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Altitude-dependent role of nitric acid in iodic acid-iodous acid nucleation: from marine boundary layer catalyst to upper troposphere core component

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Contents

Supplementary Methods

The equations in Atmospheric Cluster Dynamics Code (ACDC).

The collision coefficient, $\beta_{i,j}$, between clusters i and j is derived from kinetic gas theory:

$$\beta_{i,j} = \left(\frac{3}{4\pi}\right)^{\frac{1}{6}} \left(\frac{6k_BT}{m_i} + \frac{6k_BT}{m_j}\right)^{\frac{1}{2}} \left(V_i^{\frac{1}{3}} + V_j^{\frac{1}{3}}\right)^2, \quad \text{(S1)}$$

where m_i is the mass of cluster i, T is temperature and V_i is the van der Waals (vdW) volume of cluster i. The volume of each molecular cluster, V_i, was calculated using the Marching Tetrahedra (MT) approach in Multiwfn 3.7 (Lu and Chen, 2012). Subsequently, the cluster diameter d_i was derived from V_i assuming a spherical geometry.

The evaporation rate coefficient is derived via the detailed balance assumption:

$$\gamma_{(i+j)\to i} = \beta_{i,j} c_{ref} \exp\left(\frac{\Delta G_{i+j} - \Delta G_i - \Delta G_j}{k_BT}\right), \quad \text{(S2)}$$

where ΔG_{i+j} is the Gibbs free energy of formation for cluster $i + j$ at reference pressure $P_{\text{ref}} = 1$ atm.

Uncertainty analysis: impact of iodine oxoacid concentrations.

To probe the uncertainty from HIO_2 concentration (Figure S9), we simulated scenarios where its concentration was reduced by one or two orders of magnitude from 2 to 14 km, relative to a base case where the concentration remained unchanged from 2 to 14 km, with all other species and environmental conditions held constant. The results reveal that the two nucleation mechanisms exhibit different sensitivities to HIO_2. The pure HIO_3-HIO_2 mechanism is most sensitive to HIO_2 changes in the mid-troposphere (4-8 km), but above 9 km, a decrease in HIO_2 concentration has little impact on its rate; this aligns with our cluster analysis (Figure 5(c)), which shows this mechanism relies primarily on HIO_3 for growth at high altitudes. In contrast, the HNO_3-HIO_3-HIO_2 mechanism shows a strong dependence on HIO_2 in high-altitude regions, where a one or two order of magnitude reduction in HIO_2 causes the maximum nucleation rate to drop by 10-fold and 50-fold, respectively, even as HNO_3 still provides a promotional effect.

For HIO_3, we tested the effect in Scenario C (Figure S10) by reducing its concentration by one order of magnitude. Consistent with the previous findings, the pure HIO_3-HIO_2 mechanism is highly sensitive to the HIO_3 concentration, whereas the HNO_3-HIO_3-HIO_2 mechanism is less affected.

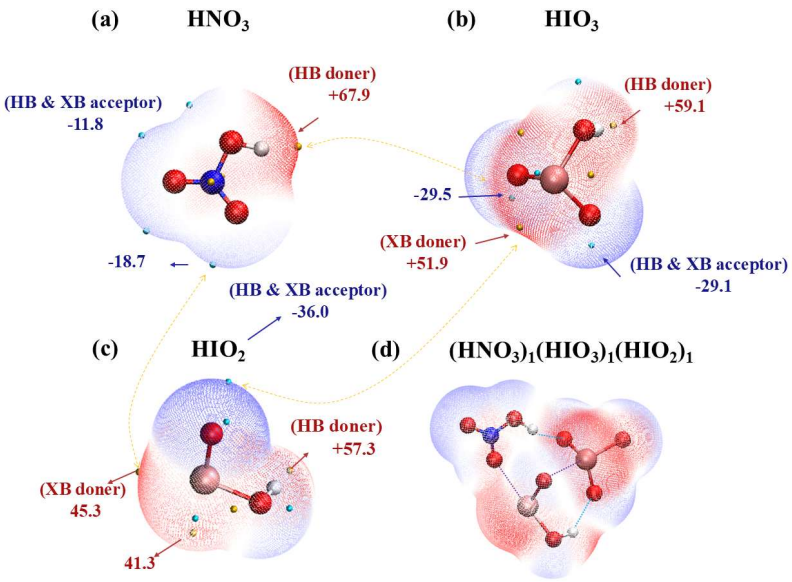
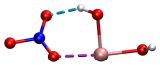
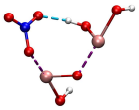


Figure S1. The electrostatic potential (ESP, kcal mol^{-1})-mapped molecular van der Waals surfaces of (a) HNO_3, (b) HIO_3, (c) HIO_2, and (d) the $(HNO_3)_1(HIO_3)_1(HIO_2)_1$ cluster. Yellow and cyan dots denote the positions of ESP maxima and minima, respectively. Yellow dashed arrows highlight the key intermolecular interaction orientations within $(HNO_3)_1(HIO_3)_1(HIO_2)_1$ cluster. Blue dashed lines represent hydrogen bonds, and purple dashed lines represent halogen bonds. White, blue, red, and pink spheres represent H, N, O, and I atoms, respectively.



$(HNO_3)_1(HIO_2)_1$



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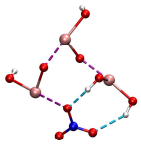

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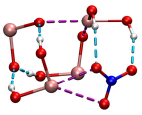

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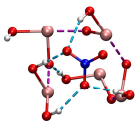

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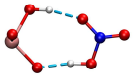

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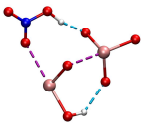

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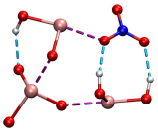

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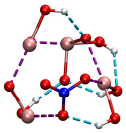

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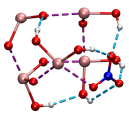

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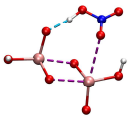

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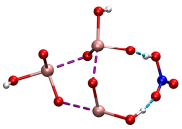

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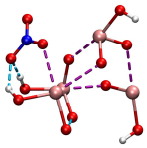

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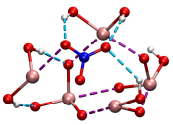

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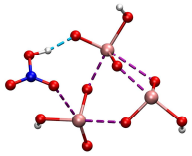

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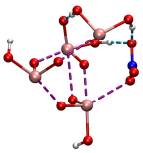

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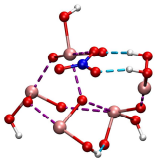

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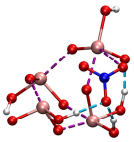

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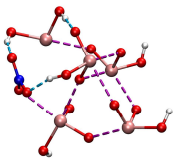

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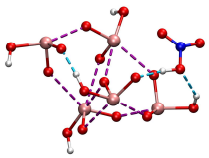

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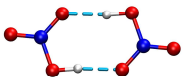

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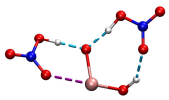

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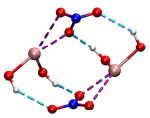

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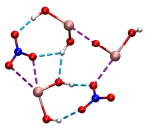

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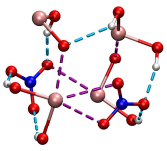
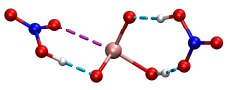


$(HNO_3)_2(HIO_2)_4$



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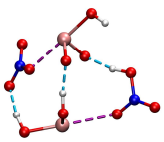

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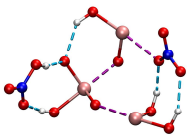

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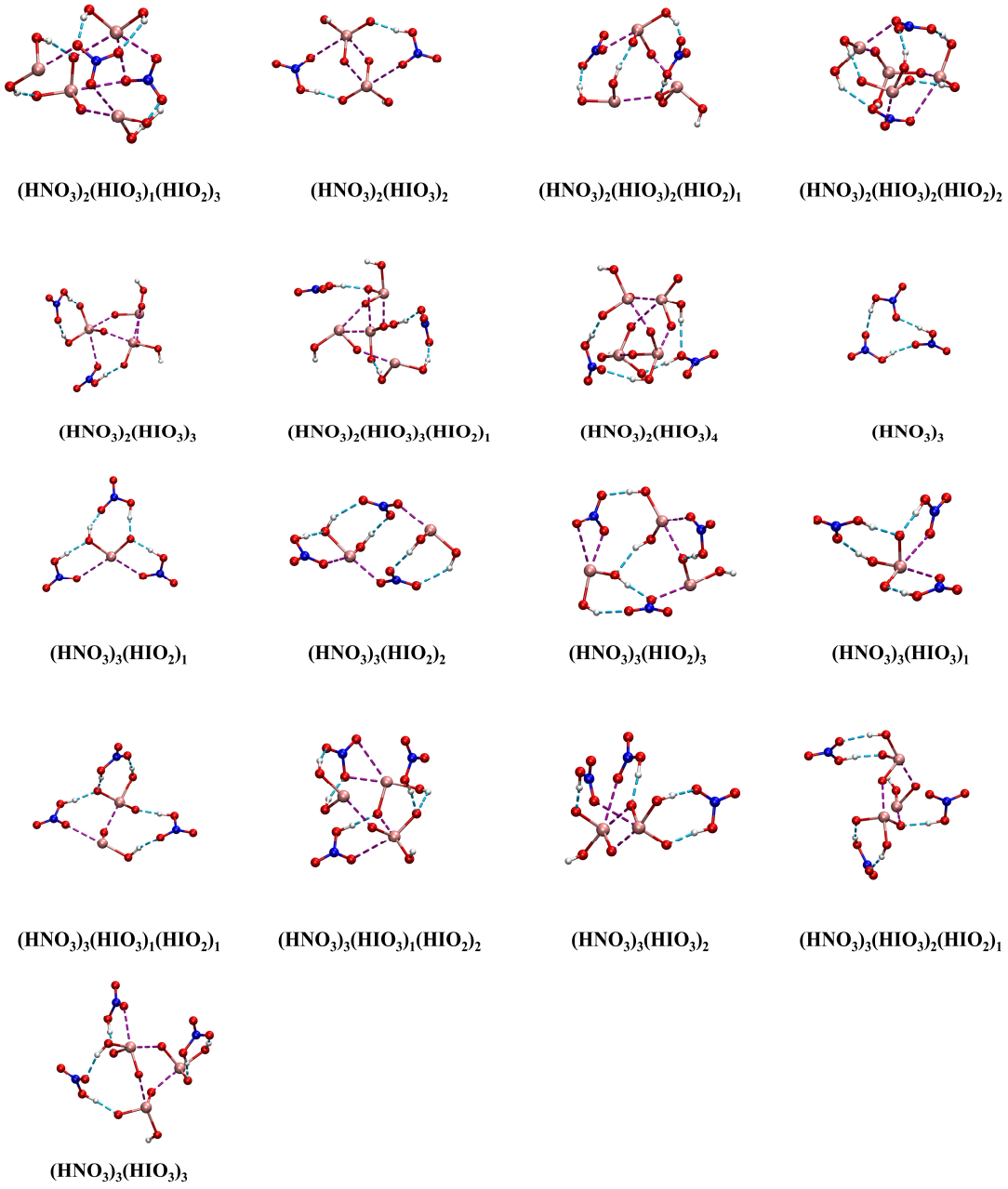


Figure S2. The most stable configurations of $(HNO_3)_x(HIO_3)_y(HIO_2)_z$ clusters ($2 \leq x + y + z \leq 6$, $1 \leq x \leq 3$) identified at the ωB97X-D/6-311++G(3df, 3pd) (for H, N, and O) and aug-cc-pVTZ-PP with ECP28MDF (for I) level of theory. The white, blue, red, and pink balls represent the H, N, O, and I atoms, respectively. Blue and purple dashed lines represent hydrogen bonds and halogen bonds, respectively.

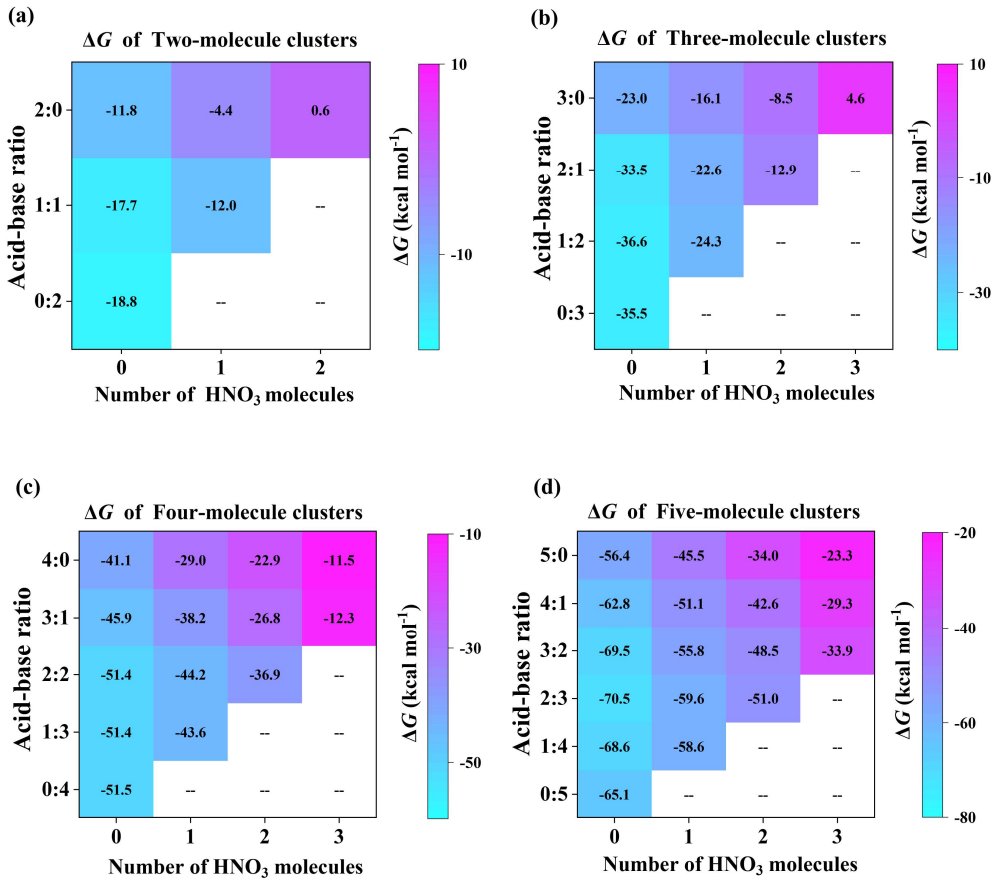


Figure S3. Gibbs free energies of formation (ΔG, in kcal mol^{-1}) at 288 K for the most stable HNO_3–HIO_3–HIO_2 clusters with varying sizes: (a) two-, (b) three-, (c) four-, and (d) five-molecule clusters. All values were calculated at the DLPNO-CCSD(T)/aug-cc-pVTZ(-PP)//ωB97X-D/6-311++G(3df,3pd) + aug-cc-pVTZ-PP level of theory.

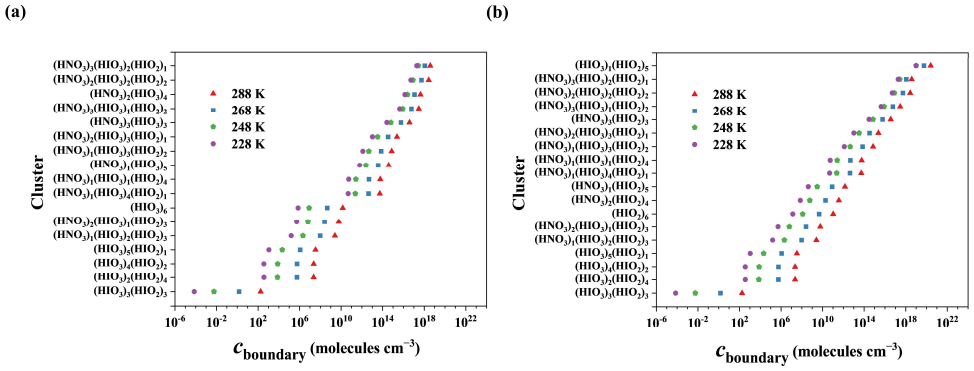


Figure S4. The minimum concentration, $c_{boundary}$, required for a six-molecule cluster to form a boundary cluster upon collision with (a) HIO_3, and (b) HIO_2 at different temperatures. Clusters are sorted in ascending order of $c_{boundary}$. This concentration is determined by the condition $\beta c_{boundary}/\Sigma\gamma = 1$. Evaluating all 141 distinct temperatures (204–288 K in 0.6 K increments) yields a dataset too large to conveniently tabulate. Therefore, to ensure full reproducibility, the complete set of $c_{boundary}$ files has been deposited to a public repository, accessible at: https://doi.org/10.5281/zenodo.20712556.

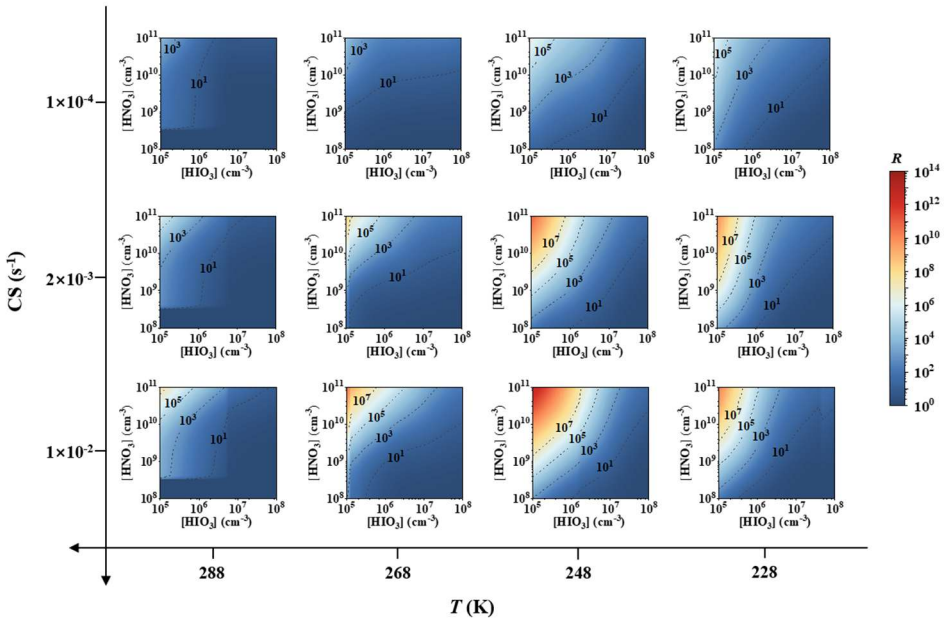


Figure S5. Heatmaps of HNO_3 enhancement factor (R) as a function of HNO_3 and HIO_3 concentrations, simulated under various temperature (T) and condensation sink (CS) conditions. The HIO_2 concentration was set to $[HIO_2] = [HIO_3]/50$. R is represented by a color gradient from blue (10^0) to red (10^{14}), with contour lines indicating R values of 10^1, 10^3, 10^5 and 10^7.

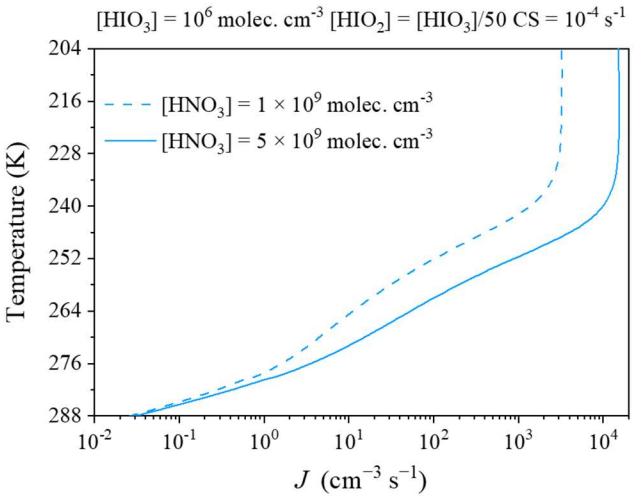


Figure S6. Temperature dependence of cluster formation rates J (cm^{-3} s^{-1}) for the HNO_3–HIO_3–HIO_2 nucleation mechanism over the tropospheric temperature range (204–288 K). Simulation conditions were fixed at $[HIO_3] = 10^6$ molecules cm^{-3}, $[HIO_2] = [HIO_3]/50$, and CS = 10^{-4} s^{-1}. The dashed and solid lines represent $[HNO_3] = 1 \times 10^9$ molecules cm^{-3} and 5×10^9 molecules cm^{-3}, respectively.

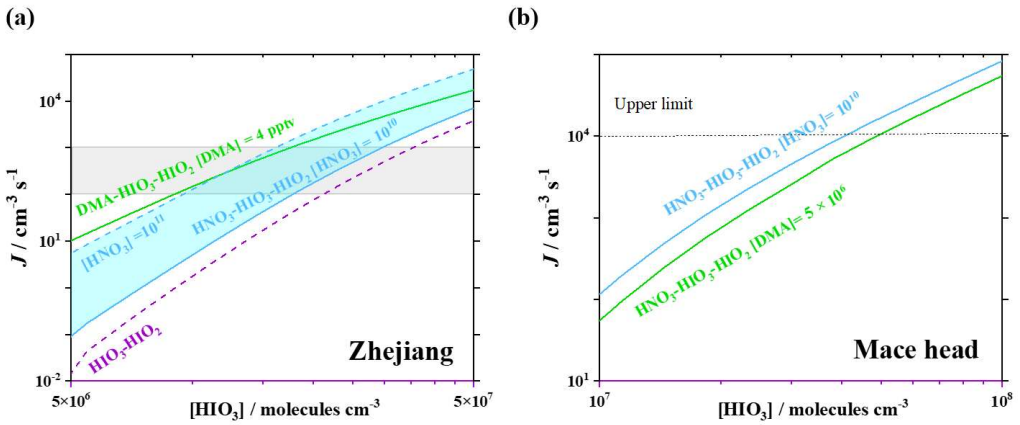


Figure S7. Cluster formation rates (J, cm^{-3} s^{-1}) for the HIO_3–HIO_2 (purple dashed line), HNO_3–HIO_3–HIO_2 (blue) and HIO_3–HIO_2–DMA (green) (Zu et al., 2024) systems under the corresponding atmospheric conditions of (a) Zhejiang, where gray shaded areas represent locally observed cluster formation rates (Yu et al., 2019); and (b) Mace Head, where the dashed line marks the upper limit of cluster formation rates reported in field observations (Sipilä et al., 2016).

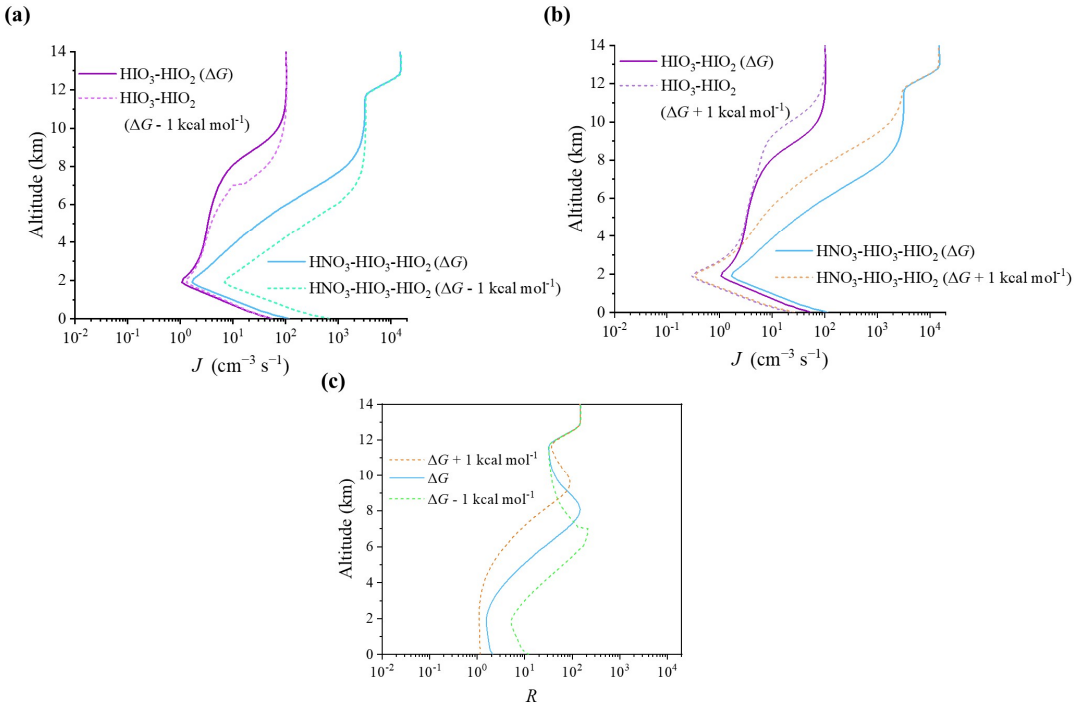


Figure S8. Sensitivity of cluster formation rates J ($cm^{-3}s^{-1}$) and enhancement factor of HNO_3 (R) to uncertainties in binding free energy (ΔG) at different altitudes. The simulations compare the Base scenario (ΔG) (solid lines) with two tests where the ΔG of all clusters (excluding monomers) was systematically shifted by ± 1 kcal mol^{-1}. (a) J for the ΔG - 1 kcal mol^{-1} scenario compared to the Base scenario for the HIO_3–HIO_2 and HNO_3–HIO_3–HIO_2 mechanisms. (b) J for the ΔG + 1 kcal mol^{-1} scenario compared to the Base scenario for both mechanisms. (c) Corresponding enhancement factor (R) of HNO_3 for all three scenarios (Base ΔG, ΔG - 1 kcal mol^{-1}, and ΔG + 1 kcal mol^{-1}).

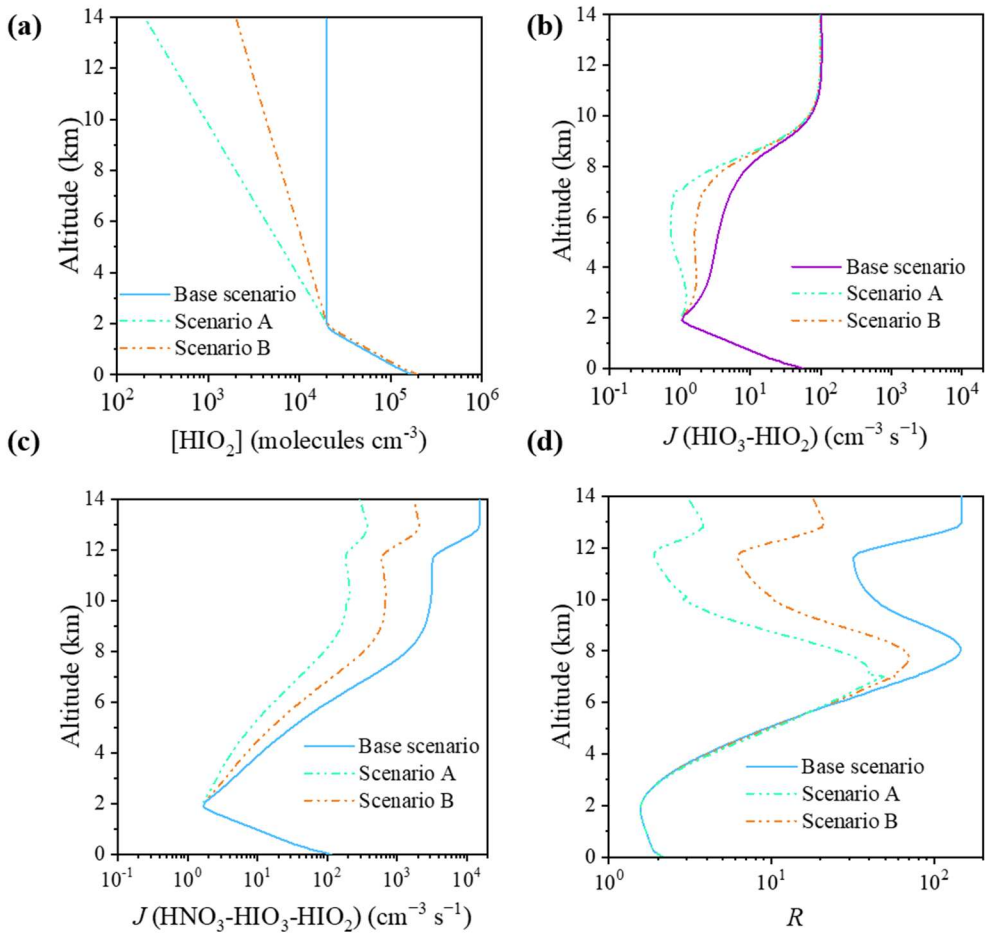


Figure S9. Sensitivity of cluster formation rates J ($cm^{-3}s^{-1}$) and enhancement factor of HNO_3 (R) to the vertical profile of HIO_2 concentration. The simulations are run for three different scenarios based on the [HIO_2] profile: the Base scenario (solid lines), Scenario A (brown dash-dotted lines, with [HIO_2] reduced by one order of magnitude from 2–14 km relative to the base), and Scenario B (cyan dash-dotted lines, with [HIO_2] reduced by two orders of magnitude from 2–14 km). (a) The assumed vertical concentration profiles for [HIO_2] in the three scenarios. (b, c) J at different altitudes for the (b) HIO_3-HIO_2 and (c) HNO_3−HIO_3−HIO_2 mechanisms. (d) Corresponding enhancement factor of HNO_3 (R), calculated as the ratio of J(HNO_3−HIO_3−HIO_2) to J(HIO_3−HIO_2).

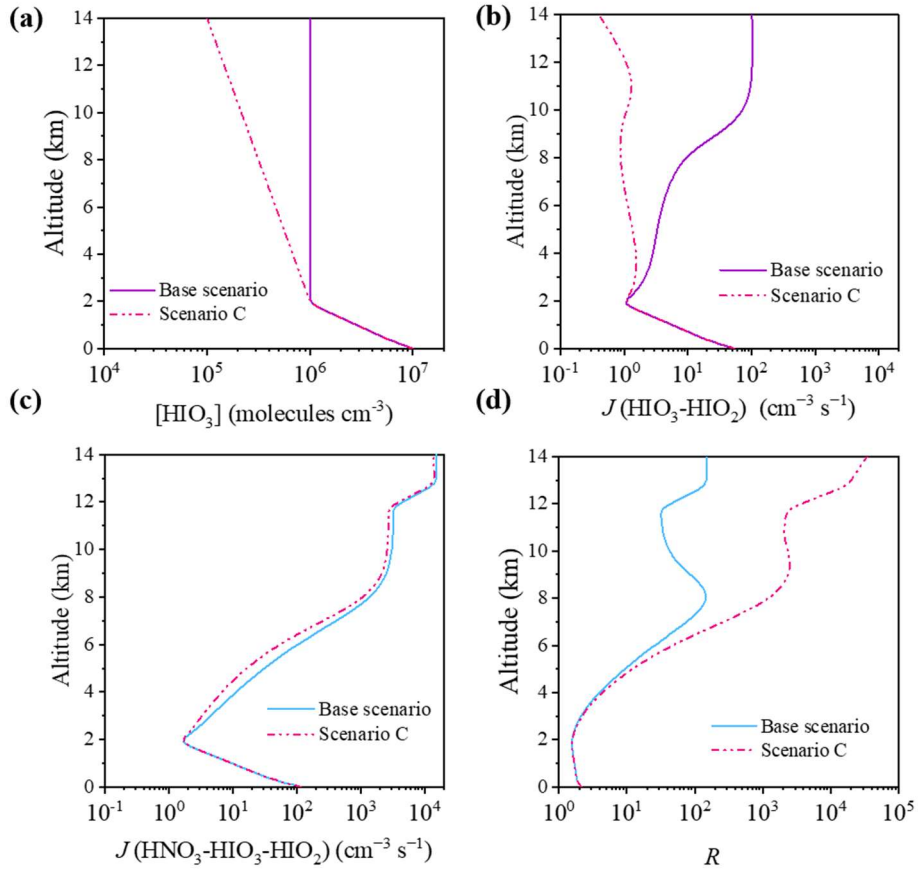


Figure S10. Sensitivity of cluster formation rates J ($cm^{-3}s^{-1}$) and enhancement factor of HNO_3 (R) to the vertical profile of HIO_3 concentration. The simulations are run for two different [HIO_3] profile scenarios: the Base scenario (solid lines) and Scenario C (pink dash-dotted lines, with [HIO_3] reduced by one order of magnitude from 2–14 km relative to the base). (a) The assumed vertical concentration profiles for [HIO_3] in the two scenarios. (b, c) J at different altitudes for the (b) HIO_3–HIO_2 and (c) HNO_3–HIO_3–HIO_2 mechanisms. (d) Corresponding enhancement factor of HNO_3 (R), calculated as the ratio of J(HNO_3–HIO_3–HIO_2) to J(HIO_3–HIO_2).

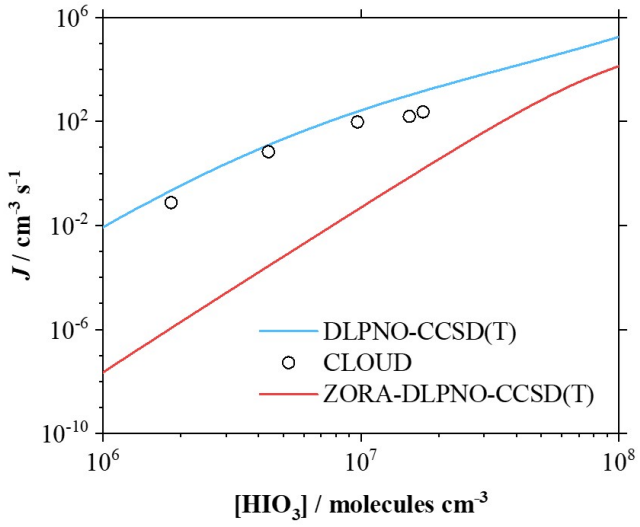


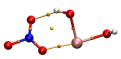
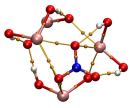
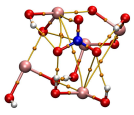
Figure S11. Cluster formation rates (J, cm^{-3} s^{-1}) of the HIO_3–HIO_2 system obtained from the CLOUD experiment (He et al., 2021) and from theoretical simulations at the DLPNO-CCSD(T) and ZORA-DLPNO-CCSD(T) (Lenthe et al., 1993) levels of theory. Simulations were performed under the same conditions as the CLOUD experiment: [HIO_3] = 10^6–10^8, [HIO_2] = 2×10^4–2×10^6 molecules cm^{-3}, T = 263 K, and CS = 2.2×10^{-3} s^{-1}. Circles represent the CLOUD experimental results. ACDC simulations are evaluated at the DLPNO-CCSD(T)/aug-cc-pVTZ (for H, N, O) + aug-cc-pVTZ-PP with ECP28MDF (for I) level of theory (blue line) and the ZORA-DLPNO-CCSD(T)/ma-ZORA-def2-TZVPP (for H, N, O) (Neese, 2012) + SARC-ZORA-TZVPP (for I) (Rolfes et al., 2020) level of theory (red line), both based on geometries optimized at the B97X-D/6-311++G(3df,3pd) +aug-cc-pVTZ-PP level.

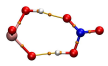
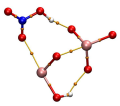
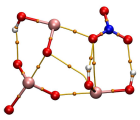
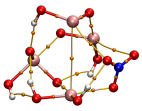
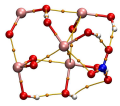
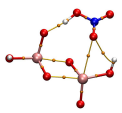
Table S1. The Gibbs free energies of formation (ΔG, kcal mol^{-1}) of the $(HNO_3)_x(HIO_3)_y(HIO_2)_z$ clusters ($2 \leqslant x + y + z \leqslant 6$, $1 \leqslant x \leqslant 3$) at the DLPNO-CCSD(T)/aug-cc-pVTZ(-PP)//ωB97X-D/6-311++G(3df,3pd) + aug-cc-pVTZ-PP level of theory at 288 K, 268 K, 248 K and 228 K.

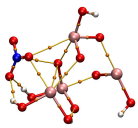
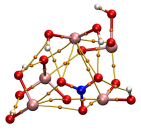
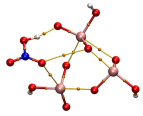
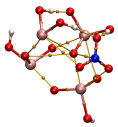
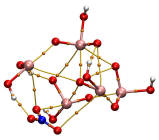
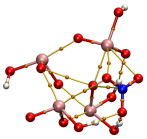
Clusters	ΔG (kcal mol^{-1})			
	288 K	268 K	248 K	228 K
$(HNO_3)_1(HIO_2)_1$	-12.0	-12.8	-13.6	-14.4
$(HNO_3)_1(HIO_2)_2$	-24.3	-25.9	-27.5	-29.1
$(HNO_3)_1(HIO_2)_3$	-43.6	-46.1	-48.6	-51.1
$(HNO_3)_1(HIO_2)_4$	-58.6	-62.0	-65.4	-68.8
$(HNO_3)_1(HIO_2)_5$	-74.8	-79.1	-83.3	-87.6
$(HNO_3)_1(HIO_3)_1$	-4.4	-5.1	-5.8	-6.4
$(HNO_3)_1(HIO_3)_1(HIO_2)_1$	-22.6	-24.2	-25.8	-27.4
$(HNO_3)_1(HIO_3)_1(HIO_2)_2$	-44.2	-46.7	-49.2	-51.7
$(HNO_3)_1(HIO_3)_1(HIO_2)_3$	-59.6	-63.0	-66.3	-69.7
$(HNO_3)_1(HIO_3)_1(HIO_2)_4$	-76.2	-80.5	-84.9	-89.2
$(HNO_3)_1(HIO_3)_2$	-16.1	-17.7	-19.2	-20.8
$(HNO_3)_1(HIO_3)_2(HIO_2)_1$	-38.2	-40.6	-42.9	-45.3
$(HNO_3)_1(HIO_3)_2(HIO_2)_2$	-55.8	-59.1	-62.5	-65.9
$(HNO_3)_1(HIO_3)_2(HIO_2)_3$	-83.9	-88.1	-92.3	-96.6
$(HNO_3)_1(HIO_3)_3$	-29.0	-31.4	-33.7	-36.1
$(HNO_3)_1(HIO_3)_3(HIO_2)_1$	-51.1	-54.5	-57.9	-61.3
$(HNO_3)_1(HIO_3)_3(HIO_2)_2$	-75.7	-79.9	-84.2	-88.5
$(HNO_3)_1(HIO_3)_4$	-45.6	-49.0	-52.4	-55.8
$(HNO_3)_1(HIO_3)_4(HIO_2)_1$	-70.5	-74.6	-78.8	-83.0
$(HNO_3)_1(HIO_3)_5$	-63.0	-67.1	-71.2	-75.4
$(HNO_3)_2$	0.6	-0.1	-0.8	-1.5
$(HNO_3)_2(HIO_2)_1$	-12.9	-14.4	-15.9	-17.4
$(HNO_3)_2(HIO_2)_2$	-36.9	-39.4	-41.9	-44.4
$(HNO_3)_2(HIO_2)_3$	-51.0	-54.2	-57.5	-60.7
$(HNO_3)_2(HIO_2)_4$	-69.1	-73.4	-77.7	-82.0
$(HNO_3)_2(HIO_3)_1$	-8.5	-9.9	-11.3	-12.8
$(HNO_3)_2(HIO_3)_1(HIO_2)_1$	-26.8	-29.2	-31.5	-33.9

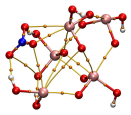
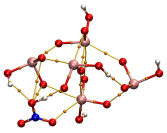
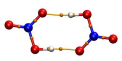
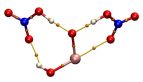
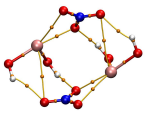
$(HNO_3)_2(HIO_3)_1(HIO_2)_2$	-48.5	-51.6	-54.8	-57.9
$(HNO_3)_2(HIO_3)_1(HIO_2)_3$	-72.5	-76.6	-80.9	-85.1
$(HNO_3)_2(HIO_3)_2$	-22.9	-25.2	-27.4	-29.7
$(HNO_3)_2(HIO_3)_2(HIO_2)_1$	-42.6	-45.9	-49.2	-52.5
$(HNO_3)_2(HIO_3)_2(HIO_2)_2$	-57.2	-61.4	-65.5	-69.7
$(HNO_3)_2(HIO_3)_3$	-34.0	-37.0	-40.1	-43.2
$(HNO_3)_2(HIO_3)_3(HIO_2)_1$	-56.6	-60.7	-64.8	-69.0
$(HNO_3)_2(HIO_3)_4$	-48.0	-52.0	-56.0	-60.1
$(HNO_3)_3$	4.6	3.3	1.9	0.5
$(HNO_3)_3(HIO_2)_1$	-12.3	-14.5	-16.8	-19.0
$(HNO_3)_3(HIO_2)_2$	-33.9	-37.0	-40.1	-43.3
$(HNO_3)_3(HIO_2)_3$	-54.9	-58.9	-62.9	-66.9
$(HNO_3)_3(HIO_3)_1$	-11.5	-13.6	-15.7	-17.8
$(HNO_3)_3(HIO_3)_1(HIO_2)_1$	-29.3	-32.3	-35.2	-38.2
$(HNO_3)_3(HIO_3)_1(HIO_2)_2$	-51.2	-55.0	-58.9	-62.8
$(HNO_3)_3(HIO_3)_2$	-23.3	-26.3	-29.2	-32.2
$(HNO_3)_3(HIO_3)_2(HIO_2)_1$	-43.9	-47.7	-51.6	-55.5
$(HNO_3)_3(HIO_3)_3$	-37.9	-41.7	-45.5	-49.4

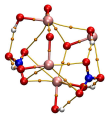
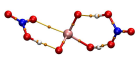
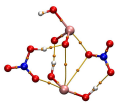
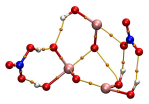
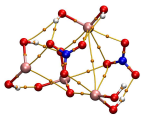
Table S2. The bond types, corresponding weakly interacting species (with proton transfer indicated by the ionic forms of the molecules), bond lengths (Å), electron density $\rho(r)$ (a.u.), Laplacian electron density $\nabla^2\rho(r)$ (a.u.), and energy density $H(r)$ (a.u.) at the bond critical points (BCPs) of the respective weak interactions. The orange spheres denote the bond critical points (BCPs) in the Atoms in Molecules (AIM) theory analysis. HB (hydrogen bond), XB (halogen bond).

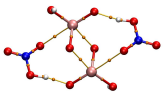
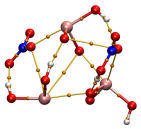
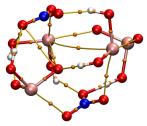
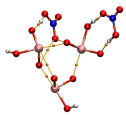
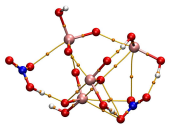
Cluster	Bond	Bond type	Bond lengths (Å)	$\rho(r)$ (a.u.)	$\nabla^2\rho(r)$ (a.u.)	$H(r)$ (a.u.)
 $(HNO_3)_1(HIO_2)_1$	NO_3^- (O)···(I) $H_2IO_2^+$	XB	2.22	0.0806	0.1772	0.0221
	NO_3^- (O)···(H) $H_2IO_2^+$	HB	1.86	0.0391	0.1111	0.0037
 $(HNO_3)_1(HIO_2)_2$	HIO_2 (O)···(I) $H_2IO_2^+$	XB	2.19	0.0841	0.1786	-0.0240
	HIO_2 (I)···(O) NO_3^-	XB	2.32	0.0645	0.1490	-0.0124
	$H_2IO_2^+$ (H)···(O) NO_3^-	HB	1.68	0.0460	0.1140	-0.0088
 $(HNO_3)_1(HIO_2)_3$	$H_2IO_2^+$ (I)···(O) HIO_2	XB	2.24	0.0764	0.1650	-0.0190
	HIO_2 (O)···(I) HIO_2	XB	2.24	0.0745	0.1639	-0.0178
	NO_3^- (O)···(I) HIO_2	XB	2.42	0.0527	0.1240	-0.0073
	NO_3^- (O)···(H) $H_2IO_2^+$	HB	1.74	0.0413	0.1117	-0.0056
	NO_3^- (O)···(H) $H_2IO_2^+$	HB	2.24	0.0123	0.0464	0.0018
 $(HNO_3)_1(HIO_2)_4$	HIO_2 (H)···(O) IO_2^-	HB	1.54	0.0701	0.1053	-0.0252
	IO_2^- (O)···(H) $H_2IO_2^+$	HB	1.65	0.0529	0.1092	-0.0133
	NO_3^- (O)···(I) $H_2IO_2^+$	XB	2.46	0.0502	0.1185	-0.0065
	HIO_2 (O)···(I) $H_2IO_2^+$	XB	2.46	0.0490	0.1260	-0.0051
	$H_2IO_2^+$ (I)···(O) IO_2^-	XB	2.53	0.0411	0.1121	-0.0023
	IO_2^- (O)···(H) $H_2IO_2^+$	HB	1.76	0.0404	0.1058	-0.0056
	$H_2IO_2^+$ (H)···(O) NO_3^-	HB	1.95	0.0232	0.0854	0.0017
	NO_3^- (O)···(I) $H_2IO_2^+$	XB	2.87	0.0220	0.0693	0.0004
	$H_2IO_2^+$ (H)···(O) NO_3^-	HB	2.06	0.0196	0.0704	0.0018
 $(HNO_3)_1(HIO_2)_5$	HIO_2 (I)···(O) HIO_2	XB	2.22	0.0794	0.1711	-0.0211
	HIO_2 (O)···(I) $H_2IO_2^+$	XB	2.29	0.0683	0.1531	-0.0142
	HIO_2 (I)···(O) HIO_2	XB	2.31	0.0654	0.1533	-0.0125
	$H_2IO_2^+$ (H)···(O) NO_3^-	HB	1.61	0.0584	0.1086	-0.0170
	HIO_2 (H)···(O) HIO_2	HB	1.64	0.0533	0.1077	-0.0141
	HIO_2 (O)···(I) HIO_2	XB	2.40	0.0532	0.1332	-0.0067
	NO_3^- (O)···(H) HIO_2	HB	1.92	0.0271	0.0849	-0.0003
	$H_2IO_2^+$ (H)···(O) NO_3^-	HB	2.09	0.0180	0.0684	0.0021
	HIO_2 (H)···(O) NO_3^-	HB	2.11	0.0179	0.0635	0.0016
	HIO_3 (O)···(H) HNO_3	HB	1.64	0.0512	0.1088	-0.0129

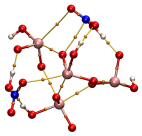
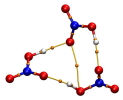
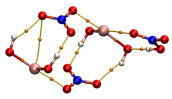
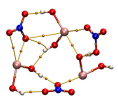
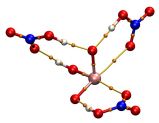
 $(HNO_3)_1(HIO_3)_1$	HNO_3 (O)···(H) HIO_3	HB	1.82	0.0301	0.1013	-0.0006
 $(HNO_3)_1(HIO_3)_1(HIO_2)_1$	HIO_2 (O)···(I) HIO_3	XB	2.26	0.0756	0.1457	-0.0195
	HIO_3 (O)···(H) HNO_3	HB	1.54	0.0668	0.1069	-0.0231
	HIO_2 (I)···(O) HNO_3	XB	2.67	0.0271	0.0909	0.0011
	HIO_2 (H)···(O) HIO_3	HB	2.05	0.0207	0.0761	0.0019
 $(HNO_3)_1(HIO_3)_1(HIO_2)_2$	HIO_3 (I)···(O) HIO_2	XB	2.19	0.0866	0.1653	-0.0262
	HIO_3 (O)···(I) $H_2IO_2^+$	XB	2.33	0.0589	0.1576	-0.0084
	NO_3^- (O)···(I) HIO_2	XB	2.42	0.0526	0.1265	-0.0073
	$H_2IO_2^+$ (H)···(O) NO_3^-	HB	1.90	0.0272	0.0914	0.0004
	$H_2IO_2^+$ (H)···(O) NO_3^-	HB	1.90	0.0269	0.0965	0.0011
	HIO_3 (O)···(H) HIO_2	HB	1.97	0.0243	0.0891	0.0017
 $(HNO_3)_1(HIO_3)_1(HIO_2)_3$	HIO_2 (O)···(I) HIO_3	XB	2.16	0.0934	0.1714	-0.0315
	HIO_2 (O)···(I) HIO_2	XB	2.31	0.0660	0.1523	-0.0129
	NO_3^- (O)···(I) $H_2IO_2^+$	XB	2.43	0.0522	0.1275	-0.0068
	HIO_2 (H)···(O) HIO_3	HB	1.76	0.0381	0.1083	-0.0042
	HIO_3 (O)···(I) $H_2IO_2^+$	XB	2.67	0.0310	0.0899	-0.0003
	NO_3^- (O)···(H) $H_2IO_2^+$	HB	1.98	0.0254	0.0857	0.0009
	HIO_3 (O)···(H) $H_2IO_2^+$	HB	2.01	0.0231	0.0806	0.0014
	HIO_2 (I)···(O) NO_3^-	XB	2.96	0.0182	0.0531	0.0008
	HIO_2 (H)···(O) HIO_3	HB	2.35	0.0122	0.0416	0.0010
 $(HNO_3)_1(HIO_3)_1(HIO_2)_4$	HIO_3 (I)···(O) IO_2^-	XB	2.23	0.0799	0.1553	-0.0217
	$H_2IO_2^+$ (I)···(O) HIO_2	XB	2.30	0.0685	0.1533	-0.0142
	IO_2^- (O)···(I) HIO_2	XB	2.50	0.0430	0.1203	-0.0025
	HIO_3 (O)···(I) $H_2IO_2^+$	XB	2.50	0.0420	0.1267	-0.0017
	$H_2IO_2^+$ (H)···(O) IO_2^-	HB	1.76	0.0399	0.1039	-0.0056
	HIO_3 (O)···(I) $H_2IO_2^+$	XB	2.52	0.0395	0.1237	-0.0008
	NO_3^- (O)···(I) $H_2IO_2^+$	XB	2.62	0.0348	0.0964	-0.0012
	NO_3^- (O)···(H) $H_2IO_2^+$	HB	1.88	0.0310	0.0977	-0.0008
	NO_3^- (O)···(H) $H_2IO_2^+$	HB	1.86	0.0308	0.1045	-0.0001
	NO_3^- (O)···(H) HIO_2	HB	2.01	0.0202	0.0765	0.0021
	HIO_3 (H)···(O) $H_2IO_2^+$	HB	2.04	0.0202	0.0668	0.0011
 $(HNO_3)_1(HIO_3)_2$	HIO_3 (I)···(O) HIO_3	XB	2.24	0.0782	0.1505	-0.0217
	HIO_3 (O)···(H) HNO_3	HB	1.58	0.0589	0.1112	-0.0177
	HIO_3 (O)···(I) HIO_3	XB	2.45	0.0514	0.1190	-0.0070
 $(HNO_3)_1(HIO_3)_2(HIO_2)_1$	HIO_2 (O)···(I) HIO_3	XB	2.15	0.0947	0.1734	-0.0325
	HIO_3 (I)···(O) HIO_3	XB	2.30	0.0680	0.1463	-0.0146
	HNO_3 (H)···(O) HIO_3	HB	1.60	0.0567	0.1131	-0.0161
	HIO_2 (I)···(O) HIO_3	XB	2.44	0.0472	0.1301	-0.0040
	HIO_2 (H)···(O) HNO_3	HB	1.99	0.0188	0.0817	0.0030
	HIO_3 (I)···(O) HIO_2	XB	2.21	0.0844	0.1572	-0.0251

 $(HNO_3)_1(HIO_3)_2(HIO_2)_2$	HIO_3 (O)···(I) HIO_3	XB	2.36	0.0560	0.1484	-0.0068
	HIO_2 (I)···(O) HIO_3	XB	2.45	0.0473	0.1265	-0.0044
	$H_2IO_2^+$ (I)···(O) NO_3^-	XB	2.50	0.0465	0.1167	-0.0046
	HIO_3 (H)···(O) NO_3^-	HB	1.80	0.0335	0.0980	-0.0028
	$H_2IO_2^+$ (H)···(O) NO_3^-	HB	1.91	0.0290	0.0970	0.0003
	$H_2IO_2^+$ (I)···(O) HIO_3	XB	2.72	0.0278	0.0851	0.0006
	$H_2IO_2^+$ (H)···(O) HIO_3	HB	1.93	0.0246	0.0884	0.0015
 $(HNO_3)_1(HIO_3)_2(HIO_2)_3$	HIO_2 (O)···(I) HIO_3	XB	2.16	0.0920	0.1717	-0.0303
	IO_3^- (O)···(I) HIO_2	XB	2.41	0.0497	0.1405	-0.0045
	HIO_3 (O)···(I) $H_2IO_2^+$	XB	2.49	0.0433	0.1197	-0.0028
	$H_2IO_2^+$ (I)···(O) NO_3^-	XB	2.53	0.0424	0.1072	-0.0037
	IO_3^- (O)···(H) $H_2IO_2^+$	HB	1.73	0.0417	0.1065	-0.0065
	IO_3^- (O)···(H) $H_2IO_2^+$	HB	1.78	0.0371	0.1027	-0.0038
	IO_3^- (O)···(I) $H_2IO_2^+$	XB	2.64	0.0321	0.0964	0.0001
	IO_3^- (I)···(O) HIO_3	XB	2.73	0.0260	0.0833	0.0012
	NO_3^- (O)···(H) $H_2IO_2^+$	HB	2.09	0.0177	0.0661	0.0020
 $(HNO_3)_1(HIO_3)_3$	HIO_3 (O)···(I) HIO_3	XB	2.28	0.0691	0.1600	-0.0140
	HIO_3 (I)···(O) HIO_3	XB	2.30	0.0677	0.1441	-0.0147
	HNO_3 (H)···(O) HIO_3	HB	1.62	0.0520	0.1126	-0.0133
	HIO_3 (O)···(I) HIO_3	XB	2.47	0.0457	0.1238	-0.0031
 $(HNO_3)_1(HIO_3)_3(HIO_2)_1$	HIO_3 (I)···(O) HIO_3	XB	2.28	0.0707	0.1511	-0.0163
	HIO_3 (O)···(I) HIO_3	XB	2.31	0.0646	0.1527	-0.0114
	HIO_3 (O)···(H) $H_2IO_2^+$	HB	1.63	0.0520	0.1101	-0.0132
	HIO_3 (I)···(O) HIO_3	XB	2.46	0.0455	0.1215	-0.0035
	NO_3^- (O)···(H) $H_2IO_2^+$	HB	1.73	0.0444	0.1014	-0.0082
	HIO_3 (H)···(O) NO_3^-	HB	1.84	0.0330	0.0896	-0.0029
 $(HNO_3)_1(HIO_3)_3(HIO_2)_2$	HIO_3 (O)···(I) HIO_3	XB	2.21	0.0800	0.1687	-0.0214
	HIO_3 (O)···(I) HIO_2	XB	2.40	0.0525	0.1367	-0.0064
	NO_3^- (O)···(I) HIO_3	XB	2.47	0.0505	0.1154	-0.0062
	HIO_3 (I)···(O) HIO_2	XB	2.45	0.0497	0.1232	-0.0052
	HIO_2 (O)···(I) HIO_3	XB	2.48	0.0475	0.1132	-0.0049
	$H_2IO_2^+$ (I)···(O) HIO_3	XB	2.46	0.0450	0.1320	-0.0029
	HIO_3 (O)···(H) $H_2IO_2^+$	HB	1.71	0.0433	0.1110	-0.0075
	NO_3^- (O)···(H) $H_2IO_2^+$	HB	1.77	0.0387	0.1033	-0.0048
	HIO_3 (O)···(I) HIO_3	XB	2.96	0.0170	0.0533	0.0013
	HIO_2 (H)···(O) HIO_3	HB	2.19	0.0159	0.0565	0.0015
 $(HNO_3)_1(HIO_3)_4$	$H_2IO_3^+$ (I)···(O) HIO_3	XB	2.21	0.0828	0.1632	-0.0236
	HIO_3 (O)···(I) HIO_3	XB	2.33	0.0609	0.1496	-0.0094
	HIO_3 (I)···(O) $H_2IO_3^+$	XB	2.35	0.0576	0.1467	-0.0081
	$H_2IO_3^+$ (I)···(O) HIO_3	XB	2.44	0.0492	0.1270	-0.0047
	NO_3^- (O)···(H) $H_2IO_3^+$	HB	1.69	0.0464	0.1033	-0.0096
	NO_3^- (O)···(H) HIO_3	HB	1.72	0.0448	0.1060	-0.0081
	HIO_3 (O)···(H) $H_2IO_3^+$	HB	1.73	0.0417	0.1069	-0.0067
	HIO_3 (I)···(O) HIO_3	XB	2.74	0.0260	0.0804	0.0012

	HIO_3 (I)···(O) HIO_3	XB	2.38	0.0548	0.1436	-0.0064
	HIO_3 (O)···(I) HIO_3	XB	2.45	0.0506	0.1192	-0.0066
	HIO_3 (H)···(O) NO_3^-	HB	1.67	0.0473	0.1102	-0.0097
	HIO_3 (I)···(O) HIO_3	XB	2.48	0.0471	0.1148	-0.0052
	HIO_3 (O)···(H) $H_2IO_2^+$	HB	1.67	0.0465	0.1111	-0.0098
	HIO_3 (O)···(I) $H_2IO_2^+$	XB	2.50	0.0410	0.1219	-0.0018
	$H_2IO_2^+$ (H)···(O) NO_3^-	HB	1.76	0.0398	0.1075	-0.0050
	HIO_3 (O)···(I) HIO_3	XB	2.53	0.0389	0.1126	-0.0012
	HIO_3 (I)···(O) HIO_3	XB	2.73	0.0279	0.0860	0.0010
	HIO_3 (I)···(O) NO_3^-	XB	2.78	0.0275	0.0740	-0.0002
$(HNO_3)_1(HIO_3)_4(HIO_2)_1$	HIO_3 (I)···(O) HIO_3	XB	2.73	0.0272	0.0843	0.0009
	HIO_3 (I)···(O) HIO_3	XB	2.35	0.0591	0.1471	-0.0086
	HIO_3 (O)···(H) HIO_3	HB	1.59	0.0572	0.1103	-0.0168
	HNO_3 (H)···(O) HIO_3	HB	1.62	0.0533	0.1091	-0.0142
	HIO_3 (O)···(I) HIO_3	XB	2.41	0.0530	0.1253	-0.0073
	HIO_3 (I)···(O) HIO_3	XB	2.42	0.0506	0.1344	-0.0050
	HIO_3 (O)···(I) HIO_3	XB	2.44	0.0477	0.1299	-0.0036
	HIO_3 (I)···(O) HIO_3	XB	2.57	0.0352	0.1038	-0.0003
	HIO_3 (I)···(O) HIO_3	XB	2.83	0.0241	0.0695	0.0001
	HIO_3 (I)···(O) HIO_3	XB	2.80	0.0232	0.0748	0.0015
	HIO_3 (O)···(I) HIO_3	XB	2.92	0.0197	0.0587	0.0009
	HIO_3 (O)···(I) HIO_3	XB	2.94	0.0177	0.0572	0.0015
$(HNO_3)_1(HIO_3)_5$	HNO_3 (O)···(H) HIO_3	HB	2.19	0.0142	0.0515	0.0017
	HNO_3 (O)···(H) HNO_3	HB	1.73	0.0401	0.1056	-0.0061
	HNO_3 (H)···(O) HNO_3	HB	1.73	0.0401	0.1056	-0.0061
$(HNO_3)_2$						
	HIO_2 (O)···(H) HNO_3	HB	1.55	0.0680	0.1082	-0.0233
	HIO_2 (O)···(H) HNO_3	HB	1.58	0.0617	0.1062	-0.0196
	HIO_2 (I)···(O) HNO_3	XB	2.67	0.0289	0.0890	0.0002
$(HNO_3)_2(HIO_2)_1$	HIO_2 (H)···(O) HNO_3	HB	1.97	0.0221	0.0870	0.0023
	NO_3^- (O)···(I) $H_2IO_2^+$	XB	2.41	0.0551	0.1264	-0.0085
	$H_2IO_2^+$ (I)···(O) NO_3^-	XB	2.41	0.0551	0.1264	-0.0085
	$H_2IO_2^+$ (H)···(O) NO_3^-	HB	1.78	0.0381	0.1070	-0.0040
	NO_3^- (O)···(H) $H_2IO_2^+$	HB	1.78	0.0381	0.1070	-0.0040
	$H_2IO_2^+$ (I)···(O) NO_3^-	XB	2.91	0.0201	0.0665	0.0006
	NO_3^- (O)···(I) $H_2IO_2^+$	XB	2.91	0.0201	0.0665	0.0006
	NO_3^- (O)···(H) $H_2IO_2^+$	HB	2.27	0.0113	0.0430	0.0016
$(HNO_3)_2(HIO_2)_2$	$H_2IO_2^+$ (H)···(O) NO_3^-	HB	2.27	0.0113	0.0430	0.0016
	HIO_2 (O)···(I) $H_2IO_2^+$	XB	2.28	0.0692	0.1597	-0.0144
	$H_2IO_2^+$ (I)···(O) NO_3^-	XB	2.33	0.0643	0.1394	-0.0130
	NO_3^- (O)···(H) $H_2IO_2^+$	HB	1.64	0.0531	0.1090	-0.0138
	NO_3^- (O)···(I) HIO_2	XB	2.44	0.0494	0.1266	-0.0054
	NO_3^- (O)···(H) $H_2IO_2^+$	HB	1.88	0.0297	0.0914	-0.0010
$(HNO_3)_2(HIO_2)_3$	NO_3^- (O)···(H) $H_2IO_2^+$	HB	1.94	0.0240	0.0896	0.0018

	$H_2IO_2^+$ (O)···(H) $H_2IO_2^+$	HB	1.96	0.0239	0.0817	0.0009
	$H_2IO_2^+$ (I)···(O) NO_3^-	XB	2.88	0.0211	0.0730	0.0006
	HIO_2 (O)···(I) $H_2IO_2^+$	XB	2.30	0.0686	0.1513	-0.0146
	NO_3^- (O)···(I) $H_2IO_2^+$	XB	2.57	0.0393	0.1011	-0.0028
	$H_2IO_2^+$ (I)···(O) HIO_2	XB	2.56	0.0389	0.1042	-0.0020
	NO_3^- (O)···(H) HIO_2	HB	1.79	0.0378	0.0999	-0.0046
	NO_3^- (O)···(H) $H_2IO_2^+$	HB	1.79	0.0369	0.1038	-0.0037
	HIO_2 (I)···(O) NO_3^-	XB	2.71	0.0293	0.0808	-0.0005
	$H_2IO_2^+$ (H)···(O) NO_3^-	HB	1.89	0.0281	0.0990	0.0007
	HIO_2 (H)···(O) NO_3^-	HB	1.90	0.0280	0.0929	0.0002
 $(HNO_3)_2(HIO_2)_4$	$H_2IO_2^+$ (I)···(O) NO_3^-	XB	2.97	0.0176	0.0582	0.0007
	HIO_3 (O)···(H) HNO_3	HB	1.61	0.0574	0.1109	-0.0162
	HIO_3 (O)···(H) HNO_3	HB	1.65	0.0493	0.1091	-0.0117
	HIO_3 (H)···(O) HNO_3	HB	1.79	0.0330	0.1042	-0.0020
 $(HNO_3)_2(HIO_3)_1$	HIO_3 (I)···(O) HNO_3	XB	2.69	0.0287	0.0849	0.0003
	NO_3^- (O)···(I) HIO_3	XB	2.34	0.0637	0.1305	-0.0127
	HIO_3 (O)···(H) HNO_3	HB	1.58	0.0615	0.1081	-0.0194
	$H_2IO_2^+$ (H)···(O) HIO_3	HB	1.62	0.0555	0.1064	-0.0156
	NO_3^- (O)···(H) $H_2IO_2^+$	HB	1.74	0.0428	0.1029	-0.0073
 $(HNO_3)_2(HIO_3)_1(HIO_2)_1$	$H_2IO_2^+$ (I)···(O) HNO_3	XB	2.74	0.0231	0.0815	0.0017
	HIO_3 (I)···(O) HIO_2	XB	2.18	0.0888	0.1688	-0.0279
	$H_2IO_2^+$ (I)···(O) HIO_3	XB	2.36	0.0557	0.1524	-0.0069
	NO_3^- (O)···(I) HIO_2	XB	2.41	0.0532	0.1275	-0.0074
	HNO_3 (H)···(O) HIO_3	HB	1.64	0.0511	0.1088	-0.0127
	$H_2IO_2^+$ (H)···(O) NO_3^-	HB	1.81	0.0340	0.1081	-0.0016
	HNO_3 (O)···(H) HIO_3	HB	1.88	0.0262	0.0925	0.0006
	$H_2IO_2^+$ (H)···(O) NO_3^-	HB	1.99	0.0216	0.0790	0.0018
 $(HNO_3)_2(HIO_3)_1(HIO_2)_2$	HIO_3 (O)···(H) HIO_2	HB	2.06	0.0201	0.0747	0.0020
	$H_2IO_2^+$ (I)···(O) IO_3^-	XB	2.38	0.0535	0.1493	-0.0059
	NO_3^- (O)···(I) $H_2IO_2^+$	XB	2.52	0.0431	0.1090	-0.0038
	$H_2IO_2^+$ (I)···(O) NO_3^-	XB	2.53	0.0424	0.1080	-0.0036
	$H_2IO_2^+$ (H)···(O) NO_3^-	HB	1.77	0.0388	0.1078	-0.0045
	$H_2IO_2^+$ (H)···(O) IO_3^-	HB	1.80	0.0351	0.1006	-0.0030
	IO_3^- (O)···(H) $H_2IO_2^+$	HB	1.82	0.0334	0.0998	-0.0020
	IO_3^- (O)···(I) $H_2IO_2^+$	XB	2.65	0.0310	0.0920	0.0000
	NO_3^- (O)···(H) $H_2IO_2^+$	HB	1.93	0.0259	0.0886	0.0007
	$H_2IO_2^+$ (I)···(O) NO_3^-	XB	2.79	0.0244	0.0736	0.0007
	NO_3^- (O)···(I) $H_2IO_2^+$	XB	2.96	0.0184	0.0603	0.0006
 $(HNO_3)_2(HIO_3)_1(HIO_2)_3$	IO_3^- (I)···(O) NO_3^-	XB	2.87	0.0174	0.0645	0.0020
	HIO_3 (O)···(I) HIO_3	XB	2.27	0.0742	0.1440	-0.0192
	HIO_3 (I)···(O) HIO_3	XB	2.27	0.0742	0.1440	-0.0192
	HNO_3 (H)···(O) HIO_3	HB	1.63	0.0516	0.1111	-0.0130
	HIO_3 (O)···(H) HNO_3	HB	1.63	0.0516	0.1111	-0.0130

	HNO_3 (O)···(I) HIO_3	XB	2.84	0.0207	0.0696	0.0017
	HIO_3 (I)···(O) HNO_3	XB	2.84	0.0207	0.0696	0.0017
$(HNO_3)_2(HIO_3)_2$						
	NO_3^- (O)···(I) HIO_3	XB	2.33	0.0655	0.1316	-0.0137
	HIO_3 (O)···(H) HNO_3	HB	1.62	0.0552	0.1078	-0.0152
	HIO_3 (I)···(O) HIO_3	XB	2.43	0.0484	0.1296	-0.0040
	$H_2IO_2^+$ (H)···(O) HIO_3	HB	1.67	0.0476	0.1076	-0.0105
	$H_2IO_2^+$ (H)···(O) NO_3^-	HB	1.79	0.0374	0.0997	-0.0044
	$H_2IO_2^+$ (I)···(O) HIO_3	XB	2.64	0.0324	0.0922	-0.0007
$(HNO_3)_2(HIO_3)_2(HIO_2)_1$	HNO_3 (O)···(H) HIO_3	HB	1.96	0.0235	0.0844	0.0014
	HIO_3 (H)···(O) NO_3^-	HB	1.49	0.0784	0.0920	-0.0316
	$H_2IO_2^+$ (I)···(O) NO_3^-	XB	2.50	0.0437	0.1213	-0.0029
	$H_2IO_2^+$ (H)···(O) HIO_3	HB	1.73	0.0404	0.1132	-0.0053
	NO_3^- (O)···(H) $H_2IO_2^+$	HB	1.76	0.0399	0.1037	-0.0054
	HIO_3 (O)···(H) $H_2IO_2^+$	HB	1.78	0.0368	0.1174	-0.0023
	NO_3^- (O)···(H) HIO_3	HB	1.80	0.0340	0.1010	-0.0024
	HIO_3 (O)···(I) $H_2IO_2^+$	XB	2.62	0.0328	0.1017	0.0002
	HIO_3 (I)···(O) NO_3^-	XB	2.70	0.0271	0.0810	0.0005
	$H_2IO_2^+$ (I)···(O) HIO_3	XB	2.72	0.0255	0.0861	0.0015
	NO_3^- (O)···(I) $H_2IO_2^+$	XB	2.91	0.0186	0.0561	0.0010
$(HNO_3)_2(HIO_3)_2(HIO_2)_2$	$H_2IO_2^+$ (H)···(O) NO_3^-	HB	2.06	0.0181	0.0723	0.0025
	HIO_3 (I)···(O) HIO_3	XB	2.31	0.0664	0.1429	-0.0140
	HIO_3 (O)···(I) HIO_3	XB	2.30	0.0644	0.1559	-0.0113
	HNO_3 (H)···(O) HIO_3	HB	1.62	0.0529	0.1103	-0.0138
	HIO_3 (O)···(H) HNO_3	HB	1.63	0.0512	0.1120	-0.0128
	HIO_3 (O)···(I) HIO_3	XB	2.46	0.0469	0.1269	-0.0035
	HNO_3 (O)···(H) HIO_3	HB	1.82	0.0306	0.1005	-0.0010
	HIO_3 (O)···(I) HIO_3	XB	2.85	0.0236	0.0703	0.0002
$(HNO_3)_2(HIO_3)_3$	HIO_3 (I)···(O) HNO_3	XB	2.82	0.0218	0.0705	0.0013
	HIO_3 (I)···(O) HIO_3	XB	2.27	0.0724	0.1496	-0.0176
	HIO_3 (O)···(I) HIO_3	XB	2.41	0.0518	0.1332	-0.0053
	HIO_3 (O)···(H) HNO_3	HB	1.64	0.0500	0.1138	-0.0117
	NO_3^- (O)···(H) $H_2IO_2^+$	HB	1.69	0.0481	0.1068	-0.0102
	HIO_3 (H)···(O) NO_3^-	HB	1.70	0.0453	0.1024	-0.0088
	HIO_3 (O)···(H) $H_2IO_2^+$	HB	1.70	0.0446	0.1054	-0.0087
	HIO_3 (I)···(O) HIO_3	XB	2.52	0.0401	0.1140	-0.0015
	$H_2IO_2^+$ (I)···(O) HIO_3	XB	2.63	0.0309	0.0990	0.0007
	HIO_3 (O)···(I) HIO_3	XB	2.86	0.0230	0.0696	0.0002
	HIO_3 (I)···(O) NO_3^-	XB	3.09	0.0155	0.0435	0.0005
	HIO_3 (O)···(I) $H_2IO_2^+$	XB	3.12	0.0154	0.0458	0.0011
$(HNO_3)_2(HIO_3)_3(HIO_2)_1$	NO_3^- (O)···(O) HIO_3	HB	2.79	0.0153	0.0566	0.0008

	HIO_3 (O)···(I) HIO_3	XB	2.24	0.0735	0.1693	-0.0165
	HNO_3 (H)···(O) HIO_3	HB	1.58	0.0604	0.1086	-0.0187
	HIO_3 (O)···(I) HIO_3	XB	2.35	0.0581	0.1481	-0.0080
	HIO_3 (O)···(H) HNO_3	HB	1.61	0.0545	0.1108	-0.0150
	HIO_3 (O)···(I) HIO_3	XB	2.42	0.0492	0.1387	-0.0039
	HIO_3 (I)···(O) HIO_3	XB	2.53	0.0395	0.1165	-0.0009
	HIO_3 (I)···(O) HIO_3	XB	2.77	0.0251	0.0812	0.0014
	HIO_3 (H)···(O) HNO_3	HB	1.92	0.0244	0.0868	0.0011
$(HNO_3)_2(HIO_3)_4$	HIO_3 (H)···(O) HNO_3	HB	2.03	0.0197	0.0696	0.0015
	HNO_3 (H)···(O) HNO_3	HB	1.75	0.0376	0.1039	-0.0047
	HNO_3 (O)···(H) HNO_3	HB	1.76	0.0357	0.1061	-0.0036
$(HNO_3)_3$	HNO_3 (H)···(O) HNO_3	HB	1.80	0.0318	0.1003	-0.0018
	HNO_3 (H)···(O) HIO_2	HB	1.54	0.0690	0.1081	-0.0240
	HIO_2 (O)···(H) HNO_3	HB	1.57	0.0639	0.1059	-0.0210
	HNO_3 (H)···(O) HIO_2	HB	1.73	0.0421	0.1060	-0.0069
	HNO_3 (O)···(I) HIO_2	XB	2.61	0.0326	0.0982	-0.0004
	HIO_2 (H)···(O) HNO_3	HB	1.84	0.0301	0.1055	0.0000
$(HNO_3)_3(HIO_2)_1$	HNO_3 (O)···(I) HIO_2	XB	2.86	0.0195	0.0652	0.0014
	NO_3^- (O)···(I) $H_2IO_2^+$	XB	2.35	0.0614	0.1352	-0.0113
	$H_2IO_2^+$ (I)···(O) NO_3^-	XB	2.42	0.0531	0.1243	-0.0074
	HNO_3 (H)···(O) $H_2IO_2^+$	HB	1.68	0.0486	0.1086	-0.0105
	$H_2IO_2^+$ (H)···(O) NO_3^-	HB	1.79	0.0363	0.1062	-0.0031
	NO_3^- (O)···(H) $H_2IO_2^+$	HB	1.80	0.0352	0.1054	-0.0025
	HNO_3 (O)···(I) $H_2IO_2^+$	XB	2.82	0.0211	0.0686	0.0012
	$H_2IO_2^+$ (H)···(O) NO_3^-	HB	2.02	0.0200	0.0760	0.0021
$(HNO_3)_3(HIO_2)_2$	NO_3^- (O)···(H) $H_2IO_2^+$	HB	2.20	0.0135	0.0512	0.0019
	$H_2IO_2^+$ (I)···(O) NO_3^-	XB	2.32	0.0653	0.1397	-0.0135
	HIO_2 (O)···(H) HNO_3	HB	1.60	0.0587	0.1077	-0.0177
	NO_3^- (O)···(I) HIO_2	XB	2.41	0.0533	0.1319	-0.0072
	NO_3^- (O)···(H) $H_2IO_2^+$	HB	1.66	0.0502	0.1083	-0.0120
	HIO_2 (O)···(I) $H_2IO_2^+$	XB	2.43	0.0501	0.1311	-0.0052
	NO_3^- (O)···(H) $H_2IO_2^+$	HB	1.82	0.0338	0.0968	-0.0028
	$H_2IO_2^+$ (O)···(H) $H_2IO_2^+$	HB	1.94	0.0250	0.0839	0.0006
	$H_2IO_2^+$ (H)···(O) NO_3^-	HB	1.96	0.0236	0.0871	0.0018
	$H_2IO_2^+$ (I)···(O) NO_3^-	XB	2.87	0.0215	0.0738	0.0006
$(HNO_3)_3(HIO_2)_3$	$H_2IO_2^+$ (I)···(O) HNO_3	XB	2.93	0.0171	0.0565	0.0014
	HNO_3 (H)···(O) HIO_3	HB	1.61	0.0569	0.1114	-0.0158
	HIO_3 (O)···(H) HNO_3	HB	1.67	0.0483	0.1086	-0.0107
	HNO_3 (H)···(O) HIO_3	HB	1.70	0.0444	0.1054	-0.0087
	HNO_3 (O)···(I) HIO_3	XB	2.66	0.0304	0.0890	0.0001
	HNO_3 (O)···(H) HIO_3	HB	1.82	0.0295	0.1004	-0.0005
$(HNO_3)_3(HIO_3)_1$	HIO_3 (I)···(O) HNO_3	XB	2.86	0.0212	0.0667	0.0012

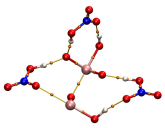
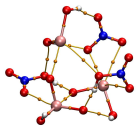
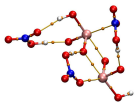
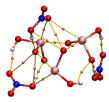
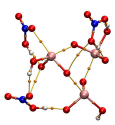
 $(HNO_3)_3(HIO_3)_1(HIO_2)_1$	HIO_2 (O)···(I) HIO_3	XB	2.22	0.0823	0.1548	-0.0238
	HNO_3 (H)···(O) HIO_3	HB	1.61	0.0558	0.1090	-0.0158
	HNO_3 (H)···(O) HIO_3	HB	1.61	0.0526	0.1155	-0.0136
	HIO_3 (O)···(H) HNO_3	HB	1.67	0.0477	0.1071	-0.0107
	HIO_2 (H)···(O) HNO_3	HB	1.79	0.0328	0.1028	-0.0022
	HIO_3 (H)···(O) HNO_3	HB	1.88	0.0258	0.0922	0.0008
	HIO_2 (I)···(O) HNO_3	XB	2.70	0.0253	0.0865	0.0014
 $(HNO_3)_3(HIO_3)_1(HIO_2)_2$	HIO_2 (O)···(I) HIO_3	XB	2.27	0.0725	0.1494	-0.0167
	HIO_2 (I)···(O) NO_3^-	XB	2.43	0.0523	0.1244	-0.0072
	HIO_2 (O)···(H) HNO_3	HB	1.65	0.0512	0.1087	-0.0127
	HIO_3 (O)···(H) HNO_3	HB	1.65	0.0503	0.1106	-0.0118
	HIO_3 (O)···(I) $H_2IO_2^+$	XB	2.41	0.0493	0.1439	-0.0041
	NO_3^- (O)···(H) $H_2IO_2^+$	HB	1.80	0.0358	0.1066	-0.0026
	NO_3^- (O)···(H) $H_2IO_2^+$	HB	1.96	0.0223	0.0833	0.0019
	HIO_2 (I)···(O) NO_3^-	XB	2.93	0.0194	0.0647	0.0006
	HIO_3 (I)···(O) HNO_3	XB	2.97	0.0163	0.0528	0.0014
	HIO_2 (H)···(O) HIO_3	HB	2.23	0.0148	0.0533	0.0014
 $(HNO_3)_3(HIO_3)_2$	HIO_3 (O)···(I) HIO_3	XB	2.32	0.0665	0.1371	-0.0144
	HIO_3 (I)···(O) HIO_3	XB	2.32	0.0658	0.1387	-0.0141
	HIO_3 (O)···(H) HNO_3	HB	1.64	0.0508	0.1101	-0.0126
	HNO_3 (H)···(O) HIO_3	HB	1.64	0.0507	0.1104	-0.0125
	HIO_3 (O)···(H) HNO_3	HB	1.71	0.0412	0.1072	-0.0068
	HIO_3 (H)···(O) HNO_3	HB	1.82	0.0313	0.1025	-0.0011
	HNO_3 (O)···(I) HIO_3	XB	2.81	0.0223	0.0733	0.0015
	HIO_3 (I)···(O) HNO_3	XB	2.97	0.0158	0.0527	0.0015
 $(HNO_3)_3(HIO_3)_2(HIO_2)_1$	HIO_2 (O)···(I) HIO_3	XB	2.19	0.0877	0.1603	-0.0277
	HIO_3 (I)···(O) HIO_3	XB	2.34	0.0596	0.1503	-0.0087
	HNO_3 (H)···(O) HIO_3	HB	1.65	0.0503	0.1094	-0.0120
	HNO_3 (H)···(O) HIO_3	HB	1.66	0.0499	0.1094	-0.0116
	HIO_3 (O)···(H) HNO_3	HB	1.68	0.0481	0.1072	-0.0105
	HIO_2 (I)···(O) HIO_3	XB	2.52	0.0406	0.1138	-0.0024
	HNO_3 (O)···(H) HIO_3	HB	1.90	0.0249	0.0902	0.0011
	HNO_3 (O)···(H) HIO_3	HB	2.02	0.0184	0.0720	0.0024
 $(HNO_3)_3(HIO_3)_3$	HIO_3 (O)···(I) HIO_3	XB	2.32	0.0653	0.1460	-0.0129
	HIO_3 (I)···(O) HIO_3	XB	2.30	0.0648	0.1575	-0.0114
	HIO_3 (O)···(H) HNO_3	HB	1.62	0.0546	0.1109	-0.0145
	HIO_3 (O)···(H) HNO_3	HB	1.68	0.0478	0.1060	-0.0105
	HIO_3 (O)···(H) HNO_3	HB	1.66	0.0471	0.1114	-0.0104
	HIO_3 (I)···(O) HIO_3	XB	2.49	0.0437	0.1213	-0.0025
	HNO_3 (O)···(H) HIO_3	HB	1.79	0.0341	0.1061	-0.0021
	HNO_3 (O)···(H) HIO_3	HB	1.91	0.0244	0.0884	0.0012
	HIO_3 (I)···(O) HNO_3	XB	2.83	0.0224	0.0690	0.0010

Table S3. Representative boundary conditions applied in the ACDC simulations include $[HIO_3]$ concentrations of 10^6 or 10^8 molecules cm^{-3} and $[HNO_3]$ concentrations of 10^8 or 10^{10} molecules cm^{-3}, with $[HIO_2] = [HIO_3]/50$, within the temperature range of 228 to 288 K. To simplify cluster names, we abbreviate $(HNO_3)_x(HIO_3)_y(HIO_2)_z$ as "*xyz*". For instance, $(HNO_3)_0(HIO_3)_3(HIO_2)_4$ is simply written as "034", and $(HNO_3)_2(HIO_3)_2(HIO_2)_3$ as "223".

Temperature (K)	Boundary Cluster		
	$[HIO_3]$	$[HNO_3] = 10^8$	$[HNO_3] = 10^{10}$
288	10^6	034 043	034 043 223 313
	10^8	034 043 052 061	034 043 052 061 223 313
278	10^6	034 043	034 043 223 313
	10^8	034 043 052 061	034 043 052 061 223 313
268	10^6	034 043 052 223	034 043 052 223 313
	10^8	025 034 043 052 061 133 223	025 034 043 052 061 133 223 313
258	10^6	034 043 052 061 223 313	034 043 052 061 223 313 304
	10^8	034 043 052 061 070 133 223 313	034 043 052 061 223 313 304 070 133
248	10^6	025 034 043 052 061 223 313	025 034 043 052 061 223 313 304 205
	10^8	025 034 043 052 061 070 133 223 313	025 034 043 052 061 223 313 304 205 070 133
238	10^6	025 034 043 052 061 070 133 223 313 304	025 034 043 052 061 070 133 223 313 304 205
	10^8	025 034 043 052 061 070 124 214 133 223 313 304	025 034 043 052 061 070 133 223 313 304 205 124 214
228	10^6	025 034 043 052 061 070 133 223 313 304 205	025 034 043 052 061 070 133 223 313 304 205 241 214
	10^8	025 034 043 052 061 070 313 214 007 124 133 223 304 205	025 034 043 052 061 070 133 223 313 304 205 241 214 007 124

Table S4. Comparison of binding free energies (ΔG, kcal mol^{-1}) for HNO_3–HIO_3–HIO_2 clusters and the corresponding H_2SO_4–HNO_3–NH_3 clusters at 228 K. All values were calculated at the DLPNO-CCSD(T)/aug-cc-pVTZ(-PP)//ωB97X-D/6-311++G(3df,3pd) + aug-cc-pVTZ-PP level of theory.

Clusters	ΔG_{228}	Clusters	ΔG_{228}
$(HNO_3)_1$ $(HIO_2)_1$	-14.4	$(HNO_3)_1$ $(NH_3)_1$	-5.7
$(HNO_3)_1(HIO_3)_1(HIO_2)_1$	-27.4	$(HNO_3)_1(H_2SO_4)_1(NH_3)_1$	-14.9
$(HNO_3)_1(HIO_3)_1(HIO_2)_2$	-51.7	$(HNO_3)_1(H_2SO_4)_1(NH_3)_2$	-25.8
$(HNO_3)_1(HIO_3)_2(HIO_2)_1$	-45.3	$(HNO_3)_1(H_2SO_4)_2(NH_3)_1$	-31.5
$(HNO_3)_1(HIO_3)_2(HIO_2)_2$	-65.9	$(HNO_3)_1(H_2SO_4)_2(NH_3)_2$	-41.8
$(HNO_3)_1(HIO_3)_2(HIO_2)_3$	-96.6	$(HNO_3)_1(H_2SO_4)_2(NH_3)_3$	-58.2
$(HNO_3)_1(HIO_3)_3(HIO_2)_1$	-61.3	$(HNO_3)_1(H_2SO_4)_3(NH_3)_1$	-43.3
$(HNO_3)_1(HIO_3)_3(HIO_2)_2$	-88.5	$(HNO_3)_1(H_2SO_4)_3(NH_3)_2$	-63.7
$(HNO_3)_2(HIO_2)_1$	-17.4	$(HNO_3)_2(NH_3)_1$	-7.9
$(HNO_3)_2(HIO_2)_2$	-44.4	$(HNO_3)_2(NH_3)_2$	-14.8
$(HNO_3)_2(HIO_3)_1(HIO_2)_1$	-33.9	$(HNO_3)_2(H_2SO_4)_1(NH_3)_1$	-22.7
$(HNO_3)_2(HIO_3)_1(HIO_2)_2$	-57.9	$(HNO_3)_2(H_2SO_4)_1(NH_3)_2$	-32.0
$(HNO_3)_2(HIO_3)_1(HIO_2)_3$	-85.1	$(HNO_3)_2(H_2SO_4)_1(NH_3)_3$	-46.6
$(HNO_3)_2(HIO_3)_2(HIO_2)_1$	-52.5	$(HNO_3)_2(H_2SO_4)_2(NH_3)_1$	-36.5
$(HNO_3)_2(HIO_3)_2(HIO_2)_2$	-69.7	$(HNO_3)_2(H_2SO_4)_2(NH_3)_2$	-54.5
$(HNO_3)_3(HIO_2)_1$	-19.0	$(HNO_3)_3(NH_3)_1$	-11.9
$(HNO_3)_3(HIO_2)_2$	-43.3	$(HNO_3)_3(NH_3)_2$	-22.5
$(HNO_3)_3(HIO_2)_3$	-66.9	$(HNO_3)_3(NH_3)_3$	-30.1
$(HNO_3)_3(HIO_3)_1(HIO_2)_1$	-38.2	$(HNO_3)_3(H_2SO_4)_1(NH_3)_1$	-28.1
$(HNO_3)_3(HIO_3)_1(HIO_2)_2$	-62.8	$(HNO_3)_3(H_2SO_4)_1(NH_3)_2$	-39.7

Table S5. Comparison of evaporation rate sums ($\Sigma\gamma$, s^{-1}) for HNO_3–HIO_3–HIO_2 clusters and the corresponding H_2SO_4–HNO_3–NH_3 clusters at 228 K. All values were calculated at the DLPNO-CCSD(T)/aug-cc-pVTZ(-PP)//ωB97X-D/6-311++G(3df,3pd) + aug-cc-pVTZ-PP level of theory.

Clusters	$\Sigma\gamma$ (s^{-1})	Clusters	$\Sigma\gamma$ (s^{-1})
$(HNO_3)_1(HIO_2)_1$	7.97×10^{-4}	$(HNO_3)_1(NH_3)_1$	4.28×10^{4}
$(HNO_3)_1(HIO_3)_1(HIO_2)_1$	7.00×10^{3}	$(HNO_3)_1(H_2SO_4)_1(NH_3)_1$	1.30×10^{4}
$(HNO_3)_1(HIO_3)_1(HIO_2)_2$	1.74×10^{1}	$(HNO_3)_1(H_2SO_4)_1(NH_3)_2$	6.25×10^{-1}
$(HNO_3)_1(HIO_3)_2(HIO_2)_1$	1.62×10^{4}	$(HNO_3)_1(H_2SO_4)_2(NH_3)_1$	1.65×10^{5}
$(HNO_3)_1(HIO_3)_2(HIO_2)_2$	1.59×10^{4}	$(HNO_3)_1(H_2SO_4)_2(NH_3)_2$	1.77×10^{4}
$(HNO_3)_1(HIO_3)_2(HIO_2)_3$	4.83×10^{-5}	$(HNO_3)_1(H_2SO_4)_2(NH_3)_3$	5.08×10^{-6}
$(HNO_3)_1(HIO_3)_3(HIO_2)_1$	2.39×10^{3}	$(HNO_3)_1(H_2SO_4)_3(NH_3)_1$	3.22×10^{5}
$(HNO_3)_1(HIO_3)_3(HIO_2)_2$	3.87×10^{2}	$(HNO_3)_1(H_2SO_4)_3(NH_3)_2$	2.83×10^{0}
$(HNO_3)_2(HIO_2)_1$	5.92×10^{7}	$(HNO_3)_2(NH_3)_1$	8.33×10^{7}
$(HNO_3)_2(HIO_2)_2$	2.30×10^{-4}	$(HNO_3)_2(NH_3)_2$	2.77×10^{6}
$(HNO_3)_2(HIO_3)_1(HIO_2)_1$	3.83×10^{4}	$(HNO_3)_2(H_2SO_4)_1(NH_3)_1$	3.47×10^{2}
$(HNO_3)_2(HIO_3)_1(HIO_2)_2$	5.63×10^{4}	$(HNO_3)_2(H_2SO_4)_1(NH_3)_2$	1.58×10^{4}
$(HNO_3)_2(HIO_3)_1(HIO_2)_3$	1.61×10^{-4}	$(HNO_3)_2(H_2SO_4)_1(NH_3)_3$	2.40×10^{-4}
$(HNO_3)_2(HIO_3)_2(HIO_2)_1$	1.33×10^{4}	$(HNO_3)_2(H_2SO_4)_2(NH_3)_1$	1.91×10^{5}
$(HNO_3)_2(HIO_3)_2(HIO_2)_2$	1.61×10^{7}	$(HNO_3)_2(H_2SO_4)_2(NH_3)_2$	9.05×10^{-3}
$(HNO_3)_3(HIO_2)_1$	1.77×10^{9}	$(HNO_3)_3(NH_3)_1$	1.78×10^{6}
$(HNO_3)_3(HIO_2)_2$	5.68×10^{11}	$(HNO_3)_3(NH_3)_2$	5.48×10^{2}
$(HNO_3)_3(HIO_2)_3$	9.21×10^{4}	$(HNO_3)_3(NH_3)_3$	1.01×10^{3}
$(HNO_3)_3(HIO_3)_1(HIO_2)_1$	3.32×10^{6}	$(HNO_3)_3(H_2SO_4)_1(NH_3)_1$	8.40×10^{4}
$(HNO_3)_3(HIO_3)_1(HIO_2)_2$	1.35×10^{6}	$(HNO_3)_3(H_2SO_4)_1(NH_3)_2$	4.70×10^{2}

Table S6. Gibbs free energies (ΔG) evaluated at 263 K (kcal mol^{-1}) of the $(HNO_3)_x(HIO_3)_y(HIO_2)_z$ clusters ($2 \le x + y + z \le 6$, $0 \le x \le 3$). DLPNO-CCSD(T) values were computed at the DLPNO-CCSD(T)/aug-cc-pVTZ (for H, N, O) + aug-cc-pVTZ-PP (for I); ZORA-DLPNO-CCSD(T) values were computed at the ZORA-DLPNO-CCSD(T)/ma-ZORA-def2-TZVPP (for H, N, O) + SARC-ZORA-TZVPP (for I) level of theory, both based on geometries optimized at the ωB97X-D/6-311++G(3df,3pd) + aug-cc-pVTZ-PP level.

Clusters	ΔG_{263K} (kcal mol^{-1})	
	DLPNO-CCSD(T)	ZORA-DLPNO-CCSD(T)
$(HIO_2)_2$	-19.9	-16.0
$(HIO_2)_3$	-37.7	-30.3
$(HIO_2)_4$	-54.7	-44.4
$(HIO_2)_5$	-69.3	-54.8
$(HIO_2)_6$	-87.3	-69.3
$(HIO_3)_1(HIO_2)_1$	-18.8	-15.7
$(HIO_3)_1(HIO_2)_2$	-38.7	-32.8
$(HIO_3)_1(HIO_2)_3$	-54.6	-43.1
$(HIO_3)_1(HIO_2)_4$	-73.0	-58.5
$(HIO_3)_1(HIO_2)_5$	-76.1	-57.3
$(HIO_3)_2$	-12.8	-8.7
$(HIO_3)_2(HIO_2)_1$	-35.6	-26.8
$(HIO_3)_2(HIO_2)_2$	-54.5	-44.4
$(HIO_3)_2(HIO_2)_3$	-74.7	-60.1
$(HIO_3)_2(HIO_2)_4$	-94.0	-74.9
$(HIO_3)_3$	-25.0	-16.4
$(HIO_3)_3(HIO_2)_1$	-49.0	-39.0
$(HIO_3)_3(HIO_2)_2$	-73.7	-58.4
$(HIO_3)_3(HIO_2)_3$	-98.8	-77.7
$(HIO_3)_4$	-44.1	-31.6
$(HIO_3)_4(HIO_2)_1$	-66.9	-48.8
$(HIO_3)_4(HIO_2)_2$	-90.7	-68.9
$(HIO_3)_5$	-60.5	-42.3

$(HIO_3)_5(HIO_2)_1$	-83.5	-61.8
$(HIO_3)_6$	-74.0	-50.3
$(HNO_3)_1(HIO_2)_1$	-13.0	-10.0
$(HNO_3)_1(HIO_2)_2$	-26.3	-19.9
$(HNO_3)_1(HIO_2)_3$	-46.7	-37.2
$(HNO_3)_1(HIO_2)_4$	-62.9	-51.2
$(HNO_3)_1(HIO_2)_5$	-80.1	-64.0
$(HNO_3)_1(HIO_3)_1$	-5.3	-3.8
$(HNO_3)_1(HIO_3)_1(HIO_2)_1$	-24.6	-18.7
$(HNO_3)_1(HIO_3)_1(HIO_2)_2$	-47.3	-37.0
$(HNO_3)_1(HIO_3)_1(HIO_2)_3$	-63.8	-48.9
$(HNO_3)_1(HIO_3)_1(HIO_2)_4$	-81.6	-63.5
$(HNO_3)_1(HIO_3)_2$	-18.1	-11.2
$(HNO_3)_1(HIO_3)_2(HIO_2)_1$	-41.2	-30.7
$(HNO_3)_1(HIO_3)_2(HIO_2)_2$	-60.0	-44.8
$(HNO_3)_1(HIO_3)_2(HIO_2)_3$	-89.2	-69.2
$(HNO_3)_1(HIO_3)_3$	-32.0	-20.8
$(HNO_3)_1(HIO_3)_3(HIO_2)_1$	-55.4	-39.2
$(HNO_3)_1(HIO_3)_3(HIO_2)_2$	-81.0	-59.7
$(HNO_3)_1(HIO_3)_4$	-49.8	-31.7
$(HNO_3)_1(HIO_3)_4(HIO_2)_1$	-75.7	-55.1
$(HNO_3)_1(HIO_3)_5$	-68.1	-47.7
$(HNO_3)_2$	-0.3	1.1
$(HNO_3)_2(HIO_2)_1$	-14.8	-11.2
$(HNO_3)_2(HIO_2)_2$	-40.0	-31.4
$(HNO_3)_2(HIO_2)_3$	-55.0	-43.7
$(HNO_3)_2(HIO_2)_4$	-74.5	-58.6
$(HNO_3)_2(HIO_3)_1$	-10.3	-6.3
$(HNO_3)_2(HIO_3)_1(HIO_2)_1$	-29.7	-21.6
$(HNO_3)_2(HIO_3)_1(HIO_2)_2$	-52.4	-40.6
$(HNO_3)_2(HIO_3)_1(HIO_2)_3$	-77.7	-60.5
$(HNO_3)_2(HIO_3)_2$	-25.7	-16.4
$(HNO_3)_2(HIO_3)_2(HIO_2)_1$	-46.7	-34.0
$(HNO_3)_2(HIO_3)_2(HIO_2)_2$	-62.4	-47.9
$(HNO_3)_2(HIO_3)_3$	-37.8	-25.1

$(HNO_3)_2(HIO_3)_3(HIO_2)_1$	-61.7	-43.7
$(HNO_3)_2(HIO_3)_4$	-53.0	-36.8
$(HNO_3)_3$	2.9	4.5
$(HNO_3)_3(HIO_2)_1$	-15.1	-9.2
$(HNO_3)_3(HIO_2)_2$	-37.8	-27.3
$(HNO_3)_3(HIO_2)_3$	-59.9	-46.6
$(HNO_3)_3(HIO_3)_1$	-14.1	-7.9
$(HNO_3)_3(HIO_3)_1(HIO_2)_1$	-33.0	-24.2
$(HNO_3)_3(HIO_3)_1(HIO_2)_2$	-56.0	-41.7
$(HNO_3)_3(HIO_3)_2$	-27.0	-16.4
$(HNO_3)_3(HIO_3)_2(HIO_2)_1$	-48.7	-34.6
$(HNO_3)_3(HIO_3)_3$	-42.6	-28.3

Table S7. Cartesian coordinates of $(HNO_3)_x(HIO_3)_y(HIO_2)_z$ clusters ($2 \leqslant x+y+z \leqslant 6$, $1 \leqslant x \leqslant 3$) in the present study calculated at the ωB97X-D/6-311++G(3df, 3pd) (for H, N, and O atoms) and aug-cc-pVTZ-PP with ECP28MDF (for I atom) levels of theory.

$(HNO_3)_1(HIO_2)_1$	X	Y	Z
O	0.430565	1.463463	0.686532
I	0.787082	-0.291332	-0.015048
O	2.635613	0.243640	-0.436589
H	3.165780	0.301811	0.362746
H	-0.396934	1.724221	0.233685
N	-2.267582	0.014152	-0.079652
O	-3.390296	-0.394462	-0.039701
O	-1.918406	1.072684	-0.607341
O	-1.333863	-0.720889	0.491930

$(HNO_3)_1(HIO_2)_2$	X	Y	Z
I	-1.822661	-0.470866	-0.258089
O	-1.150974	-0.134475	1.505491
O	-3.634537	0.146428	0.246900
H	-4.077767	-0.506937	0.794137
I	1.810791	-0.447402	-0.036907
O	0.207530	-1.124829	-0.748199
O	2.461160	-2.225289	0.521509
H	2.063051	-2.465776	1.362480
H	-0.700719	0.744251	1.450594
N	0.644079	2.533070	0.010189
O	0.113807	2.167480	1.073111
O	1.123630	1.631805	-0.792244
O	0.733885	3.684526	-0.312038

$(HNO_3)_1(HIO_2)_3$	X	Y	Z
H	0.979335	-0.772235	1.482792
I	-2.166914	-0.943320	-0.088293
O	-1.666417	0.552975	0.909124
O	-3.713408	-0.107396	-0.982256
H	-3.422911	0.322526	-1.790709
I	-0.383850	2.276575	0.259485
O	0.506729	1.092304	-0.897093
O	0.837868	3.795228	-0.137656
H	0.651497	4.150077	-1.010233
I	2.263669	-0.206021	-0.418091

O	1.669326	-0.075246	1.398367
O	3.682716	-1.468788	0.066219
H	3.261362	-2.325619	0.214198
N	0.116749	-2.986408	0.348034
O	-0.239552	-1.920911	1.003445
O	1.278028	-3.345111	0.423196
O	-0.739101	-3.549716	-0.314172

$(HNO_3)_1(HIO_2)_4$	X	Y	Z
H	-1.428569	1.949293	2.077297
I	2.535812	-1.041280	0.965910
O	2.329711	-0.740676	-0.871255
O	1.178177	0.024423	1.705353
H	1.281125	1.623587	1.313082
I	-1.317100	-0.396259	1.619295
O	-1.327206	1.214153	2.702694
O	-3.250943	-0.527111	1.568017
H	-3.544668	0.156027	0.942981
I	0.731885	2.296150	-0.917228
O	1.298771	2.528302	0.891545
O	2.479147	1.860236	-1.620363
H	2.593762	0.894869	-1.453281
I	-0.986412	-2.057853	-1.658891
O	-1.225480	-2.369031	0.150348
O	0.845910	-2.521732	-1.944976
H	1.437742	-1.787701	-1.564300
N	-2.285048	2.088740	-0.741843
O	-1.948831	2.104368	-1.922720
O	-3.335496	1.597613	-0.353668
O	-1.474492	2.592276	0.119465

$(HNO_3)_1(HIO_2)_5$	X	Y	Z
N	-2.022976	2.781292	-0.247648
O	-1.431846	2.890349	0.853086
H	-1.752665	2.279455	2.824230
O	-2.864969	1.850325	-0.399981
O	-1.763076	3.521198	-1.174910
I	-0.152234	0.847334	-2.184586
O	-0.084514	-1.012172	-1.832901
O	-1.938167	0.761098	-3.013700
H	-2.548500	1.145522	-2.365925
I	-1.291492	0.000073	2.229495
O	-1.760356	1.494444	3.392412
O	-3.015201	-0.027025	1.402563

H	-3.010978	0.729463	0.743353
I	2.135328	1.750099	0.508245
O	1.938164	1.061441	-1.224303
O	1.304877	3.488680	0.201168
H	0.349255	3.431634	0.390700
I	2.846202	-1.884137	0.032727
O	3.229757	-0.340358	0.971684
O	1.574371	-2.773225	1.165081
H	0.664479	-2.416988	0.972531
I	-1.756347	-2.050317	-0.806754
O	-0.815110	-1.732798	0.808504
O	-3.151342	-3.094319	0.136966
H	-3.738714	-2.481084	0.589614

$(HNO_3)_1(HIO_3)_1$	X	Y	Z
I	-1.389839	-0.077570	-0.087919
O	-0.526817	1.449337	-0.852732
H	0.413899	1.421772	-0.582378
O	-1.370848	0.245701	1.648874
O	-0.161574	-1.342818	-0.403486
N	2.871843	0.093884	0.082144
O	2.444631	-1.160264	-0.120647
H	1.447746	-1.136542	-0.184306
O	2.031180	0.977799	0.131304
O	4.045545	0.226343	0.203112

$(HNO_3)_1(HIO_3)_1(HIO_2)_1$	X	Y	Z
I	1.731370	0.420553	0.247837
O	0.749387	1.467663	-0.843102
O	1.825937	-1.149740	-0.605364
O	3.447336	1.103332	-0.364708
H	3.497848	1.078698	-1.326513
I	-1.213164	-1.353959	-0.087321
O	-0.235167	-0.300111	1.100664
O	-0.223297	-2.997348	0.129239
H	0.657755	-2.786156	-0.228186
H	-0.578716	2.076627	-0.351294
N	-2.489044	2.043526	-0.060133
O	-1.321466	2.664729	0.029616
O	-2.511398	0.929455	-0.577465
O	-3.433644	2.631606	0.358565

$(HNO_3)_1(HIO_3)_1(HIO_2)_2$	X	Y	Z
H	1.380709	-0.233226	1.598421

I	-2.018095	-1.078948	0.207136
O	-0.505562	-1.795566	-0.514970
O	-2.636185	-0.028251	-1.096824
O	-3.115327	-2.607188	-0.312504
H	-3.244831	-2.617409	-1.267005
I	1.803975	-1.631181	-0.243761
O	1.403294	-1.208677	1.576937
O	3.714846	-1.471431	0.002857
H	3.910375	-0.516160	-0.021329
I	-0.560814	2.192815	0.029651
O	-0.962384	0.647671	1.046488
O	-2.419313	2.656499	-0.308095
H	-2.784921	1.915306	-0.819967
N	2.542920	1.930862	-0.092725
O	2.271203	2.967013	-0.670897
O	3.615356	1.351149	-0.199217
O	1.635290	1.407919	0.667299

$(HNO_3)_1(HIO_3)_1(HIO_2)_3$	X	Y	Z
H	-2.015927	2.988790	0.355648
I	2.497560	-0.557915	0.346596
O	1.918401	0.443172	-1.045472
O	1.441430	-0.033984	1.718108
O	3.929390	0.696695	0.784851
H	3.626055	1.608701	0.699230
I	-0.372842	-1.760528	-1.396613
O	1.069834	-2.075206	-0.210377
O	0.795398	-1.642728	-2.971046
H	1.241463	-0.788377	-2.928024
I	0.095444	2.295796	-0.417513
O	-1.208488	3.530436	0.291941
O	1.376917	2.724850	0.988218
H	1.348483	1.972302	1.603911
I	-1.858766	-0.716583	1.767556
O	-1.759129	-2.000459	0.430802
O	-0.538067	-1.353057	3.010493
H	0.311843	-0.994049	2.666332
N	-2.598352	1.019111	-1.369591
O	-3.143981	0.120561	-1.965789
O	-2.865013	1.280438	-0.171217
O	-1.701379	1.716542	-1.949424

$(HNO_3)_1(HIO_3)_1(HIO_2)_4$	X	Y	Z
H	3.214318	-1.689238	-1.648287

O	2.656371	-1.519278	-2.429296
I	1.646588	2.072546	-0.676137
O	3.555766	1.818720	-0.946042
H	3.799160	1.017450	-0.454565
O	-1.570845	-0.929888	-1.272883
I	-2.565426	-1.476969	0.129810
O	-2.196218	-3.349031	-0.210858
H	-1.312196	-3.448123	-0.608279
O	-1.529913	-1.340120	1.591167
O	-0.625684	1.455282	2.711475
I	0.467386	-0.101267	2.486407
O	2.054954	0.805246	3.129098
H	2.733591	0.597447	2.458267
O	-3.121997	0.672540	0.306675
I	-2.357068	2.077423	-0.686208
O	-0.696529	2.350903	0.135810
H	-0.697882	1.885023	1.828803
O	1.038014	1.021080	-2.093586
I	0.859639	-1.250657	-1.780719
O	0.561835	-3.191028	-1.382548
H	1.158606	-3.424997	-0.660634
N	3.019239	-1.531304	0.988270
O	3.409225	-0.341448	0.978940
O	2.259936	-1.923994	1.896570
O	3.362643	-2.308417	0.096694

$(HNO_3)_1(HIO_3)_2$	X	Y	Z
I	-1.848277	0.145043	-0.287611
O	-1.405319	1.743304	0.386349
O	-1.218908	-1.050698	0.926901
O	-3.648899	0.112313	0.419932
H	-3.643741	0.161093	1.382596
I	1.118082	-1.198515	0.209347
O	2.873538	-0.853101	-0.516814
O	0.250741	-0.131698	-1.030830
O	0.967160	-2.829847	-0.426404
N	1.880498	2.468278	0.166501
O	0.741699	3.047546	-0.193491
O	2.878536	2.939639	-0.282018
O	1.815488	1.511403	0.928954
H	-0.022947	2.466296	0.117557
H	3.171207	0.017809	-0.218325

$(HNO_3)_1(HIO_3)_2(HIO_2)_1$	X	Y	Z

N	3.817881	-0.104040	1.674226
O	3.312860	-1.328095	1.466786
H	2.787637	-1.306828	0.611120
O	3.597481	0.745322	0.832657
O	4.441420	0.032286	2.679851
I	0.152873	-1.618999	-0.853661
O	1.935322	-1.580396	-0.709472
O	-0.342428	-0.907840	0.767115
O	-0.051464	-3.448687	-0.201829
H	0.458269	-3.600956	0.600673
I	-2.395075	0.123123	0.847142
O	-1.583529	1.670158	0.364049
O	-2.710233	-0.753753	-0.672240
O	-4.160333	0.906205	1.028217
H	-4.497017	1.175961	0.165982
I	0.649497	1.879277	-0.605290
O	0.147292	0.386234	-1.630543
O	2.403923	2.103249	-1.396084
H	3.016811	1.542388	-0.899577

$(HNO_3)_1(HIO_3)_2(HIO_2)_2$	X	Y	Z
H	-3.857594	-1.370692	0.214044
I	0.151898	2.186925	-0.357146
O	-0.270178	1.586682	1.272782
O	1.951041	1.987632	-0.341058
O	0.160270	4.067697	0.078009
H	0.572519	4.213678	0.937640
I	0.530101	-1.674390	-1.362841
O	0.522105	-2.241409	0.337005
O	-0.085273	0.040090	-1.310080
O	-1.198267	-2.351144	-1.879575
H	-1.918284	-1.692621	-1.780991
I	-2.123399	-0.400923	1.471298
O	-3.776685	-1.346290	1.186646
O	-1.258378	-1.795169	2.497205
H	-0.669704	-2.231519	1.854321
I	2.902696	-0.040956	0.648027
O	2.544428	-0.841467	-1.004845
O	3.674770	-1.634785	1.472382
H	2.948585	-2.232495	1.683738
N	-2.989765	0.643532	-1.399883
O	-2.763754	1.273059	-2.402973
O	-2.912717	1.214396	-0.260470
O	-3.286843	-0.576276	-1.429334

$(HNO_3)_1(HIO_3)_2(HIO_2)_3$	X	Y	Z
H	0.680378	3.623919	-0.744833
O	1.124909	3.278699	-1.535188
I	0.533226	1.451904	-1.677598
O	-1.024432	1.911652	-2.727729
H	-1.725925	2.145785	-2.102346
O	2.324576	-0.632865	1.881932
I	0.637215	0.130000	2.215061
O	1.322389	1.728554	3.094337
H	1.186951	2.465834	2.486295
O	2.155205	-1.668323	-0.765107
O	2.585117	1.080387	-0.310710
I	3.339113	-0.539162	-0.024916
O	4.491077	-0.499303	-1.612375
H	3.978271	-0.539104	-2.425738
O	-0.348632	-1.789425	1.135495
I	-0.469564	-2.392168	-0.575250
O	-2.142445	-3.041542	-0.552964
H	-3.565546	-2.273292	0.051873
O	-0.719121	-0.867463	-1.556489
O	-4.287892	-1.624095	0.248868
I	-3.455180	0.100891	0.234598
O	-3.236696	0.194987	-1.661766
H	-2.364445	-0.235121	-1.832866
N	-1.512062	2.477503	0.995971
O	-1.820647	1.895367	2.038708
O	-2.235675	2.299577	-0.033694
O	-0.512761	3.189021	0.917352

$(HNO_3)_1(HIO_3)_3$	X	Y	Z
N	-3.524129	0.526733	1.376055
O	-3.623357	1.593044	0.574295
H	-2.693721	1.846501	0.306399
O	-2.403381	0.080449	1.567200
O	-4.543966	0.118536	1.830197
I	-1.157957	-1.650311	-0.365330
O	-0.752041	-0.094444	-1.236211
O	-0.748591	-2.881885	-1.559272
O	-3.054229	-1.573477	-0.745283
H	-3.195155	-1.900043	-1.642735
I	0.245267	1.858864	-0.628072
O	-1.328220	2.573705	-0.188775
O	0.727628	1.047314	0.939326

O	1.253805	3.477848	-0.285398
H	0.848588	3.964118	0.442356
I	2.424451	-0.488997	0.686918
O	1.154775	-1.756581	0.485768
O	2.593590	0.281104	-0.917003
O	3.929852	-1.694422	0.517756
H	3.938957	-2.103703	-0.355590

$(HNO_3)_1(HIO_3)_3(HIO_2)_1$	X	Y	Z
N	-1.423636	-2.698310	-0.694533
O	-2.307883	-2.479478	0.192182
H	-3.463335	-1.350934	-0.420432
O	-1.527458	-2.162108	-1.798536
O	-0.457094	-3.406055	-0.406340
I	0.128259	-0.463731	2.063180
O	-1.236722	0.610766	2.466912
O	-0.081852	-0.593434	0.257305
O	-0.678259	-2.132042	2.451476
H	-1.303112	-2.389014	1.726962
I	1.683429	-1.469941	-0.884957
O	2.155038	0.272005	-1.211152
O	2.307344	-1.757657	0.764366
O	3.229312	-2.210844	-1.777956
H	3.989353	-2.173174	-1.185363
I	1.431282	2.285476	-0.342879
O	-0.179373	2.136734	-1.099706
O	1.322942	1.555752	1.309121
O	1.216336	4.098829	0.312989
H	0.492815	4.151181	0.948076
I	-2.561593	0.754263	-0.991891
O	-3.935507	-0.540428	-0.754766
O	-2.784900	1.700997	0.639112
H	-2.198666	1.284253	1.329439

$(HNO_3)_1(HIO_3)_3(HIO_2)_2$	X	Y	Z
H	-0.304658	2.536235	-1.583672
O	-0.605154	3.150571	-0.892490
I	0.111726	2.442144	0.765931
O	1.795911	3.321583	0.554531
H	2.404723	2.662232	0.150868
O	-0.721319	-2.458554	-0.897560
I	-1.354768	-2.366866	0.887264
O	0.148052	-3.135860	1.792578
H	0.701670	-2.392694	2.144869

O	-1.388844	0.072022	-1.763442
O	0.925230	-0.503413	-0.118346
I	0.228683	-0.751422	-1.772157
O	0.933853	0.969570	-2.420401
H	1.827794	1.129888	-2.060841
O	-3.453228	-1.146287	-0.019128
I	-3.321450	0.579697	-0.498902
O	-5.050634	1.132099	0.169311
H	-5.106478	0.985627	1.121067
O	-2.344257	1.320945	0.799521
I	3.334093	-0.360117	-0.098542
O	5.265206	-0.428666	-0.071673
H	5.611076	-0.273724	-0.958775
O	3.095277	-1.282949	-1.614504
O	3.163801	1.329753	-0.700269
N	1.078709	0.020368	2.613568
O	-0.125118	0.105722	2.826288
O	1.675130	-1.074613	2.642897
O	1.736832	1.054045	2.320320

$(HNO_3)_1(HIO_3)_4$	X	Y	Z
N	0.441001	-2.985928	-0.868172
O	1.444110	-3.190919	-0.110081
H	1.192887	-2.566310	1.438299
O	-0.661742	-3.403633	-0.531871
O	0.603411	-2.327669	-1.899484
I	-0.834512	2.589558	-0.188792
O	-0.521761	1.862150	1.436380
O	0.411502	1.896652	-1.262853
O	0.086005	4.254996	0.158548
H	1.037544	4.115264	0.237427
I	0.404381	-0.329622	1.981247
O	-0.152236	-0.672097	0.291413
O	1.160804	-2.024830	2.277697
O	-1.255166	-0.750578	2.796319
H	-1.917628	-1.085831	2.143348
I	-2.226107	-0.938503	-0.785576
O	-2.936438	-1.388901	0.784247
O	-2.326038	0.885268	-0.751632
O	-3.847515	-1.187946	-1.790233
H	-4.604398	-1.109004	-1.195938
I	2.417845	0.052254	-0.948102
O	3.720788	1.173973	-1.311192
O	2.218917	0.291843	0.879390

O	3.435565	-1.540089	-0.840848
H	2.797811	-2.283836	-0.667456

$(HNO_3)_1(HIO_3)_4(HIO_2)_1$	X	Y	Z
N	2.252174	2.434297	1.046334
O	3.213185	1.938829	1.639223
H	4.432410	1.222741	0.583474
O	2.272360	2.576644	-0.192086
O	1.230371	2.777181	1.681824
I	-3.614825	0.153836	0.045401
O	-2.854951	-1.072182	-1.010317
O	-2.673836	0.071391	1.563979
O	-5.113992	-0.941535	0.611702
H	-4.818236	-1.837257	0.811371
I	-0.109891	-0.695147	2.078654
O	1.540252	-1.275708	2.406783
O	0.116511	0.072417	0.413731
O	-0.066256	0.923816	3.049731
H	0.553132	1.596907	2.657835
I	-0.390687	2.187621	-0.879372
O	0.198647	1.088040	-2.149514
O	-2.173170	1.821216	-0.839436
O	-0.524425	3.759147	-1.983773
H	-0.542753	3.477797	-2.907582
I	-0.226526	-1.793823	-1.184623
O	1.540130	-1.974624	-1.464881
O	-0.425340	-2.511583	0.469429
O	-0.757542	-3.388132	-2.116294
H	-0.328975	-4.153125	-1.712402
I	3.415903	-0.539392	-0.635007
O	4.851163	0.574875	-0.028832
O	3.527701	-1.851118	0.738867
H	2.812129	-1.650557	1.394138

$(HNO_3)_1(HIO_3)_5$	X	Y	Z
N	-2.909959	-2.951893	0.784056
O	-3.160359	-1.975891	1.692021
H	-2.275966	-1.644369	2.032925
O	-1.760130	-3.291116	0.645616
O	-3.875801	-3.367216	0.222218
I	0.443484	2.181988	-0.938658
O	0.424420	2.924872	0.686556
O	-1.334928	2.078343	-1.322031
O	0.725426	3.832706	-1.901540

H	0.337239	4.561359	-1.402219
I	3.753885	-0.693269	0.075910
O	3.129817	-0.953455	1.731572
O	3.015100	0.828203	-0.483568
O	5.487825	0.036795	0.558214
H	5.379649	0.825123	1.102927
I	-0.322799	0.619117	2.148715
O	0.182690	0.210720	0.430322
O	-0.954602	-0.963566	2.678143
O	1.385304	0.547583	2.928603
H	2.029548	-0.056778	2.452111
I	-3.126058	0.801062	-0.509190
O	-2.481198	1.081907	1.157515
O	-2.383766	-0.724591	-1.051138
O	-4.795742	0.050859	0.083486
H	-4.625137	-0.716814	0.651589
I	0.216960	-1.734775	-1.253949
O	1.932019	-2.070154	-0.790109
O	0.401177	-0.362760	-2.369943
O	0.052668	-3.103966	-2.598028
H	0.435051	-2.767966	-3.418856

$(HNO_3)_2$	X	Y	Z
N	2.008830	-0.073401	-0.000004
O	1.480241	1.165502	0.000064
H	0.501255	1.048347	0.000020
O	1.228135	-1.013575	-0.000071
O	3.190652	-0.130721	0.000008
N	-2.008830	0.073401	-0.000004
O	-1.480240	-1.165501	0.000064
H	-0.501254	-1.048347	0.000019
O	-1.228135	1.013575	-0.000072
O	-3.190653	0.130720	0.000009

$(HNO_3)_2(HIO_2)_1$	X	Y	Z
O	0.041622	0.467921	0.854239
I	0.240003	-1.148935	-0.050464
O	-1.347658	-2.033782	0.595426
H	-2.100416	-1.571060	0.194164
N	3.004440	1.081376	-0.175573
O	2.296099	1.685373	0.775380
H	1.399335	1.205468	0.834075
O	2.511749	0.089083	-0.714092
O	4.064080	1.548482	-0.428560

N	-3.026033	1.208334	-0.235726
O	-2.097910	1.866991	0.465544
H	-1.289181	1.265188	0.551281
O	-2.735403	0.093408	-0.645910
O	-4.054921	1.778275	-0.405253

$(HNO_3)_2(HIO_2)_2$	X	Y	Z
N	0.045943	2.389347	-0.489043
O	0.374242	1.754316	0.599910
H	-0.984017	1.039673	1.495783
O	-1.105063	2.761982	-0.609871
O	0.919583	2.547814	-1.326721
N	-0.045936	-2.389280	-0.489353
O	1.105072	-2.761902	-0.610213
H	3.161981	-1.792894	-0.611758
O	-0.374247	-1.754386	0.599676
O	-0.919563	-2.547639	-1.327064
I	-2.239966	-0.342710	0.039701
O	-1.719755	0.423607	1.709379
O	-3.608878	0.987511	-0.317806
H	-3.162008	1.792961	-0.611538
I	2.239964	0.342703	0.039753
O	3.608863	-0.987482	-0.317937
O	1.719759	-0.423818	1.709339
H	0.984017	-1.039852	1.495669

$(HNO_3)_2(HIO_2)_3$	X	Y	Z
N	-3.016938	1.853557	0.536427
O	-2.217854	1.211602	-0.255632
H	-0.245762	0.768234	-1.385693
O	-2.782210	3.030063	0.746063
O	-3.949830	1.236747	1.026597
N	0.606287	-2.942433	0.811650
O	0.817593	-2.076780	-0.145381
H	-0.476743	-1.432639	-0.922669
O	-0.546054	-3.323771	0.976768
O	1.546145	-3.314195	1.469844
I	-2.759343	-1.055242	-0.253869
O	-1.204433	-0.943445	-1.393063
O	-2.926628	-2.970103	-0.522901
H	-2.207392	-3.385969	-0.020107
I	0.814742	2.248687	0.206736
O	0.563490	1.308338	-1.448495
O	-0.263889	3.770153	-0.331097

H	-1.187919	3.594463	-0.070008
I	2.911887	-0.829641	-0.175246
O	1.995977	0.414181	0.864344
O	4.546899	0.233397	-0.437589
H	5.092496	0.186911	0.352380

$(HNO_3)_2(HIO_2)_4$	X	Y	Z
N	1.231410	-0.776436	2.328894
O	0.359631	0.039415	2.624449
H	2.579107	1.313993	1.982440
O	2.435961	-0.443650	2.297660
O	0.915510	-1.944117	2.013093
N	-0.607041	-1.438517	-2.239246
O	-0.076174	-2.516958	-1.977285
H	-0.666663	-3.612246	-0.161314
O	0.119388	-0.426541	-2.462579
O	-1.834763	-1.294759	-2.265125
I	-2.797961	1.497451	-0.520316
O	-2.130182	0.763793	1.030665
O	-1.198704	1.794522	-1.576161
H	-0.915931	0.959600	-2.022374
I	-1.454496	-1.708362	1.054863
O	-1.068921	-3.575418	0.718621
O	-3.148320	-1.851470	0.121902
H	-2.926584	-1.839367	-0.825640
I	1.207787	2.133539	0.207108
O	2.598604	2.179124	1.517547
O	-0.099722	3.059405	1.342936
H	-0.577537	2.379181	1.836596
I	2.432865	-0.893951	-1.131261
O	2.632875	0.962265	-1.169216
O	3.874761	-1.365828	0.063980
H	3.523124	-1.254658	0.967986

$(HNO_3)_2(HIO_3)_1$	X	Y	Z
I	-0.311449	-0.929552	-0.164173
O	0.432211	0.339391	-1.175086
O	-0.649593	-0.148939	1.410087
O	1.231765	-1.938995	0.293530
H	1.958832	-1.313965	0.500749
N	3.527701	0.987124	0.104615
O	2.796112	1.476918	-0.907226
H	1.920552	0.999774	-0.909933
O	3.041683	0.085849	0.770769

O	4.591181	1.488718	0.262194
N	-3.309047	1.005473	0.006416
O	-2.775074	1.350056	1.179814
H	-1.951915	0.784724	1.303754
O	-2.734860	0.135129	-0.647399
O	-4.302329	1.567816	-0.308012

$(HNO_3)_2(HIO_3)_1(HIO_2)_1$	X	Y	Z
N	-0.741666	-2.616878	-0.682143
O	-0.675619	-1.829570	0.345404
H	1.577280	-2.763854	0.061456
O	0.247616	-3.309280	-0.910582
O	-1.748634	-2.624658	-1.354810
N	1.146825	3.141673	-0.607421
O	-0.167543	3.002610	-0.790544
H	-0.378747	2.026822	-0.962258
O	1.846405	2.147184	-0.748080
O	1.524890	4.234533	-0.339012
I	-2.091241	0.026468	0.197753
O	-1.169886	0.484461	1.667056
O	-1.035307	0.604378	-1.136517
O	-3.291374	1.549331	0.275397
H	-2.837598	2.321137	0.634801
I	2.162184	-0.446339	0.075558
O	2.376912	-2.304057	0.425517
O	1.420653	0.145914	1.710037
H	0.418071	0.188683	1.656550

$(HNO_3)_2(HIO_3)_1(HIO_2)_2$	X	Y	Z
H	2.232570	-0.438083	-1.290641
I	-1.491796	-0.023449	-1.361548
O	-0.689693	-1.238963	-0.275958
O	-2.270365	1.062941	-0.152208
O	-3.066197	-1.100614	-1.633049
H	-3.507514	-1.279742	-0.784626
I	1.443297	-2.176213	0.071149
O	1.897091	-1.315297	-1.571252
O	3.222229	-2.867618	0.373206
H	3.740323	-2.123629	0.725308
I	0.727443	2.357679	0.156107
O	0.230153	1.312967	-1.339074
O	-0.819963	3.536107	0.050278
H	-1.600548	2.976974	0.180927
N	-3.980375	-0.923299	2.072551

O	-3.272627	0.218970	2.123836
H	-2.952868	0.422685	1.199848
O	-4.105896	-1.460474	0.988469
O	-4.419219	-1.300364	3.111373
N	3.260265	0.766037	1.071013
O	3.160132	1.700807	1.842267
O	3.953071	-0.220251	1.271903
O	2.574380	0.817753	-0.029583

$(HNO_3)_2(HIO_3)_1(HIO_2)_3$	X	Y	Z
H	2.041693	3.085921	1.628396
O	2.050842	3.497019	0.754893
I	0.983258	2.373557	-0.396735
O	-0.652247	3.261070	0.119017
H	-0.989617	2.803740	0.909334
O	2.547522	-2.841217	-0.274939
I	1.505960	-1.911041	1.031890
O	2.830349	-2.078744	2.452002
H	3.430028	-1.326930	2.422084
O	-0.214774	-1.774812	-0.601075
I	-0.659727	-0.867525	-2.116284
O	-2.363952	-1.385391	-2.291354
H	-3.578651	-1.424603	-0.969107
O	-0.865843	0.846179	-1.528269
O	-4.098899	-1.203673	-0.161638
I	-2.924920	-0.161254	0.942638
O	-3.109677	1.462539	-0.043991
H	-2.380999	1.437072	-0.705316
N	3.092559	0.255790	-1.239297
O	3.918070	-0.640066	-1.065708
H	3.095626	-2.168138	-0.737211
O	2.047835	0.053967	-1.889581
O	3.279529	1.385449	-0.735273
N	-0.240079	0.680311	2.489406
O	-0.348864	-0.551603	2.608169
O	0.810139	1.264346	2.684770
O	-1.270998	1.336457	2.128111

$(HNO_3)_2(HIO_3)_2$	X	Y	Z
N	-3.740984	0.567886	0.166542
O	-3.352500	1.673584	-0.478151
H	-2.400323	1.848868	-0.226889
O	-2.920492	0.029034	0.894571
O	-4.859897	0.218129	-0.027062

N	3.740986	-0.567884	-0.166526
O	3.352495	-1.673581	0.478163
H	2.400321	-1.848866	0.226891
O	2.920503	-0.029037	-0.894570
O	4.859896	-0.218125	0.027094
I	-0.609236	-1.486097	0.227845
O	-0.581143	-0.230848	-1.120740
O	0.892617	-2.409666	-0.039698
O	-1.767669	-2.654074	-0.774407
H	-1.404539	-2.826590	-1.651184
I	0.609236	1.486096	-0.227852
O	-0.892616	2.409666	0.039691
O	0.581140	0.230848	1.120734
O	1.767665	2.654072	0.774408
H	1.404530	2.826589	1.651184

$(HNO_3)_2(HIO_3)_2(HIO_2)_1$	X	Y	Z
N	-3.089710	1.029282	-0.971113
O	-2.354734	1.160056	0.092025
H	-3.688871	-0.967483	0.427968
O	-3.931820	0.139478	-0.953926
O	-2.901419	1.777351	-1.906318
N	2.834733	0.967806	1.837969
O	2.296890	-0.095736	2.426975
H	1.868636	-0.637501	1.698592
O	2.862907	0.970316	0.606856
O	3.251562	1.819419	2.548793
I	1.633506	-1.146911	-1.178677
O	0.435513	-2.096084	-2.066245
O	1.135644	-1.498604	0.539195
O	3.107035	-2.403223	-1.219413
H	2.779907	-3.307047	-1.135636
I	-0.313038	2.206359	-0.309503
O	0.116013	0.753008	-1.297977
O	-0.040944	1.680266	1.379608
O	1.363820	3.133528	-0.511331
H	2.088906	2.615367	-0.122548
I	-1.472869	-1.746862	0.868790
O	-3.374294	-1.675960	1.038189
O	-1.019548	-0.605748	2.315506
H	-0.759440	0.285455	1.955807

$(HNO_3)_2(HIO_3)_2(HIO_2)_2$	X	Y	Z
N	0.153740	0.393962	-2.531328

O	1.319600	0.315347	-2.930221
H	-0.113728	-2.596098	-1.609131
O	-0.413005	1.470871	-2.379950
O	-0.471211	-0.680626	-2.276179
N	1.529025	0.135340	2.595250
O	2.657945	-0.302898	2.366826
H	1.319933	2.681210	0.037532
O	1.327543	1.337988	2.786019
O	0.548801	-0.659103	2.640617
I	-3.636917	-0.537242	-0.254806
O	-3.318207	1.162232	0.213092
O	-2.483051	-1.506017	0.697345
O	-2.976459	-0.634060	-2.000019
H	-1.946362	-0.564936	-2.080640
I	3.188224	0.315896	-0.978651
O	1.724036	0.963031	-0.188761
O	3.042944	-1.457173	-0.909938
O	4.387390	0.648876	0.461574
H	3.889328	0.457025	1.294366
I	-0.982821	2.347655	0.338108
O	0.620660	3.363445	0.098108
O	-1.067349	2.468175	2.240863
H	-0.318974	1.918938	2.587931
I	0.136479	-2.228875	0.743817
O	-0.319262	-3.195323	-0.875312
O	1.864268	-3.007225	0.928134
H	2.470194	-2.465547	0.376162

$(HNO_3)_2(HIO_3)_3$	X	Y	Z
N	-1.432455	-3.111090	-1.678444
O	-1.439656	-3.683006	-0.470804
H	-0.723710	-3.240480	0.068441
O	-0.640951	-2.193855	-1.852339
O	-2.195597	-3.554000	-2.472791
N	-4.359548	1.774398	1.662438
O	-3.558675	2.759243	1.232676
H	-2.947421	2.379759	0.537380
O	-4.224698	0.671229	1.159956
O	-5.135392	2.074638	2.511104
I	-1.249664	0.433630	-1.033175
O	-0.679096	-0.145201	0.594013
O	-1.877303	2.053447	-0.640291
O	-2.913362	-0.497256	-1.003957
H	-3.461823	-0.127880	-0.283413

I	2.540999	1.290831	-0.576266
O	0.939909	1.485672	-1.388388
O	2.216031	1.427609	1.175219
O	3.121139	3.116622	-0.836823
H	2.558187	3.724835	-0.343144
I	1.192258	-1.222226	1.400501
O	0.430540	-2.812097	1.136561
O	1.986153	-0.923720	-0.218030
O	2.781746	-1.930663	2.242632
H	3.002015	-2.787145	1.856708

$(HNO_3)_2(HIO_3)_3(HIO_2)_1$	X	Y	Z
N	2.654750	-2.228315	-0.383436
O	3.515124	-1.756003	0.378770
H	4.218653	-0.321425	-0.166399
O	2.529149	-1.810010	-1.537524
O	1.876535	-3.113690	0.047533
N	-4.358646	-0.048937	0.443344
O	-3.887199	-1.167341	1.021776
H	-3.113539	-1.470353	0.470150
O	-3.882363	0.251740	-0.636979
O	-5.203208	0.528913	1.047630
I	-1.401697	1.985521	-0.557188
O	0.305392	2.477127	-0.762891
O	-1.458646	1.102844	1.013735
O	-2.050671	3.649136	0.172774
H	-1.624838	3.841557	1.017095
I	-0.553939	-1.709343	-1.353282
O	-0.991840	-0.018681	-1.837734
O	-1.664629	-2.095859	0.015742
O	-1.646973	-2.508832	-2.729659
H	-2.514639	-2.089305	-2.767176
I	-0.069491	-0.769021	1.977707
O	1.011038	0.386996	2.788003
O	0.600239	-0.646810	0.284119
O	0.774040	-2.410671	2.382957
H	1.338078	-2.715289	1.614803
I	2.728757	1.496042	-0.503244
O	4.420343	0.631934	-0.374457
O	2.543565	2.021007	1.314170
H	2.012038	1.351679	1.816843

$(HNO_3)_2(HIO_3)_4$	X	Y	Z
N	-3.272930	-1.352569	1.897361

O	-3.678291	-1.159113	0.617741
H	-3.501053	-0.190132	0.388298
O	-2.807997	-0.392010	2.471827
O	-3.419568	-2.455538	2.313854
N	1.049753	3.611651	0.013109
O	1.550360	3.011749	-1.074464
H	2.271784	2.387769	-0.760936
O	1.659219	3.475342	1.052632
O	0.039698	4.227104	-0.159917
I	3.224509	-0.453743	-0.185271
O	3.414451	1.301036	-0.451003
O	1.776805	-0.875736	-1.160927
O	4.542121	-1.024926	-1.479605
H	4.401106	-0.592832	-2.330163
I	-1.944678	1.536800	-1.315337
O	-3.271774	1.279945	-0.140901
O	-1.616079	-0.115511	-1.907511
O	-3.023394	2.139812	-2.800286
H	-3.740094	1.517753	-2.973236
I	-0.286830	-2.319327	-0.872178
O	-0.527786	-1.554968	0.784875
O	0.658874	-3.759509	-0.513177
O	-2.019022	-3.145295	-0.862168
H	-2.679489	-2.530543	-0.500249
I	0.076198	0.287028	1.916839
O	-0.312536	1.245042	0.441364
O	1.825692	-0.109421	1.670719
O	0.375789	1.832477	3.005992
H	0.809972	2.540358	2.495853

$(HNO_3)_3$	X	Y	Z
N	-2.489276	-0.713745	0.162763
O	-2.398031	0.205547	-0.823552
H	-1.472085	0.538452	-0.810951
O	-1.464310	-0.983554	0.766807
O	-3.570133	-1.161214	0.344516
N	0.463351	2.118792	-0.105470
O	1.545555	2.046011	0.687115
H	1.800271	1.095137	0.694689
O	0.183815	1.104882	-0.731087
O	-0.102866	3.158567	-0.125761
N	2.008011	-1.421074	-0.029051
O	0.830266	-1.944684	-0.419609
H	0.136136	-1.496610	0.111776

O	1.974090	-0.638960	0.907788
O	2.959248	-1.789693	-0.630369

$(HNO_3)_3(HIO_2)_1$	X	Y	Z
I	-0.121056	-0.419199	0.141625
O	1.466136	0.276226	0.823495
O	-1.262009	0.994258	0.883032
H	-0.951623	1.817551	0.463107
N	-3.883616	-0.703047	-0.227538
O	-3.888910	0.384064	0.574045
H	-2.940403	0.631445	0.698096
O	-2.794441	-1.125900	-0.577937
O	-4.947995	-1.139153	-0.509877
N	2.708106	-2.454000	-0.242749
O	3.224558	-1.569594	0.604288
H	2.535660	-0.827403	0.724204
O	1.552464	-2.267224	-0.635553
O	3.399023	-3.362641	-0.556717
N	1.253358	3.375986	-0.390138
O	2.215895	2.656150	0.188467
H	1.846817	1.731479	0.383708
O	0.172449	2.829095	-0.579220
O	1.535404	4.491208	-0.683055

$(HNO_3)_3(HIO_2)_2$	X	Y	Z
N	-0.583904	-2.175846	-0.202999
O	-0.942653	-1.748911	-1.316678
H	0.253204	-0.897108	-2.339812
O	0.522854	-2.652319	-0.011985
O	-1.400537	-2.097134	0.762132
N	4.326665	0.244516	1.736782
O	4.746063	-0.839355	1.056418
H	4.074273	-0.995626	0.339918
O	3.315687	0.799242	1.333970
O	4.989019	0.558860	2.667961
N	-0.740333	2.115456	-0.299089
O	-1.834957	2.588115	-0.532888
H	-3.857566	1.854156	-0.073679
O	-0.422315	1.664015	0.812177
O	0.124615	2.064059	-1.238908
I	1.692607	0.339634	-0.931857
O	0.973110	-0.276568	-2.586322
O	2.906645	-1.235459	-0.838073
H	2.331182	-1.984685	-0.612550

I	-3.054848	-0.364387	0.416828
O	-4.343470	1.076214	0.235755
O	-2.380155	0.247390	2.091853
H	-1.650576	0.861068	1.856476

$(HNO_3)_3(HIO_2)_3$	X	Y	Z
N	0.092000	-2.692309	1.287032
O	0.168920	-2.416272	0.006736
H	-1.152444	-1.681039	-0.685388
O	-1.029172	-2.798443	1.765390
O	1.115753	-2.823053	1.909426
N	2.992474	1.771915	2.506795
O	3.078389	0.440844	2.343842
H	2.609822	0.221224	1.482033
O	2.381543	2.400385	1.659636
O	3.526991	2.210074	3.473553
N	-2.988404	2.255918	0.205509
O	-2.432429	1.331400	-0.513206
H	-0.721573	0.270518	-1.785155
O	-2.555877	3.390135	0.101034
O	-3.902113	1.930435	0.945546
I	0.759786	1.861038	-0.723292
O	0.111164	0.677694	-2.088543
O	-0.168547	3.426552	-1.349185
H	-1.051231	3.460414	-0.924993
I	2.294720	-1.687334	-0.852071
O	1.920838	-0.114189	0.080473
O	3.899829	-1.012150	-1.757844
H	4.652916	-1.043010	-1.161016
I	-3.198495	-0.747801	0.190565
O	-1.862730	-1.163575	-1.146621
O	-3.571561	-2.626422	0.501814
H	-2.826516	-2.976940	1.017025

$(HNO_3)_3(HIO_3)_1$	X	Y	Z
I	0.319295	-0.038131	-0.879329
O	0.057382	-1.799977	-1.020847
O	-0.333469	0.306001	0.768247
O	-1.148490	0.574312	-1.906580
H	-1.969167	0.232505	-1.496060
N	0.744014	3.398110	0.544910
O	0.089682	2.814971	1.565071
H	-0.062728	1.871322	1.289438
O	1.002326	2.696762	-0.423170

O	1.010452	4.543805	0.685402
N	2.734185	-2.068560	0.746246
O	1.855886	-3.021763	0.428954
H	1.148617	-2.591476	-0.141642
O	2.525947	-0.932976	0.315702
O	3.651391	-2.396352	1.417451
N	-3.543551	-0.929740	0.663596
O	-2.599812	-0.846671	1.620497
H	-1.795481	-0.436171	1.211335
O	-3.261619	-0.508748	-0.444785
O	-4.572981	-1.411102	1.001319

$(HNO_3)_3(HIO_3)_1(HIO_2)_1$	X	Y	Z
N	4.126821	-1.406677	0.468529
O	3.887445	-0.437612	-0.429248
H	2.908901	-0.245471	-0.402887
O	3.164803	-1.891424	1.042318
O	5.267242	-1.698152	0.621856
N	0.711768	3.544201	1.736156
O	-0.348173	2.723336	1.869679
H	-0.532192	2.326575	0.976689
O	1.211456	3.640821	0.631473
O	1.055531	4.099215	2.728350
N	-3.940224	-0.148087	0.454791
O	-3.612535	0.838847	-0.381100
H	-2.625760	1.007826	-0.296822
O	-3.043666	-0.622376	1.144072
O	-5.081956	-0.469459	0.465436
I	0.098112	0.748939	-1.496358
O	-1.099775	1.513687	-0.368379
O	1.338099	0.123857	-0.362751
O	0.982703	2.401171	-1.916404
H	1.124786	2.922200	-1.106179
I	-0.796436	-1.992418	0.529966
O	-0.981371	-1.156704	-1.133948
O	0.793567	-3.010236	0.212838
H	1.579931	-2.472588	0.438071

$(HNO_3)_3(HIO_3)_1(HIO_2)_2$	X	Y	Z
N	3.264047	1.519962	1.585686
O	2.187255	1.295448	2.368973
H	1.723211	0.505875	1.976400
O	3.465740	0.724350	0.687990
O	3.912330	2.474241	1.864502

N	-2.824600	-1.712660	-1.622039
O	-1.665272	-1.257286	-2.170067
H	-0.928221	-1.769915	-1.735262
O	-2.728577	-2.617280	-0.828016
O	-3.807984	-1.152140	-1.992910
N	-2.348768	1.496315	1.660523
O	-1.077408	1.231610	1.717801
H	0.135574	2.266969	0.877395
O	-2.696030	2.551683	1.156949
O	-3.115884	0.660124	2.101154
I	1.812500	-1.270311	-0.773555
O	1.220859	0.232802	-1.583012
O	0.419287	-2.383555	-1.002750
O	2.804741	-1.866240	-2.327354
H	2.271916	-1.832051	-3.129571
I	-0.423635	1.977118	-1.384548
O	0.612016	2.603562	0.086735
O	-1.673472	3.446652	-1.367426
H	-2.251318	3.319218	-0.596176
I	-0.873912	-1.186748	1.734033
O	0.889632	-0.699711	1.223529
O	-0.538542	-3.096269	1.683912
H	-0.547982	-3.362458	0.753630

$(HNO_3)_3(HIO_3)_2$	X	Y	Z
N	4.249982	0.784096	-0.725577
O	4.026855	-0.236877	-1.567254
H	3.215318	-0.720661	-1.244914
O	3.494549	0.904449	0.227103
O	5.167460	1.485603	-0.996150
N	-0.491014	3.421160	0.006324
O	0.427630	2.803010	0.778504
H	0.371584	1.844613	0.552128
O	-1.127432	2.723572	-0.762752
O	-0.579673	4.594336	0.155667
N	-1.369981	-0.186641	3.082152
O	-2.101914	0.750891	2.466093
H	-2.326724	0.403352	1.556998
O	-1.133097	-1.209179	2.452422
O	-1.025004	0.065216	4.188710
I	0.758156	-1.470384	0.394391
O	0.088126	0.224197	0.075968
O	1.923555	-1.679805	-0.935961
O	1.975131	-0.862398	1.730772

H	2.614526	-0.246395	1.321233
I	-1.720714	-0.129703	-1.335143
O	-2.838529	0.062231	0.037803
O	-1.008197	-1.796970	-1.078458
O	-3.034181	-0.731023	-2.604483
H	-3.624233	-1.384641	-2.209745

$(HNO_3)_3(HIO_3)_2(HIO_2)_1$	X	Y	Z
N	-3.599671	-2.299757	0.562939
O	-2.296448	-2.668676	0.578982
H	-1.916321	-2.435657	-0.315905
O	-4.061861	-1.943269	-0.498585
O	-4.156721	-2.374461	1.611502
N	3.385192	-2.816821	-0.934938
O	2.890672	-2.651255	0.306376
H	2.898213	-1.673598	0.504834
O	3.770284	-1.824553	-1.522669
O	3.400031	-3.936195	-1.333934
N	-1.082409	3.580558	-0.281302
O	-2.084684	3.022707	0.417145
H	-2.041689	2.049119	0.216486
O	-0.525241	2.875012	-1.110007
O	-0.840677	4.714842	-0.031644
I	-1.266755	-0.010907	-1.701878
O	-1.067692	-1.776835	-1.579892
O	-1.818787	0.400283	-0.007713
O	-3.043312	0.027994	-2.427219
H	-3.606993	-0.585036	-1.926834
I	2.085499	1.117378	0.030709
O	2.698661	-0.160295	1.138428
O	0.964385	0.151729	-1.030222
O	3.544156	1.003610	-1.215747
H	3.742753	0.070790	-1.408879
I	-0.429792	-0.196259	2.006050
O	0.432435	1.374168	1.448310
O	0.674607	-0.503662	3.569729
H	1.549317	-0.763897	3.251997

$(HNO_3)_3(HIO_3)_3$	X	Y	Z
N	-1.735728	3.881068	-1.450434
O	-2.236201	2.858292	-2.157862
H	-2.127326	2.040748	-1.589572
O	-1.286472	3.631374	-0.340237
O	-1.775659	4.945574	-1.973755

N	3.122607	1.777699	2.179018
O	2.313059	0.696712	2.259975
H	2.555941	0.084400	1.510057
O	3.955332	1.784502	1.295231
O	2.930073	2.615808	2.998101
N	-4.256091	-0.901639	0.191089
O	-3.833526	-1.774559	-0.728209
H	-3.002946	-2.186570	-0.366961
O	-3.687140	-0.930976	1.272740
O	-5.150977	-0.190191	-0.131296
I	2.177265	-0.135266	-1.316767
O	2.638029	-0.974916	0.209815
O	1.053624	1.151594	-0.745227
O	3.730040	0.974916	-1.437609
H	3.940027	1.344303	-0.561305
I	-0.900287	1.064791	0.790594
O	-0.392110	-0.615762	1.268092
O	-1.908290	0.738492	-0.645522
O	-2.276782	1.258583	2.082899
H	-2.959559	0.568461	1.936372
I	0.083804	-2.596724	0.197143
O	0.426049	-1.649441	-1.322599
O	-1.626873	-3.033518	-0.008264
O	0.791504	-4.261869	-0.485590
H	0.247512	-4.586666	-1.213197

Supplementary Reference

Lenthe, E. V., Baerends, E. J., and Snijders, J. G.: Relativistic regular two-component Hamiltonians, The Journal of Chemical Physics, 99, 4597–4610, https://doi.org/10.1063/1.466059, 1993.

Lu, T. and Chen, F.: Multiwfn: A multifunctional wavefunction analyzer, J. Comput. Chem., 33, 580–592, https://doi.org/10.1002/jcc.22885, 2012.

Neese, F.: The ORCA program system, WIREs Comput. Mol. Sci., 2, 73–78, https://doi.org/10.1002/wcms.81, 2012.

Rolfes, J. D., Neese, F., and Pantazis, D. A.: All-electron scalar relativistic basis sets for the elements Rb–Xe, J Comput Chem, 41, 1842–1849, https://doi.org/10.1002/jcc.26355, 2020.

Sipilä, M., Sarnela, N., Jokinen, T., Henschel, H., Junninen, H., Kontkanen, J., Richters, S., Kangasluoma, J., Franchin, A., Peräkylä, O., Rissanen, M. P., Ehn, M., Vehkamäki, H., Kurten, T., Berndt, T., Petäjä, T., Worsnop, D., Ceburnis, D., Kerminen, V.-M., Kulmala, M., and O'Dowd, C.: Molecular-scale evidence of aerosol particle formation via sequential addition of HIO_3, Nature, 537, 532–534, https://doi.org/10.1038/nature19314, 2016.

Yu, H., Ren, L., Huang, X., Xie, M., He, J., and Xiao, H.: Iodine speciation and size distribution in ambient aerosols at a coastal new particle formation hotspot in China, Atmos. Chem. Phys., 19, 4025–4039, https://doi.org/10.5194/acp-19-4025-2019, 2019.

Zu, H., Chu, B., Lu, Y., Liu, L., and Zhang, X.: Rapid iodine oxoacid nucleation enhanced by dimethylamine in broad marine regions, Atmos. Chem. Phys., 24, 5823–5835, https://doi.org/10.5194/acp-24-5823-2024, 2024.