Supplement of

Mechanistic insights into nitric acid-enhanced iodic acid particle formation in the upper troposphere and lower stratosphere

Jing Li et al.

Corresponding author: An Ning (anning@bit.edu.cn) and Xiuhui Zhang (zhangxiuhui@bit.edu.cn)

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Table S4. The Gibbs formation free energies ΔG_{ref} (kcal mol^{-1}) of the IA–NA–NH_3 and SA–NA–NH_3 systems at the DLPNO-CCSD(T)/aug-cc-pVTZ(-PP)//ωB97X-D/6-311++G(3df,3pd) + aug-cc-pVTZ-PP with ECP28MDF (for I) level of theory, P = 1 atm, and T = 220 K.

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Supplementary Methods

Multi-step cluster conformational searching method.

First, the artificial bee colony algorithm combined with UFF force field (Rappé et al., 1992) was employed to yield more than 5000 configurations for each cluster by ABCluster (Zhang and Dolg, 2015). Then up to 1000 relatively stable structures were selected to pre-optimize at PM7 method (Stewart, 2013) by MOPAC 2016 (Stewart, 2016). Next, up to 100 low-energy ones were re-optimized with at the ωB97X-D/6-31+G* (for C, H, O, and N) + Lanl2DZ (for I) level of theory (Elm and Kristensen, 2017), due to best performance of ωB97X-D functional in studying atmospheric clusters. Finally, the top 10 isomers with the low energy were optimized at ωB97X-D/6-311++G(3df,3pd) (for C, H, O, and N) + aug-cc-pVTZ-PP with ECP28MDF (for I) level of theory (Francl et al., 1982; Peterson et al., 2003) to obtain the global minimum one.

The equations in Atmospheric Cluster Dynamics Code (ACDC).

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

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

where m_i and V_i are the mass and volume of cluster i, respectively. Equation (1) is derived from the hard-sphere collision theory where the volume of molecule clusters $V_i = 3/4 \times \pi \times (d_i/2)^3$. The diameter d_i of cluster i is derived from the cluster volume V_i calculated by Multiwfn 3.7 (Lu and Chen, 2012). Evaporation rate coefficient $\gamma_{(i+j)\to i}$ is derived from the collision coefficients based on the detailed balance assumption:

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

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

Boundary setting in ACDC simulation.

In general, a lower evaporation rate translates into a higher cluster stability. Table S2 display the total evaporation rates ($\Sigma\gamma$, s^{-1}) of IA–NA–NH_3 clusters at temperatures ranging from 220 to 260 K. In ACDC simulations, the stability of clusters within the simulated system depends on the ratio of collision frequencies between the clusters and monomer molecule at the concentration C to the total evaporation frequencies of clusters ($\beta C/\Sigma\gamma$). If $\beta C/\Sigma\gamma$ of a cluster is greater than 1, the cluster is stable and may continue to grow. In this study, we systematically considered the collisions involving all monomer species, namely IA, NA, and NH_3. The boundary cluster settings for the system at different temperatures (220 – 260 K) are shown in Table S3.

Enhancement of NA on Nucleation.

Despite the identified NA's effective role in IA nucleation, the specific strength, particularly across a broader range of atmospheric conditions, remains unclear. Herein, we have calculated the enhancement strength *R* (Eq. (S3)) to quantify the impacts of NA on IA–NH_3 nucleation.

$$R = \frac{J\left(\left[\mathrm{IA}\right]=10^6, \left[\mathrm{NA}\right]=x, \left[\mathrm{NH_3}\right]=y\right)}{J\left(\left[\mathrm{IA}\right]=10^6, \left[\mathrm{NA}\right]=0, \left[\mathrm{NH_3}\right]=y\right)}, \tag{S3}$$

where *J* denotes the cluster formation rate. Due to the potentially low concentration of IA in the UTLS and the lack of available field measurement, here the [IA] is set to a lower value of 10^6 molec. cm^{-3}. *R* is shown in Fig. S5 as a function of [NA].

As expected, NH_3 level is a key factor influencing *R* due to the vital base-stabilization on both acidic NA and IA. Additionally, *R* is sensitive to temperature variation, showing a negative correlation. At low temperatures, entropy effects are decreased, and all cluster formation free energies are more negative (Bork et al., 2014), resulting in more stable clusters and a higher *R*. At high NH_3 levels, NH_3 is in large excess compared to IA, and the growth of clusters is thus limited by acid collisions. Consequently, the introduction of an additional acid source, such as increased NA concentrations, would have a more significant impact. When the [NA] is below 10^{10} molec. cm^{-3}, its variation exerts a minimal impact on changes in *R*. However, once [NA] exceeds 10^{10} molec. cm^{-3}, further increases in [NA] can enhance *J* by up to 120%. Overall, the enhancing effect of NA on the IA–NH_3 system is stronger in regions with lower temperatures and higher concentrations of NA and NH_3, which corresponds to the real environmental conditions in the UTLS.

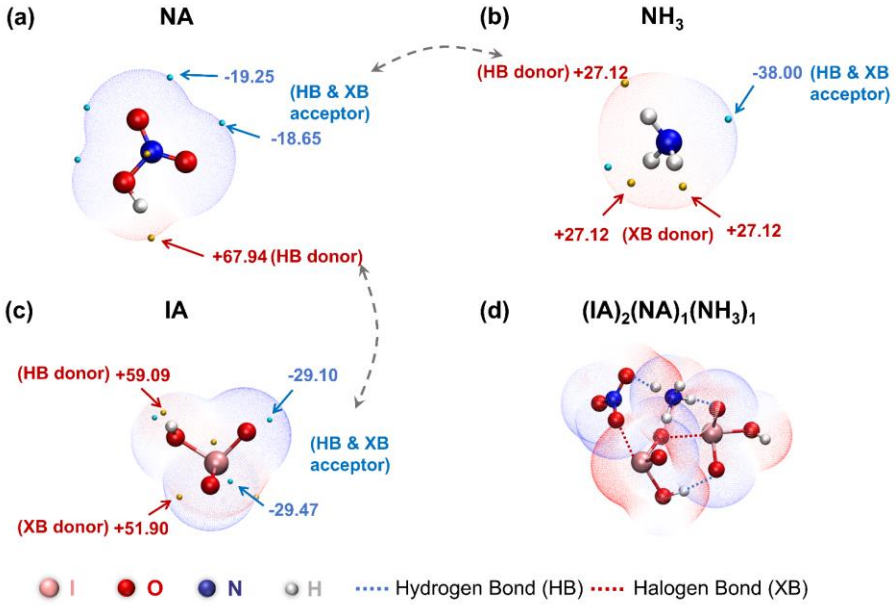

Figure S1. The ESP-mapped molecular vdW surface of **(a)** NA, **(b)** NH_3, **(c)** IA, and **(d)** $(IA)_2(NA)_1(NH_3)_1$. The golden and cyan dots represent the positions of maximums and minimums of ESP (unit: kcal mol^{-1}), respectively. The gray dashed arrows signify the site-to-site interaction tendencies.

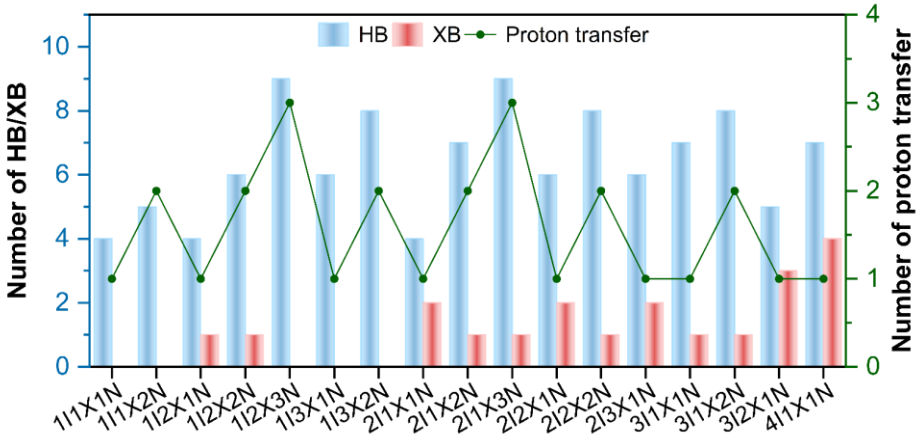

Figure S2. The number of hydrogen bonds (HB), halogen bonds (XB), and proton transfers in the IA–NA–NH_3 clusters, where I represents iodic acid (IA), X represents nitric acid (NA), and N represents ammonia (NH_3).

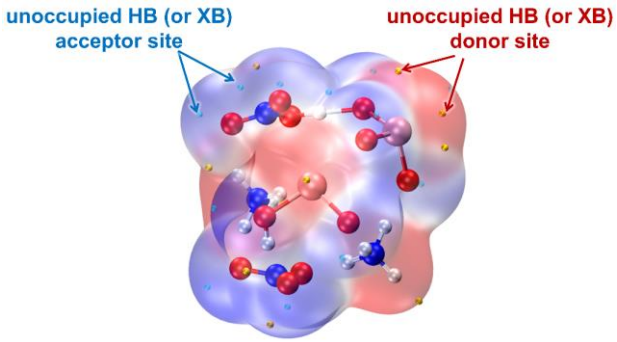

Figure S3. The ESP-mapped molecular vdW surfaces of the $(IA)_2(NA)_2(NH_3)_2$ cluster. The red region is the electron-deficient region, and the blue region is the electron-rich region.

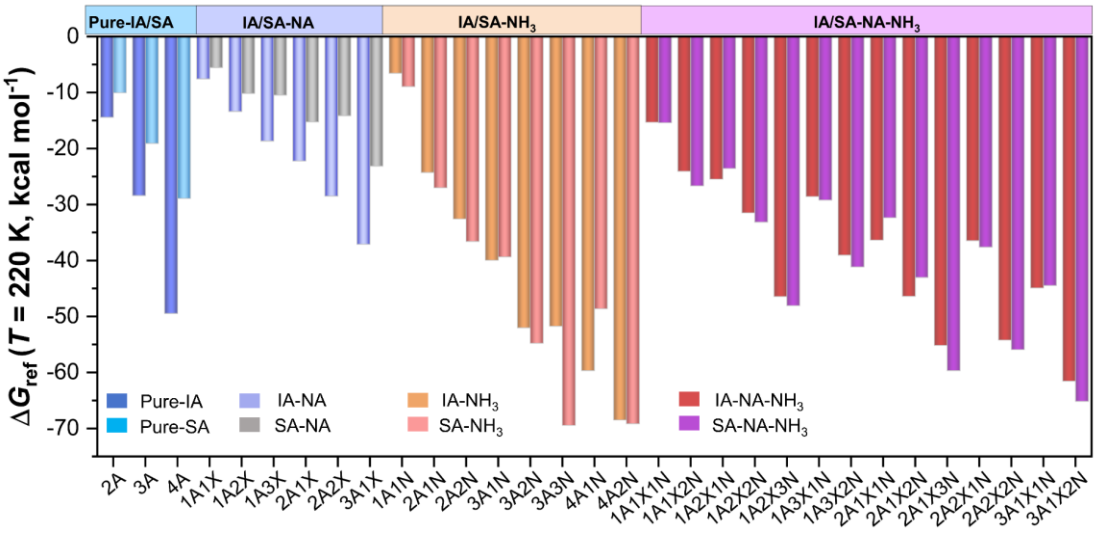

Figure S4. The Gibbs free energy (ΔG_{ref}, kcal mol^{-1}) of IA–NA–NH_3 and SA–NA–NH_3 system at T = 220 K, where A represents iodic acid (IA) or sulfuric acid (SA), X represents nitric acid (NA), and N represents ammonia (NH_3).

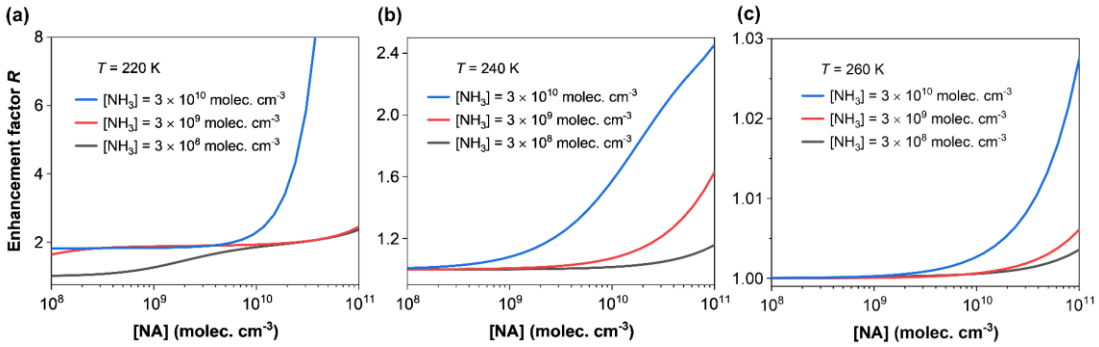

Figure S5. Enhancement strength (R) of NA on the IA–NH_3 nucleation. The ACDC simulations were performed at the conditions of CS = 10^{-4} s^{-1}, [IA] = 10^6 molec. cm^{-3}, [NH_3] = 3 × 10^8 – 3 × 10^{10} molec. cm^{-3}, **(a)** T = 220 K, **(b)** T = 240 K, and **(c)** T = 260 K.

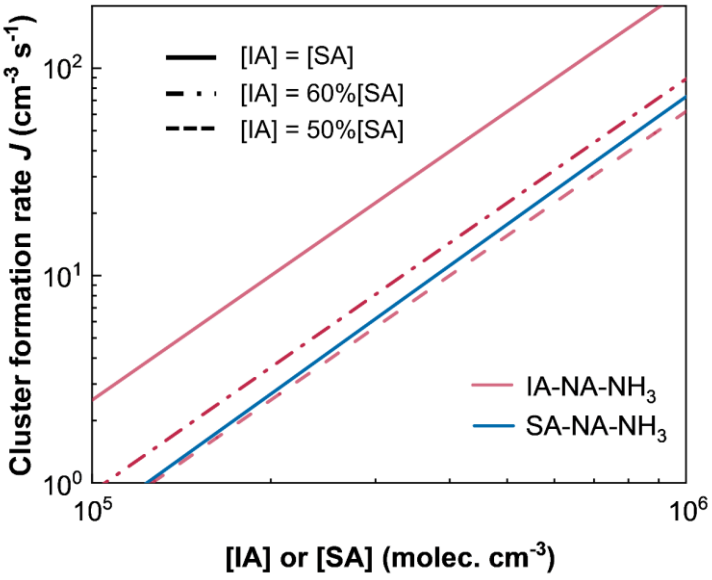

Figure S6. Cluster formation rate J (cm^{-3} s^{-1}) as a function of [IA] or [SA] of IA–NA–NH_3 and SA–NA–NH_3 system at T = 220 K, CS = 10^{-4} s^{-1}, [IA] (or [SA]) = 10^5 – 10^6 molec. cm^{-3}, [NA] = 10^{10} molec. cm^{-3}, and [NH_3] = 3 × 10^8 molec. cm^{-3}.

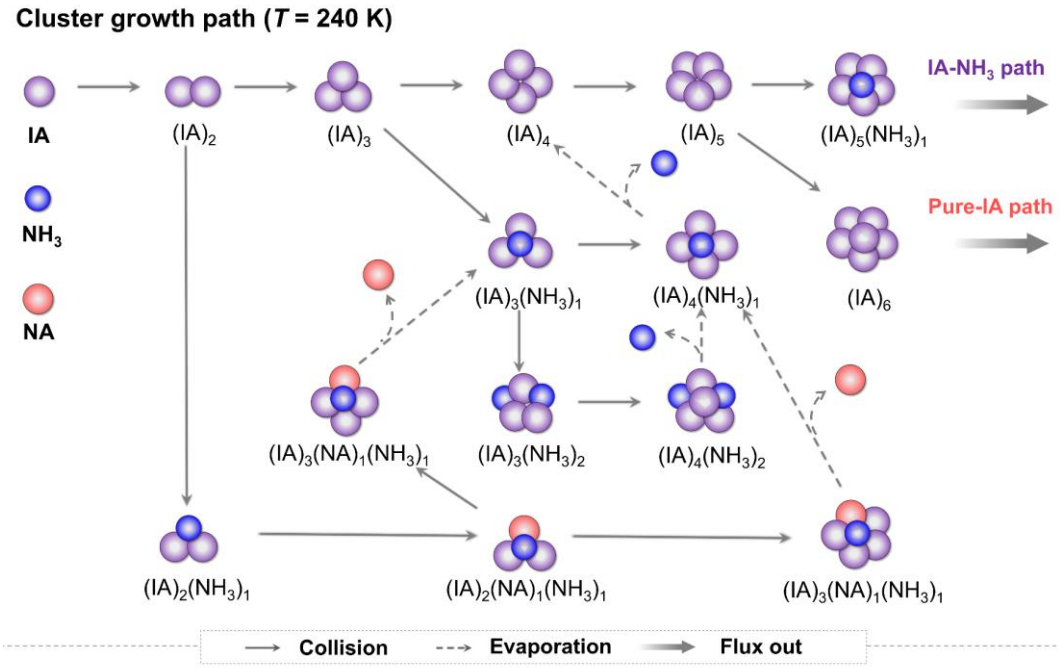

Figure S7. Main cluster formation pathways of the IA–NA–NH_3 system at T = 240 K, CS = 10^{-4} s^{-1}, [IA] = 10^6 molec. cm^{-3}, [NA] = 10^9 molec. cm^{-3}, and [NH_3] = 5.5 × 10^8 molec. cm^{-3}.

Table S1. The Gibbs formation free energies ΔG_{ref} (kcal mol^{-1}) of the studied IA–NA–NH_3 clusters at the DLPNO-CCSD(T)/aug-cc-pVTZ(-PP)//ωB97X-D/6-311++G(3df,3pd) + aug-cc-pVTZ-PP with ECP28MDF (for I) level of theory, P = 1 atm, and T = 210, 220, 230, 240, and 260 K.

Clusters	**Δ*G* (kcal mol^{-1})**				
	210K	**220K**	**230K**	**240K**	**260K**
$(IA)_1(NA)_1$	-7.91	-7.57	-7.22	-6.88	-6.20
$(IA)_1(NA)_2$	-14.11	-13.38	-12.65	-11.93	-10.48
$(IA)_1(NA)_3$	-19.71	-18.65	-17.59	-16.54	-14.44
$(IA)_2(NA)_1$	-22.94	-22.22	-21.51	-20.80	-19.39
$(IA)_2(NA)_2$	-29.66	-28.50	-27.35	-26.21	-23.93
$(IA)_2(NA)_3$	-35.89	-34.38	-32.87	-31.36	-28.37
$(IA)_3(NA)_1$	-38.31	-37.09	-35.89	-34.69	-32.30
$(IA)_3(NA)_2$	-45.94	-44.39	-42.83	-41.29	-38.22
$(IA)_3(NA)_3$	-51.80	-49.88	-47.96	-46.05	-42.24
$(IA)_4(NA)_1$	-54.55	-52.98	-51.41	-49.86	-46.76
$(IA)_4(NA)_2$	-64.53	-62.50	-60.47	-58.46	-54.45
$(NA)_2$	-2.12	-1.77	-1.42	-1.07	-0.36
$(NA)_3$	-0.71	-0.02	0.67	1.35	2.71
$(IA)_2$	-14.79	-14.41	-14.02	-13.64	-12.89
$(IA)_3$	-29.22	-28.40	-27.59	-26.79	-25.19
$(IA)_4$	-50.71	-49.46	-48.21	-46.97	-44.50
$(IA)_5$	-69.38	-67.70	-66.02	-64.35	-61.02
$(IA)_6$	-87.32	-85.18	-83.05	-80.94	-76.73
$(IA)_1(NH_3)_1$	-6.82	-6.55	-6.28	-6.02	-5.50
$(IA)_1(NH_3)_2$	-11.38	-10.72	-10.06	-9.40	-8.07
$(IA)_1(NH_3)_3$	-16.40	-15.46	-14.50	-13.56	-11.66
$(IA)_2(NH_3)_1$	-25.00	-24.26	-23.52	-22.78	-21.31
$(IA)_2(NH_3)_2$	-33.62	-32.55	-31.48	-30.41	-28.28
$(IA)_2(NH_3)_3$	-33.56	-32.21	-30.86	-29.51	-26.82
$(IA)_3(NH_3)_1$	-41.08	-39.94	-38.79	-37.65	-35.38
$(IA)_3(NH_3)_2$	-53.57	-52.02	-50.47	-48.92	-45.84
$(IA)_3(NH_3)_3$	-53.51	-51.71	-49.92	-48.13	-44.58

$(IA)_4(NH_3)_1$	-61.23	-59.67	-58.11	-56.56	-53.48
$(IA)_4(NH_3)_2$	-70.44	-68.49	-66.54	-64.60	-60.73
$(IA)_5(NH_3)_1$	-81.43	-79.36	-77.29	-75.24	-71.14
$(NH_3)_2$	2.29	2.51	2.72	2.94	3.38
$(NH_3)_3$	3.14	3.66	4.18	4.70	5.73
$(NA)_1(NH_3)_1$	-6.21	-5.92	-5.63	-5.35	-4.78
$(NA)_2(NH_3)_1$	-8.97	-8.36	-7.75	-7.13	-5.92
$(NA)_2(NH_3)_2$	-16.71	-15.66	-14.61	-13.55	-11.46
$(NA)_3(NH_3)_1$	-13.71	-12.71	-11.71	-10.71	-8.72
$(NA)_3(NH_3)_2$	-24.94	-23.58	-22.21	-20.85	-18.13
$(NA)_3(NH_3)_3$	-33.24	-31.48	-29.72	-27.96	-24.45
$(NA)_4(NH_3)_1$	-17.88	-16.43	-14.98	-13.53	-10.64
$(NA)_4(NH_3)_2$	-30.24	-28.48	-26.73	-24.98	-21.49
$(NA)_5(NH_3)_1$	-21.73	-19.90	-18.07	-16.25	-12.63
$(IA)_1(NA)_1(NH_3)_1$	-15.99	-15.29	-14.58	-13.88	-12.47
$(IA)_1(NA)_1(NH_3)_2$	-25.08	-24.05	-23.01	-21.98	-19.91
$(IA)_2(NA)_1(NH_3)_1$	-37.52	-36.35	-35.18	-34.02	-31.71
$(IA)_2(NA)_1(NH_3)_2$	-47.94	-46.38	-44.81	-43.25	-40.13
$(IA)_2(NA)_1(NH_3)_3$	-57.00	-55.16	-53.32	-51.48	-47.82
$(IA)_3(NA)_1(NH_3)_1$	-46.36	-44.89	-43.43	-41.97	-39.06
$(IA)_3(NA)_1(NH_3)_2$	-63.43	-61.53	-59.63	-57.73	-53.95
$(IA)_4(NA)_1(NH_3)_1$	-71.39	-69.35	-67.31	-65.28	-61.23
$(IA)_1(NA)_2(NH_3)_1$	-26.54	-25.46	-24.37	-23.29	-21.13
$(IA)_1(NA)_2(NH_3)_2$	-32.99	-31.48	-29.97	-28.46	-25.46
$(IA)_1(NA)_2(NH_3)_3$	-48.27	-46.42	-44.56	-42.71	-39.02
$(IA)_2(NA)_2(NH_3)_1$	-38.02	-36.46	-34.89	-33.32	-30.21
$(IA)_2(NA)_2(NH_3)_2$	-56.17	-54.20	-52.23	-50.27	-46.35
$(IA)_3(NA)_2(NH_3)_1$	-57.29	-55.32	-53.35	-51.38	-47.47
$(IA)_1(NA)_3(NH_3)_1$	-30.08	-28.56	-27.05	-25.53	-22.52
$(IA)_1(NA)_3(NH_3)_2$	-40.88	-39.04	-37.21	-35.37	-31.72
$(IA)_2(NA)_3(NH_3)_1$	-45.39	-43.50	-41.62	-39.75	-36.02

Table S2. The total evaporation rate coefficients ($\Sigma\gamma$, s^{-1}) of IA–NA–NH_3 clusters calculated at 220 – 260 K.

Clusters	$\Sigma\gamma$ (s^{-1})		
	220 K	**240 K**	**260 K**
$(IA)_2$	1.77×10^{-5}	1.33×10^{-3}	4.91×10^{-2}
$(IA)_3$	9.97×10^{-5}	8.00×10^{-3}	3.32×10^{-1}
$(IA)_4$	1.03×10^{-11}	3.47×10^{-9}	4.65×10^{-7}
$(IA)_5$	7.04×10^{-9}	1.32×10^{-6}	1.11×10^{-4}
$(IA)_6$	4.27×10^{-8}	7.39×10^{-6}	5.66×10^{-4}
$(NA)_2$	8.30×10^{7}	4.83×10^{8}	2.18×10^{9}
$(NA)_3$	5.65×10^{11}	1.58×10^{12}	3.62×10^{12}
$(NH_3)_2$	2.01×10^{12}	2.94×10^{12}	4.12×10^{12}
$(NH_3)_3$	1.97×10^{11}	5.45×10^{11}	1.23×10^{12}
$(IA)_1(NA)_1$	5.38×10^{2}	9.27×10^{3}	1.01×10^{5}
$(IA)_1(NA)_2$	1.73×10^{4}	2.47×10^{5}	2.38×10^{6}
$(IA)_1(NA)_3$	6.58×10^{4}	6.87×10^{5}	4.88×10^{6}
$(IA)_2(NA)_1$	1.83×10^{2}	3.03×10^{3}	3.31×10^{4}
$(IA)_2(NA)_2$	6.68×10^{3}	1.31×10^{5}	1.62×10^{6}
$(IA)_2(NA)_3$	1.80×10^{4}	2.44×10^{5}	2.13×10^{6}
$(IA)_3(NA)_1$	2.78×10^{1}	7.31×10^{2}	1.16×10^{4}
$(IA)_3(NA)_2$	7.18×10^{2}	1.20×10^{4}	1.25×10^{5}
$(IA)_3(NA)_3$	4.83×10^{4}	6.08×10^{5}	5.27×10^{6}
$(IA)_4(NA)_1$	4.19×10^{6}	2.94×10^{7}	1.52×10^{8}
$(IA)_4(NA)_2$	4.88×10^{0}	1.98×10^{2}	4.42×10^{3}
$(IA)_1(NH_3)_1$	8.20×10^{3}	8.32×10^{4}	5.77×10^{5}
$(IA)_1(NH_3)_2$	1.07×10^{6}	1.19×10^{7}	9.46×10^{7}
$(IA)_1(NH_3)_3$	3.13×10^{5}	2.50×10^{6}	1.41×10^{7}
$(IA)_2(NH_3)_1$	2.72×10^{0}	7.53×10^{1}	1.27×10^{3}
$(IA)_2(NH_3)_2$	1.03×10^{2}	1.90×10^{3}	2.25×10^{4}
$(IA)_2(NH_3)_3$	4.09×10^{10}	1.19×10^{11}	2.91×10^{11}
$(IA)_3(NH_3)_1$	6.66×10^{-2}	2.40×10^{0}	4.85×10^{1}
$(IA)_3(NH_3)_2$	2.04×10^{-2}	1.07×10^{0}	3.02×10^{1}

$(IA)_3(NH_3)_3$	4.30×10^{10}	1.06×10^{11}	2.23×10^{11}
$(IA)_4(NH_3)_1$	1.57×10^{0}	3.85×10^{1}	5.66×10^{2}
$(IA)_4(NH_3)_2$	3.94×10^{1}	1.04×10^{3}	1.69×10^{4}
$(IA)_5(NH_3)_1$	6.22×10^{-2}	2.76×10^{0}	6.82×10^{1}
$(NA)_1(NH_3)_1$	3.25×10^{4}	3.18×10^{5}	2.18×10^{6}
$(NA)_2(NH_3)_1$	3.91×10^{7}	2.38×10^{8}	1.05×10^{9}
$(NA)_2(NH_3)_2$	9.12×10^{2}	2.22×10^{4}	3.30×10^{5}
$(NA)_3(NH_3)_1$	5.28×10^{5}	5.83×10^{6}	4.51×10^{7}
$(NA)_3(NH_3)_2$	1.57×10^{2}	2.51×10^{3}	2.66×10^{4}
$(NA)_3(NH_3)_3$	2.73×10^{0}	6.19×10^{3}	8.63×10^{4}
$(NA)_4(NH_3)_1$	2.40×10^{6}	3.08×10^{7}	2.66×10^{8}
$(NA)_4(NH_3)_2$	1.69×10^{5}	2.07×10^{6}	1.72×10^{7}
$(NA)_5(NH_3)_1$	4.55×10^{6}	4.06×10^{7}	2.49×10^{8}
$(IA)_1(NA)_1(NH_3)_1$	3.62×10^{2}	7.16×10^{3}	9.30×10^{4}
$(IA)_1(NA)_1(NH_3)_2$	3.35×10^{1}	6.80×10^{2}	8.65×10^{3}
$(IA)_2(NA)_1(NH_3)_1$	1.10×10^{-2}	6.35×10^{-1}	1.93×10^{1}
$(IA)_2(NA)_1(NH_3)_2$	2.12×10^{0}	7.33×10^{1}	1.50×10^{3}
$(IA)_2(NA)_1(NH_3)_3$	3.86×10^{1}	6.25×10^{2}	6.44×10^{3}
$(IA)_3(NA)_1(NH_3)_1$	1.51×10^{5}	1.40×10^{6}	9.31×10^{6}
$(IA)_3(NA)_1(NH_3)_2$	4.62×10^{0}	1.18×10^{2}	1.81×10^{3}
$(IA)_4(NA)_1(NH_3)_1$	3.33×10^{0}	1.51×10^{2}	3.87×10^{3}
$(IA)_1(NA)_2(NH_3)_1$	8.77×10^{-1}	2.89×10^{1}	5.45×10^{2}
$(IA)_1(NA)_2(NH_3)_2$	2.02×10^{4}	3.67×10^{5}	4.19×10^{6}
$(IA)_1(NA)_2(NH_3)_3$	2.83×10^{-5}	1.98×10^{-3}	7.22×10^{-2}
$(IA)_2(NA)_2(NH_3)_1$	9.38×10^{9}	5.01×10^{10}	2.02×10^{11}
$(IA)_2(NA)_2(NH_3)_2$	2.14×10^{2}	4.88×10^{3}	6.84×10^{4}
$(IA)_3(NA)_2(NH_3)_1$	8.96×10^{-1}	4.86×10^{1}	1.40×10^{3}
$(IA)_1(NA)_3(NH_3)_1$	9.88×10^{6}	1.04×10^{8}	7.41×10^{8}
$(IA)_1(NA)_3(NH_3)_2$	3.82×10^{2}	6.04×10^{3}	6.24×10^{4}
$(IA)_2(NA)_3(NH_3)_1$	1.33×10^{3}	1.78×10^{4}	1.63×10^{5}

Table S3. Boundary conditions of the ACDC simulations at 220 K, 240 K, and 260 K, respectively.

Temperature (K)	Boundary cluster
220 K	$(IA)_7$
	$(IA)_6(NA)_1$
	$(IA)_6(NH_3)_1$
	$(IA)_5(NH_3)_2$
	$(IA)_2(NA)_2(NH_3)_3$
	$(IA)_5(NA)_1(NH_3)_1$
	$(IA)_1(NA)_3(NH_3)_3$
240 K	$(IA)_7$
	$(IA)_6(NA)_1$
	$(IA)_6(NH_3)_1$
	$(IA)_1(NA)_3(NH_3)_3$
260 K	$(IA)_6(NA)_1$
	$(IA)_6(NH_3)_1$
	$(IA)_1(NA)_3(NH_3)_3$

Table S4. The Gibbs formation free energies ΔG_{ref} (kcal mol^{-1}) of the IA–NA–NH_3 and SA–NA–NH_3 systems at the DLPNO-CCSD(T)/aug-cc-pVTZ(-PP)//ωB97X-D/6-311++G(3df,3pd) + aug-cc-pVTZ-PP with ECP28MDF (for I) level of theory, P = 1 atm, and T = 220 K.

Cluster		ΔG (kcal mol^{-1})	
		Pure-IA	Pure-SA
Pure-IA/SA	2	-14.41	-10.04
	3	-28.40	-19.08
	4	-49.46	-28.91
		IA–NA	SA–NA
IA/SA–NA	1-1	-7.57	-5.53
	1-2	-13.38	-10.15
	1-3	-18.65	-10.46
	2-1	-22.22	-15.22
	2-2	-28.50	-14.13
	3-1	-37.09	-23.12
		IA–NH_3	SA–NH_3
IA/SA–NH_3	1-1	-6.55	-8.93
	2-1	-24.26	-26.99
	2-2	-32.55	-36.58
	3-1	-39.94	-39.35
	3-2	-52.02	-54.77
	3-3	-51.71	-69.42
	4-1	-59.67	-48.61
	4-2	-68.49	-69.14
	5-1	-79.36	-55.71
		IA–NA–NH_3	SA–NA–NH_3
IA/SA–NA–NH_3	1-1-1	-15.29	-15.39
	1-1-2	-24.05	-26.65
	1-2-1	-25.46	-23.55
	1-2-2	-31.48	-33.14
	1-2-3	-46.42	-48.06
	1-3-1	-28.56	-29.19

	1-3-2	-39.04	-41.14
	2-1-1	-36.35	-32.33
	2-1-2	-46.38	-43.02
	2-1-3	-55.16	-59.66
	2-2-1	-36.46	-37.60
	2-2-2	-54.20	-55.90
	3-1-1	-44.89	-44.44
	3-1-2	-61.53	-65.15

Table S5. The total evaporation rate coefficients ($\Sigma\gamma$, s^{-1}) of SA–NA–NH_3 clusters calculated at 220 – 260 K.

Clusters	$\Sigma\gamma$ (s^{-1})		
	220 K	**240 K**	**260 K**
$(SA)_2$	5.12×10^{-1}	1.44×10^{1}	2.42×10^{2}
$(SA)_3$	1.09×10^{1}	3.12×10^{2}	5.22×10^{3}
$(SA)_4$	1.94×10^{0}	8.34×10^{1}	2.00×10^{3}
$(NA)_2$	8.37×10^{7}	4.87×10^{8}	2.20×10^{9}
$(NA)_3$	5.68×10^{11}	1.59×10^{12}	3.63×10^{12}
$(NH_3)_2$	2.01×10^{12}	2.94×10^{12}	4.12×10^{12}
$(NH_3)_3$	1.97×10^{11}	5.45×10^{11}	1.24×10^{12}
$(SA)_1(NA)_1$	6.27×10^{4}	7.16×10^{5}	5.61×10^{6}
$(SA)_1(NA)_2$	2.75×10^{5}	3.00×10^{6}	2.17×10^{7}
$(SA)_1(NA)_3$	5.73×10^{9}	2.42×10^{10}	8.18×10^{10}
$(SA)_2(NA)_1$	7.88×10^{4}	8.78×10^{5}	6.61×10^{6}
$(SA)_2(NA)_2$	1.45×10^{11}	5.57×10^{11}	1.73×10^{12}
$(SA)_3(NA)_1$	1.19×10^{6}	1.70×10^{7}	1.60×10^{8}
$(SA)_1(NH_3)_1$	3.64×10^{1}	6.19×10^{2}	6.78×10^{3}
$(SA)_2(NH_3)_1$	2.54×10^{-7}	3.05×10^{-5}	1.78×10^{-3}
$(SA)_2(NH_3)_2$	5.26×10^{0}	1.22×10^{2}	1.72×10^{3}
$(SA)_3(NH_3)_1$	5.70×10^{-3}	2.77×10^{-1}	7.12×10^{0}
$(SA)_3(NH_3)_2$	9.79×10^{-6}	8.03×10^{-4}	3.40×10^{-2}
$(SA)_3(NH_3)_3$	5.93×10^{-5}	4.20×10^{-3}	1.54×10^{-1}
$(SA)_4(NH_3)_1$	7.44×10^{0}	1.88×10^{2}	2.89×10^{3}
$(SA)_4(NH_3)_2$	6.45×10^{-5}	6.30×10^{-3}	2.98×10^{-1}
$(SA)_5(NH_3)_1$	1.12×10^{3}	3.45×10^{4}	6.26×10^{5}
$(NA)_1(NH_3)_1$	3.26×10^{4}	3.19×10^{5}	2.19×10^{6}
$(NA)_2(NH_3)_1$	3.93×10^{7}	2.39×10^{8}	1.06×10^{9}
$(NA)_2(NH_3)_2$	9.13×10^{2}	2.22×10^{4}	3.31×10^{5}
$(NA)_3(NH_3)_1$	5.30×10^{5}	5.85×10^{6}	4.53×10^{7}
$(NA)_3(NH_3)_2$	1.58×10^{2}	2.52×10^{3}	2.67×10^{4}
$(NA)_3(NH_3)_3$	2.74×10^{2}	6.19×10^{3}	8.64×10^{4}

$(NA)_4(NH_3)_1$	2.40×10^{6}	3.09×10^{7}	2.67×10^{8}
$(NA)_4(NH_3)_2$	1.69×10^{5}	2.07×10^{6}	1.72×10^{7}
$(NA)_5(NH_3)_1$	4.56×10^{6}	4.08×10^{7}	2.49×10^{8}
$(SA)_1(NA)_1(NH_3)_1$	4.02×10^{3}	6.36×10^{4}	6.68×10^{5}
$(SA)_1(NA)_1(NH_3)_2$	1.11×10^{-1}	4.11×10^{0}	8.54×10^{1}
$(SA)_1(NA)_2(NH_3)_1$	8.86×10^{1}	2.29×10^{3}	3.37×10^{4}
$(SA)_1(NA)_2(NH_3)_2$	4.25×10^{3}	1.01×10^{5}	1.46×10^{6}
$(SA)_1(NA)_2(NH_3)_3$	2.98×10^{-5}	2.47×10^{-3}	1.01×10^{-1}
$(SA)_1(NA)_3(NH_3)_1$	3.05×10^{4}	3.42×10^{5}	2.63×10^{6}
$(SA)_1(NA)_3(NH_3)_2$	1.43×10^{2}	2.41×10^{3}	2.52×10^{4}
$(SA)_2(NA)_1(NH_3)_1$	5.73×10^{4}	7.47×10^{5}	6.54×10^{6}
$(SA)_2(NA)_1(NH_3)_2$	4.87×10^{3}	1.05×10^{5}	1.41×10^{6}
$(SA)_2(NA)_1(NH_3)_3$	6.02×10^{-7}	5.48×10^{-5}	2.44×10^{-3}
$(SA)_2(NA)_2(NH_3)_1$	7.25×10^{4}	7.10×10^{5}	4.79×10^{6}
$(SA)_2(NA)_2(NH_3)_2$	2.07×10^{-3}	6.72×10^{-2}	1.25×10^{0}
$(SA)_3(NA)_1(NH_3)_1$	1.13×10^{5}	1.37×10^{6}	1.16×10^{7}
$(SA)_3(NA)_1(NH_3)_2$	6.50×10^{-1}	2.17×10^{1}	4.12×10^{2}

Table S6. Cartesian coordinates of all IA–NA–NH_3 clusters in the present study at the ωB97X-D/6-311++G(3df,3pd) + aug-cc-pVTZ-PP with ECP28MDF (for I) level of theory.

$(IA)_1(NA)_1(NH_3)_1$:

Atoms	X	Y	Z
N	2.915478	-0.186698	-0.059097
O	2.159906	0.697102	-0.435162
O	4.081342	-0.069885	0.167650
O	2.396832	-1.394593	0.108645
H	1.389981	-1.338087	-0.074451
I	-1.428830	-0.356142	0.026980
O	-1.283892	0.887506	-1.281094
O	-0.103788	-1.541462	-0.285673
O	-0.877765	0.584324	1.474969
H	-0.063073	2.000503	0.901473
N	0.275421	2.585119	0.097605
H	1.266500	2.391695	-0.047734
H	0.087406	3.571932	0.218204
H	-0.270162	2.156577	-0.691691

$(IA)_1(NA)_1(NH_3)_2$:

Atoms	X	Y	Z
N	3.387294	-0.110091	-0.093397
O	2.547301	-0.033475	0.892035
O	3.706174	-1.219004	-0.487385
O	3.797114	0.935511	-0.580391
H	1.833445	1.418646	0.712443
I	-1.891077	0.006567	-0.157118
O	-1.254990	1.676503	0.140329
O	-0.725236	-0.691063	-1.349123
O	-1.493821	-0.910383	1.346041
H	0.060869	-1.969062	1.082832
N	0.860706	-2.083841	0.440991
H	1.610919	-1.396423	0.705809
H	0.476606	-1.780235	-0.472568
H	1.228003	-3.026070	0.412275
N	1.316304	2.290735	0.408032
H	1.742237	2.583698	-0.465348
H	1.422586	3.023975	1.098323
H	0.289964	2.055093	0.272055

$(IA)_1(NA)_2(NH_3)_1$:

Atoms	X	Y	Z
N	3.241715	-0.839752	-0.162451
O	2.802255	-0.629110	0.960324
O	4.356798	-0.649723	-0.531189
O	2.403464	-1.348112	-1.061528
H	1.488647	-1.409317	-0.640605
N	-0.226449	2.265392	-0.690746
O	0.275395	1.067099	-0.693189
O	-1.319532	2.443594	-1.184642
O	0.440312	3.147380	-0.153926
H	1.115930	2.209279	1.273751
I	-1.371813	-0.516967	-0.133947
O	-1.248066	0.193790	1.508955
O	-0.011921	-1.680746	-0.221661
O	-2.717245	-1.844037	0.297093
H	-2.392609	-2.441838	0.980191
N	1.155148	1.429000	1.952763
H	1.373881	1.756329	2.885717
H	1.853421	0.748547	1.625839
H	0.222235	0.952681	1.915441

$(IA)_1(NA)_2(NH_3)_2$:

Atoms	X	Y	Z
N	0.917410	2.434360	-0.028051
O	0.178348	2.723457	0.933570
O	1.927359	1.722744	0.150940
O	0.622662	2.835969	-1.159607
H	-1.106815	2.358317	-1.211626
N	-2.542395	-0.905800	0.091380
O	-2.745431	0.188210	0.728303
O	-2.932696	-0.996347	-1.060778
O	-1.937322	-1.814457	0.667963
H	-1.551756	0.364451	1.930351
I	1.268487	-0.845965	-0.284205
O	1.297431	-0.970791	1.496392
O	-0.178116	0.073097	-0.752266
O	0.558797	-2.579953	-0.690012
H	-0.370244	-2.576739	-0.375193
N	-2.021701	1.876324	-1.333629
H	-1.895446	1.121385	-2.004640
H	-2.322642	1.394352	-0.454027
H	-2.737201	2.518524	-1.652151
N	-0.694771	0.612890	2.479425
H	-0.901551	0.723888	3.463424
H	0.012760	-0.127544	2.316535
H	-0.294960	1.479695	2.070274

$(IA)_1(NA)_2(NH_3)_3$:

Atoms	X	Y	Z
N	-0.231034	2.745955	-0.043725
O	-1.321880	2.578957	0.559505
O	0.834315	2.482878	0.534445
O	-0.247799	3.137619	-1.215110
H	-1.873616	2.089967	-1.681251
N	-2.603400	-1.334435	0.170184
O	-3.200014	-0.266849	0.385258
O	-2.587091	-1.838041	-0.955406
O	-1.991089	-1.884818	1.122631
H	-1.545509	-0.248433	2.082103
I	1.730297	-0.144791	-0.144545
O	1.506161	-0.377824	1.628463
O	0.021030	-0.177289	-0.750715
O	2.229387	-1.807904	-0.664004
H	0.897001	-2.707951	-0.506240
N	-2.082302	1.089141	-1.778007
H	-2.763892	0.774781	-1.068671
H	-2.397798	0.851192	-2.709248
H	-1.188981	0.590967	-1.541547
N	-0.061506	-3.169985	-0.430399
H	-0.611435	-2.765051	0.352268
H	-0.617013	-2.927729	-1.248952
H	0.007727	-4.175526	-0.333802
N	-0.936426	0.533422	2.354713
H	0.054143	0.231076	2.185652
H	-1.124770	1.356225	1.736064
H	-1.083050	0.781853	3.324590

$(IA)_1(NA)_3(NH_3)_1$:

Atoms	X	Y	Z
N	0.984744	-2.181626	-1.259174
O	0.764039	-1.132634	-1.847938
O	2.069065	-2.673025	-1.099446
O	-0.039048	-2.829127	-0.745353
H	-0.873477	-2.220338	-0.801272
N	2.179960	-0.615847	1.851665
O	1.335111	-0.129297	0.932824
O	1.753939	-0.937544	2.916920
O	3.335184	-0.672383	1.472337
H	3.376895	-0.169815	-0.319992
N	1.143410	2.747967	-0.456310
O	0.416052	3.358438	0.266036
O	2.359461	2.837406	-0.508825
O	0.626292	1.868825	-1.315148
H	-0.370304	1.713061	-1.082507
I	-2.358084	0.044142	0.245444
O	-2.159644	-1.481016	-0.699873
O	-1.784748	1.350252	-0.860219
O	-1.086643	-0.062622	1.527458
H	0.357732	-0.142587	1.281932
N	3.188608	0.243886	-1.248048
H	3.965639	0.084844	-1.878108
H	2.329089	-0.196969	-1.617962
H	3.003328	1.253438	-1.117771

$(IA)_1(NA)_3(NH_3)_2$:

Atoms	X	Y	Z
N	0.405580	-1.885811	-1.678967
O	0.186390	-0.712847	-1.886186
O	1.441022	-2.464578	-1.927473
O	-0.539936	-2.618843	-1.141189
H	-1.348464	-2.000233	-0.900412
N	1.826048	-1.045045	2.011372
O	1.216270	-0.621436	0.891421
O	1.242408	-0.964030	3.047822
O	2.942129	-1.486224	1.829497
H	3.524499	-1.106320	0.115285
N	2.686540	2.030661	-0.076821
O	3.495505	1.656298	0.753017
O	2.703532	1.527608	-1.248033
O	1.822653	2.886531	0.178570
H	-0.975438	1.976172	-1.345894
I	-2.646376	0.232467	0.424257
O	-2.561975	-1.343399	-0.462062
O	-2.482507	1.490405	-0.853598
O	-1.085326	0.343420	1.320200
H	0.291342	-0.261328	1.133772
N	3.653741	-0.916086	-0.889983
H	4.618327	-1.070135	-1.155918
H	3.022433	-1.528165	-1.416469
H	3.367841	0.096216	-1.066417
N	-0.029778	2.251403	-1.708308
H	0.445653	1.423454	-2.063912
H	0.595968	2.625749	-0.952398
H	-0.120459	2.934773	-2.450174

$(IA)_2(NA)_1(NH_3)_1$:

Atoms	X	Y	Z
N	-2.625495	1.689453	-0.678585
O	-2.213277	2.753768	-0.210411
O	-2.852164	1.508431	-1.847922
O	-2.815449	0.719984	0.170289
H	-1.365475	2.264776	1.290985
I	-1.420240	-1.144816	-0.022772
O	-1.293550	-0.951201	1.745383
O	-0.246137	0.071177	-0.703035
O	-0.256684	-2.654603	-0.226248
H	0.652551	-2.381532	0.033523
I	2.102504	0.297093	-0.316848
O	2.096343	-1.364700	0.341769
O	1.765753	1.368211	1.075661
O	4.029799	0.501681	-0.325985
H	4.404610	0.082665	0.457711
N	-0.778782	1.805458	2.016800
H	-0.824322	2.306806	2.894961
H	0.203419	1.737328	1.676842
H	-1.117865	0.832944	2.122337

$(IA)_2(NA)_1(NH_3)_2$:

Atoms	X	Y	Z
N	2.904083	1.698666	0.132322
O	2.083109	2.466318	0.738890
O	3.197588	1.938837	-1.028755
O	3.352356	0.721437	0.743864
H	1.293027	1.453556	1.901499
I	-2.567497	0.193527	0.003358
O	-1.630242	-1.336609	-0.328821
O	-1.899533	0.855192	1.538807
O	-2.067167	1.389579	-1.249955
H	-0.569497	2.161046	-1.279823
I	0.814317	-1.546938	-0.325249
O	0.816180	-1.730110	1.454433
O	0.702205	0.208783	-0.615330
O	2.706512	-1.687313	-0.638634
H	3.139418	-0.893880	-0.255932
N	0.347520	2.654832	-1.416027
H	0.223653	3.565185	-1.841371
H	0.939910	2.066221	-1.997538
H	0.874800	2.733626	-0.519578
N	0.681335	0.824642	2.466227
H	0.777563	1.018693	3.454483
H	0.927833	-0.160045	2.249806
H	-0.306798	0.930480	2.155061

$(IA)_2(NA)_1(NH_3)_3$:

Atoms	X	Y	Z
N	-2.226050	2.522677	0.186169
O	-1.119380	3.014940	0.579678
O	-2.805461	1.711519	0.927850
O	-2.663648	2.830942	-0.910575
H	-0.177891	2.837469	-1.019260
I	3.225204	-0.038694	-0.003587
O	2.519635	-1.503240	-0.789590
O	2.660935	1.358361	-0.992399
O	2.304422	0.080868	1.545371
H	0.797072	0.767322	1.968816
I	-2.398287	-0.933157	-0.159285
O	-1.600107	-1.174570	1.465724
O	-1.077593	-0.059341	-1.023855
O	-2.217734	-2.585960	-0.855613
H	-0.437068	-2.935992	-0.486344
N	0.351350	-2.798923	0.176281
H	0.682808	-3.688384	0.528677
H	-0.078200	-2.245758	0.935368
H	1.147131	-2.257851	-0.248478
N	-0.168577	1.028626	2.254530
H	-0.511060	1.847192	1.706201
H	-0.200403	1.240856	3.243589
H	-0.796002	0.220951	2.038112
N	0.173893	2.180244	-1.732023
H	0.099479	2.579729	-2.658136
H	-0.427181	1.331825	-1.638035
H	1.151841	1.894218	-1.505714

$(IA)_2(NA)_2(NH_3)_1$:

Atoms	X	Y	Z
N	2.103338	-2.450728	1.062798
O	3.029829	-1.739059	0.737903
O	1.743690	-2.688274	2.182795
O	1.399456	-3.033183	0.087572
H	1.529600	-2.462142	-0.731386
N	0.669854	2.750928	0.755536
O	1.906318	2.881694	0.917164
O	0.205304	2.751567	-0.396535
O	-0.064583	2.563033	1.732568
H	2.350135	1.540279	2.103996
I	-2.293101	-0.500162	0.300152
O	-4.016643	-0.753986	0.038727
O	-1.612706	-0.271663	-1.370647
O	-2.393027	1.291017	0.934641
H	-1.520534	1.710466	1.138883
I	0.751142	0.247378	-1.358902
O	1.309522	-1.353771	-1.911707
O	0.419842	-0.065018	0.405496
O	2.524377	0.955614	-1.075129
H	2.453867	1.830912	-0.646232
N	2.210426	0.537915	2.318062
H	1.925869	0.400247	3.280409
H	3.031775	-0.025043	2.098534
H	1.456736	0.232223	1.651964

$(IA)_2(NA)_2(NH_3)_2$:

Atoms	X	Y	Z
N	3.487066	-0.631799	1.239746
O	3.453231	-1.488469	0.346679
O	4.141118	0.414289	1.089463
O	2.827798	-0.798504	2.291137
H	1.512358	-1.889632	1.863016
N	-0.167701	3.073128	-0.281086
O	-0.692866	2.870446	0.926848
O	-0.741701	2.628548	-1.240496
O	0.869719	3.696343	-0.284511
H	1.936480	2.894626	1.337325
I	0.586069	-0.411621	-1.460778
O	0.641682	-2.183089	-1.246867
O	0.628565	0.219072	0.225752
O	2.438569	-0.123879	-1.867652
H	2.996394	-0.597341	-1.211892
I	-2.744491	-0.490052	0.411716
O	-1.786474	-0.543126	-1.136344
O	-1.843973	-1.519871	1.575105
O	-2.557511	1.197214	1.020941
H	-1.440749	2.165922	0.845840
N	2.040465	1.968400	1.751600
H	3.009406	1.593183	1.667175
H	1.441078	1.311780	1.202577
H	1.741587	1.968902	2.718928
N	0.743612	-2.493063	1.505238
H	-0.185253	-2.047833	1.642630
H	0.772761	-3.403134	1.947535
H	0.862945	-2.576243	0.478244

$(IA)_2(NA)_3(NH_3)_1$:

Atoms	X	Y	Z
N	-3.474957	0.628776	-0.976909
O	-2.306535	0.978580	-0.911754
O	-4.415615	1.333896	-1.159676
O	-3.728264	-0.671123	-0.839671
H	-2.849505	-1.130097	-0.658152
N	-1.998756	-1.061183	2.545963
O	-0.829180	-1.241918	2.844247
O	-2.896504	-1.817453	2.711005
O	-2.326402	0.117441	1.993598
H	-1.492129	0.628749	1.802753
N	4.108135	-0.718460	0.104806
O	3.821520	-0.474747	1.268615
O	4.737540	-1.652807	-0.279991
O	3.698124	0.136169	-0.828568
H	3.086734	0.819469	-0.396377
N	1.565148	0.270703	2.757968
H	2.320629	0.057213	2.089154
H	1.946405	0.467962	3.675549
H	1.008921	1.065019	2.385785
I	0.331745	1.779471	-0.288524
O	2.092620	1.945300	0.040625
O	-0.300502	1.748632	1.406665
O	0.034037	3.668275	-0.564970
H	0.477284	4.188783	0.114415
I	0.053744	-1.845219	-0.961764
O	0.747424	-0.470160	0.072425
O	-1.600313	-2.038742	-0.279699
O	-0.130450	-1.054905	-2.543627
H	0.893761	-0.502811	2.795502

$(IA)_3(NA)_1(NH_3)_1$:

Atoms	X	Y	Z
N	-0.302532	3.087877	-1.128785
O	-0.030972	2.619907	-0.042589
O	-1.218594	2.437396	-1.862345
O	0.148610	4.074455	-1.621876
I	3.605863	0.170217	0.520747
O	3.302569	-1.566446	0.232991
O	2.817548	0.987406	-0.987827
O	2.566836	0.685481	1.869712
H	0.042024	0.202109	1.782081
I	-3.487672	0.027151	0.399087
O	-3.394931	-1.708207	0.786081
O	-2.920253	0.935435	1.846557
O	-2.061520	0.187115	-0.768718
H	-1.451678	1.600027	-1.368619
I	-0.224388	-1.495554	-0.832964
O	0.030146	-1.215120	0.909843
O	0.591733	-0.133698	-1.669657
O	1.151712	-2.808317	-1.047440
H	1.959724	-2.480097	-0.595691
H	1.939119	0.546919	-1.225245
N	-0.232384	1.057487	2.312176
H	0.186712	1.855118	1.842129
H	0.107076	0.991832	3.263292
H	-1.273237	1.107143	2.256378

$(IA)_3(NA)_1(NH_3)_2$:

Atoms	X	Y	Z
N	0.749358	2.365446	1.800145
O	-0.335725	2.845911	1.441800
O	1.759541	2.561485	1.076481
O	0.836568	1.698750	2.831030
H	-0.904812	1.051338	2.862547
I	-3.670478	0.318301	-0.851790
O	-3.164674	-1.359524	-0.409330
O	-3.310417	1.280067	0.630604
O	-2.443749	0.880267	-2.048259
H	-1.010489	1.610316	-1.564779
I	3.569665	0.103307	-0.891416
O	2.793380	-1.494188	-0.706072
O	2.446725	1.143400	-1.808715
O	3.516417	0.778804	0.861116
H	2.764823	1.469537	1.023934
I	0.274559	-1.841522	0.644309
O	0.218590	-0.085876	0.335982
O	-0.688848	-2.008877	2.147642
O	-0.891859	-2.510307	-0.676622
H	-1.786628	-2.031564	-0.623380
N	-1.763168	0.490561	2.739159
H	-1.474569	-0.495243	2.586155
H	-2.287007	0.823003	1.896272
H	-2.353770	0.569047	3.557666
N	-0.177853	2.185186	-1.297805
H	-0.290618	2.513448	-0.322377
H	-0.099748	2.984923	-1.914367
H	0.688310	1.632970	-1.355842

$(IA)_3(NA)_2(NH_3)_1$:

Atoms	X	Y	Z
N	-0.870445	-1.748378	-2.318798
O	-1.406140	-1.966133	-1.181800
O	0.334003	-1.883719	-2.470815
O	-1.621788	-1.422910	-3.240613
H	-3.151945	-0.975903	-2.244197
N	0.904346	1.603534	2.697389
O	1.167452	0.481237	3.075939
O	0.064359	2.335534	3.124621
O	1.622613	2.093935	1.671977
H	2.223794	1.363424	1.293655
I	2.317938	-0.762230	-0.633437
O	1.253676	-1.513280	0.584125
O	3.112614	0.528042	0.330148
O	3.761592	-2.044064	-0.537370
H	4.024757	-2.170592	0.382328
I	-1.341094	-1.342672	1.226922
O	-3.109373	-1.466595	1.087750
O	-1.086886	0.426105	0.879025
O	-1.276319	-1.099363	3.133291
H	-0.495467	-0.562248	3.361204
I	-0.544250	2.063770	-0.645443
O	-2.055346	1.769521	-1.548511
O	0.627263	0.905066	-1.372072
O	0.034966	3.581352	-1.693575
H	0.060110	3.350961	-2.629754
N	-3.681764	-0.418763	-1.550060
H	-3.644702	-0.903222	-0.638314
H	-4.635802	-0.251661	-1.844434
H	-3.154656	0.476676	-1.463388

$(IA)_4(NA)_1(NH_3)_1$:

Atoms	X	Y	Z
N	-3.817829	-1.658823	1.459851
O	-3.868573	-0.360482	1.536259
O	-4.504810	-2.233114	0.651476
O	-3.038264	-2.224126	2.229980
H	-1.824126	-0.915462	2.603334
I	0.992561	2.416697	-0.150962
O	0.129236	1.405032	-1.363849
O	0.867228	1.572603	1.427210
O	-0.448090	3.628675	0.141438
H	-1.246617	3.095547	0.376175
I	3.434293	-0.496945	0.285563
O	5.185190	-0.336715	0.379425
O	2.877163	1.013766	-0.565433
O	2.971164	0.037946	2.054938
H	2.171840	0.616387	1.958875
I	0.074295	-2.324062	-0.746623
O	0.706834	-1.458718	0.708368
O	1.289488	-3.573818	-1.041414
O	0.693655	-1.094035	-2.061940
H	0.458709	-0.163355	-1.807239
I	-3.151801	0.704747	-0.416298
O	-2.347745	1.787471	0.780801
O	-2.053852	-0.702358	-0.564560
O	-2.556896	1.638846	-1.988430
H	-1.580204	1.687307	-1.956725
N	-1.072625	-0.213746	2.472989
H	-0.631678	0.033084	3.350483
H	-0.365784	-0.601696	1.818892
H	-1.478228	0.625208	2.033167

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