm⁻³, (c) [HIO₃] = 10⁸, [HIO₂] = 5 × 10⁶ cm⁻³ at 278.15 K and CS = 0.002 s⁻¹ on the relative contribution of the HIO₃-HIO₂, HIO₃-EDA, and the HIO₃-HIO₂-EDA clustering route to the system flux. Others indicate that the route contribution of the cluster growing out of the studied system is less than 5%.

Figure S15 The influence of [EDA] (0.01-10 ppt), [HIO₃] and [HIO₂] ((a) [HIO₃] = 10⁶, [HIO₂] = 10⁴ cm⁻³, (b) [HIO₃] = 10⁷, [HIO₂] = 10⁵ cm⁻³, (c) [HIO₃] = 10⁸, [HIO₂] = 10⁶ cm⁻³ at 278.15 K and CS = 0.002 s⁻¹ on the relative contribution of the HIO₃-HIO₂, HIO₃-EDA, and the HIO₃-HIO₂-EDA clustering route to the system flux. Others indicate that the route contribution of the cluster growing out of the studied system is less than 5%.

Table S1 The number of HBs/XBs and the number of proton transfer for (HIO₂)₁₋₃(EDA)₁₋₃ clusters and (HIO₃)_x(HIO₂)_y(EDA)_z (x = 1–3, y+z = 2–3) clusters.

Table S2 The formation free energy (ΔG, kcal mol⁻¹) for all clusters of HIO₃-HIO₂-EDA system at the DLPNO-CCSD(T)/aug-cc-pVTZ(-pp)//ωB97X-D/aug-cc-pVDZ(-pp) level of theory and T = 298.15 K, 288.15 K, 278.15K, 268.15 K, and 258.15 K.

Table S3 The total evaporation rate coefficients (γ, s⁻¹) for all clusters of HIO₃-HIO₂-EDA system at T = 298.15 K, 288.15 K, 278.15K, 268.15 K, and 258.15 K.

Table S4 The Cartesian coordinates of all optimized (HIO₂)_x(EDA)_y (x=1-3, y=1-3), (HIO₂)_z (z=1-6) and (HIO₃)_x(HIO₂)_y(EDA)_z (x = 1–3, y+z = 2–3) clusters in the present study calculated DLPNO-CCSD(T)/aug-cc-pVTZ(-pp)//ωB97X-D/aug-cc-pVDZ(-pp) level of theory.

Text S1 Selection of boundary clusters

In ACDC simulations, the stability of a cluster determines whether it can grow out of the simulation system and contribute to the nucleation rate[McGrath *et al.*, 2012; Olenius *et al.*, 2013; F. Yu, 2006; F. Yu *et al.*, 2018; F. Yu and Turco, 2001]. Clusters with low total evaporation rates ($\sum\gamma$) are more prone to collide with other monomers or clusters under ambient atmospheric conditions and undergo continuous growth into larger clusters. This growth propensity is quantified by the ratio of the cluster's collision frequency to its total evaporation rate, denoted as $\beta C/\sum\gamma$. The β represents the collision rate of a cluster with monomers at a given monomer concentration C . When the ratio $\beta C/\sum\gamma$ exceeds 1, the cluster is sufficiently stable such that its collisional growth can overcome evaporation, thereby contributing to nucleation. Therefore, clusters that are sufficiently stable and large enough to nucleate are set as boundary clusters in ACDC simulations.

In the HIO_3 - HIO_2 -EDA ternary system, the constituent HIO_3 - HIO_2 and HIO_3 -EDA binary systems have been extensively investigated[Bai *et al.*, 2025; Zhang *et al.*, 2022], and the $(\text{HIO}_3)_4(\text{HIO}_2)_3$, $(\text{HIO}_3)_3(\text{HIO}_2)_4$, $(\text{HIO}_3)_4(\text{HIO}_2)_4$, $(\text{HIO}_3)_7$, $(\text{HIO}_2)_7$, $(\text{HIO}_3)_4(\text{EDA})_3$, and $(\text{HIO}_3)_4(\text{EDA})_4$ clusters have been identified as boundary clusters for ACDC simulations. As discussed in Section 3.2, for the HIO_2 -EDA binary system, the calculated $\sum\gamma$ and $\beta C/\sum\gamma$ values indicate that the clusters exhibit poor stability and thus cannot further grow. For the $(\text{HIO}_3)_x(\text{HIO}_2)_y(\text{EDA})_z$ ($x = 1-3$, $y+z = 2-3$) ternary clusters, the larger $(\text{HIO}_3)_3(\text{HIO}_2)_1(\text{EDA})_2$ cluster exhibits a $\sum\gamma$ of $8.33 \times 10^{-10} \text{ s}^{-1}$ at 278.15 K. Under marine-relevant atmospheric conditions and at the specified low concentrations of the three precursors, this cluster satisfies the $\beta C/\sum\gamma > 1$ criterion for all monomer interactions. Accordingly, $(\text{HIO}_3)_4(\text{HIO}_2)_1(\text{EDA})_2$, $(\text{HIO}_3)_3(\text{HIO}_2)_2(\text{EDA})_2$, and $(\text{HIO}_3)_3(\text{HIO}_2)_1(\text{EDA})_3$ clusters are also set as boundary clusters for ACDC simulations in this work.

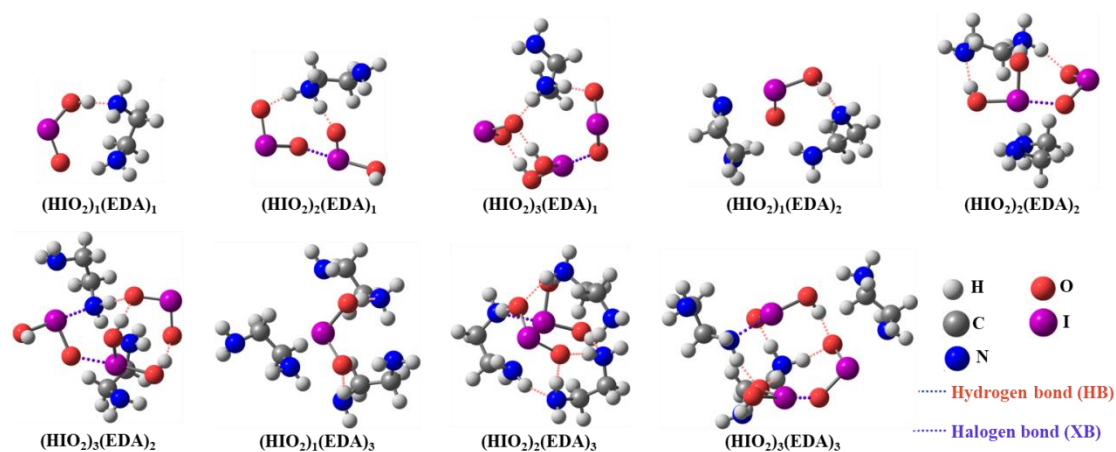


Figure S1 Identified global minimum configurations of (HIO₂)₀₋₃(EDA)₀₋₃ clusters at the DLPNO-CCSD(T)/aug-cc-pVTZ(-pp)//ωB97X-D/aug-cc-pVDZ(-pp) level of theory. The dashed red and purple lines indicate HBs and XBs, respectively.

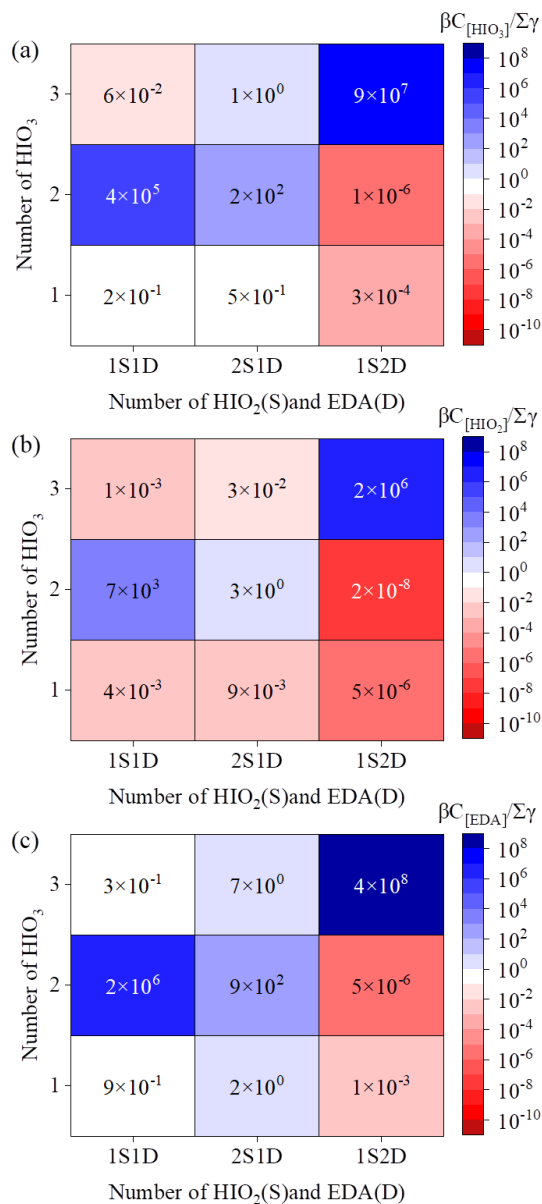


Figure S2 The ratio of the collision frequency between the cluster and monomer molecule at the concentration C to the total evaporation frequency of the cluster ($\beta C / \Sigma \gamma$) for $(\text{HIO}_3)_x(\text{HIO}_2)_y(\text{EDA})_z$ ($x = 1-3$, $y + z = 2-3$) clusters at (a) $C_{[\text{HIO}_3]} = 10^6 \text{ cm}^{-3}$, (b) $C_{[\text{HIO}_2]} = 2 \times 10^4 \text{ cm}^{-3}$, and (c) $C_{[\text{EDA}]} = 0.1 \text{ ppt}$ and $T = 258.15 \text{ K}$.

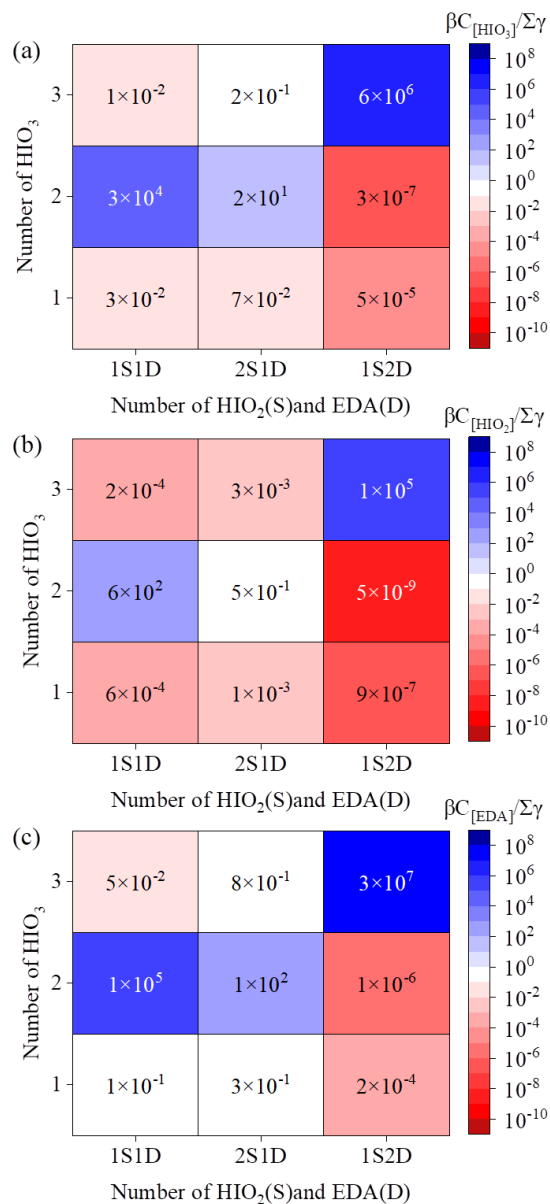


Figure S3 The ratio of the collision frequency between the cluster and monomer molecule at the concentration C to the total evaporation frequency of the cluster ($\beta C / \Sigma \gamma$) for $(\text{HIO}_3)_x(\text{HIO}_2)_y(\text{EDA})_z$ ($x = 1-3$, $y + z = 2-3$) clusters at (a) $C_{[\text{HIO}_3]} = 10^6 \text{ cm}^{-3}$, (b) $C_{[\text{HIO}_2]} = 2 \times 10^4 \text{ cm}^{-3}$, and (c) $C_{[\text{EDA}]} = 0.1 \text{ ppt}$ and $T = 268.15 \text{ K}$.

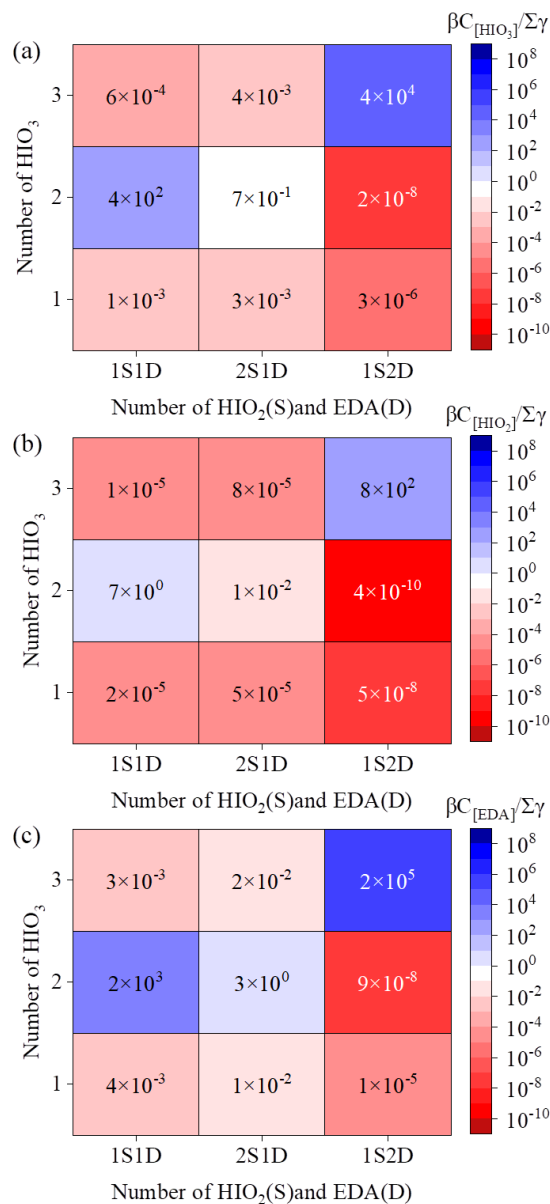


Figure S4 The ratio of the collision frequency between the cluster and monomer molecule at the concentration C to the total evaporation frequency of the cluster ($\beta C / \Sigma \gamma$) for $(\text{HIO}_3)_x(\text{HIO}_2)_y(\text{EDA})_z$ ($x = 1-3$, $y + z = 2-3$) clusters at (a) $C_{[\text{HIO}_3]} = 10^6 \text{ cm}^{-3}$, (b) $C_{[\text{HIO}_2]} = 2 \times 10^4 \text{ cm}^{-3}$, and (c) $C_{[\text{EDA}]} = 0.1 \text{ ppt}$ and $T = 288.15 \text{ K}$.

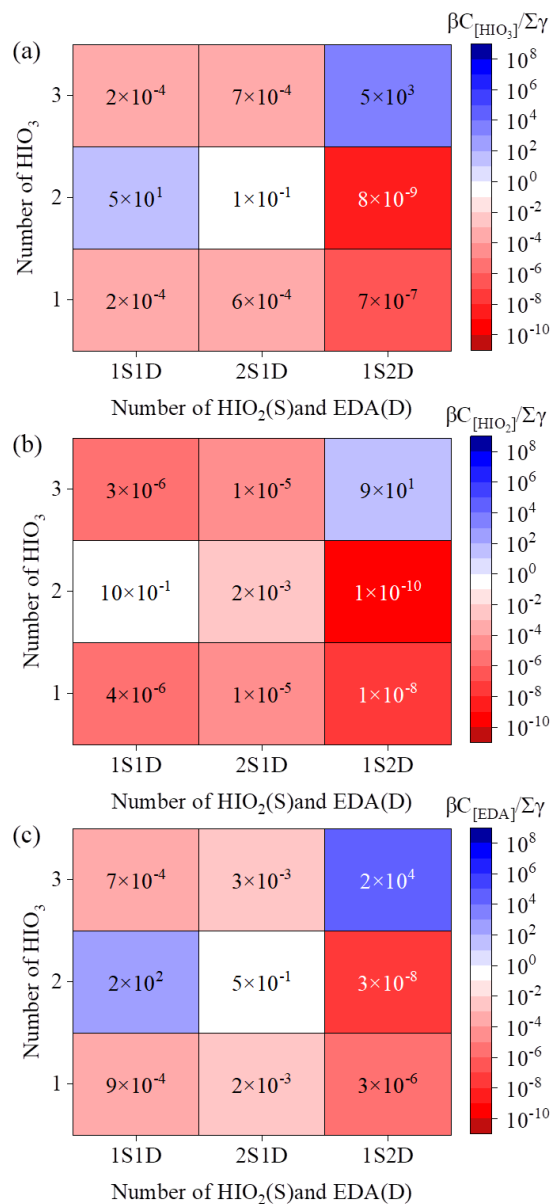


Figure S5 The ratio of the collision frequency between the cluster and monomer molecule at the concentration C to the total evaporation frequency of the cluster ($\beta C/\Sigma\gamma$) for $(\text{HIO}_3)_x(\text{HIO}_2)_y(\text{EDA})_z$ ($x = 1-3$, $y + z = 2-3$) clusters at (a) $C_{[\text{HIO}_3]} = 10^6 \text{ cm}^{-3}$, (b) $C_{[\text{HIO}_2]} = 2 \times 10^4 \text{ cm}^{-3}$, and (c) $C_{[\text{EDA}]} = 0.1 \text{ ppt}$ and $T = 298.15 \text{ K}$.

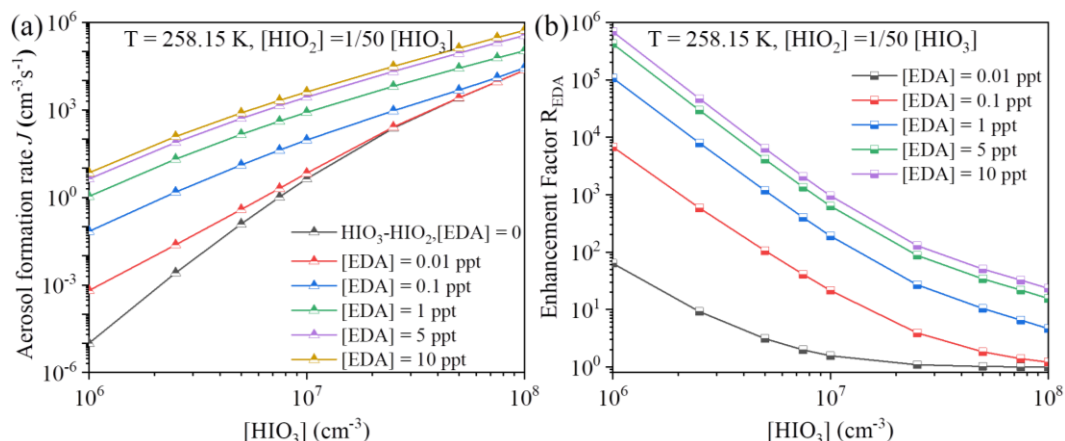


Figure S6 (a) Aerosol formation rates J (cm³ s⁻¹) of HIO₃-HIO₂ system and HIO₃-HIO₂-EDA system and (b) corresponding enhancement factor of EDA (R_{EDA}) for HIO₃-HIO₂-EDA system compared with HIO₃-HIO₂ system at T = 258.15 K, 1atm, CS = 0.002 s⁻¹, [HIO₃] = 10⁶ - 10⁸ cm⁻³, [HIO₂] = 2 × 10⁴ - 2 × 10⁶ cm⁻³, [EDA] = 0.01, 0.1, 1, 5, 10 ppt, and CS = 0.002 s⁻¹.

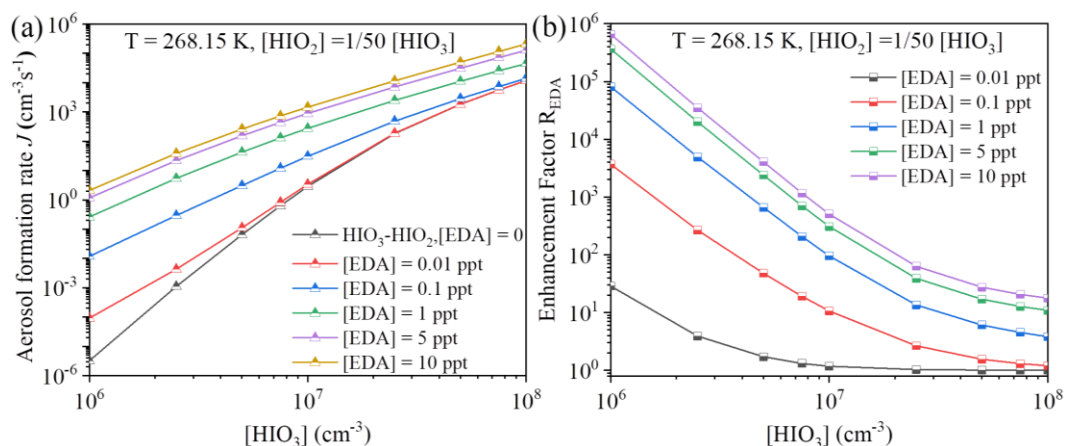


Figure S7 (a) Aerosol formation rates J (cm³ s⁻¹) of HIO₃-HIO₂ system and HIO₃-HIO₂-EDA system and (b) corresponding enhancement factor of EDA (R_{EDA}) for HIO₃-HIO₂-EDA system compared with HIO₃-HIO₂ system at T = 268.15 K, 1atm, CS = 0.002 s⁻¹, [HIO₃] = 10⁶ - 10⁸ cm⁻³, [HIO₂] = 2 × 10⁴ - 2 × 10⁶ cm⁻³, [EDA] = 0.01, 0.1, 1, 5, 10 ppt, and CS = 0.002 s⁻¹.

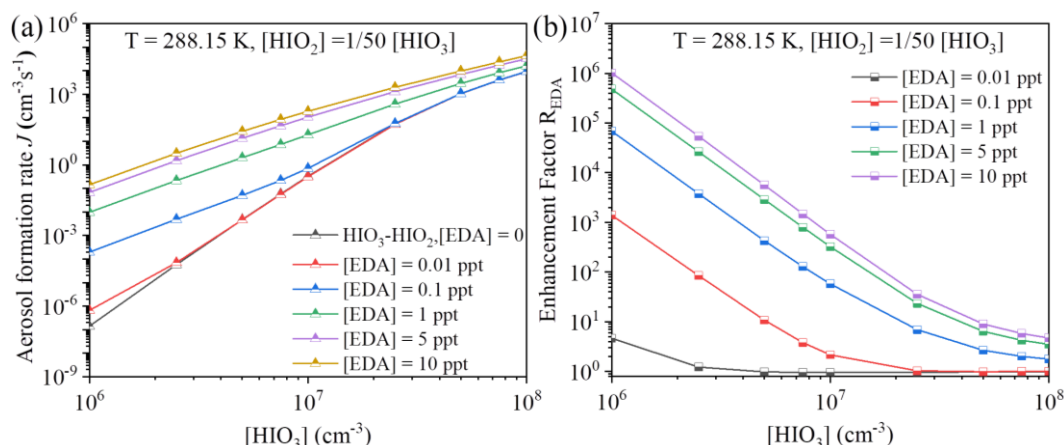


Figure S8 (a) Aerosol formation rates J (cm³ s⁻¹) of HIO₃-HIO₂ system and HIO₃-HIO₂-EDA system and (b) corresponding enhancement factor of EDA (R_{EDA}) for HIO₃-HIO₂-EDA system compared with HIO₃-HIO₂ system at $T = 288.15$ K, 1atm, $CS = 0.002$ s⁻¹, $[HIO_3] = 10^6 - 10^8$ cm⁻³, $[HIO_2] = 2 \times 10^4 - 2 \times 10^6$ cm⁻³, $[EDA] = 0.01, 0.1, 1, 5, 10$ ppt, and $CS = 0.002$ s⁻¹.

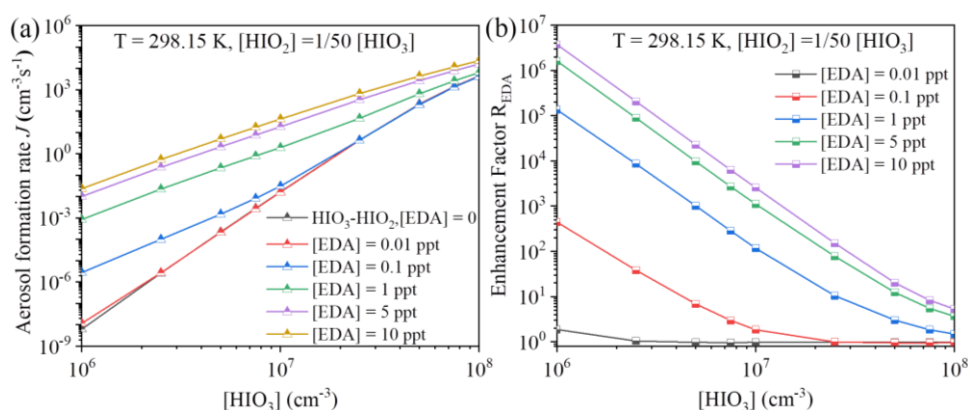


Figure S9 (a) Aerosol formation rates J (cm³ s⁻¹) of HIO₃-HIO₂ system and HIO₃-HIO₂-EDA system and (b) corresponding enhancement factor of EDA (R_{EDA}) for HIO₃-HIO₂-EDA system compared with HIO₃-HIO₂ system at $T = 298.15$ K, 1atm, $CS = 0.002$ s⁻¹, $[HIO_3] = 10^6 - 10^8$ cm⁻³, $[HIO_2] = 2 \times 10^4 - 2 \times 10^6$ cm⁻³, $[EDA] = 0.01, 0.1, 1, 5, 10$ ppt, and $CS = 0.002$ s⁻¹.

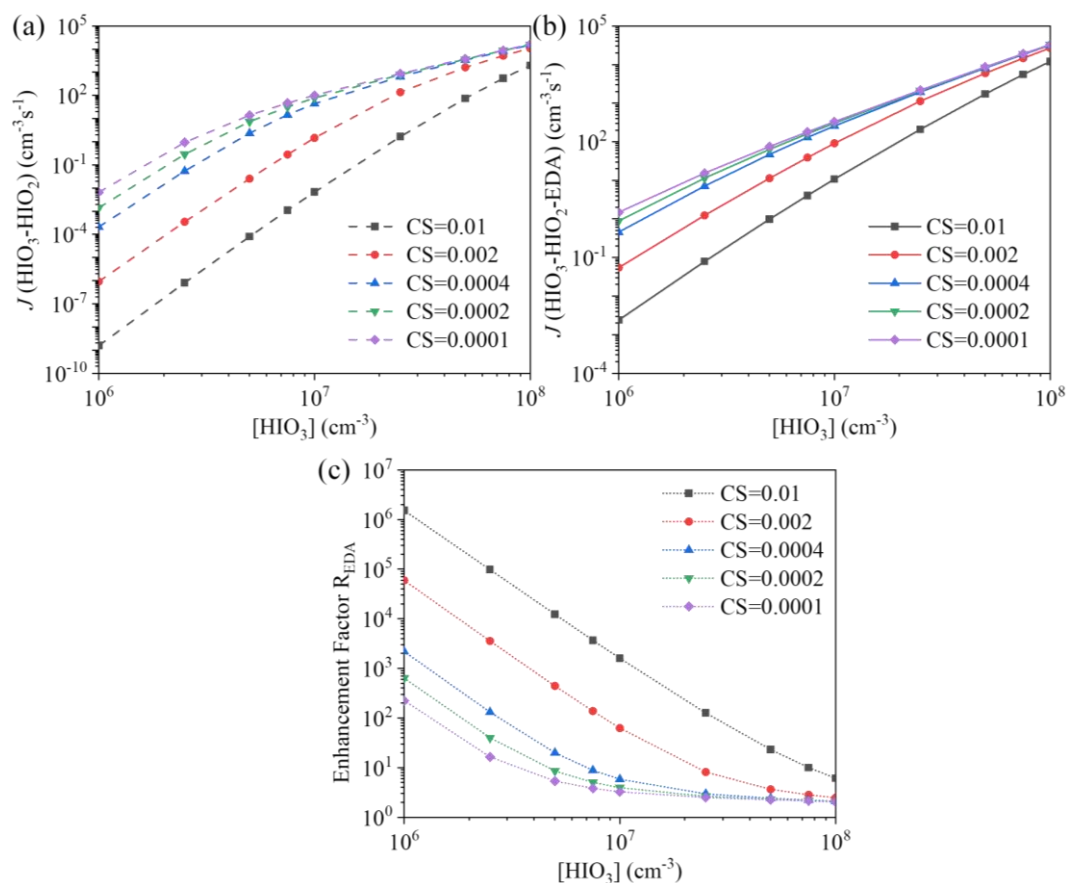


Figure S10 Variation of the aerosol formation rate J ($cm^{-3} s^{-1}$) for (a) HIO_3 - HIO_2 system and (b) HIO_3 - HIO_2 -EDA system and (c) the corresponding enhancement factor of EDA (R_{EDA}) as a function of $[HIO_3]$ at $T = 278.15$ K, $[HIO_3] = 10^6 - 10^8 cm^{-3}$, $[HIO_2] = 2 \times 10^4 - 2 \times 10^6 cm^{-3}$, $[EDA] = 1$ ppt, and $CS = 0.01 s^{-1}, 0.002 s^{-1}, 0.0004 s^{-1}, 0.0002 s^{-1}$ and $0.0001 s^{-1}$.

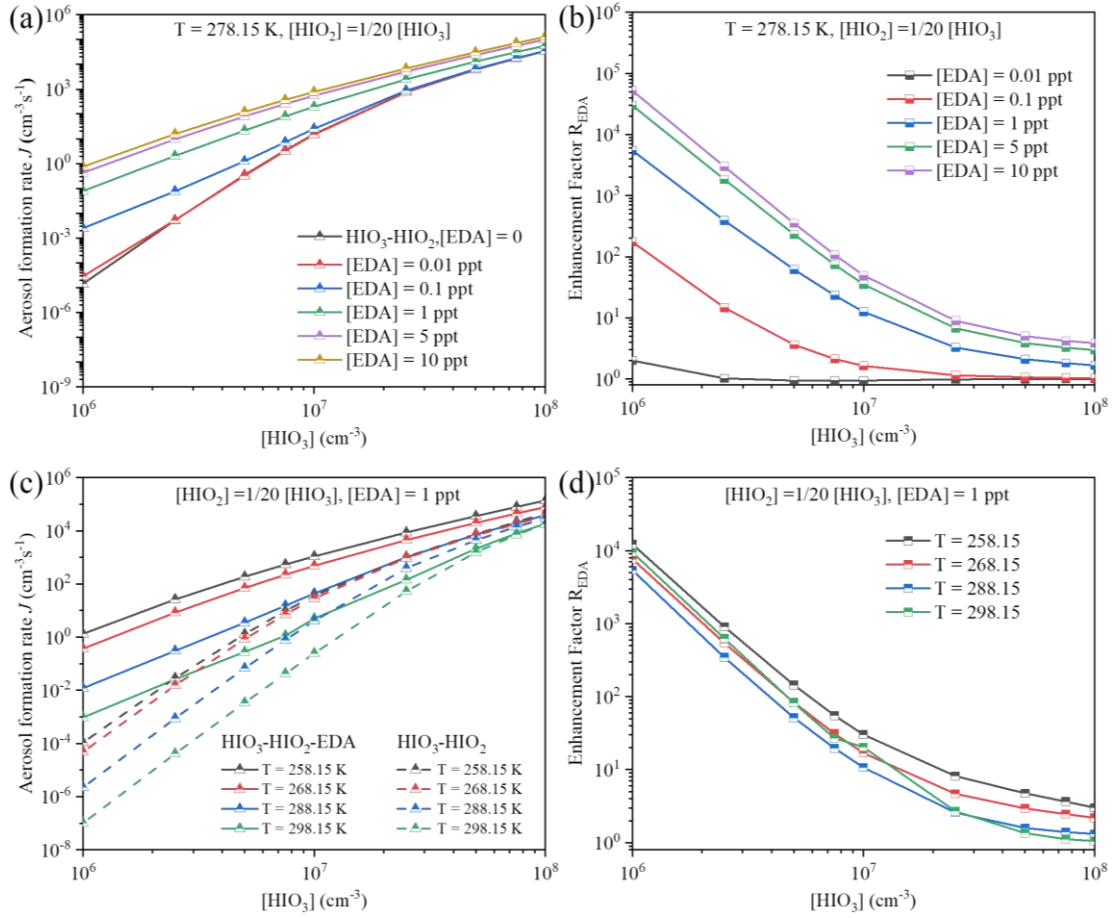


Figure S11 (a) Aerosol formation rate (J , $\text{cm}^{-3}\text{s}^{-1}$) of HIO_3 - HIO_2 system and HIO_3 - HIO_2 -EDA system and (b) corresponding enhancement factor of EDA (R_{EDA}) for HIO_3 - HIO_2 -EDA system compared with HIO_3 - HIO_2 system at $T = 278.15$ K, 1atm, $\text{CS} = 0.002 \text{ s}^{-1}$, $[\text{HIO}_3] = 10^6 - 10^8 \text{ cm}^{-3}$, $[\text{HIO}_2] = 5 \times 10^4 - 5 \times 10^6 \text{ cm}^{-3}$, $[\text{EDA}] = 0.01, 0.1, 1, 5, 10 \text{ ppt}$. (c) Aerosol formation rate (J , $\text{cm}^{-3}\text{s}^{-1}$) of HIO_3 - HIO_2 system and HIO_3 - HIO_2 -EDA system and (d) corresponding enhancement factor of EDA (R_{EDA}) for HIO_3 - HIO_2 -EDA system compared with HIO_3 - HIO_2 system at $T = 258.15, 268.15, 288.15, 298.15$ K, 1atm, $\text{CS} = 0.002 \text{ s}^{-1}$, $[\text{HIO}_3] = 10^6 - 10^8 \text{ cm}^{-3}$, $[\text{HIO}_2] = 5 \times 10^4 - 5 \times 10^6 \text{ cm}^{-3}$, $[\text{EDA}] = 1 \text{ ppt}$.

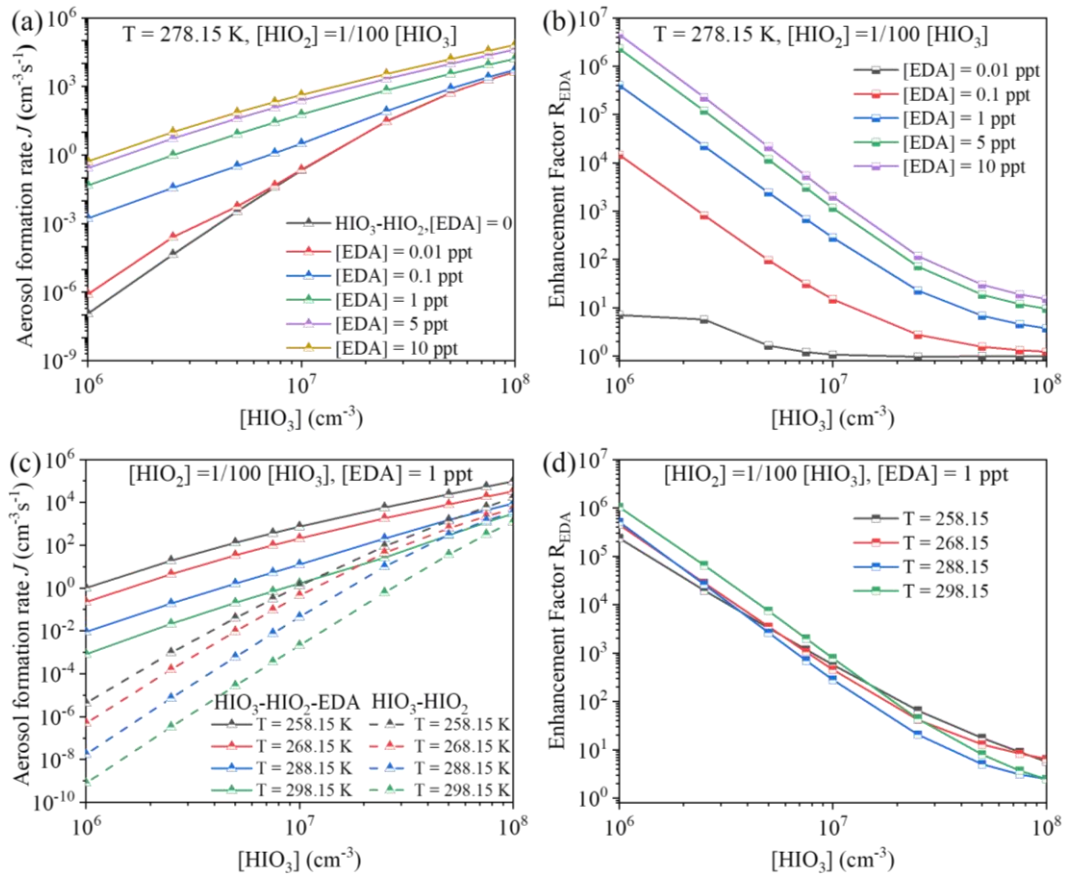


Figure S12 (a) Aerosol formation rate (J , $\text{cm}^3 \text{s}^{-1}$) of $\text{HIO}_3\text{-HIO}_2$ system and $\text{HIO}_3\text{-HIO}_2\text{-EDA}$ system and (b) corresponding enhancement factor of EDA (R_{EDA}) for $\text{HIO}_3\text{-HIO}_2\text{-EDA}$ system compared with $\text{HIO}_3\text{-HIO}_2$ system at $T = 278.15 \text{ K}$, 1 atm , $\text{CS} = 0.002 \text{ s}^{-1}$, $[\text{HIO}_3] = 10^6 - 10^8 \text{ cm}^{-3}$, $[\text{HIO}_2] = 10^4 - 10^6 \text{ cm}^{-3}$, $[\text{EDA}] = 0.01, 0.1, 1, 5, 10 \text{ ppt}$. (c) Aerosol formation rate (J , $\text{cm}^3 \text{s}^{-1}$) of $\text{HIO}_3\text{-HIO}_2$ system and $\text{HIO}_3\text{-HIO}_2\text{-EDA}$ system and (d) corresponding enhancement factor of EDA (R_{EDA}) for $\text{HIO}_3\text{-HIO}_2\text{-EDA}$ system compared with $\text{HIO}_3\text{-HIO}_2$ system at $T = 258.15, 268.15, 288.15, 298.15 \text{ K}$, 1 atm , $\text{CS} = 0.002 \text{ s}^{-1}$, $[\text{HIO}_3] = 10^6 - 10^8 \text{ cm}^{-3}$, $[\text{HIO}_2] = 10^4 - 10^6 \text{ cm}^{-3}$, $[\text{EDA}] = 1 \text{ ppt}$.

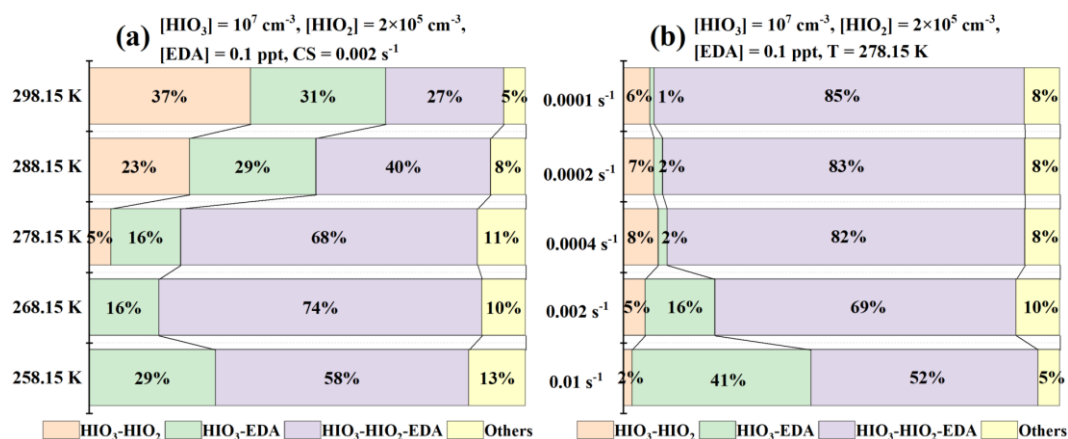


Figure S13 The influence of (a) T (258.15, 268.15, 278.15, 288.15, 298.15 K) and (b) CS (0.01, 0.002, 0.0004, 0.0002, 0.0001 s^{-1}) at $[\text{HIO}_3] = 10^7$, $[\text{HIO}_2] = 2 \times 10^5 \text{ cm}^{-3}$, $[\text{EDA}] = 0.1 \text{ ppt}$ at CS = 0.002 s^{-1} and T = 278.15 K, respectively, on the relative contribution of the $\text{HIO}_3\text{-HIO}_2$, $\text{HIO}_3\text{-EDA}$, and the $\text{HIO}_3\text{-HIO}_2\text{-EDA}$ clustering route to the system flux. Others indicate that the route contribution of the cluster growing out of the studied system is less than 5%.

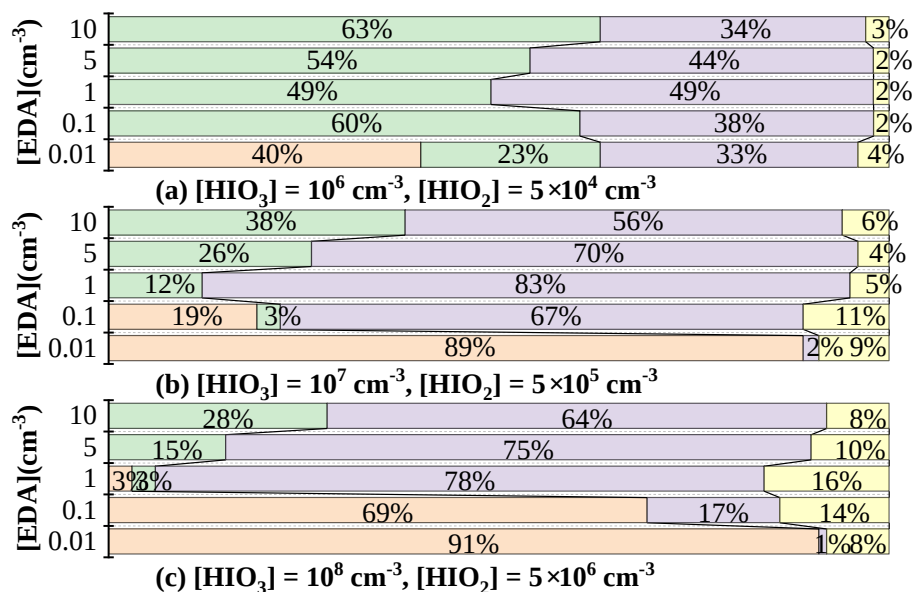


Figure S14 The influence of [EDA] (0.01-10 ppt), [HIO₃] and [HIO₂] ((a) [HIO₃] = 10⁶, [HIO₂] = 5 × 10⁴ cm⁻³, (b) [HIO₃] = 10⁷, [HIO₂] = 5 × 10⁵ cm⁻³, (c) [HIO₃] = 10⁸, [HIO₂] = 5 × 10⁶ cm⁻³ at 278.15 K and CS = 0.002 s⁻¹ on the relative contribution of the HIO₃-HIO₂, HIO₃-EDA, and the HIO₃-HIO₂-EDA clustering route to the system flux. Others indicate that the route contribution of the cluster growing out of the studied system is less than 5%.

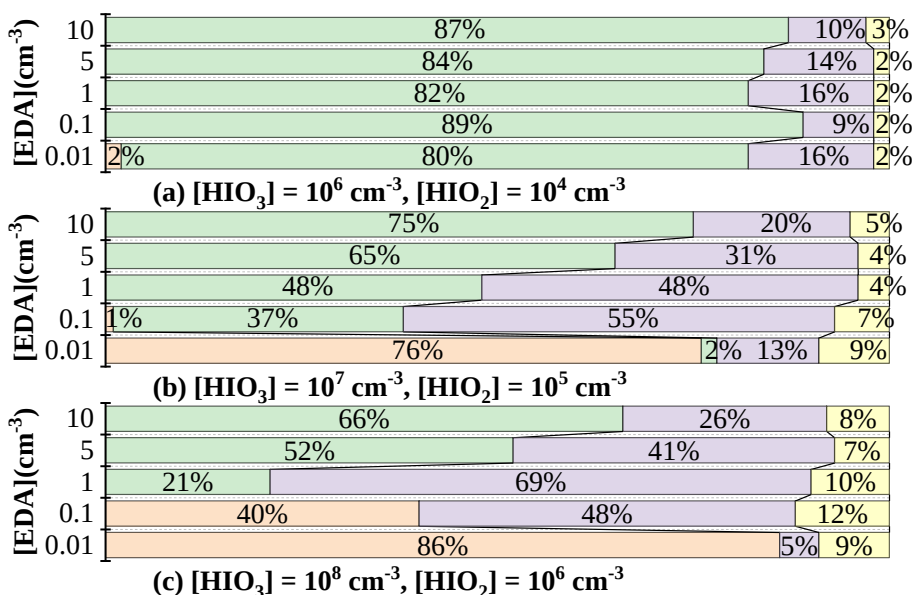


Figure S15 The influence of [EDA] (0.01-10 ppt), [HIO₃] and [HIO₂] ((a) [HIO₃] = 10⁶, [HIO₂] = 10⁴ cm⁻³, (b) [HIO₃] = 10⁷, [HIO₂] = 10⁵ cm⁻³, (c) [HIO₃] = 10⁸, [HIO₂] = 10⁶ cm⁻³ at 278.15 K and CS = 0.002 s⁻¹ on the relative contribution of the HIO₃-HIO₂, HIO₃-EDA, and the HIO₃-HIO₂-EDA clustering route to the system flux. Others indicate that the route contribution of the cluster growing out of the studied system is less than 5%.

Table S1 The number of HBs/XBs and the number of proton transfer for $(\text{HIO}_2)_{1-3}(\text{EDA})_{1-3}$ clusters and $(\text{HIO}_3)_x(\text{HIO}_2)_y(\text{EDA})_z$ ($x = 1-3$, $y+z = 2-3$) clusters.

Cluster	HBs	XBs	n
$(\text{HIO}_2)_1(\text{EDA})_1$	0	1	0
$(\text{HIO}_2)_2(\text{EDA})_1$	2	1	1
$(\text{HIO}_2)_3(\text{EDA})_1$	4	1	2
$(\text{HIO}_2)_1(\text{EDA})_2$	1	0	0
$(\text{HIO}_2)_2(\text{EDA})_2$	3	1	1
$(\text{HIO}_2)_3(\text{EDA})_2$	3	2	1
$(\text{HIO}_2)_1(\text{EDA})_3$	2	0	0
$(\text{HIO}_2)_2(\text{EDA})_3$	7	1	1
$(\text{HIO}_2)_3(\text{EDA})_3$	5	2	1
$(\text{HIO}_3)_1(\text{HIO}_2)_1(\text{EDA})_1$	3	1	1
$(\text{HIO}_3)_1(\text{HIO}_2)_2(\text{EDA})_1$	3	2	1
$(\text{HIO}_3)_1(\text{HIO}_2)_1(\text{EDA})_2$	5	1	1
$(\text{HIO}_3)_2(\text{HIO}_2)_1(\text{EDA})_1$	5	1	2
$(\text{HIO}_3)_2(\text{HIO}_2)_2(\text{EDA})_1$	5	2	2
$(\text{HIO}_3)_3(\text{HIO}_2)_1(\text{EDA})_1$	5	3	2
$(\text{HIO}_3)_2(\text{HIO}_2)_1(\text{EDA})_2$	7	1	2
$(\text{HIO}_3)_3(\text{HIO}_2)_2(\text{EDA})_1$	6	3	2
$(\text{HIO}_3)_3(\text{HIO}_2)_1(\text{EDA})_2$	10	0	3

251 **Table S2** The formation free energy (ΔG , kcal mol⁻¹) for all clusters of HIO₃-HIO₂-EDA system at
 252 the DLPNO-CCSD(T)/aug-cc-pVTZ(-pp)// ω B97X-D/aug-cc-pVDZ(-pp) level of theory and $T =$
 253 298.15 K, 288.15 K, 278.15K, 268.15 K, and 258.15 K.

Cluster	ΔG (kcal mol ⁻¹)				
	298.15 K	288.15 K	278.15K	268.15 K	258.15 K
(HIO ₃) ₁ (HIO ₂) ₁	-16.94	-17.34	-17.74	-18.15	-18.55
(HIO ₃) ₁ (HIO ₂) ₂	-35.22	-36.06	-36.90	-37.74	-38.57
(HIO ₃) ₁ (HIO ₂) ₃	-49.35	-50.62	-51.89	-53.16	-54.43
(HIO ₃) ₂ (HIO ₂) ₁	-31.37	-32.20	-33.04	-33.88	-34.72
(HIO ₃) ₂ (HIO ₂) ₂	-48.63	-49.87	-51.11	-52.35	-53.59
(HIO ₃) ₂ (HIO ₂) ₃	-67.56	-69.23	-70.90	-72.57	-74.24
(HIO ₃) ₃ (HIO ₂) ₁	-44.18	-45.41	-46.63	-47.85	-49.08
(HIO ₃) ₃ (HIO ₂) ₂	-65.63	-67.33	-69.03	-70.72	-72.42
(HIO ₃) ₃ (HIO ₂) ₃	-89.78	-91.94	-94.09	-96.25	-98.41
(HIO ₂) ₂	-17.59	-18.01	-18.43	-18.84	-19.26
(HIO ₂) ₃	-33.65	-34.49	-35.34	-36.18	-37.03
(HIO ₂) ₄	-48.19	-49.47	-50.75	-52.03	-53.31
(HIO ₂) ₅	-61.09	62.79	-64.49	-66.18	-67.88
(HIO ₂) ₆	-77.47	-79.64	-81.81	-83.98	-86.15
(HIO ₃) ₂	-10.62	-11.01	-11.41	-11.80	-12.19
(HIO ₃) ₃	-20.83	-21.62	-22.41	-23.20	-23.98
(HIO ₃) ₄	-38.01	-39.23	-40.46	-41.68	-42.90
(HIO ₃) ₅	-53.20	-54.84	-56.47	-58.11	-59.75
(HIO ₃) ₆	-68.42	-70.53	-72.65	-74.76	-76.88
(EDA) ₂	4.28	3.97	3.67	3.36	3.06
(EDA) ₃	7.02	6.28	5.54	4.80	4.06
(HIO ₃) ₁ (EDA) ₁	-10.28	-10.66	-11.04	-11.41	-11.79
(HIO ₃) ₁ (EDA) ₂	-18.48	-19.26	-20.04	-20.83	-21.61
(HIO ₃) ₁ (EDA) ₃	-19.97	-21.13	-22.30	-23.46	-24.63
(HIO ₃) ₂ (EDA) ₁	-28.80	-29.57	-30.34	-31.10	-31.87
(HIO ₃) ₂ (EDA) ₂	-42.23	-43.47	-44.71	-45.94	-47.18
(HIO ₃) ₂ (EDA) ₃	-42.38	-43.97	-45.56	-47.15	-48.75
(HIO ₃) ₃ (EDA) ₁	-45.35	-46.62	-47.89	-49.15	-50.42
(HIO ₃) ₃ (EDA) ₂	-62.57	-64.23	-65.88	-67.53	-69.19
(HIO ₃) ₃ (EDA) ₃	-79.35	-81.42	-83.49	-85.56	-87.63
(HIO ₂) ₁ (EDA) ₁	-7.35	-7.74	-8.13	-8.52	-8.91
(HIO ₂) ₂ (EDA) ₁	-21.04	-21.82	-22.60	-23.38	-24.15
(HIO ₂) ₃ (EDA) ₁	-36.79	-38.02	-39.26	-40.49	-41.73
(HIO ₂) ₁ (EDA) ₂	-11.13	-11.90	-12.68	-13.46	-14.24
(HIO ₂) ₂ (EDA) ₂	-25.84	-27.04	-28.25	-29.45	-30.66
(HIO ₂) ₃ (EDA) ₂	-45.00	-46.66	-48.32	-49.97	-51.63
(HIO ₂) ₁ (EDA) ₃	-12.24	-13.38	-14.52	-15.67	-16.81
(HIO ₂) ₂ (EDA) ₃	-31.47	-33.19	-34.90	-36.62	-38.33
(HIO ₂) ₃ (EDA) ₃	-48.04	-50.08	-52.11	-54.14	-56.18

$(\text{HIO}_3)_1(\text{HIO}_2)_1(\text{EDA})_1$	-30.43	-31.27	-32.10	-32.93	-33.76
$(\text{HIO}_3)_1(\text{HIO}_2)_2(\text{EDA})_1$	-49.28	-50.52	-51.77	-53.01	-54.26
$(\text{HIO}_3)_2(\text{HIO}_2)_1(\text{EDA})_1$	-52.28	-53.56	-54.85	-56.14	-57.42
$(\text{HIO}_3)_2(\text{HIO}_2)_2(\text{EDA})_1$	-69.26	-70.93	-72.60	-74.27	-75.94
$(\text{HIO}_3)_3(\text{HIO}_2)_1(\text{EDA})_1$	-65.34	-66.97	-68.60	-70.23	-71.86
$(\text{HIO}_3)_3(\text{HIO}_2)_2(\text{EDA})_1$	-83.56	-85.76	-87.95	-90.15	-92.34
$(\text{HIO}_3)_1(\text{HIO}_2)_1(\text{EDA})_2$	-40.51	-41.77	-43.04	-44.31	-45.57
$(\text{HIO}_3)_2(\text{HIO}_2)_1(\text{EDA})_2$	-59.69	-61.38	-63.06	-64.75	-66.44
$(\text{HIO}_3)_3(\text{HIO}_2)_1(\text{EDA})_2$	-88.87	-91.00	-93.12	-95.25	-97.38

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258 **Table S3** The total evaporation rate coefficients (γ , s^{-1}) for all clusters of HIO_3 - HIO_2 -EDA system
 259 at $T = 298.15 \text{ K}$, 288.15 K , 278.15 K , 268.15 K , and 258.15 K .

Cluster	$\Sigma \gamma (\text{s}^{-1})$				
	298.15 K	288.15 K	278.15K	268.15 K	258.15 K
$(\text{HIO}_3)_1(\text{HIO}_2)_1$	2.22×10^{-3}	4.13×10^{-4}	6.81×10^{-5}	9.80×10^{-6}	1.21×10^{-6}
$(\text{HIO}_3)_1(\text{HIO}_2)_2$	9.84×10^{-4}	1.68×10^{-4}	2.53×10^{-5}	3.30×10^{-6}	3.68×10^{-7}
$(\text{HIO}_3)_1(\text{HIO}_2)_3$	3.91×10^{-1}	8.03×10^{-2}	1.41×10^{-2}	2.39×10^{-3}	3.36×10^{-4}
$(\text{HIO}_3)_2(\text{HIO}_2)_1$	1.78×10^{-1}	3.65×10^{-2}	6.68×10^{-3}	1.08×10^{-3}	1.50×10^{-4}
$(\text{HIO}_3)_2(\text{HIO}_2)_2$	1.11×10^0	2.53×10^{-1}	5.21×10^{-2}	9.53×10^{-3}	1.53×10^{-3}
$(\text{HIO}_3)_2(\text{HIO}_2)_3$	3.46×10^{-2}	6.78×10^{-3}	1.18×10^{-3}	1.80×10^{-4}	2.38×10^{-5}
$(\text{HIO}_3)_3(\text{HIO}_2)_1$	3.06×10^0	7.48×10^{-1}	1.65×10^{-1}	3.26×10^{-2}	5.68×10^{-3}
$(\text{HIO}_3)_3(\text{HIO}_2)_2$	4.18×10^{-3}	7.03×10^{-4}	1.04×10^{-4}	1.33×10^{-5}	1.46×10^{-6}
$(\text{HIO}_3)_3(\text{HIO}_2)_3$	5.35×10^{-7}	6.24×10^{-8}	6.23×10^{-9}	5.25×10^{-10}	3.65×10^{-11}
$(\text{HIO}_2)_2$	3.18×10^{-4}	5.58×10^{-5}	8.64×10^{-6}	1.16×10^{-6}	1.34×10^{-7}
$(\text{HIO}_2)_3$	9.45×10^{-3}	1.77×10^{-3}	2.95×10^{-4}	4.29×10^{-5}	5.36×10^{-6}
$(\text{HIO}_2)_4$	9.55×10^{-1}	2.05×10^{-1}	3.95×10^{-2}	6.72×10^{-3}	9.96×10^{-4}
$(\text{HIO}_2)_5$	3.59×10^2	9.55×10^1	2.31×10^1	5.01×10^0	9.65×10^{-1}
$(\text{HIO}_2)_6$	1.21×10^2	2.91×10^1	8.64×10^{-6}	1.22×10^0	2.09×10^{-1}
$(\text{HIO}_3)_2$	5.39×10^1	1.48×10^1	3.69×10^0	8.31×10^{-1}	1.66×10^{-1}
$(\text{HIO}_3)_3$	2.34×10^2	6.59×10^1	1.69×10^1	3.93×10^0	8.12×10^{-1}
$(\text{HIO}_3)_4$	3.87×10^{-3}	6.82×10^{-4}	1.06×10^{-4}	1.44×10^{-5}	1.66×10^{-6}
$(\text{HIO}_3)_5$	6.33×10^{-2}	1.28×10^{-2}	2.32×10^{-3}	3.69×10^{-4}	5.07×10^{-5}
$(\text{HIO}_3)_6$	6.54×10^{-2}	1.18×10^{-2}	1.89×10^{-3}	2.64×10^{-4}	3.15×10^{-5}
$(\text{EDA})_2$	7.92×10^{12}	6.09×10^{12}	4.59×10^{12}	3.38×10^{12}	2.43×10^{12}
$(\text{EDA})_3$	1.33×10^{12}	7.40×10^{11}	3.95×10^{11}	2.01×10^{11}	9.71×10^{10}
$(\text{HIO}_3)_1(\text{EDA})_1$	2.72×10^2	7.84×10^1	2.06×10^1	4.92×10^0	1.05×10^0
$(\text{HIO}_3)_1(\text{EDA})_2$	1.14×10^4	3.53×10^3	1.01×10^3	2.61×10^2	6.09×10^1
$(\text{HIO}_3)_1(\text{EDA})_3$	1.08×10^9	5.16×10^8	2.34×10^8	1.00×10^8	3.99×10^7
$(\text{HIO}_3)_2(\text{EDA})_1$	7.27×10^{-4}	1.31×10^{-4}	2.09×10^{-5}	2.91×10^{-6}	3.48×10^{-7}
$(\text{HIO}_3)_2(\text{EDA})_2$	1.86×10^0	3.78×10^{-1}	6.87×10^{-2}	1.10×10^{-2}	1.52×10^{-3}
$(\text{HIO}_3)_2(\text{EDA})_3$	1.13×10^{10}	6.14×10^9	3.18×10^9	1.57×10^9	7.32×10^8
$(\text{HIO}_3)_3(\text{EDA})_1$	6.12×10^{-3}	9.87×10^{-4}	1.39×10^{-4}	1.70×10^{-5}	1.76×10^{-6}
$(\text{HIO}_3)_3(\text{EDA})_2$	3.40×10^{-3}	6.41×10^{-4}	1.07×10^{-4}	1.57×10^{-5}	1.98×10^{-6}
$(\text{HIO}_3)_3(\text{EDA})_3$	7.81×10^{-3}	1.44×10^{-3}	2.35×10^{-4}	3.34×10^{-5}	4.09×10^{-6}
$(\text{HIO}_2)_1(\text{EDA})_1$	3.36×10^4	1.13×10^4	3.47×10^3	9.82×10^2	2.52×10^2
$(\text{HIO}_2)_2(\text{EDA})_1$	2.80×10^7	1.24×10^7	5.16×10^6	2.01×10^6	7.30×10^5
$(\text{HIO}_2)_3(\text{EDA})_1$	5.30×10^7	2.27×10^7	9.14×10^6	3.44×10^6	1.20×10^6
$(\text{HIO}_2)_1(\text{EDA})_2$	1.84×10^7	7.64×10^6	2.97×10^6	1.08×10^6	3.61×10^5
$(\text{HIO}_2)_2(\text{EDA})_2$	3.57×10^6	1.30×10^6	4.39×10^5	1.37×10^5	3.88×10^4
$(\text{HIO}_2)_3(\text{EDA})_2$	1.19×10^4	3.59×10^3	9.90×10^2	2.48×10^2	5.58×10^1
$(\text{HIO}_2)_1(\text{EDA})_3$	1.96×10^9	9.89×10^8	4.73×10^8	2.14×10^8	9.13×10^7
$(\text{HIO}_2)_2(\text{EDA})_3$	9.93×10^5	2.99×10^5	8.23×10^4	2.06×10^4	4.63×10^3
$(\text{HIO}_2)_3(\text{EDA})_3$	8.34×10^7	3.68×10^7	1.53×10^7	5.96×10^6	2.16×10^6
$(\text{HIO}_3)_1(\text{HIO}_2)_1(\text{EDA})_1$	1.32×10^0	2.88×10^{-1}	5.65×10^{-2}	9.81×10^{-3}	1.49×10^{-3}

$(\text{HIO}_3)_1(\text{HIO}_2)_2(\text{EDA})_1$	5.61×10^{-1}	1.23×10^{-1}	2.43×10^{-2}	4.25×10^{-3}	6.47×10^{-4}
$(\text{HIO}_3)_2(\text{HIO}_2)_1(\text{EDA})_1$	6.50×10^{-6}	8.77×10^{-7}	1.03×10^{-7}	1.02×10^{-8}	8.54×10^{-10}
$(\text{HIO}_3)_2(\text{HIO}_2)_2(\text{EDA})_1$	2.84×10^{-3}	5.46×10^{-4}	9.32×10^{-5}	1.40×10^{-5}	1.80×10^{-6}
$(\text{HIO}_3)_3(\text{HIO}_2)_1(\text{EDA})_1$	2.28×10^0	5.93×10^{-1}	1.40×10^{-1}	2.96×10^{-2}	5.55×10^{-3}
$(\text{HIO}_3)_3(\text{HIO}_2)_2(\text{EDA})_1$	5.27×10^{-1}	9.42×10^{-2}	1.49×10^{-2}	2.04×10^{-3}	2.40×10^{-4}
$(\text{HIO}_3)_1(\text{HIO}_2)_1(\text{EDA})_2$	5.08×10^2	1.34×10^2	3.22×10^1	6.94×10^0	1.33×10^0
$(\text{HIO}_3)_2(\text{HIO}_2)_1(\text{EDA})_2$	5.04×10^4	1.65×10^4	4.98×10^3	1.37×10^3	3.43×10^2
$(\text{HIO}_3)_3(\text{HIO}_2)_1(\text{EDA})_2$	8.54×10^{-8}	9.14×10^{-9}	8.33×10^{-10}	6.35×10^{-11}	3.96×10^{-12}

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Table S4 The Cartesian coordinates of all optimized $(\text{HIO}_2)_x(\text{EDA})_y$ ($x=1-3$, $y=1-3$), $(\text{HIO}_2)_z$ ($z=1-6$) and $(\text{HIO}_3)_x(\text{HIO}_2)_y(\text{EDA})_z$ ($x = 1-3$, $y+z = 2-3$) clusters calculated at the DLPNO-CCSD(T)/aug-cc-pVTZ(-pp)// ω B97X-D/aug-cc-pVDZ(-pp) level of theory.

HIO₂:

Atmos	X	Y	Z
O	-1.35249	1.069015	-0.01094
I	-0.08818	-0.27341	0.004599
O	1.696973	0.622363	-0.11499
H	1.917501	0.959488	0.763597
O	-1.35249	1.069015	-0.01094

(HIO₂)₂:

Atmos	X	Y	Z
O	3.244039	-0.78824	0.105738
I	1.588428	0.34617	-0.0041
O	0.455333	-1.22623	0.017495
H	3.371744	-1.25137	-0.73079
O	-0.45535	1.226247	-0.01753
I	-1.58843	-0.34617	0.004125
O	-3.24405	0.788234	-0.10587
H	-3.37171	1.251542	0.730563

(HIO₂)₃:

Atmos	X	Y	Z
O	3.048161	-2.010702	-0.08532
I	1.03769	-1.803775	-0.138876
O	1.068548	-0.311967	1.077594
H	3.311629	-2.395675	0.758584
O	-0.28467	1.057315	-0.977512
I	1.073261	1.728978	0.213154
O	0.824717	3.618488	-0.448751
H	1.16255	3.694797	-1.348999
O	-1.163745	-1.601721	-0.199251
I	-2.088567	0.084305	-0.084514
O	-3.748602	-0.837477	0.587156
H	-3.615799	-1.114519	1.501594

(HIO₂)₄:

Atmos	X	Y	Z
I	0.82646	2.150394	0.799592
O	-0.090446	1.674674	-0.813968
O	-0.090446	3.951291	0.929598
H	0.269138	4.542849	0.258227
I	-0.82646	-2.150394	0.799592
O	0.090446	-1.674674	-0.813968
O	0.090446	-3.951291	0.929598
H	-0.269138	-4.542849	0.258227

	I	-2.150394	0.82646	-0.799592
	O	-1.674674	-0.090446	0.813968
	O	-3.951291	-0.090446	-0.929598
	H	-4.542849	0.269138	-0.258227
	I	2.150394	-0.82646	-0.799592
	O	1.674674	0.090446	0.813968
	O	3.951291	0.090446	-0.929598
	H	4.542849	-0.269138	-0.258227
269	(HIO ₂) ₅ :			
	Atmos	X	Y	Z
	I	-0.099876	2.383876	-0.037157
	O	-1.046122	1.338324	-1.33142
	O	-1.746792	3.310572	0.650484
	H	-2.183921	2.682502	1.243536
	I	-2.962006	0.300962	-0.823107
	O	-2.341406	0.257359	0.987818
	O	-4.596801	-0.810003	-0.423402
	H	-5.233508	-0.279147	0.069266
	I	0.963086	-1.929919	-1.305599
	O	1.923002	-1.387837	0.272562
	O	2.626454	-1.852262	-2.447818
	H	3.149622	-2.64842	-2.297742
	I	-0.897265	-1.329046	1.767493
	O	-0.855672	-2.032309	-0.010599
	O	0.392939	-2.688836	2.471898
	H	1.242976	-2.475929	2.05617
	I	2.983463	0.601829	0.379215
	O	1.718269	1.286922	-0.872141
	O	3.841671	2.403149	0.703779
	H	4.368242	2.652235	-0.065271
270	(HIO ₂) ₆ :			
	Atmos	X	Y	Z
	I	-3.24539	1.452838	0.011253
	O	-1.432407	1.741087	-0.507897
	O	-3.865518	3.27504	-0.562996
	H	-3.565203	3.935943	0.072393
	I	-2.312994	-2.185823	-0.321535
	O	-2.65698	-0.619822	0.772623
	O	-2.738199	-3.366965	1.238619
	H	-2.004195	-3.319133	1.86859
	I	2.204511	1.988503	0.235098
	O	2.296091	0.678451	1.643604
	O	0.645614	2.949709	1.052113
	H	-0.156136	2.604233	0.604836

I	-0.362344	0.247959	-2.031775
O	-1.99185	-0.767098	-2.009293
O	0.713009	-1.023392	-3.09026
H	1.305018	-1.436856	-2.419138
I	0.39083	-0.249841	2.383255
O	0.953404	-1.884607	1.480535
O	-1.23307	-1.181605	3.04418
H	-1.925612	-0.998964	2.372232
I	3.91966	-1.085238	-0.561438
O	3.873841	0.828059	-0.726694
O	2.122879	-1.631784	-0.829532
H	1.355107	-1.686944	0.573545

271 (HIO₂)₁(EDA)₁:

Atmos	X	Y	Z
H	0.604261	-1.433715	0.256398
O	-0.261515	-1.395681	0.780949
I	-1.402484	-0.070513	-0.112810
O	-0.806100	1.602268	0.439945
C	3.067923	-0.603370	0.198348
C	2.503436	0.761206	0.593071
N	2.019963	1.476791	-0.587481
N	2.060569	-1.316002	-0.601580
H	2.426367	-2.196179	-0.951069
H	1.855952	-0.722054	-1.406090
H	3.289681	-1.190754	1.099767
H	4.008934	-0.470557	-0.362103
H	3.275000	1.317728	1.147853
H	1.659023	0.610996	1.277811
H	2.655252	2.209569	-0.878856
H	1.106219	1.886935	-0.397022
H	0.604261	-1.433715	0.256398
O	-0.261515	-1.395681	0.780949

272 (HIO₂)₂(EDA)₁:

Atmos	X	Y	Z
H	0.966481	2.165603	-0.656801
O	2.459562	1.533308	-0.430126
I	2.343993	-0.304840	-0.030409
O	0.712814	-0.463613	0.991956
H	-3.060808	-2.391265	-1.189363
O	-3.093279	-1.962057	-0.326625
I	-1.239844	-1.279580	0.139898
O	-1.237371	0.064628	-1.187638
C	-0.522635	2.842120	0.679940
C	-2.025544	2.618546	0.848780

N	-2.732995	2.973343	-0.382996
N	-0.075309	2.341338	-0.638842
H	-0.367817	2.979347	-1.375772
H	-0.532173	1.389156	-0.839943
H	0.044037	2.296641	1.442504
H	-0.271802	3.907492	0.740786
H	-2.372592	3.256815	1.671009
H	-2.205230	1.575025	1.150240
H	-3.668390	3.306862	-0.181964
H	-2.838237	2.143667	-0.963579

273 (HIO₂)₃(EDA)₁:

Atmos	X	Y	Z
H	0.318353	-1.048299	-1.194165
O	-0.263889	-1.828739	-0.901606
I	-0.489770	-1.659484	1.020432
O	1.305911	-2.362003	1.439937
H	1.951850	-1.606713	1.339997
O	2.841840	-0.223728	0.960495
I	3.029790	-0.181851	-0.918471
O	1.237597	0.187759	-1.505525
H	-0.899120	2.220741	-0.265210
O	-2.453693	1.993148	-0.151694
I	-3.013534	0.314367	-0.811983
O	-2.591719	-0.959243	0.563798
C	0.525006	2.190424	1.273345
C	0.498609	3.590102	1.870438
N	1.369465	4.462272	1.080988
N	0.165910	2.266524	-0.162583
H	0.595204	1.472899	-0.715231
H	0.531141	3.152967	-0.523028
H	-0.205745	1.544845	1.770483
H	1.513720	1.720478	1.362727
H	0.771030	3.523639	2.935662
H	-0.524403	3.987184	1.813491
H	2.347858	4.278881	1.285729
H	1.198710	5.440350	1.285912

274 (HIO₂)₁(EDA)₂:

Atmos	X	Y	Z
H	-2.132696	-1.215498	0.344469
O	-1.576641	-1.842260	-0.195052
I	0.286854	-1.183229	-0.076965
O	0.278871	0.137732	-1.409261
C	3.133544	0.718382	1.059832
C	2.240722	1.902880	0.697178

N	2.359530	2.200159	-0.728944
N	2.858405	-0.420750	0.168175
H	3.490605	-1.190331	0.371184
H	3.048726	-0.128782	-0.790507
H	2.937049	0.404460	2.094539
H	4.188262	1.028965	0.986117
H	2.578989	2.768591	1.282501
H	1.201254	1.690611	1.001166
H	2.161455	3.176465	-0.913986
H	1.667893	1.645958	-1.238915
C	-3.698727	0.974789	0.381436
C	-2.753434	1.471535	-0.710086
N	-1.555614	2.077684	-0.124706
N	-2.957555	0.076720	1.275684
H	-3.540286	-0.236713	2.045325
H	-2.189243	0.618467	1.670601
H	-4.528303	0.417131	-0.074968
H	-4.126744	1.835784	0.924438
H	-3.302215	2.161998	-1.369930
H	-2.439951	0.615370	-1.321358
H	-1.570580	3.088371	-0.186437
H	-0.731317	1.724292	-0.612198

275 (HIO₂)₂(EDA)₂:

Atmos	X	Y	Z
H	-3.156601	0.312823	-0.535835
O	-2.716477	0.919547	-1.174176
I	-0.755757	0.525414	-1.083460
O	-0.986636	-1.367733	-1.607571
H	-1.044687	-1.839458	-0.732160
O	1.457173	-1.070601	1.553370
I	2.432360	-1.017405	-0.056520
O	1.547759	0.324947	-1.122920
C	-3.456587	-1.829527	1.564297
C	-1.996055	-1.600552	1.923258
N	-1.087416	-2.315811	1.020655
N	-3.763643	-1.320551	0.224999
H	-4.753481	-1.423746	0.023531
H	-3.269345	-1.864072	-0.479705
H	-4.082060	-1.288792	2.287272
H	-3.692434	-2.904791	1.670438
H	-1.846068	-1.886837	2.978054
H	-1.767022	-0.529057	1.840492
H	-1.154047	-3.317786	1.180825
H	-0.120927	-2.033933	1.250377

C	0.811512	3.234473	0.438300
C	0.899289	2.446218	1.740162
N	-0.222315	2.797265	2.615961
N	-0.491266	3.002315	-0.199530
H	-0.668249	3.666895	-0.946215
H	-1.221552	3.114504	0.503690
H	1.605507	2.896601	-0.240825
H	0.967280	4.307800	0.644225
H	1.887346	2.632353	2.192832
H	0.844702	1.369980	1.533584
H	-0.050700	3.676456	3.095292
H	-0.348681	2.091127	3.332721

276 (HIO₂)₃(EDA)₂:

Atmos	X	Y	Z
H	-0.462101	0.563797	-1.875238
O	-0.141888	-0.290218	-2.278188
I	-0.444445	-1.639577	-0.884348
O	-2.361029	-1.907785	-1.307051
H	-2.816855	-1.229312	-0.743526
O	-3.069296	0.016750	0.430069
I	-2.800573	1.749384	-0.298688
O	-0.966007	1.810547	-0.829536
H	4.030263	-0.701275	-2.173069
O	4.311102	-0.571928	-1.259672
I	2.745743	0.174678	-0.193995
O	1.798930	-1.481224	-0.169437
C	1.195582	2.198009	1.975409
C	1.684576	3.378272	1.148834
N	2.989220	3.076940	0.550425
N	0.912785	1.041603	1.120401
H	0.190095	1.316614	0.426117
H	0.483157	0.287365	1.676768
H	0.287668	2.495988	2.523906
H	1.953171	1.916558	2.722428
H	1.698290	4.279980	1.783421
H	0.967202	3.553816	0.335450
H	3.733083	3.169902	1.236566
H	3.202167	3.719968	-0.205257
C	-1.017790	-1.996812	3.216527
C	-0.191235	-2.990969	2.410975
N	-0.843719	-3.374490	1.147618
N	-1.076101	-0.662983	2.618683
H	-1.456610	-0.014079	3.301976
H	-1.735347	-0.614838	1.833588

H	-0.535711	-1.905262	4.199498
H	-2.020944	-2.429159	3.396654
H	-0.015966	-3.874155	3.046276
H	0.784159	-2.548351	2.163285
H	-1.842475	-3.525008	1.273981
H	-0.458257	-4.247859	0.800002

277 (HIO₂)₁(EDA)₃:

Atmos	X	Y	Z
H	-1.498534	1.723556	-1.210191
O	-0.856430	1.536351	-1.939049
I	0.313198	0.111708	-1.165519
O	-0.626526	-1.407681	-1.746776
C	-0.709110	3.274102	1.587693
C	-1.556624	2.009463	1.644830
N	-2.359577	1.826767	0.432248
N	0.325420	3.185594	0.556401
H	0.908128	4.016602	0.573586
H	-0.099662	3.150180	-0.367768
H	-0.212028	3.398238	2.560298
H	-1.380370	4.145175	1.456414
H	-2.176753	2.042882	2.557645
H	-0.887567	1.142857	1.731892
H	-3.147315	2.468405	0.428168
H	-2.734299	0.868892	0.401479
C	-2.908268	-2.096464	1.178173
C	-1.444211	-2.291854	1.574591
N	-0.635860	-3.084944	0.649742
N	-3.035314	-1.146434	0.070956
H	-3.952305	-1.219168	-0.358261
H	-2.350058	-1.343760	-0.667676
H	-3.461545	-1.700923	2.044443
H	-3.336513	-3.089671	0.945395
H	-1.400994	-2.764262	2.565939
H	-0.977061	-1.298938	1.672102
H	-0.705124	-2.693754	-0.297328
H	-0.977600	-4.040632	0.614409
C	2.296883	-0.890127	1.436467
C	3.341468	0.190680	1.189498
N	4.508551	-0.391811	0.525754
N	1.879809	-1.501951	0.175549
H	1.257526	-2.298336	0.350835
H	2.702720	-1.812277	-0.336180
H	1.416444	-0.441172	1.917429
H	2.702927	-1.641079	2.136966

	H	3.574703	0.684360	2.148547
	H	2.918091	0.959808	0.528755
	H	5.072633	-0.919535	1.185948
	H	5.106665	0.327322	0.134220
278	(HIO₂)₂(EDA)₃:			
	Atmos	X	Y	Z
	H	-1.311565	-0.387144	-2.521985
	O	-1.352043	-1.696631	-1.011233
	I	-2.319153	-1.261685	0.566031
	O	-1.684807	0.421969	1.168563
	H	1.537652	2.420030	-0.075490
	O	2.370906	2.043646	-0.480927
	I	1.994612	0.115906	-0.747796
	O	1.691031	0.200383	-2.676124
	N	-0.952296	0.484113	-2.928987
	C	-1.284291	1.585502	-2.022415
	C	-2.776347	1.833426	-1.810586
	N	-2.957070	2.657842	-0.616137
	H	0.692241	0.317680	-2.839513
	H	-1.370055	0.614448	-3.845655
	H	-0.789163	2.503723	-2.364948
	H	-0.851097	1.326429	-1.051124
	H	-3.286351	0.853444	-1.747466
	H	-3.198750	2.361282	-2.678937
	H	-2.758274	2.077995	0.201754
	H	-3.919921	2.967672	-0.536945
	C	1.807208	-3.140684	0.163734
	C	1.480195	-2.488652	1.501160
	N	2.205246	-1.228588	1.680926
	N	1.371771	-2.289080	-0.948499
	H	0.333843	-2.190764	-0.962175
	H	1.667867	-2.661732	-1.846170
	H	1.325215	-4.130679	0.121115
	H	2.893358	-3.297143	0.084288
	H	1.682245	-3.213851	2.306602
	H	0.405823	-2.261826	1.538748
	H	3.167805	-1.396623	1.958830
	H	1.748681	-0.656703	2.406469
	C	0.471167	3.120511	2.277390
	C	1.270809	1.967553	2.883107
	N	0.521644	0.731158	3.130628
	N	0.080907	2.807116	0.898024
	H	-0.477570	3.556386	0.496907
	H	-0.541919	1.994945	0.896160

H	1.106928	4.017363	2.260220
H	-0.399596	3.338114	2.920972
H	1.712718	2.298179	3.833008
H	2.110613	1.746955	2.206601
H	-0.186671	0.561980	2.404703
H	0.002088	0.807345	3.999295

279 (HIO₂)₃(EDA)₃:

Atmos	X	Y	Z
H	0.848019	-1.327299	1.382856
O	1.639637	1.556523	1.819454
I	0.848942	1.897373	0.140609
O	-0.922658	2.540373	0.849156
H	2.581017	-2.390174	-2.927985
O	1.963336	-1.650834	-2.932944
I	0.486298	-1.997484	-1.538475
O	1.683666	-1.660237	-0.106714
H	-1.390258	1.712671	1.119773
O	-1.930052	0.068580	1.512433
I	-2.591671	-0.982308	0.077237
O	-1.137063	-2.280448	-0.075479
C	4.155871	1.197554	0.003687
C	4.622894	2.607477	-0.324131
N	4.843614	2.739408	-1.765753
N	2.930567	0.879535	-0.730952
H	2.665197	-0.108306	-0.608906
H	3.075205	1.055427	-1.724676
H	3.935964	1.119063	1.074988
H	4.950299	0.472841	-0.243261
H	5.513089	2.836150	0.286409
H	3.837542	3.318789	-0.033529
H	5.699959	2.267632	-2.043187
H	4.943529	3.712281	-2.034082
C	2.440967	-2.024708	3.395929
C	0.970105	-1.638338	3.464412
N	0.575839	-0.859415	2.275678
N	2.656932	-3.081934	2.414391
H	3.625432	-3.383407	2.427185
H	2.457598	-2.761639	1.464421
H	2.730140	-2.407329	4.384338
H	3.033845	-1.107350	3.215359
H	0.775585	-1.019702	4.348505
H	0.350910	-2.541709	3.511672
H	1.053805	0.088880	2.230319
H	-0.441291	-0.669605	2.198681

	C	-4.874342	1.567084	-0.899386
	C	-3.753971	2.601206	-0.990449
	N	-3.690293	3.379277	0.241597
	N	-4.632175	0.709214	0.266794
	H	-5.475755	0.218556	0.548337
	H	-4.356250	1.317593	1.041381
	H	-4.894794	0.949899	-1.809665
	H	-5.844507	2.086251	-0.823214
	H	-3.906588	3.213836	-1.893658
	H	-2.795981	2.077728	-1.112581
	H	-4.190421	4.256987	0.168951
	H	-2.725944	3.564216	0.504994
280	(HIO₃)₁(HIO₂)₁(EDA)₁:			
	Atmos	X	Y	Z
	I	-2.259493	-0.284864	-0.091657
	O	-1.281124	-1.735805	0.494085
	H	0.219011	-1.672935	1.290356
	O	-1.866038	1.032970	1.132388
	O	-1.427300	0.279333	-1.621456
	H	1.859568	-2.603245	-1.341273
	O	2.564035	-2.067991	-0.954853
	I	1.749046	-0.459225	-0.053260
	O	1.178951	-1.497393	1.501326
	C	0.638873	2.964624	-0.428108
	C	1.267027	2.647087	0.923371
	N	0.894605	1.282926	1.328756
	N	1.045995	1.976088	-1.435018
	H	1.526883	2.403938	-2.217066
	H	0.223437	1.480144	-1.787681
	H	0.934287	3.981209	-0.720590
	H	-0.454198	2.954530	-0.318657
	H	0.925105	3.373748	1.675935
	H	2.362730	2.708566	0.858187
	H	-0.143482	1.179880	1.339930
	H	1.232573	1.058612	2.261828
281	(HIO₃)₁(HIO₂)₂(EDA)₁:			
	Atmos	X	Y	Z
	I	1.299145	2.304470	-0.079588
	O	0.240890	1.852597	1.368181
	H	-0.781878	0.685964	1.509750
	O	2.774265	1.234846	0.068972
	O	0.352993	1.697060	-1.530414
	H	-3.181530	2.288001	0.813096
	O	-3.677781	1.463242	0.880249

I	-2.602516	-0.042846	0.063631
O	-1.440723	-0.073752	1.630961
H	0.475207	0.117099	-2.442036
O	0.464568	-0.852613	-2.607435
I	0.446284	-1.626893	-0.788670
O	-1.487328	-1.771743	-0.592707
N	3.039600	-1.656602	0.193544
C	3.018127	-2.055334	1.603145
C	1.710933	-1.636793	2.262546
N	0.563857	-2.322760	1.644972
H	3.822924	-2.077388	-0.295250
H	3.125625	-0.636889	0.116654
H	3.849077	-1.615740	2.178952
H	3.125513	-3.149275	1.660715
H	1.558648	-0.556716	2.130745
H	1.765389	-1.837345	3.343254
H	-0.314853	-1.927541	1.979170
H	0.567841	-3.319734	1.843947

282 (HIO₃)₂(HIO₂)₁(EDA)₁:

Atmos	X	Y	Z
I	-3.402693	-0.869474	-0.323580
O	-2.861182	0.305692	-1.613943
H	-1.889049	1.901149	-1.637976
O	-2.140305	-2.212026	-0.332342
O	-3.085926	-0.013260	1.276142
I	3.588535	-0.247868	-0.516211
O	3.448600	-2.065906	-0.507248
H	-0.547877	-1.989686	-0.175515
O	1.870210	0.233118	-1.062962
O	3.581417	0.252062	1.245432
H	-2.176574	1.370223	1.415371
O	-1.488689	2.091903	1.452390
I	-0.206993	1.626686	0.057693
O	-1.203254	2.548872	-1.368606
C	0.789912	-2.018832	1.466426
C	0.178801	-0.886510	2.277916
N	0.791788	0.424893	1.999882
N	0.494489	-1.940954	0.010640
H	0.970547	-2.706112	-0.469133
H	0.906821	-1.083412	-0.424146
H	0.372133	-2.964781	1.827451
H	1.879880	-2.050318	1.576666
H	0.321976	-1.157637	3.334078
H	-0.903495	-0.819109	2.098185

		H	1.816173	0.360749	1.892565
		H	0.587272	1.064525	2.763048
283	(HIO₃)₂(HIO₂)₂(EDA)₁:				
		Atmos	X	Y	Z
		I	-3.187899	-0.090933	-0.790549
		O	-3.032799	0.939528	0.713116
		H	-1.947452	0.833486	2.283589
		O	-1.905130	0.591520	-1.912814
		O	-2.531638	-1.751482	-0.319787
		I	3.209063	1.068513	-0.087001
		O	3.125823	-0.616088	-0.850169
		H	-0.863553	1.815565	-1.359615
		O	2.446465	2.169632	-1.340568
		O	1.979614	1.076354	1.271101
		H	-1.262187	-2.645097	-1.220942
		O	-0.458519	-3.123957	-1.524404
		I	1.086800	-1.973489	-1.126173
		O	1.130754	-2.238961	0.758737
		H	-1.921626	-2.089931	1.326911
		O	-1.389891	-2.105242	2.155142
		I	-0.075578	-0.686322	1.921705
		O	-1.210467	0.636419	2.894107
		C	-0.481983	3.110154	0.265216
		C	-1.729933	3.980431	0.269942
		N	-1.592972	5.020108	-0.753079
		N	-0.238139	2.619616	-1.112799
		H	0.765696	2.351322	-1.241559
		H	-0.459803	3.397007	-1.745252
		H	-0.590827	2.256318	0.936376
		H	0.405576	3.675971	0.571699
		H	-1.882494	4.365511	1.289636
		H	-2.596656	3.353863	0.026468
		H	-1.014533	5.787199	-0.422828
		H	-2.492989	5.413644	-1.003039
284	(HIO₃)₃(HIO₂)₁(EDA)₁:				
		Atmos	X	Y	Z
		I	3.258472	-0.764552	-0.769380
		O	2.287802	-2.215186	-1.301291
		H	1.045212	-2.928601	-0.377210
		O	2.592782	0.682659	-1.659909
		O	2.815992	-0.487554	1.033020
		I	0.754658	0.132133	1.937019
		O	0.089542	-0.267912	0.248945
		H	0.499622	2.441176	0.015582

O	1.164989	1.886848	1.758820
O	-0.992855	0.270652	2.758909
I	-3.328547	1.211180	-0.445317
O	-2.547793	1.677183	1.147898
H	-1.614184	0.778815	2.158357
O	-2.128773	1.760608	-1.716786
O	-3.290585	-0.634066	-0.510320
H	-2.713334	-4.159818	-0.267257
O	-2.270695	-3.705749	-0.994660
I	-1.269888	-2.151270	-0.275337
O	0.306586	-3.207203	0.220250
N	2.273047	4.358759	0.135387
C	2.223529	4.054785	-1.291080
C	0.823268	3.614002	-1.691103
N	0.449900	2.352988	-1.009872
H	3.095585	4.906979	0.359598
H	2.320823	3.514776	0.702824
H	2.946297	3.285638	-1.613657
H	2.445854	4.972991	-1.850436
H	0.761560	3.432716	-2.770063
H	0.086679	4.373722	-1.408062
H	1.112653	1.592178	-1.254556
H	-0.522972	2.055246	-1.249833

285 (HIO₃)₃(HIO₂)₂(EDA)₁:

Atmos	X	Y	Z
I	-3.715716	0.701454	-0.574566
O	-2.447444	1.283177	-1.751780
H	-0.428463	-0.858068	-0.861057
O	-3.739033	-1.156766	-0.939887
O	-2.977145	0.712804	1.093838
I	3.225524	2.154603	-0.552551
O	1.824443	2.840141	-1.515029
H	0.297752	2.739995	-0.744151
O	2.551003	1.985820	1.143008
O	3.544290	0.441130	-1.195582
I	0.898308	-0.132128	1.799811
O	-0.520224	1.188295	2.349255
H	-1.387367	0.849420	2.043624
O	-0.031704	-1.620520	2.293324
O	0.438712	0.132233	0.036612
H	1.143317	-3.693580	-0.437637
O	2.107043	-3.678449	-0.613526
I	2.681027	-1.801918	-0.802402
O	2.580855	-1.360915	1.051271

H	-0.172509	-3.043402	1.239062
O	-0.528086	-3.580055	0.489713
I	-2.066487	-2.471967	-0.149653
O	-0.921112	-1.547950	-1.401619
N	-0.635841	2.695608	-0.273042
C	-1.187700	4.030335	0.020171
C	-2.485510	3.979544	0.816696
N	-3.636281	3.522245	0.020279
H	-1.272920	2.130720	-0.879789
H	-0.501849	2.155025	0.593193
H	-1.323503	4.558639	-0.932430
H	-0.436946	4.575983	0.602362
H	-2.650897	4.988453	1.226743
H	-2.367471	3.289193	1.662357
H	-3.721627	4.077325	-0.828849
H	-4.486945	3.682187	0.554089

286 (HIO₃)₁(HIO₂)₁(EDA)₂:

Atmos	X	Y	Z
I	-2.302829	-1.159938	-0.071918
O	-0.801943	-2.217335	-0.181476
O	-2.218818	-0.029514	-1.508965
O	-2.002393	-0.102852	1.404904
H	2.440351	-0.425820	-1.703705
O	2.670192	0.538023	-1.587407
I	1.412540	1.206842	-0.209447
O	2.441068	0.551627	1.328616
C	-1.658427	3.026248	-0.106218
C	-0.808155	3.272517	1.134747
N	-0.128724	2.028159	1.517230
N	-0.857309	2.491000	-1.214716
H	-0.707298	3.177371	-1.945090
H	-1.328435	1.671123	-1.609013
H	-2.166641	3.962612	-0.378887
H	-2.433681	2.290614	0.143059
H	-1.451962	3.642349	1.948591
H	-0.045859	4.038964	0.932113
H	-0.807225	1.252941	1.608978
H	0.387992	2.121791	2.386951
C	2.929049	-2.530356	-0.305150
N	1.982233	-2.119972	-1.358524
C	2.275512	-3.025123	0.980080
N	1.472654	-1.965071	1.613752
H	1.012765	-2.109482	-1.029447
H	2.004644	-2.763155	-2.141083

	H	3.584975	-3.322874	-0.690183
	H	3.574245	-1.674421	-0.054936
	H	3.075808	-3.316521	1.674103
	H	1.666343	-3.920159	0.771279
	H	2.123063	-0.394906	1.489529
	H	1.287456	-2.204392	2.583156
	H	0.554093	-1.930067	1.156633
287	(HIO₃)₂(HIO₂)₁(EDA)₂:			
	Atmos	X	Y	Z
	I	2.819151	-0.037081	-1.036727
	O	1.058395	0.290802	-1.543698
	O	2.977674	-1.791356	-1.512540
	O	2.781467	-0.129218	0.810937
	I	-3.684799	0.140744	-0.475070
	O	-2.610457	-0.770691	0.721110
	O	-3.104732	-0.537788	-2.079712
	O	-3.094914	1.874950	-0.430526
	H	-1.784554	-0.527905	2.368751
	O	-1.075099	-0.531630	3.042013
	I	0.606471	-0.216832	2.038232
	O	0.614490	1.674642	2.067456
	C	1.609028	3.599656	-1.040176
	N	2.472323	2.762869	-0.196296
	C	0.168122	3.671234	-0.547206
	N	-0.366959	2.322770	-0.261184
	H	2.056642	2.534343	0.710209
	H	3.358679	3.217258	-0.009035
	H	1.982072	4.631788	-1.109732
	H	1.605362	3.188503	-2.062010
	H	-0.454115	4.152563	-1.310180
	H	0.098006	4.256520	0.377964
	H	0.063310	1.613095	-0.883341
	H	-1.401710	2.248922	-0.335082
	H	-0.066357	2.042298	0.739607
	C	0.175693	-3.848964	-0.284472
	N	1.091773	-3.079917	0.549418
	C	-0.196251	-3.075064	-1.540818
	N	-0.745974	-1.734285	-1.217830
	H	1.926075	-2.822438	0.016925
	H	1.394063	-3.631648	1.345325
	H	0.581893	-4.819885	-0.618243
	H	-0.735278	-4.059900	0.295853
	H	-0.948757	-3.631012	-2.110324
	H	0.687579	-2.918826	-2.170642

	H	-1.517600	-1.424127	-1.838658
	H	-0.003415	-0.995062	-1.268685
	H	-1.177810	-1.675408	-0.282802
288	(HIO₃)₃(HIO₂)₁(EDA)₂:			
	Atmos	X	Y	Z
	I	-1.725924	2.302714	0.086217
	O	-0.576560	3.550086	0.785879
	H	1.008049	3.359256	0.384450
	O	-1.534309	2.442809	-1.725264
	O	-0.675617	0.788578	0.366368
	I	2.703308	-2.598480	-0.293244
	O	3.401605	-0.936959	-0.662414
	O	1.370153	-2.802617	-1.529413
	O	1.817615	-2.390612	1.307062
	I	-3.980376	-1.410948	-0.059108
	O	-2.930757	-1.819329	-1.510678
	O	-3.744250	0.388803	0.214846
	O	-3.155227	-2.218449	1.374759
	H	2.954178	1.002846	2.314538
	O	3.524801	1.478194	1.651314
	I	2.566716	1.479648	-0.061327
	O	1.961440	3.322642	0.075329
	C	0.529579	0.309584	3.467930
	N	1.906378	-0.132276	3.230712
	C	-0.536358	-0.784345	3.395321
	N	-0.686126	-1.291537	2.010252
	H	1.952961	-0.880374	2.533807
	H	2.318233	-0.509442	4.078292
	H	0.477480	0.778560	4.457850
	H	0.279222	1.089550	2.735981
	H	-1.509545	-0.376286	3.693434
	H	-0.296199	-1.628215	4.053595
	H	-0.750598	-0.465530	1.361331
	H	-1.583849	-1.808187	1.853482
	H	0.125219	-1.855865	1.704947
	C	1.156752	0.567200	-3.259565
	N	1.272877	1.709561	-2.332953
	C	-0.208321	-0.103382	-3.192904
	N	-0.451951	-0.757993	-1.891076
	H	0.346674	2.114768	-2.137030
	H	1.822223	2.453174	-2.753845
	H	1.301180	0.892216	-4.299848
	H	1.943431	-0.166513	-3.030771
	H	-0.270053	-0.874922	-3.968159

H	-1.009875	0.626790	-3.349057
H	0.240404	-1.516650	-1.716020
H	-1.412025	-1.175171	-1.827639
H	-0.423841	-0.079328	-1.099393

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