



Supplement of

Perchloric acid (HClO_4) drives atmospheric new particle formation enhanced by dimethylamine, ammonia and sulfuric acid: mechanisms and implications

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Figure S2. The formation free energy (ΔG) (in kcal mol⁻¹) of $(\text{PA})_m(\text{NH}_3)_n$ clusters ($m = 0-4$ and $n = 0-4$) calculated at the DLPNO-CCSD(T)/aug-cc-pVTZ// ω B97X-D/6-31++G(d,p) level of theory. The calculations are performed at 278 K and 1 atm.

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Figure S9. (A) Gibbs formation free energies (ΔG) of the $(PA)_{1-4}(DMA)_{1-4}$ clusters identified at the DLPNO-CCSD(T)/aug-cc-pVTZ// ω B97X-D/6-31++G(d,p) level of theory, $T = 298$ K, $p = 1$ atm. (B) Total evaporation rate coefficients ($\Sigma\gamma$ in s^{-1}) and the ratios of collision frequencies with (C) DMA monomer or (D) PA monomer versus total evaporation rate coefficients ($\beta_{DMA}C_{DMA}/\Sigma\gamma$ or $\beta_{PA}C_{PA}/\Sigma\gamma$) of the corresponding clusters.

Figure S10. The most stable configurations of $(PA)_m(SA)_n$ ($m = 0-4$ and $n = 0-4$) clusters calculated at the DLPNO-CCSD(T)/aug-cc-pVTZ// ω B97X-D/6-31++G(d,p) level of theory. The dashed white lines indicate hydrogen bonds. The white, red, gray,

yellow and green spheres denote the H, O, S, N and Cl atoms, respectively.

Figure S11. The simulated cluster formation rate J ($\text{cm}^{-3} \text{ s}^{-1}$) of PA–SA system at 278 K with different $[\text{SA}]$ (10^6 – 10^8 cm^{-3}), and $\text{CS} = 2 \times 10^{-3} \text{ s}^{-1}$.

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Figure S15. Evaporation rates for $(\text{CA})_m(\text{PA})_n$ clusters ($m = 0$ – 3 and $n = 0$ – 3), at 278 K and 1 atm.

Figure S16. The simulated cluster formation rate J ($\text{cm}^{-3} \text{ s}^{-1}$) of CA–PA system at 278 K with different $[\text{CA}]$ (10^6 – 10^8 cm^{-3}), and $\text{CS} = 2 \times 10^{-3} \text{ s}^{-1}$.

Figure S17. The simulated steady-state CA dimer concentration of CA–PA cluster system at 278 K with different $[\text{PA}]$ (10^6 – 10^8 cm^{-3}), and $\text{CS} = 2 \times 10^{-3} \text{ s}^{-1}$.

Figure S18. Main clustering pathways of $(\text{CA})_m(\text{PA})_n$ ($m = 0$ – 3 and $n = 0$ – 3) clusters at 278 K, $[\text{CA}] = 10^7 \text{ cm}^{-3}$, and $[\text{PA}] = 10^7 \text{ cm}^{-3}$.

Table S1. Coordinates of all optimized clusters

Section S1. The multi-step searching method to systematically screen the most stable structures of clusters.

In order to locate the conformer of the chlorine oxoacids clusters with lowest energy, a systematic multi-step sampling scheme was employed here. First, the artificial bee colony algorithm was adopted to yield about 1000-10000 initial structures for each studied cluster by ABCcluster software^[1]. The universal force field (UFF)^[2] was used to obtain the energies of all the above structures. And then up to 1000 low-energy conformers were selected for pre-optimization by the PM7 semiempirical method^[3] in MOPAC 2016^[4]. Next, geometry optimization and frequency calculations were carried out using the Gaussian 16 package and the employed integration grid is FineGrid^[5]. Subsequently, single-point ω B97X-D/6-31++G(d,p) energies were calculated, using Gaussian16, for the clusters, and only the 100 energetically lowest structures were saved for further optimization. About 100 structures with lower energies were selected to perform optimization at the ω B97X-D/6-31+G(d,p) level of theory^[6, 7]. 10 structures with lowest energies were further optimized at the ω B97X-D/6-31++G(d,p) level of theory to obtain the global minimum one with no imaginary frequency^[6, 7]. Finally, for 10 global energy minimum structures of the molecular cluster, the single-point correction was carried out at the DLPNO-CCSD(T)/aug-cc-pVTZ-PP level. The DLPNO-CCSD(T) calculations were performed using the ORCA 4.0.0 program^[8].

Section S2. Atmospheric clusters dynamic simulations

Atmospheric Cluster Dynamics Code (ACDC)^[9] was used to study the cluster kinetic process by explicit solution of the birth–death equations, which can be written as follows:

$$\frac{dC_i}{dt} = \frac{1}{2} \sum_{j < i} \beta_{j,(i-j)} C_j C_{i-j} + \sum_j \gamma_{j,(i+j) \rightarrow i} C_{i+j} - \sum_j \beta_{i,j} C_i C_j - \frac{1}{2} \sum_{j < i} \gamma_{i \rightarrow j} C_i + Q_i - S_i$$

where C_i is the concentration of cluster i , $\beta_{i,j}$ is the rate coefficient of collision between clusters i and j , $\gamma_{(i+j) \rightarrow i}$ is the evaporating rate coefficient of cluster $(i + j)$ into clusters i and j , Q_i and S_i are the external source term and possible loss term of cluster i , respectively. The condensation sink (CS) coefficient is set to be a typical value ($2 \times 10^{-3} \text{ s}^{-1}$) in coastal regions^[10].

The kinetic gas theory was taken to calculate the collision rate coefficient between two clusters. $\beta_{i,j}$ is calculated as follows:

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

where m_i is the mass of cluster i , T is the temperature and k_B is the Boltzmann constant. V_i is the van der Waals (vdW) volume of cluster i , calculated based on the Marching Tetrahedra (MT) approach^[11] using Multiwfn. And $\gamma_{(i+j) \rightarrow i}$ is given as follows:

$$\gamma_{(i+j) \rightarrow i} = \beta_{i,j} \frac{P_{ref}}{k_B T} \exp \left(\frac{\Delta G_{i+j} - \Delta G_i - \Delta G_j}{k_B T} \right)$$

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

Section S3. The boundary clusters in the simulated system.

In ACDC simulation, the boundary clusters are ones allowed to flux out the simulation box for further growth, therefore, these clusters are required to have favorable compositions for high stability (low evaporation rate). The boundary clusters are the smallest clusters outside the simulated system. Once the boundary clusters are formed, they tend to keep growing rather than evaporate into smaller clusters^[9]. Boundary conditions require that the growing clusters could be sufficiently stable and the clusters should be more likely to grow than evaporate. For $(PA)_m(DMA)_n$ ($m = 0-4$, $n = 0-4$) clusters, clusters with roughly equal numbers of PA and DMA molecules have lower evaporation rates and higher concentrations in the simulations. This allows us to select $(PA)_5(DMA)_4$ and $(PA)_4(DMA)_5$ as the boundary clusters for chlorine oxoacid system in the 4×4 box simulation.

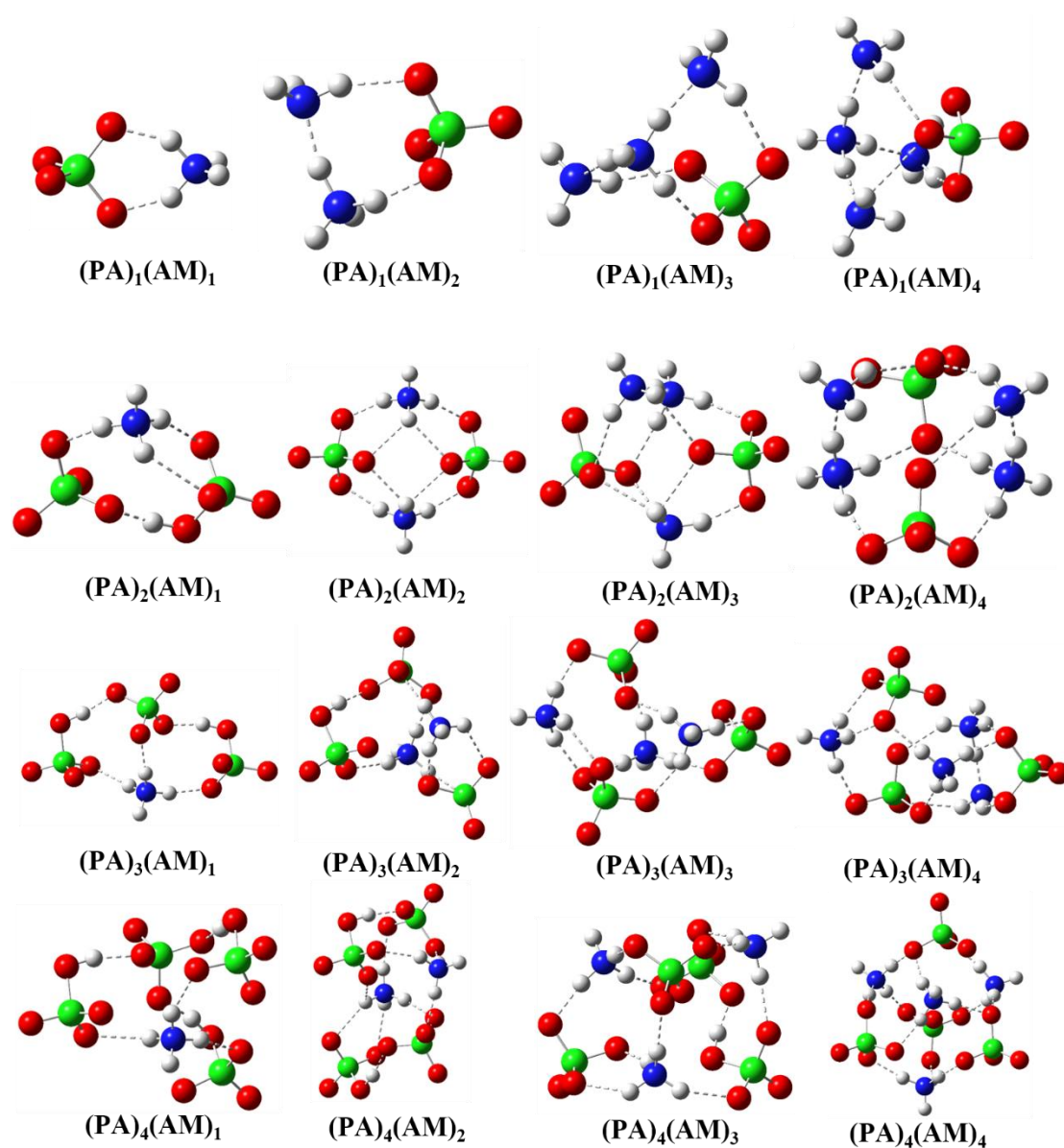


Figure S1. The most stable configurations of $(\text{PA})_m(\text{AM})_n$ ($m = 0-4$ and $n = 0-4$) clusters calculated at the DLPNO-CCSD(T)/aug-cc-pVTZ// ω B97X-D/6-31++G(d,p) level of theory. The dashed white lines indicate hydrogen bonds. The white, red, gray, blue and green spheres denote the H, O, C, N and Cl atoms, respectively.

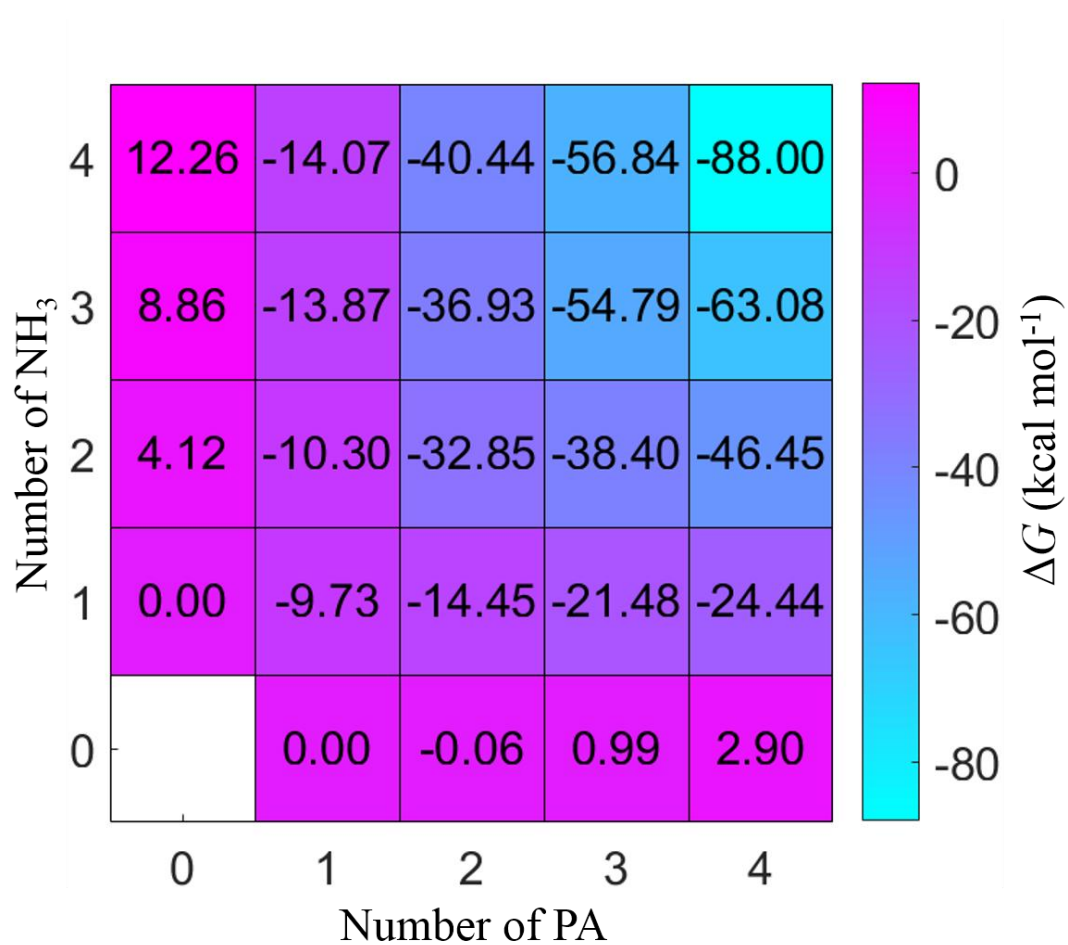


Figure S2. The formation free energy (ΔG) (in kcal mol⁻¹) of (PA)_m(NH₃)_n clusters ($m = 0-4$ and $n = 0-4$) calculated at the DLPNO-CCSD(T)/aug-cc-pVTZ// ω B97X-D/6-31++G(d,p) level of theory. The calculations are performed at 278 K and 1 atm.

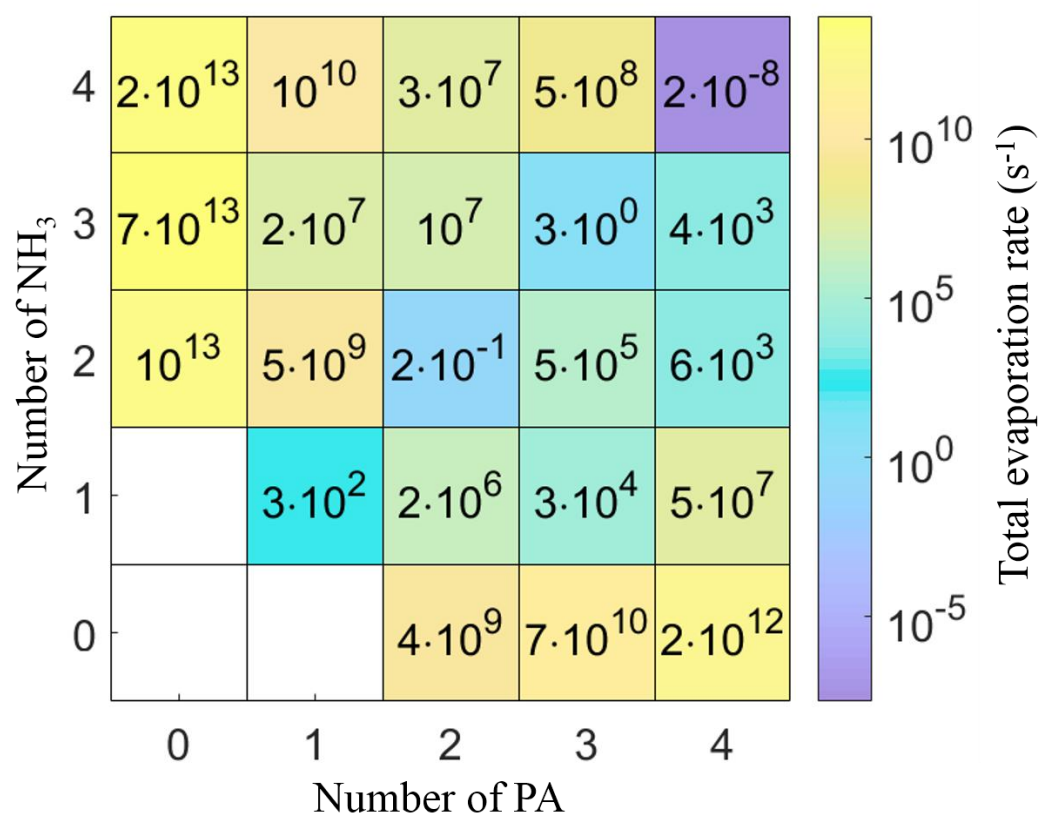


Figure S3. Evaporation rates for $(\text{PA})_m(\text{NH}_3)_n$ clusters ($m = 0-4$ and $n = 0-4$), at 278 K and 1 atm.

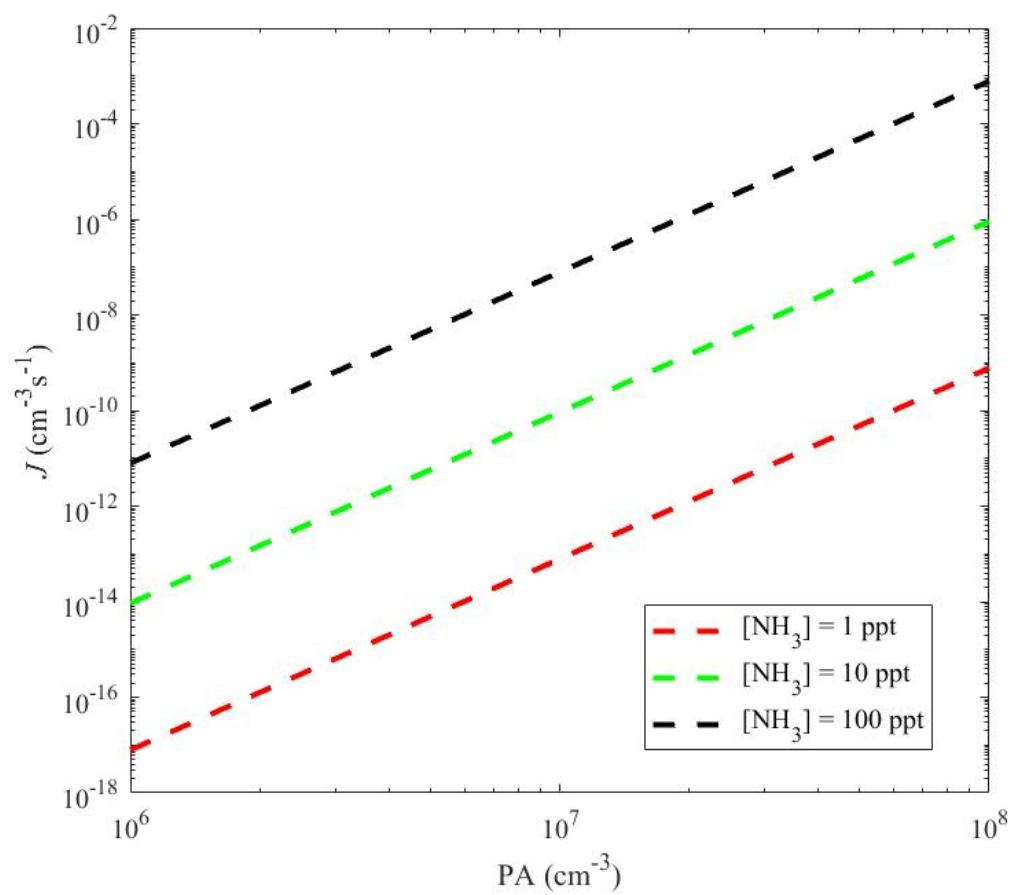


Figure S4. The simulated cluster formation rate J ($\text{cm}^{-3} \text{s}^{-1}$) of PA- NH_3 system at 278 K with different [DMA] (0.1 –10 ppt), and $\text{CS} = 2 \times 10^{-3} \text{s}^{-1}$.

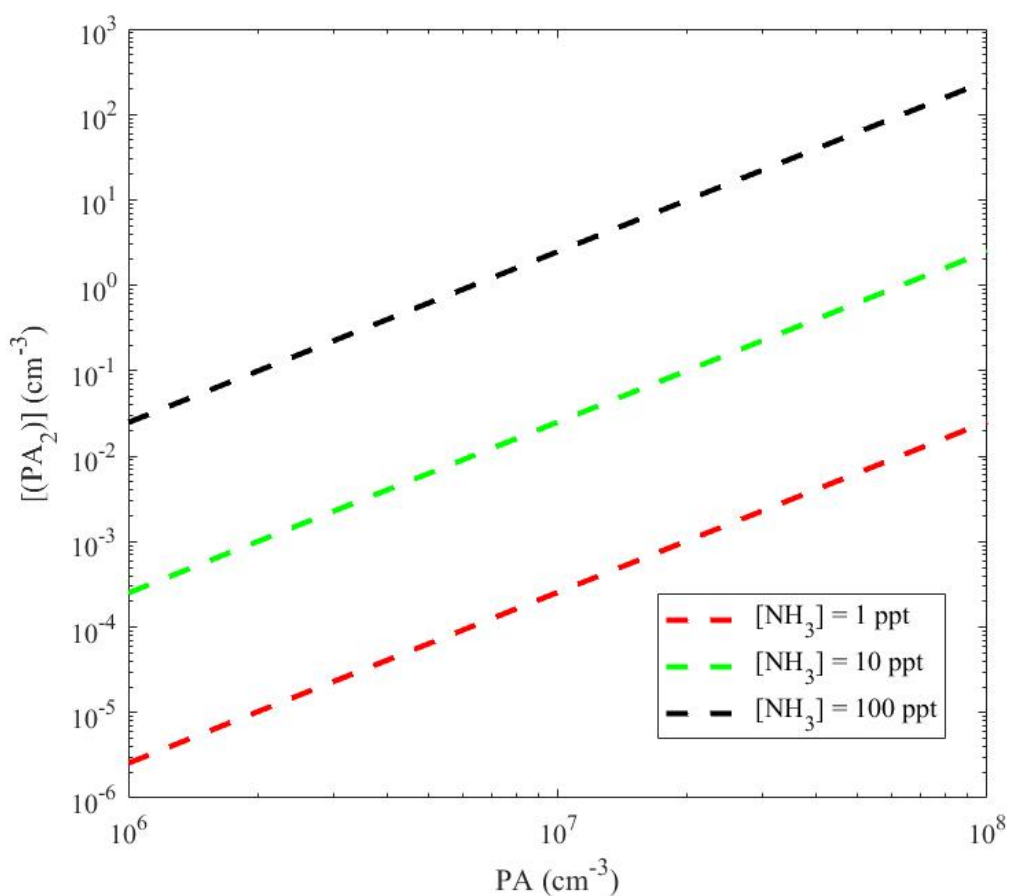


Figure S5. The simulated steady-state PA dimer concentration of PA–NH₃ cluster system at 278 K with different [NH₃] (0.1 –10 ppt), and CS = $2 \times 10^{-3} \text{ s}^{-1}$.

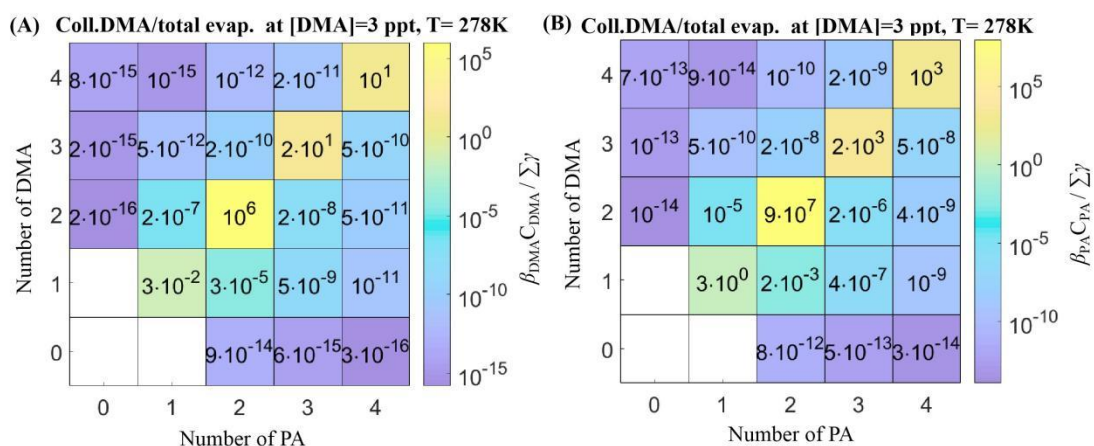


Figure S6. Ratios of collision frequencies with (A) DMA monomer or (B) PA

monomer versus total evaporation rate coefficients ($\beta_{\text{DMA}}C_{\text{DMA}}/\Sigma\gamma$ or $\beta_{\text{PA}}C_{\text{PA}}/\Sigma\gamma$) of the corresponding clusters.

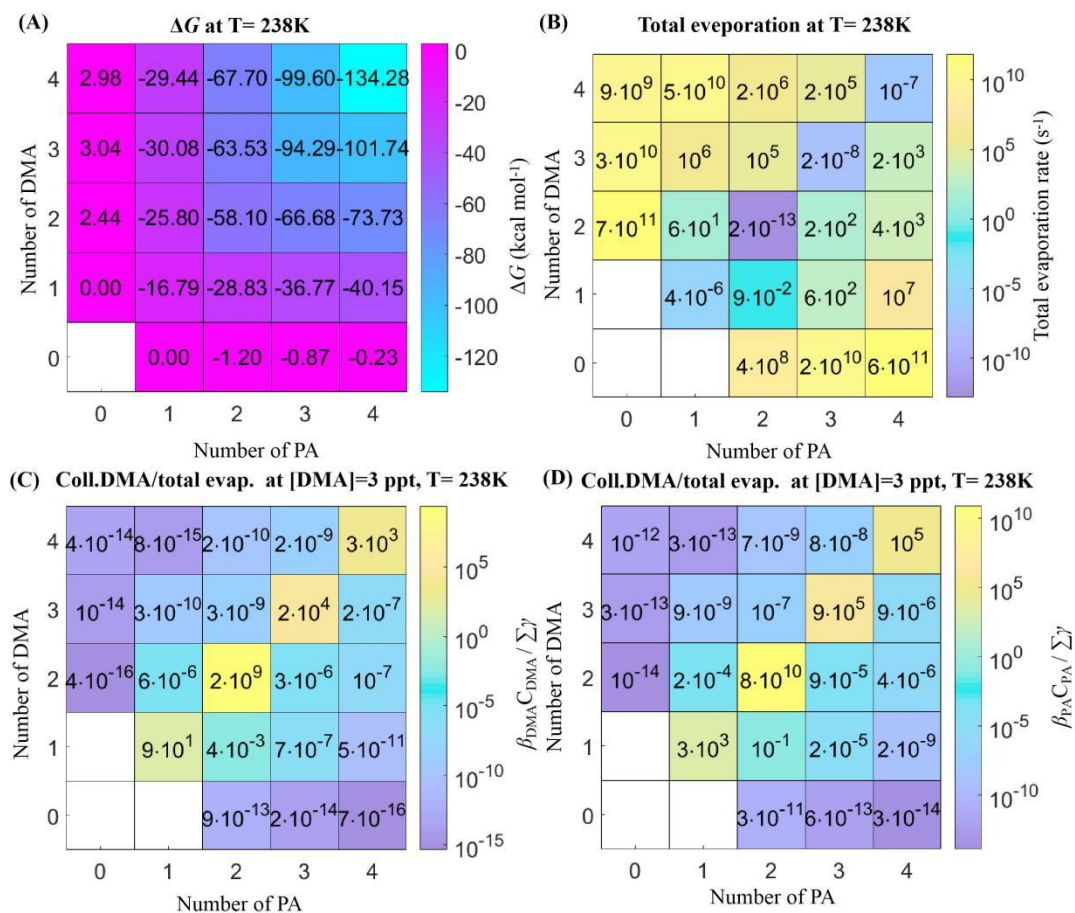


Figure S7. (A) Gibbs formation free energies (ΔG) of the $(\text{PA})_{1-4}(\text{DMA})_{1-4}$ clusters identified at the DLPNO-CCSD(T)/aug-cc-pVTZ// ω B97X-D/6-31++G(d,p) level of theory, $T = 238 \text{ K}$, $p = 1 \text{ atm}$. (B) Total evaporation rate coefficients ($\Sigma\gamma$ in s^{-1}) and the ratios of collision frequencies with (C) DMA monomer or (D) PA monomer versus total evaporation rate coefficients ($\beta_{\text{DMA}}C_{\text{DMA}}/\Sigma\gamma$ or $\beta_{\text{PA}}C_{\text{PA}}/\Sigma\gamma$) of the corresponding clusters.

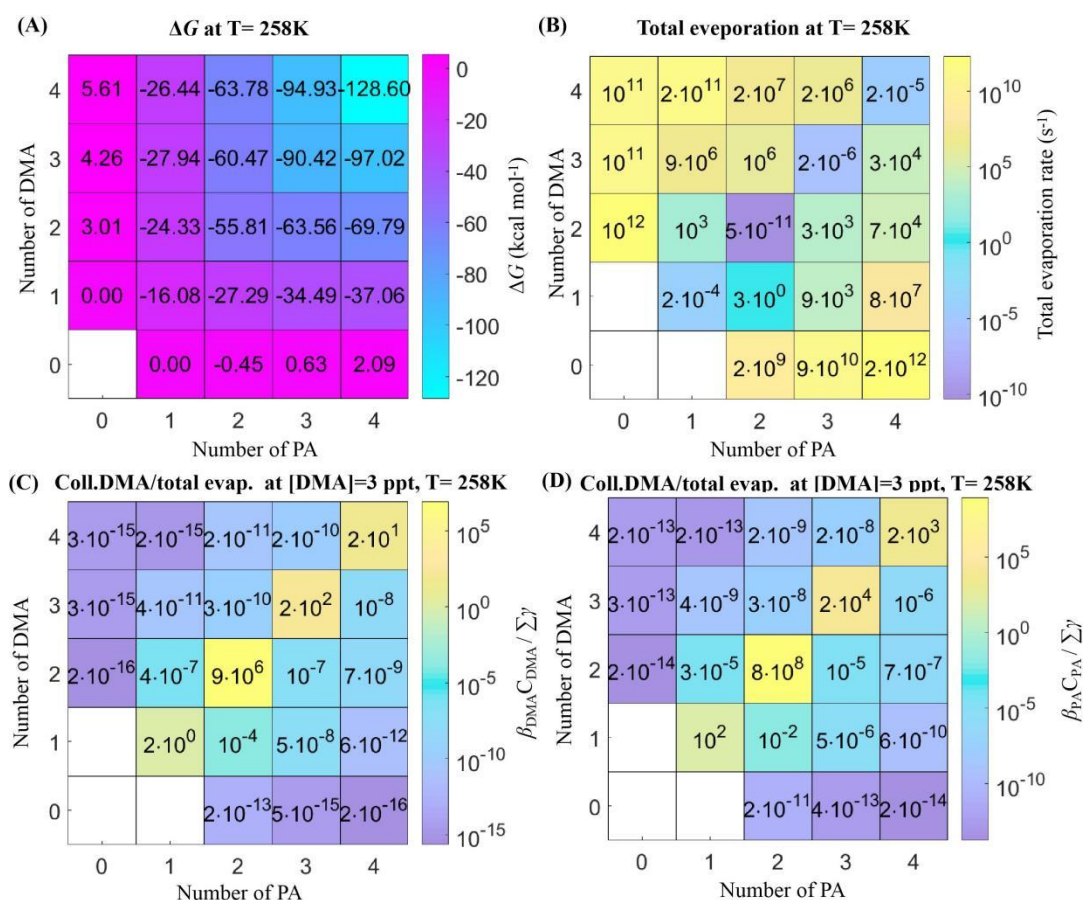


Figure S8. (A) Gibbs formation free energies (ΔG) of the $(\text{PA})_{1-4}(\text{DMA})_{1-4}$ clusters identified at the DLPNO-CCSD(T)/aug-cc-pVTZ// ω B97X-D/6-31++G(d,p) level of theory, $T = 258 \text{ K}$, $p = 1 \text{ atm}$. (B) Total evaporation rate coefficients ($\Sigma\gamma$ in s^{-1}) and the ratios of collision frequencies with (C) DMA monomer or (D) PA monomer versus total evaporation rate coefficients ($\beta_{\text{DMA}}C_{\text{DMA}}/\Sigma\gamma$ or $\beta_{\text{PA}}C_{\text{PA}}/\Sigma\gamma$) of the corresponding clusters.

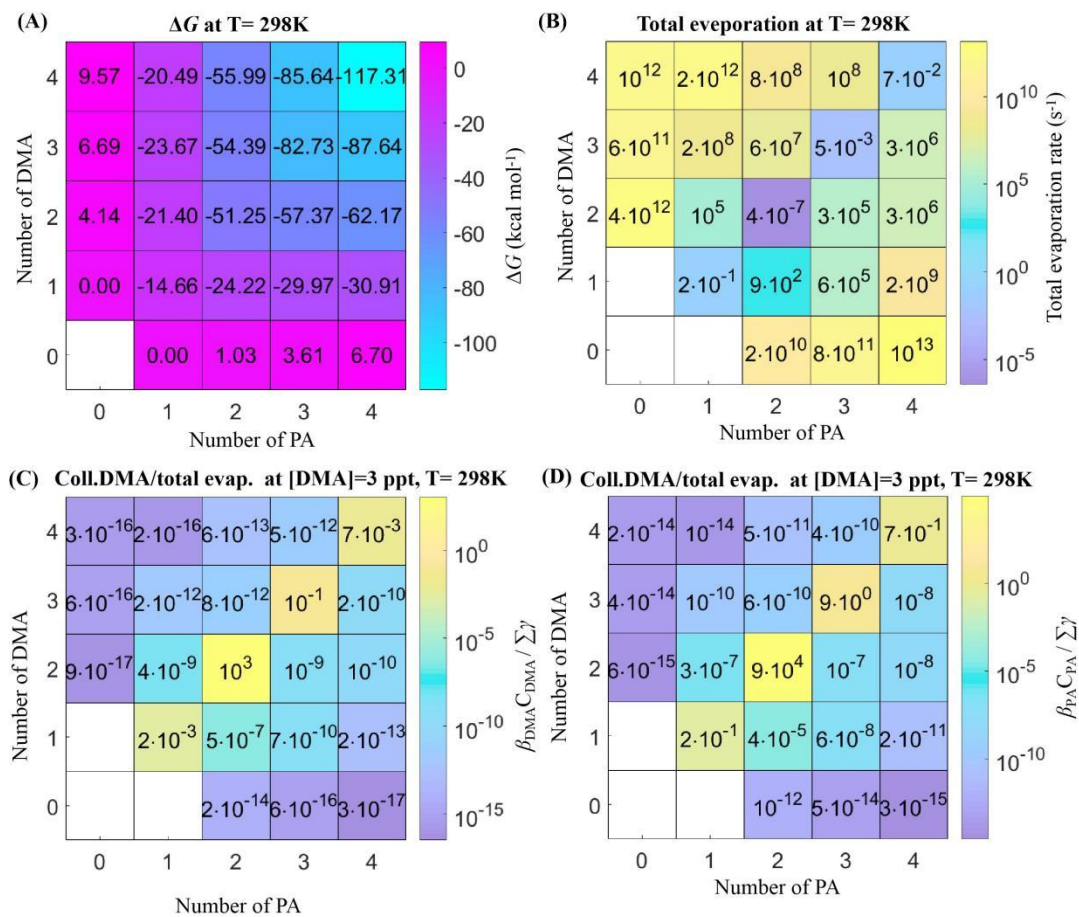


Figure S9. (A) Gibbs formation free energies (ΔG) of the $(\text{PA})_{1-4}(\text{DMA})_{1-4}$ clusters identified at the DLPNO-CCSD(T)/aug-cc-pVTZ// ω B97X-D/6-31++G(d,p) level of theory, $T = 298 \text{ K}$, $p = 1 \text{ atm}$. (B) Total evaporation rate coefficients ($\Sigma\gamma$ in s^{-1}) and the ratios of collision frequencies with (C) DMA monomer or (D) PA monomer versus total evaporation rate coefficients ($\beta_{\text{DMA}}C_{\text{DMA}}/\Sigma\gamma$ or $\beta_{\text{PA}}C_{\text{PA}}/\Sigma\gamma$) of the corresponding clusters.

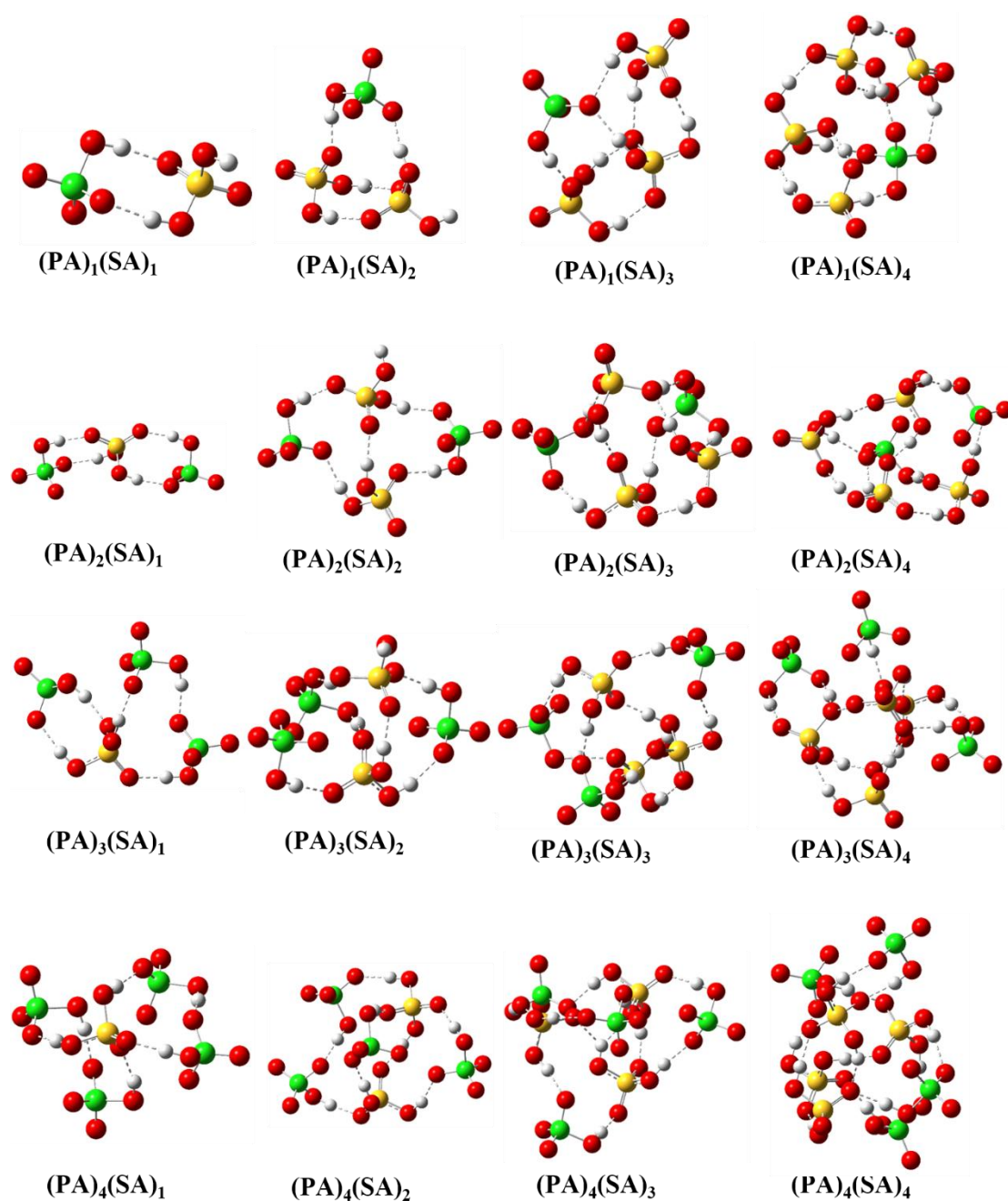


Figure S10. The most stable configurations of $(\text{PA})_m(\text{SA})_n$ ($m = 0-4$ and $n = 0-4$) clusters calculated at the DLPNO-CCSD(T)/aug-cc-pVTZ// ω B97X-D/6-31++G(d,p) level of theory. The dashed white lines indicate hydrogen bonds. The white, red, gray, yellow and green spheres denote the H, O, S, N and Cl atoms, respectively.

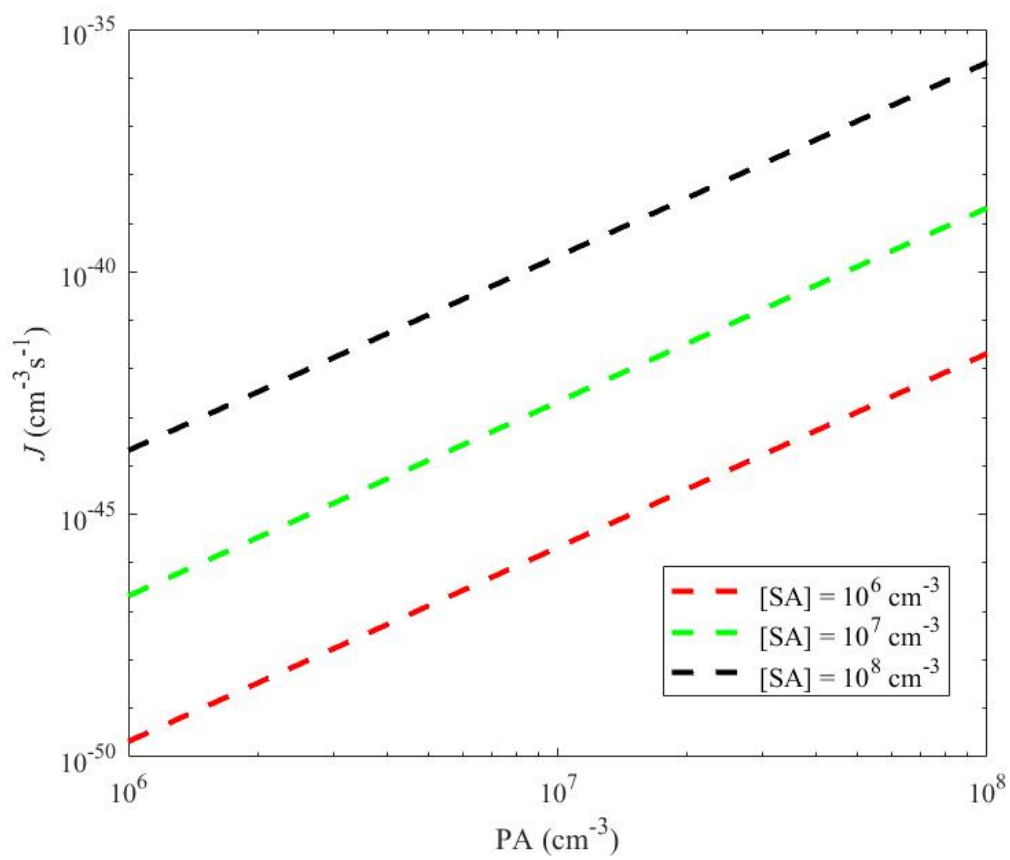


Figure S11. The simulated cluster formation rate J ($\text{cm}^{-3} \text{s}^{-1}$) of PA–SA system at 278 K with different $[\text{SA}]$ (10^6 – 10^8 cm^{-3}), and $\text{CS} = 2 \times 10^{-3} \text{ s}^{-1}$.

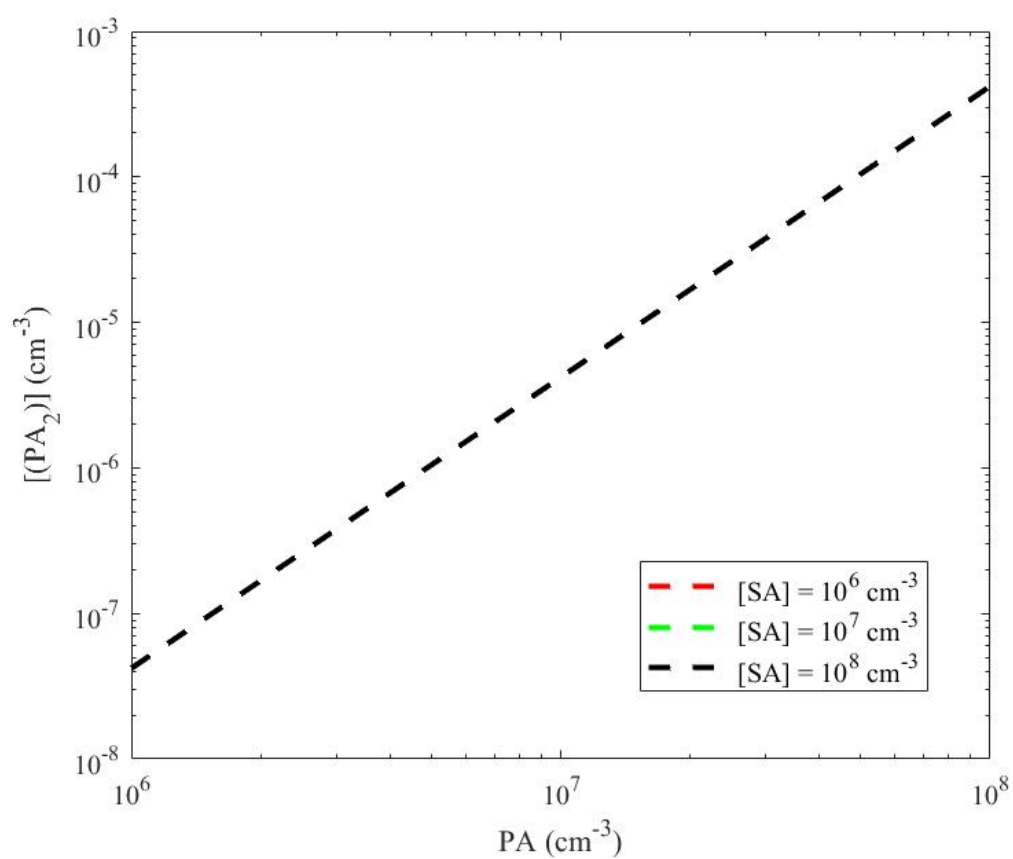


Figure S12. The simulated steady-state PA dimer concentration of PA–SA cluster system at 278 K with different [SA] (10^6 – 10^8 cm^{-3}), and $\text{CS} = 2 \times 10^{-3} \text{ s}^{-1}$.

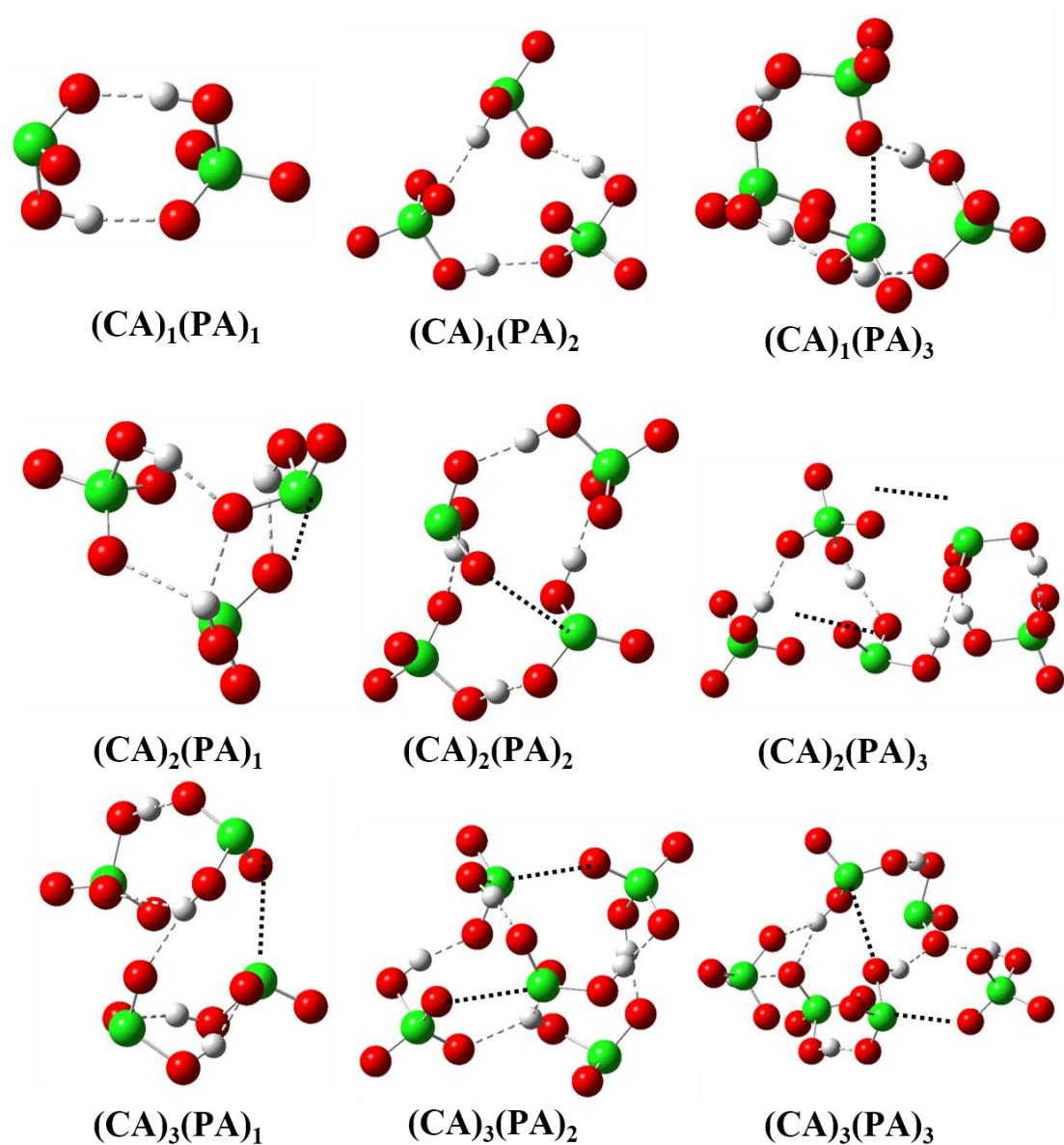


Figure S13. The most stable configurations of $(\text{CA})_m(\text{PA})_n$ ($m = 0-3$ and $n = 0-3$) clusters calculated at the DLPNO-CCSD(T)/aug-cc-pVTZ// ω B97X-D/6-31++G(d,p) level of theory. The dashed white lines indicate hydrogen bonds. The white, red, gray, and green spheres denote the H, O, C, and Cl atoms, respectively.

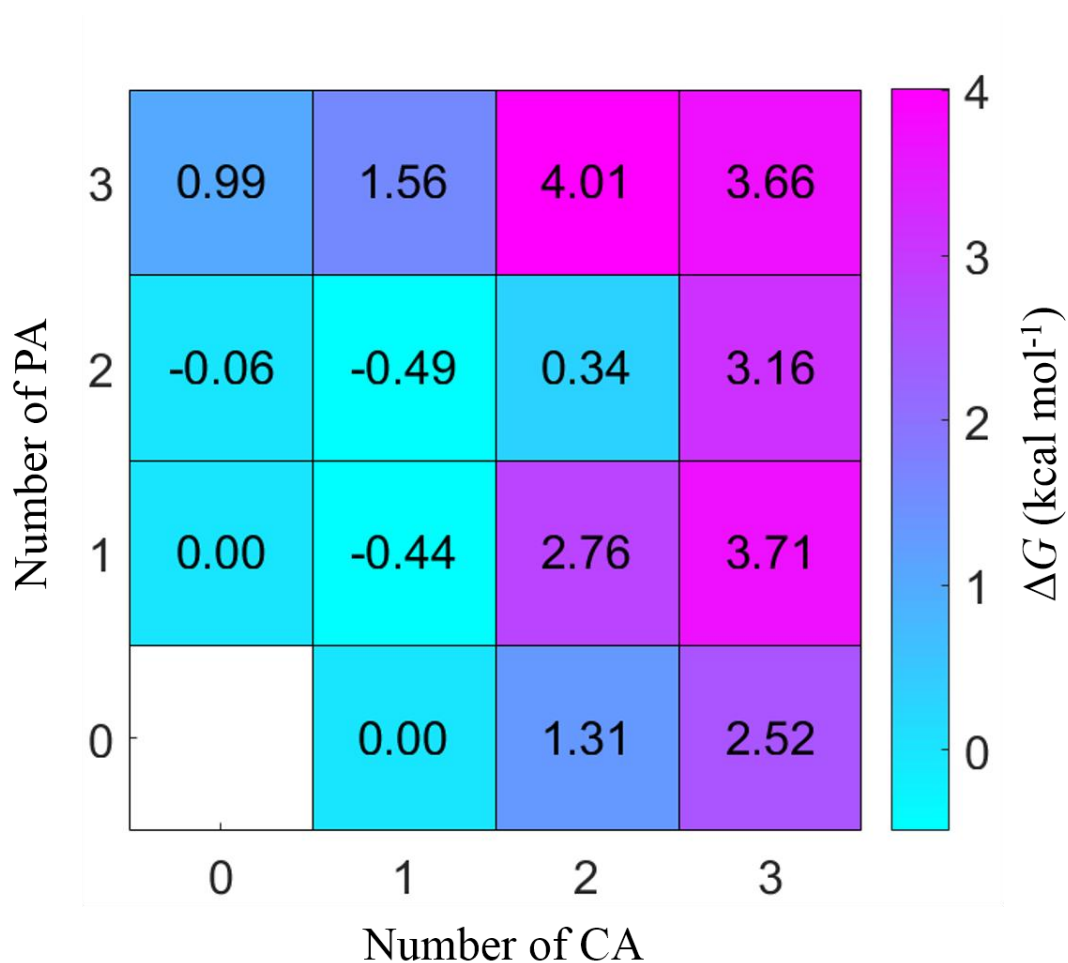


Figure S14. The formation free energy (ΔG) (in kcal mol⁻¹) of (CA)_m(PA)_n clusters ($m = 0-3$ and $n = 0-3$) calculated at the DLPNO-CCSD(T)/aug-cc-pVTZ// ω B97X-D/6-31++G(d,p) level of theory. The calculations are performed at 278 K and 1 atm.

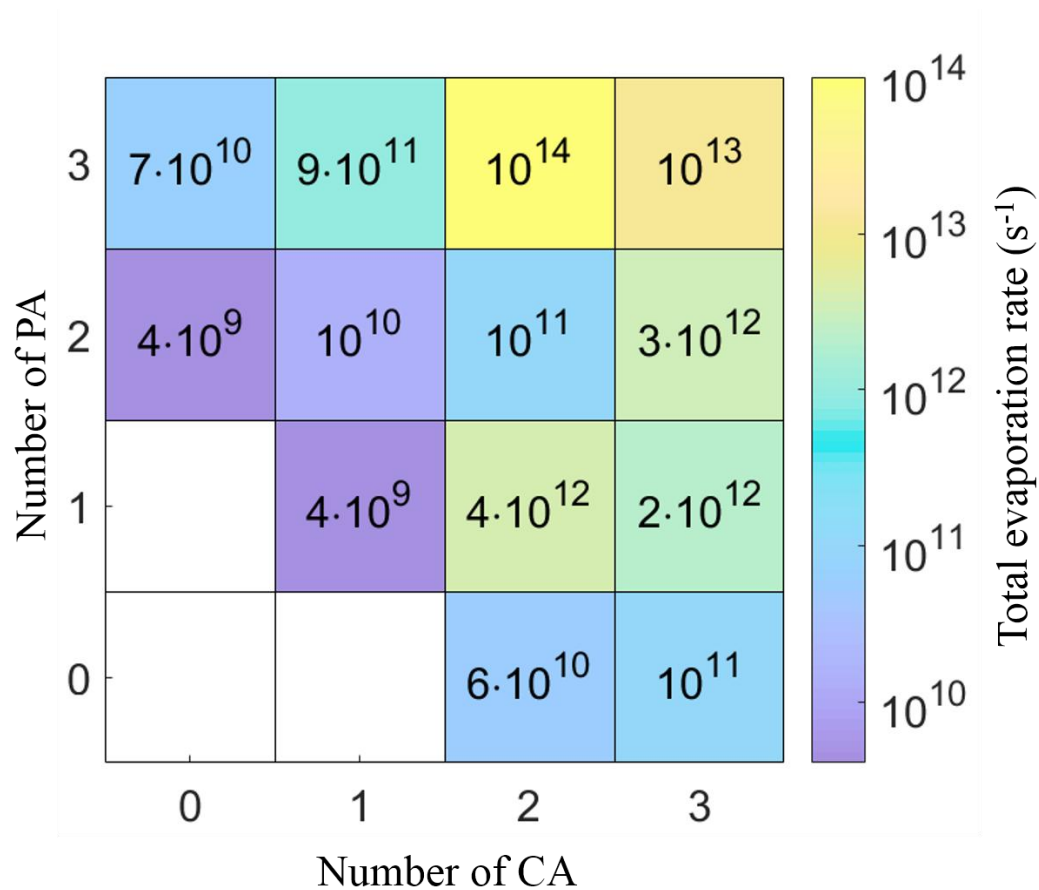


Figure S15. Evaporation rates for $(\text{CA})_m(\text{PA})_n$ clusters ($m = 0-3$ and $n = 0-3$), at 278 K and 1 atm.

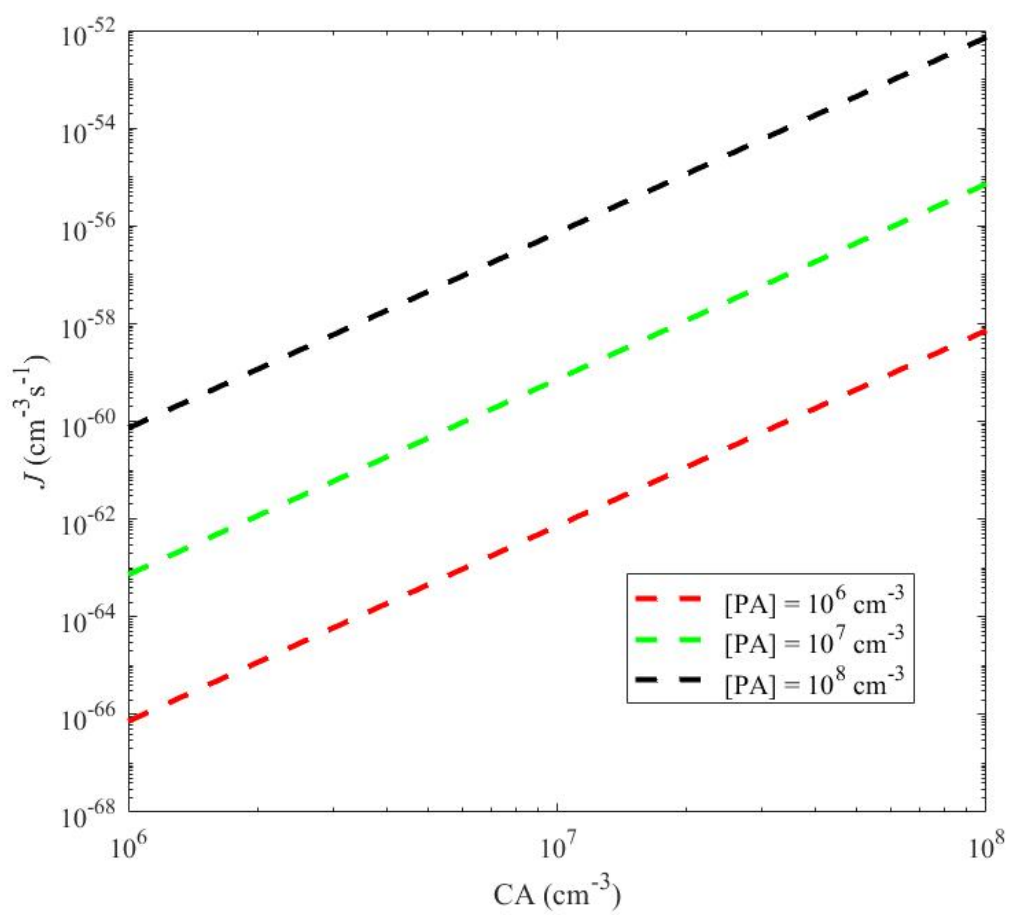


Figure S16. The simulated cluster formation rate J ($\text{cm}^{-3} \text{s}^{-1}$) of CA–PA system at 278 K with different $[\text{CA}]$ (10^6 – 10^8 cm^{-3}), and $\text{CS} = 2 \times 10^{-3} \text{ s}^{-1}$.

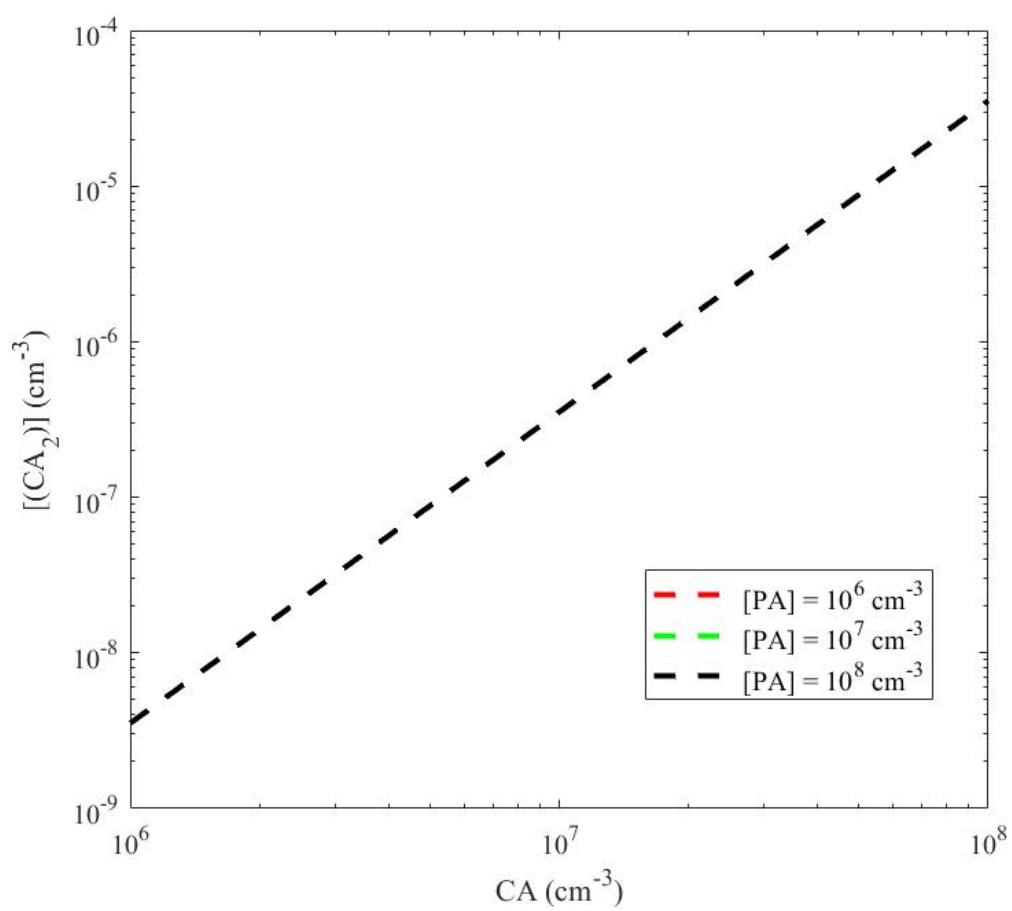


Figure S17. The simulated steady-state CA dimer concentration of CA-PA cluster system at 278 K with different [PA] (10^6 – 10^8 cm⁻³), and $CS = 2 \times 10^{-3}$ s⁻¹.

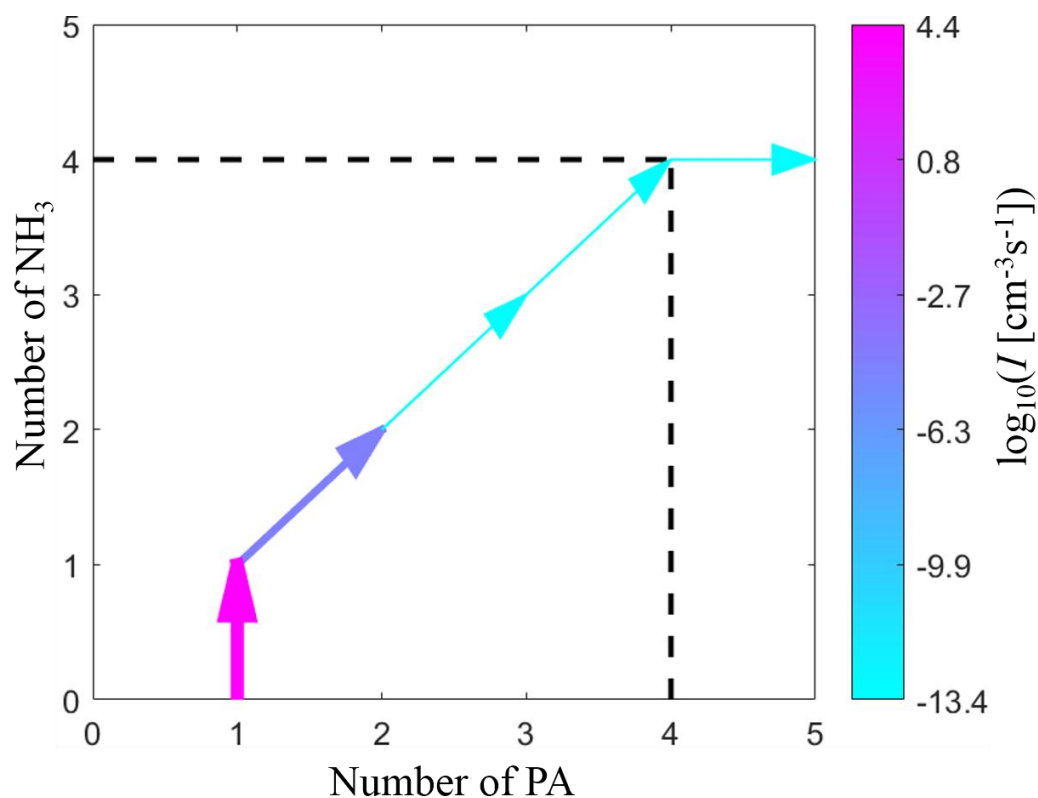


Figure S18. Main clustering pathways of $(\text{CA})_m(\text{PA})_n$ ($m = 0-3$ and $n = 0-3$) clusters at 278 K, $[\text{CA}] = 10^7 \text{ cm}^{-3}$, and $[\text{PA}] = 10^7 \text{ cm}^{-3}$.

Table S1. Coordinates of all optimized clusters

$(\text{DMA})_2$	x	y	z
C	-1.84310200	-1.20568500	-0.22374200
H	-1.00916100	-1.24346100	-0.92613900
H	-1.79434700	-2.08539200	0.41559800
H	-2.77568800	-1.24197500	-0.80161300
H	-2.41106500	0.00381100	1.31323200
C	-1.83919100	1.20255500	-0.23076900
H	-2.77142500	1.23816000	-0.80926000
H	2.53913600	1.24215600	1.01792000
H	-1.00471700	1.23383100	-0.93282500

N	-1.71465200	0.00056500	0.58008200
C	2.04890400	1.20555100	0.03443900
H	2.82818300	1.28012200	-0.72589900
H	1.40469500	2.07894100	-0.05946300
H	-1.78831600	2.08577400	0.40356300
H	0.46623900	-0.00706000	0.43535600
C	2.06200700	-1.20144500	0.02873800
H	2.55239300	-1.23754900	1.01217100
H	1.42760400	-2.08148700	-0.06980800
H	2.84229700	-1.26364800	-0.73169600
N	1.27500400	-0.00171900	-0.17910000

(DMA) ₃	x	y	z
C	-2.45662200	-0.64779100	1.19336100
H	-3.06800000	-1.53512000	1.36820100
H	-1.75697700	-0.55596600	2.02406600
H	-3.12569100	0.22530100	1.20951100
H	-1.06824100	-0.01795700	-0.14320500
C	-2.60912700	-0.82233900	-1.20041300
H	-3.28776800	0.04172100	-1.25313600
H	-2.02138000	-0.85159000	-2.11727600
H	-3.22472100	-1.72314900	-1.16905800
N	-1.72658100	-0.79009500	-0.05090800
C	1.77652600	-1.49114800	-1.19555700
H	0.72110200	-1.22162900	-1.25483900
H	2.29043700	-1.09392100	-2.06931300
H	1.84038700	-2.58626600	-1.21525400
H	3.32901100	-1.08853200	0.06160600
C	1.68074700	-1.43039100	1.20970500
H	1.74550200	-2.52257700	1.29298900
H	2.12026700	-0.98419700	2.10041400
H	0.62227300	-1.16820200	1.16698900
N	2.33476200	-0.90803500	0.01730900
C	0.25940700	2.11911600	1.22505600
H	-0.73483300	2.56575300	1.28808800
H	0.34655300	1.37948100	2.02019800
H	0.99563400	2.91337900	1.40846300
H	1.27778700	0.91671400	-0.06605600
C	0.43251900	2.41927800	-1.16298200
H	1.18371000	3.21198200	-1.04542500
H	0.62662000	1.89684000	-2.09858200
H	-0.54518400	2.89812900	-1.24189700
N	0.42507700	1.47233800	-0.06375900

(DMA) ₄		x	y	z
N	-1.00242	1.79381	-0.42657	
H	-1.37401	0.84766	-0.28175	
H	0.84838	1.37469	0.28065	
N	1.79428	1.00270	0.42607	
C	2.76803	1.93152	-0.11997	
C	2.00142	0.73230	1.83818	
C	-0.73179	2.00206	-1.83847	
C	-1.93191	2.76666	0.11996	
H	-2.15013	2.51762	1.16244	
H	-2.88834	2.81606	-0.43008	
H	-1.48390	3.76716	0.09933	
H	-0.24155	2.97196	-1.98583	
H	-1.63841	1.98551	-2.46839	
H	-0.04906	1.22534	-2.19748	
H	2.97089	0.24148	1.98636	
H	1.98498	1.63909	2.46787	
H	1.22400	0.05017	2.19685	
H	2.81764	2.88801	0.42993	
H	3.76825	1.48290	-0.09858	
H	2.51988	2.14973	-1.16267	
N	1.00279	-1.79417	-0.42569	
H	1.37476	-0.84817	-0.28094	
C	0.73122	-2.00200	-1.83748	
C	1.93222	-2.76753	0.11997	
H	0.04863	-1.22488	-2.19593	
H	1.63747	-1.98569	-2.46794	
H	0.24046	-2.97164	-1.98476	
H	1.48377	-3.76784	0.09929	
H	2.88828	-2.81718	-0.43068	
H	2.15123	-2.51895	1.16241	
N	-1.79380	-1.00257	0.42642	
H	-0.84768	-1.37455	0.28266	
C	-2.00317	-0.73093	1.83797	
C	-2.76664	-1.93192	-0.12036	
H	-2.81697	-2.88799	0.43022	
H	-3.76694	-1.48340	-0.10078	
H	-2.51692	-2.15091	-1.16251	
H	-1.98757	-1.63714	2.46850	
H	-2.97294	-0.24012	1.98421	
H	-1.22642	-0.04831	2.19720	

(CA) ₂	x	y	z
O	-1.34215900	-0.48622400	1.31847000
O	-1.28894400	1.22226200	-0.39685700
Cl	-2.15920400	0.15966800	0.08651500
H	0.40891000	1.34932700	-0.01396200
O	-2.29789900	-0.87958100	-0.88347600
O	0.92018700	-1.07550500	-0.08705900
O	1.35275300	1.27394100	0.26605500
Cl	1.93748300	-0.08996100	-0.40277800
H	-0.48465800	-0.81267000	0.94622900
O	3.13668900	-0.27010200	0.33839200

(CA) ₃	x	y	z
O	-2.04844600	-1.16000700	1.24085300
O	-0.47425900	-1.01724800	-0.66340500
Cl	-1.82263400	-1.58448200	-0.35013200
H	-2.10773300	-0.17615900	1.24428000
O	-1.80425400	-3.03995500	-0.25459000
O	1.90801000	-1.40173300	0.60540600
O	1.94134300	0.87759800	-0.33750500
Cl	2.76665700	-0.36075000	-0.36529500
H	0.98798400	-1.43531100	0.23296600
O	4.01335200	-0.23866100	0.37856600
O	-0.24892200	1.43734200	1.17357500
O	-1.01711500	3.37528300	-0.20981400
Cl	-0.92754100	1.92003500	-0.28119200
H	0.70869600	1.29741300	0.98273500
O	-2.25335400	1.26018200	-0.12276800

(PA) ₁	x	y	z
O	1.48408000	0.34314700	-0.00080400
O	-0.36646400	-0.78243600	-1.20962900
Cl	-0.15078600	-0.01401100	-0.00026500
H	1.94484000	-0.51441900	0.00217300
O	-0.36714200	-0.77556200	1.21332600
O	-0.72081500	1.30691900	-0.00417900

(PA) ₂	x	y	z
O	1.48408000	0.34314700	-0.00080400
O	-0.36646400	-0.78243600	-1.20962900
Cl	-0.15078600	-0.01401100	-0.00026500
H	1.94484000	-0.51441900	0.00217300

O	-0.36714200	-0.77556200	1.21332600
O	-0.72081500	1.30691900	-0.00417900

(PA) ₃	x	y	z
O	-0.61216400	-2.87669100	-0.38977900
O	-1.17436200	-1.01677900	1.13965200
Cl	-1.71213600	-1.72721600	-0.00274500
H	0.22796800	-2.38767500	-0.57406600
O	-1.80220400	-0.86651000	-1.18865500
O	-2.89417400	-2.50182000	0.24003200
O	-0.46309600	1.56587200	-1.26691800
O	-0.60459600	3.74286800	-0.24816400
Cl	-0.80047100	2.36894800	0.12162500
H	-0.92457200	0.69069100	-1.21984400
O	-2.14945200	1.99623500	0.48406800
O	0.19720500	1.90178900	1.08805900
O	1.82761700	-0.29219100	1.40502100
O	3.40101900	-1.65408400	0.22225200
Cl	2.47559700	-0.59188200	-0.06364400
H	1.17087800	0.44089200	1.28839700
O	1.34121700	-1.01771800	-0.90116500
O	3.05081700	0.64263700	-0.53551100

(PA) ₄	x	y	z
O	-0.55189000	-2.28845900	1.84786700
O	0.92329400	-0.29795900	1.75036700
Cl	0.97131200	-1.74029600	1.64367800
H	-1.08407400	-2.01431500	1.05948800
O	1.67746100	-2.40907500	2.69841900
O	1.35291400	-2.17489700	0.29305800
O	-0.24589200	2.39029800	1.17507800
O	-1.88976100	0.54486400	1.41126900
Cl	-1.80150200	1.94259800	1.03961800
H	0.29237600	1.91699300	0.48913200
O	-2.45809000	2.85551200	1.93008900
O	-2.14387400	2.13965100	-0.37784100
O	2.48081600	-0.45445800	-1.60820200
O	1.38669100	1.64097400	-0.88861200
Cl	2.72104500	1.04187700	-0.99363000
H	2.01484600	-0.99224700	-0.92096800
O	3.35408300	0.85984300	0.29397500
O	3.52839300	1.65678800	-2.00950600

O	-2.92361300	-0.06855000	-1.84346100
O	-0.52901400	-0.44060800	-1.42656900
Cl	-1.75920800	-1.18842400	-1.61334300
H	-2.68265600	0.71608300	-1.28520500
O	-2.14497700	-1.92001000	-0.40500400
O	-1.83841400	-1.98146700	-2.80684000

(PA) ₅	x	y	z
O	1.80267400	2.88206300	-0.79582500
O	0.12232200	1.08266600	-0.91126100
Cl	0.23729300	2.53718200	-1.12189900
H	1.98334600	2.49933400	0.09747500
O	-0.56227100	3.27813700	-0.18074400
O	0.11646900	2.92366600	-2.50076300
O	1.06449600	-0.83952800	-2.67164700
O	3.05869300	0.13739200	-1.58713800
Cl	2.42995300	-1.14468200	-1.82655400
H	0.56665900	-0.16058800	-2.15182400
O	1.98634900	-1.78017800	-0.57765200
O	3.13533900	-2.04330500	-2.69279400
O	-3.11288700	-2.56442100	-0.61648000
O	-0.99757500	-1.34233100	-0.32871700
Cl	-1.51947200	-2.71501700	-0.27239300
H	-3.45403700	-1.85823300	-0.01154300
O	-1.42716700	-3.27834500	1.05483500
O	-1.04957900	-3.55156300	-1.34038700
O	0.96027100	-0.51831900	1.58692000
O	1.72741400	0.38520800	3.69208900
Cl	2.06754300	0.46884500	2.30016100
H	1.38272600	-0.90736600	0.77490100
O	3.35949500	-0.05839600	1.92204600
O	1.80473000	1.79745200	1.74290500
O	-1.63526700	0.72222200	1.60812400
O	-3.00396100	1.17287300	-0.41079200
Cl	-3.14518700	0.81391800	0.98261100
H	-1.13387900	0.07161200	1.06364800
O	-3.71403100	-0.53144600	1.15504200
O	-3.76158600	1.79707500	1.82621700

(PA) ₆	x	y	z
O	1.95432500	2.62153500	1.46165800

O	3.36790200	0.64785100	0.97152300
Cl	2.74039000	1.77060900	0.31117900
H	1.01504500	2.30413300	1.48807500
O	1.68330600	1.34230400	-0.62058200
O	3.65090200	2.73255000	-0.24236900
O	1.10317800	-1.37644500	-0.88809900
O	2.12453500	-3.28554300	-1.94095600
Cl	2.53709500	-2.07570100	-1.28528700
H	1.26061600	-0.40224600	-0.79297000
O	3.23597900	-1.11392200	-2.10604000
O	3.20635700	-2.31818800	-0.00467700
O	2.35382800	-1.87794400	2.58608200
O	0.45634400	-1.45081200	3.97137900
Cl	0.76942200	-1.50198300	2.57328100
H	2.64476400	-1.96995600	1.64344500
O	0.64011100	-0.24737800	1.85963800
O	0.11873500	-2.60082000	1.84889800
O	-0.77033700	3.28512000	-0.76629400
O	-2.81665500	2.23668000	0.15688300
Cl	-1.63123200	2.94285400	0.58621400
H	-0.65763500	2.42373000	-1.24232200
O	-0.75131700	2.08972300	1.39216500
O	-1.85082200	4.24732600	1.14714600
O	-1.65668200	-1.89969600	-0.18966600
O	-3.51467300	-2.78162900	1.20494300
Cl	-2.97100300	-1.53560300	0.72433400
H	-0.94191500	-2.18477500	0.43197600
O	-2.50951300	-0.64248100	1.76255600
O	-3.81079200	-0.89466500	-0.28380700
O	-3.05662300	0.49715600	-2.53769300
O	-1.34967900	1.15625000	-4.07541400
Cl	-1.49322500	0.27844400	-2.94569700
H	-3.22929300	-0.00901100	-1.70196100
O	-0.72795800	0.72093500	-1.76619200
O	-1.30500900	-1.12567200	-3.20754300

(PA) _i (DMA) _i	x	y	z
C	3.12709700	-0.87752900	-0.08043500
H	3.90015700	-0.51621000	0.59934000
H	2.95048600	-1.94014300	0.08380900
H	3.43778500	-0.71211900	-1.11248900

H	1.06996600	-0.48200200	-0.46000100
C	1.97275700	1.33324500	-0.03849200
H	2.27927100	1.52000800	-1.06826300
H	0.98742700	1.76934400	0.13571700
H	2.70869700	1.74177600	0.65526100
N	1.87154800	-0.13637600	0.15895600
H	1.48838700	-0.31569700	1.09444700
O	-2.60108000	-0.70945200	0.00369200
O	-1.40733500	1.37465700	-0.33704100
Cl	-1.30839100	-0.05055000	-0.00006700
O	-0.62063400	-0.19563100	1.31431200
O	-0.40588900	-0.71773400	-1.02169000

(PA) ₁ (DMA) ₂	x	y	z
C	1.76443000	-1.75041800	1.29961000
H	2.21306300	1.85116400	1.71307700
H	0.91601400	-1.43539900	1.91039100
H	1.82970500	-2.84716600	1.32539400
H	0.65607900	-1.51600500	-0.39197500
C	2.60069000	-1.70619200	-0.99260300
H	2.66950100	-2.80277600	-1.02505700
H	2.36947900	-1.34561200	-1.99824500
H	3.58027000	-1.31384700	-0.69880300
N	1.58144700	-1.23661100	-0.05795300
C	1.92454300	2.15344800	-1.01252800
H	2.97599100	2.05895900	-0.73329500
H	1.76342600	1.70022900	-1.99135400
H	1.65016700	3.20931800	-1.05305400
H	0.08856600	1.47335300	-0.32498900
C	1.18957800	1.97594300	1.35307600
H	0.92009600	3.03385100	1.36742200
H	0.49527800	1.41108300	1.97514500
H	2.68808300	-1.34371900	1.72623100
N	1.08821300	1.45303400	-0.02305900
H	1.33875900	0.39306100	-0.02347000
O	-3.30502300	-0.33138800	0.00445300
O	-1.18276200	-0.19640200	1.19051800
Cl	-1.86243000	-0.18114600	-0.13325100
O	-1.28704400	-1.26040500	-0.97393900
O	-1.54496300	1.14133400	-0.78108700

(PA) ₁ (DMA) ₃	x	y	z
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C	-3.55464000	1.16002200	-0.25497800
H	-3.63694100	2.24422900	-0.11695900
H	-3.46348300	0.95154700	-1.32429600
H	-4.48649000	0.70154000	0.10812800
H	-2.22364300	-0.31775400	0.19722300
C	-2.44740500	0.80344800	1.88851000
H	-1.56693600	0.33476100	2.33295700
H	-2.46242400	1.86656900	2.15553100
H	-3.34668900	0.33382300	2.31365800
N	-2.37251000	0.66230500	0.43831000
C	2.44920700	0.79823900	1.88843500
H	0.89519800	3.52980200	-0.72676300
H	1.56765400	0.33140000	2.33267900
H	3.34739900	0.32652900	2.31358200
H	2.22319900	-0.32214900	0.19694300
C	3.55744900	1.15279500	-0.25487500
H	4.48824400	0.69218900	0.10824600
H	3.46593500	0.94471900	-1.32424100
H	3.64212700	2.23679200	-0.11665100
N	2.37415500	0.65755500	0.43819800
C	0.00145200	1.31896700	-2.05920100
H	0.89460700	1.74649000	-2.52093600
H	0.00056300	0.23618400	-2.18490300
H	-0.89106900	1.74789400	-2.52086400
H	-0.87651900	1.19325400	-0.17115300
C	0.00287200	3.06044200	-0.30621500
H	-0.88879800	3.53115400	-0.72664100
H	0.00304500	3.18912600	0.77743600
H	2.46655200	1.86126900	2.15567200
N	0.00174800	1.62176600	-0.61429400
H	0.87936700	1.19189600	-0.17116900
O	-0.00336800	-3.44881900	0.10141800
O	-0.00100900	-1.19596000	1.00882900
Cl	-0.00195500	-2.02629500	-0.23095400
O	1.20729300	-1.66960000	-1.02415000
O	-1.21042100	-1.66708400	-1.02421000

(PA) ₁ (DMA) ₄	x	y	z
C	-3.45107900	-1.45829700	0.62615300
H	-3.49333100	-2.33301000	1.28501200
H	-3.46629200	-0.56083100	1.24936400
H	-4.35942000	-1.46092700	0.00416600

H	-2.24438300	0.94168800	2.27323800
C	-2.19882400	-2.61823300	-1.09825100
H	-3.08172000	-2.64150100	-1.75450300
H	-1.30379700	-2.54042600	-1.71890100
H	-2.16815300	-3.56209000	-0.54126500
N	-2.22589100	-1.49505300	-0.16270000
C	3.46458200	-0.53636000	-0.03869800
H	3.84274900	-1.36987900	0.56476800
H	3.06739300	-0.92886200	-0.97719000
H	4.30893100	0.13144300	-0.26402200
H	1.98108200	0.83390800	0.04988700
C	2.82356400	0.77927600	1.91507800
H	1.96415200	1.26542300	2.38334200
H	3.21304600	0.01904400	2.60224300
H	3.61580600	1.52622600	1.75574300
N	2.38822300	0.14143700	0.67878500
C	0.15868000	3.02382800	1.18666200
H	-0.80933800	-2.06084000	2.90247300
H	0.94667300	2.90881200	0.43905600
H	-0.50140800	3.84187700	0.85375200
H	-0.83122100	1.43909200	0.42877800
C	-1.71868000	1.89907500	2.19840000
H	-2.43538800	2.65567500	1.83624300
H	-2.12739800	-0.63234700	-0.69941100
H	-1.41278700	2.18979000	3.21063600
N	-0.54382400	1.75706300	1.35327600
C	0.77873500	-2.87676900	0.77495700
H	0.04735900	-3.64370300	1.04023400
H	0.94089100	-2.87475600	-0.30303700
H	1.72153900	-3.07522100	1.28973800
H	1.02232400	-0.82411300	0.89083300
C	0.00993900	-1.40154800	2.60564500
H	0.90890300	-1.65729600	3.17135300
H	-0.25154000	-0.35818000	2.78753300
H	0.61462200	3.32554500	2.13747600
N	0.27556500	-1.54839400	1.16511200
H	-0.62529300	-1.38336200	0.63629300
O	-1.15753100	0.89766600	-1.55603500
O	0.50935700	-0.84756400	-1.69309000
Cl	0.15162100	0.51761000	-2.17167600
O	0.04634000	0.53619300	-3.62877900
O	1.18465800	1.47396100	-1.70259900

(PA) ₂ (DMA) ₁	x	y	z
O	-1.51177600	-1.80840900	-0.35554900
O	-1.72902000	0.03071900	1.25890300
Cl	-2.18803900	-0.39329200	-0.05901100
H	-0.52372100	-1.79473900	-0.03470400
O	-1.71163200	0.53496200	-1.09435100
O	-3.59919400	-0.66054000	-0.15657800
C	-0.22052600	3.00038200	0.97595800
H	-0.85628300	3.70412400	0.43734200
H	-0.82692300	2.37263600	1.62793500
H	0.52408200	3.54135700	1.56063900
H	1.05324800	1.42003900	0.50760800
C	1.34413500	2.84294300	-0.96334900
H	2.11413300	3.38223700	-0.41095200
H	1.80232200	2.10067100	-1.61593900
H	0.73887000	3.54149500	-1.54234300
N	0.47518100	2.12851400	0.00201400
H	-0.21970800	1.57042600	-0.51544100
O	0.86269500	-1.94413800	0.50576800
O	3.18760600	-1.65897900	-0.08487200
Cl	1.91962500	-0.97038800	0.05446800
O	1.46170300	-0.35025100	-1.20888000
O	2.01805700	0.11102000	1.08562100

(PA) ₂ (DMA) ₂	x	y	z
C	-0.54929500	-3.21630300	1.04909800
H	-0.03099800	-4.17601300	1.05724200
H	-0.51766400	-2.76376900	2.03980400
H	-1.58640700	-3.34455900	0.73747700
H	-1.58395000	3.34675600	0.73541900
C	0.14585700	-2.79856200	-1.30350900
H	-0.88090400	-2.90597000	-1.65243700
H	0.67518300	-2.06326200	-1.90790500
H	0.66737400	-3.75637400	-1.33166200
N	0.11843100	-2.30596500	0.09295900
H	1.08014000	-2.08326100	0.40774800
O	-2.65425500	1.21896800	-0.86713700
O	-3.74037600	0.00157500	0.92964700
Cl	-2.64732000	0.00120100	-0.03500500
O	-2.65484600	-1.21676300	-0.86683600
O	-1.32014400	0.00096600	0.72255300

C	0.14791700	2.79790100	-1.30518800
H	0.67029500	3.75522300	-1.33407700
H	0.67658000	2.06167200	-1.90903300
H	-0.87875200	2.90596800	-1.65418300
H	-0.37742300	1.39666200	0.13170900
C	-0.54691500	3.21798800	1.04709200
H	-0.37829200	-1.39582000	0.13233400
H	-0.51556200	2.76623900	2.03816500
H	-0.02789700	4.17731500	1.05442300
N	0.12006900	2.30637500	0.09165600
H	1.08159800	2.08313600	0.40660500
O	4.04394600	-0.00158800	-0.61612900
O	2.59769900	-1.21515000	0.90462800
Cl	2.75037300	-0.00079600	0.05167700
O	2.59869500	1.21433400	0.90367800
O	1.63306600	-0.00073100	-0.93943900

(PA) ₂ (DMA) ₃	x	y	z
C	-0.94039800	3.70046000	0.80656300
H	-1.52901600	4.52156300	0.39495300
H	-1.35492100	3.38648400	1.76431700
H	0.10130300	3.99686100	0.93387700
H	-0.40923900	1.78437400	0.28408300
C	-0.48082700	2.83778800	-1.48598100
H	0.55902800	3.15741600	-1.41440500
H	-0.54819600	1.91997600	-2.06915000
H	-1.09503400	3.61858900	-1.93671900
N	-0.98821200	2.55028500	-0.12313000
H	3.35412600	-2.39440000	-1.91427000
O	3.22086700	0.48545700	1.21517200
O	2.30135000	2.68297500	0.69504300
Cl	2.19867400	1.23162100	0.47057600
O	2.28646300	0.93875400	-0.97819500
O	0.84162100	0.77687000	0.95274900
C	0.67488200	-2.68876500	-2.15931600
H	-0.29729200	-4.06525400	1.02667400
H	-0.33088000	-2.27261300	-2.24792700
H	1.16940400	-2.65284600	-3.14054700
H	1.43355200	-0.95847400	-1.37230900
C	2.79183700	-2.40815100	-0.97014800
H	2.79139000	-3.43546200	-0.58876500

H	-1.95101300	2.17519700	-0.19796300
H	3.30248600	-1.76262500	-0.25190400
N	1.41243700	-1.94967800	-1.13560800
C	1.04742800	-2.08614900	2.32678800
H	1.70152000	-1.21593400	2.27490000
H	0.52637000	-2.10823100	3.28598100
H	1.63525800	-2.99862300	2.20762700
H	-0.48084100	-1.13569900	1.30392400
C	-0.86933100	-3.14540300	1.16467700
H	-1.44889100	-3.20209300	2.08748900
H	-1.54695900	-2.99980500	0.32314000
H	0.59340600	-3.73972300	-1.86098600
N	0.06544900	-2.00481800	1.22741300
H	0.59835900	-1.94091500	0.27931000
O	-1.60035700	-0.52963200	-1.05415700
O	-3.34506800	1.04123800	-0.46811400
Cl	-2.72746600	-0.27160100	-0.12257100
O	-3.71742900	-1.34469100	-0.18936500
O	-2.16112700	-0.16097100	1.25612400

(PA) ₂ (DMA) ₄	x	y	z
C	-2.87995500	1.14325000	-2.12707900
H	-3.95814000	1.24931000	-1.99010300
H	-2.36486900	1.99724500	-1.68868500
H	-2.65160000	1.07294200	-3.19246000
H	-1.41651900	-0.19660800	-1.52357200
C	-3.10621500	-1.31367100	-1.91778100
H	-4.18045800	-1.21455500	-1.74846900
H	-2.91243000	-1.44761400	-2.98375400
H	-2.71393800	-2.16808300	-1.36600100
N	-2.43645100	-0.08669300	-1.44030000
H	-2.60486700	0.01958000	-0.36187200
O	1.26767500	-3.15967600	0.02748300
O	-1.15727800	-3.26412100	-0.08479400
Cl	0.02392800	-2.38342400	-0.12475300
O	-0.07156000	-1.38280100	0.97138400
O	0.05102800	-1.65731700	-1.42880400
C	-3.27429100	-1.12755100	1.79941600
H	-4.29348100	-1.29817700	1.43549600
H	-2.63993700	-1.95367500	1.47264600
H	-3.30369500	-1.11397000	2.89829700
H	-1.78754100	0.24378600	1.50520400

C	-3.52213900	1.29889900	1.68919000
H	-3.04815200	2.20171400	1.29966500
H	-4.54643800	1.23828500	1.30515400
H	-3.57286800	1.36785200	2.78517800
N	-2.76705200	0.12764400	1.24437300
C	3.52042600	-1.29751100	-1.69089000
H	2.36670300	-1.99784000	1.68714400
H	3.57017600	-1.36563500	-2.78697500
H	4.54510200	-1.23822900	-1.30765400
H	1.78713500	-0.24043400	-1.50482300
C	3.27533600	1.12929800	-1.79870500
H	3.30428200	1.11661700	-2.89760900
H	2.64201600	1.95585300	-1.47101200
H	4.29485700	1.29851900	-1.43505000
N	2.76696500	-0.12581900	-1.24452000
C	3.10506600	1.31357400	1.91918700
H	4.17952600	1.21540500	1.75071700
H	2.71256600	2.16799800	1.36758600
H	2.91027100	1.44674200	2.98507200
H	1.41661500	0.19511900	1.52334500
C	2.88091700	-1.14377400	2.12646100
H	3.95925200	-1.24885100	1.98990500
H	2.65201300	-1.07448600	3.19179100
H	3.04591000	-2.20017300	-1.30168100
N	2.43669200	0.08634100	1.44044600
H	2.60549000	-0.01896700	0.36200700
O	1.15757600	3.26472300	0.08506800
O	-1.26742400	3.16065900	-0.02712400
Cl	-0.02375500	2.38414800	0.12441700
O	0.07146800	1.38439500	-0.97251700
O	-0.05079400	1.65705200	1.42791800

(PA) ₃ (DMA) ₁	x	y	z
O	-3.13349900	-0.98983800	-1.14068100
O	-4.92276500	0.54851000	-0.72515200
Cl	-3.56352600	0.33200700	-0.30450300
H	-2.15610700	-1.12971400	-0.94481000
O	-3.40250400	0.00880100	1.10261900
O	-2.63639000	1.38531100	-0.72305500
C	0.17738800	2.83172300	-0.22468200
H	0.72095700	3.60258300	0.32244400

H	0.72910100	2.54894900	-1.12048800
H	-0.81945800	3.18232200	-0.48955600
H	-0.40934000	0.87343200	0.11062400
C	-0.70162900	1.86790700	1.90265800
H	-1.70412900	2.21376300	1.65523000
H	-0.75470000	0.92528500	2.44536100
H	-0.17055500	2.61809400	2.48941600
N	0.04413500	1.63511400	0.64052200
H	0.98071500	1.27337600	0.86597300
O	4.79683500	0.98298200	-0.64946600
O	2.91679200	1.03447500	0.88150400
Cl	3.45994300	0.52493600	-0.38210600
O	2.50921700	0.70926900	-1.46942400
O	3.64797200	-1.06337300	-0.19545300
O	1.37476500	-2.31978900	-0.37977300
O	-0.70546800	-2.97935100	0.66286900
Cl	0.15849700	-1.85852200	0.34788400
H	2.73260900	-1.50378500	-0.22859300
O	0.56754200	-1.08607900	1.53206200
O	-0.57647200	-0.90008200	-0.57563000

(PA) ₃ (DMA) ₂	x	y	z
C	-0.74064300	-2.24795500	2.67676900
H	-1.79398600	-2.30058800	2.95294400
H	-0.53513000	-2.93791600	1.85882100
H	-0.10894600	-2.48390000	3.53382900
H	0.54010500	-0.85467800	1.88476500
C	-0.66185200	0.18303300	3.22081300
H	-0.02465900	-0.01192600	4.08458400
H	-0.41774900	1.14579200	2.77496300
H	-1.71320700	0.17934300	3.50632900
N	-0.43815700	-0.87594600	2.20960300
H	-1.03133400	-0.69757500	1.37311100
O	-4.46364100	-0.08138600	-0.16585300
O	-2.87849900	1.12076200	1.22644000
Cl	-3.07832100	0.34171300	-0.00380700
O	-2.18233200	-0.87649300	0.06705000
O	-2.63037400	1.12508400	-1.19326200
C	-1.31052000	-1.50080100	-2.93409700
H	-0.60499600	-2.24307900	-3.30877300
H	-1.95093100	-1.93749000	-2.16896700
H	-1.91626800	-1.10465400	-3.74968800

H	-1.23214300	0.28436000	-1.90704200
C	0.37421200	0.30189100	-3.23937200
H	-0.19323500	0.67476600	-4.09295800
H	0.84130400	1.13429000	-2.71593200
H	1.13679100	-0.40365100	-3.56975800
N	-0.55237700	-0.38801500	-2.31442000
H	-0.02556700	-0.77495400	-1.51602000
O	3.08397000	-2.89377700	-0.33869800
O	0.81414400	-2.04803800	-0.45213700
Cl	2.22812500	-1.75030700	-0.08559100
O	2.26065600	-1.34487000	1.34252300
O	2.67753600	-0.57656300	-0.91763100
O	2.70286700	1.69744900	0.37322400
O	1.16952700	2.91875400	-1.12362700
Cl	1.19588300	2.25818900	0.16736400
H	2.75351200	0.81261300	-0.11988700
O	0.33604400	1.07591100	0.19781100
O	1.01593300	3.13944000	1.29404700

(PA) ₃ (DMA) ₃	x	y	z
C	-1.53266500	2.49664400	1.80774000
H	-0.82526400	3.12944700	2.34517300
H	-1.57635000	2.78107600	0.75782500
H	-2.53019800	2.56900400	2.23978900
H	-1.71345000	0.48097100	1.33711800
C	-1.02146700	0.55082600	3.27177500
H	-2.02410800	0.58169900	3.69920900
H	-0.66509300	-0.47693100	3.22104300
H	-0.33921000	1.15927000	3.86712300
N	-1.07661300	1.08912500	1.89450900
H	-0.14807100	1.00865900	1.45633900
O	1.91147200	-1.82839100	-0.55337000
O	1.45064000	-3.37286400	1.26537800
Cl	1.51751600	-1.96859500	0.87601300
O	2.52285800	-1.24535000	1.71135400
O	0.19075300	-1.31920200	1.04568800
C	-1.38025800	-2.76965400	-1.31505600
H	-0.46110700	-3.35022300	-1.22968400
H	-1.92165400	-2.77504700	-0.37033600
H	-2.00933900	-3.16281500	-2.11450300
H	-1.90786100	-0.80814500	-1.66162700
C	-0.27672200	-1.19509700	-2.89399600
H	-0.88673600	-1.56567600	-3.71885400

H	-0.05879800	-0.13661500	-3.02472800
H	0.65280200	-1.75893700	-2.81932900
N	-1.03135700	-1.36473400	-1.63270100
H	-0.48885700	-0.98178100	-0.84807900
O	-5.17465600	-0.75331800	0.13512300
O	-2.80573800	-0.68575500	0.66018200
Cl	-3.92982600	-0.03696100	-0.11573200
O	-3.55643700	-0.13309200	-1.55895300
O	-4.01224400	1.37228600	0.29551700
C	4.88988400	-0.67205000	-0.76764000
H	5.62033400	-1.01750500	-0.03497700
H	4.29127400	-1.51136000	-1.11941300
H	5.39814500	-0.18670200	-1.60193000
H	3.25886000	0.61218100	-0.79954900
C	4.65168800	1.49412300	0.43830400
H	5.16861200	2.02180000	-0.36419000
H	3.88824200	2.13697700	0.87490400
H	5.36612800	1.17829100	1.19970100
N	3.98052800	0.30009800	-0.12179000
H	3.44417800	-0.18495400	0.62431400
O	0.91040800	3.46613700	-1.03928900
O	1.45165900	1.71684800	0.55374700
Cl	1.00449000	2.02381200	-0.84388700
O	-0.30429800	1.37095400	-1.05814800
O	2.01071900	1.43612600	-1.77919000

(PA) ₃ (DMA) ₄	x	y	z
C	-5.06835400	0.40782000	-1.10531700
H	-5.62248200	1.33943500	-1.22796700
H	-4.42967700	0.22123500	-1.96707900
H	-5.76260000	-0.42329000	-0.97353100
H	-3.61849000	-0.34056200	0.17994400
C	-4.95168200	0.73136100	1.35669700
H	-5.61827400	-0.11487700	1.52846600
H	-4.22769600	0.82075200	2.16514400
H	-5.53207200	1.65110600	1.27211500
N	-4.20854400	0.51207700	0.09524800
H	-3.51083000	1.27293200	-0.02708100
O	-2.34044600	-3.05808700	-1.76862500
O	-0.37060800	-1.85892800	-1.02180300
Cl	-1.84483800	-1.82617600	-1.16463200
O	-2.23636400	-0.64092100	-1.96369300

O	-2.43282500	-1.66485500	0.21545900
C	0.07071400	-2.81206600	2.08651600
H	-0.60422200	-3.02059200	2.91774900
H	-0.30978600	-3.25693800	1.16923900
H	1.07247600	-3.18779800	2.29658900
H	0.81773300	-1.16969400	1.09994700
C	0.67121900	-0.61995400	3.08268400
H	1.63228800	-1.05189200	3.36206200
H	0.80400000	0.42772400	2.82016600
H	-0.05220700	-0.71643300	3.89270100
N	0.16528500	-1.34658600	1.89255500
H	4.84128700	2.70193100	-0.86810200
O	3.67251500	0.25485000	1.47555100
O	4.59848300	-1.31573000	-0.12738100
Cl	3.50791400	-1.06230800	0.81981900
O	3.41024900	-2.12369100	1.83922700
O	2.20956800	-1.03529800	0.05197400
C	2.27000600	3.48989500	-0.65378300
H	0.67909000	2.03926500	-3.44290000
H	1.31723700	3.47880900	-0.12134600
H	2.96249700	4.16088900	-0.12502300
H	2.84877200	1.71501900	0.17456000
C	4.10812300	2.05891000	-1.37527300
H	4.03880100	2.37974300	-2.42113800
H	-0.74456800	-0.96368500	1.60884500
H	4.47310500	1.02964200	-1.34265700
N	2.78449100	2.12632200	-0.75627000
C	1.86759500	-0.38341000	-2.98231300
H	2.52940800	-0.98517900	-2.36013700
H	1.20732600	-1.03254100	-3.55995000
H	2.45166000	0.24924800	-3.65377300
H	0.54823800	-0.12357300	-1.44066400
C	0.11258200	1.35839200	-2.80377600
H	-0.57139000	0.75629300	-3.40298100
H	-0.45483800	1.92198100	-2.06326100
H	2.10644800	3.89625600	-1.65820700
N	1.06062200	0.47783400	-2.09494300
H	1.72656400	1.09824300	-1.50378600
O	-0.02284100	1.26159100	0.42031900
O	-1.87376500	0.93573100	1.92394500
Cl	-1.17079900	1.93404500	1.06825000
O	-0.71906300	3.07423300	1.86087800
O	-2.12879000	2.39198000	0.01175100

(PA) ₄ (DMA) ₁	x	y	z
O	3.43659500	-1.94741500	0.83039300
O	0.81676900	-1.88292900	1.14432400
Cl	0.05569400	-0.85311500	1.92560600
H	2.47298300	-1.91713600	1.10698400
O	-0.62945900	-1.45776200	3.04840500
O	-0.92064600	-0.25470700	0.95996400
O	-3.39407400	0.76625900	1.02493400
O	-3.91660900	-1.30270500	-0.22762700
Cl	-3.80659800	0.13318100	-0.41823100
H	-2.46719000	0.45372700	1.20913900
O	-5.04874100	0.80033700	-0.70397100
O	-2.71896100	0.47859300	-1.33227800
C	-0.95280700	-2.35574100	-1.59029600
H	-0.51194300	-3.09014500	-2.26494800
H	-0.86563100	-2.69163800	-0.55870800
H	-1.99875100	-2.18244400	-1.83970100
H	-0.59274300	-0.39089300	-1.06689900
C	-0.23494700	-0.51602600	-3.10515300
H	-1.27004600	-0.31200200	-3.37713000
H	0.34023700	0.40800500	-3.11440800
H	0.20474700	-1.24434000	-3.78701900
N	-0.21106500	-1.07732200	-1.73182200
H	0.76650000	-1.22841400	-1.44974400
O	4.91148000	-1.22652900	-0.91489500
O	2.61068000	-1.75722500	-1.48505900
Cl	3.52813600	-1.09255900	-0.54895300
O	0.99599900	0.20342400	2.36228100
O	3.09001700	0.25275800	-0.23802900
O	1.40097400	2.52491800	1.00610500
O	0.61454500	4.05866700	-0.65137200
Cl	0.23461000	2.78250600	-0.10402700
H	1.21333500	1.65370200	1.45149300
O	0.34951300	1.68324700	-1.05787200
O	-1.02609500	2.77294300	0.60962700

(PA) ₄ (DMA) ₂	x	y	z
C	0.63921200	-0.26392500	3.15973100

H	0.43890300	-0.69317800	4.14213300
H	1.05536800	-1.01649500	2.49158700
H	1.32228800	0.58170100	3.24528800
H	-0.41202100	0.58206100	1.62789700
C	-1.30254000	1.28039000	3.37116500
H	-0.64225200	2.14573400	3.42026600
H	-2.23273400	1.55390800	2.87571100
H	-1.50542400	0.89323500	4.37045400
N	-0.63347500	0.22455200	2.57440300
H	-1.27975200	-0.56451500	2.41869900
O	0.19229600	3.15393200	-0.77737100
O	0.57763200	0.95175000	0.16739600
Cl	1.00844900	2.39289800	0.15748400
O	2.43626000	2.41262200	-0.30606100
O	0.91529000	2.89967900	1.53200800
O	-4.08633200	-0.23102200	-0.73702700
O	-4.10768600	2.13784600	-1.12035400
Cl	-3.15642500	1.09938500	-0.82466200
H	-3.44118600	-1.00098400	-0.64935000
O	-2.51792600	1.23044300	0.47573900
O	-2.19783700	0.84055200	-1.89062600
C	0.80958600	-2.21262600	-2.39471400
H	1.86711500	-2.14290300	-2.64866100
H	0.66594500	-2.92174500	-1.58138900
H	0.22715800	-2.50813700	-3.26753200
H	-0.65141200	-0.92856000	-1.70192000
C	0.59095900	0.21324100	-2.91758400
H	0.07501800	-0.02734300	-3.84744800
H	0.20306800	1.14300600	-2.50518600
H	1.66538400	0.29114600	-3.08216900
N	0.34831800	-0.87833400	-1.94104500
H	0.80831700	-0.63831100	-1.05280500
O	4.96607800	-1.56068500	0.05475500
O	3.74071400	-0.39430900	-1.70322400
Cl	3.81267900	-0.77179700	-0.29641300
O	2.54986200	-1.33930200	0.16633600
O	4.04068500	0.59056700	0.53758100
O	-0.19309700	-2.11530400	0.67304700
O	-1.73162600	-3.99258700	0.58842800
Cl	-1.60544500	-2.54624600	0.59001400
H	3.37006600	1.28974900	0.21001900
O	-2.36760700	-1.92963300	1.70376600
O	-2.15303200	-1.99185800	-0.71321300

(PA) ₄ (DMA) ₃	x	y	z
C	3.35970900	2.69828100	-0.03086200
H	4.39575100	2.37319400	0.05395800
H	3.03770200	2.62071800	-1.06713100
H	-3.10983400	3.46239000	-1.97766200
H	1.52922100	2.03380500	0.65915900
C	2.87392800	1.78418300	2.22625000
H	2.69450800	2.77314600	2.64840000
H	2.26318600	1.04030700	2.73472500
H	3.92577700	1.51144300	2.31485200
N	2.51982100	1.79175300	0.78791500
H	2.61870900	0.81299100	0.44921300
O	4.96758400	-2.11738400	0.89447000
O	3.95281800	-2.05474900	-1.30851500
Cl	4.23278600	-1.30540000	-0.07150200
O	2.88029100	-0.93538700	0.53481600
O	4.93006500	-0.03728200	-0.35360900
C	0.48533700	-3.05260300	0.07550000
H	1.36968300	-3.69032200	0.08151300
H	0.33269800	-2.62525000	1.06528900
H	-0.39434000	-3.61422200	-0.23788800
H	-0.05444600	-1.26885300	-0.85153500
C	0.92952500	-2.38418400	-2.27642000
H	0.02549000	-2.88554600	-2.62387500
H	1.13827700	-1.50556100	-2.88411300
H	1.78724200	-3.05529500	-2.30237400
N	0.72091800	-1.94359100	-0.87734600
H	1.55735700	-1.42772500	-0.53986900
O	-0.00087700	2.04760200	-3.28416600
O	1.54808800	0.80612500	-1.88095600
Cl	0.22360300	1.44454100	-1.97399200
O	0.13789200	2.50965200	-0.90864500
O	-0.83436100	0.43805700	-1.67870900
C	-3.29607300	2.48457800	-1.53247700
H	3.23675300	3.71882900	0.33435200
H	-2.89761000	1.69804600	-2.17088300
H	-4.36403400	2.33467400	-1.37347800
H	-2.68429500	1.47373100	0.17506200
C	-3.08459700	3.40210900	0.77386200
H	-4.13937900	3.21284900	0.97514500
H	-2.49862900	3.28333700	1.68387900
H	-2.95531000	4.40610000	0.36806900

N	-2.60158000	2.41885500	-0.22348800
H	-1.58096400	2.54451100	-0.37419400
O	-0.51002500	0.22213000	3.62117600
O	-0.38456900	2.10621900	2.09127700
Cl	-0.67477700	0.66679900	2.24461700
O	0.17071400	-0.11089200	1.32259700
O	-2.12838100	0.47283500	1.83044000
O	-3.19468200	-1.81192600	1.37196000
O	-3.97584300	-0.31267400	-0.41334100
Cl	-3.54878000	-1.69349000	-0.20317700
H	-2.70373700	-0.95501300	1.62570300
O	-2.32781200	-2.01021600	-0.92513300
O	-4.59766800	-2.66495000	-0.38158400

(PA) ₄ (DMA) ₄	x	y	z
C	1.24478000	-2.85396300	2.49600400
H	1.97414800	-2.34889200	3.12887100
H	0.23332300	-2.65724100	2.84898700
H	1.43200200	-3.92845800	2.47821300
H	0.64577400	-2.71089000	0.51029200
C	2.69082300	-2.63465400	0.48836700
H	2.77217500	-3.71499100	0.36843600
H	2.72857200	-2.15824800	-0.49045000
H	3.48655900	-2.24792300	1.12350500
N	1.38291200	-2.32565700	1.11777900
H	1.23469600	-1.30288200	1.12493400
O	-0.89689200	-2.77439200	-3.14981100
O	1.51834600	-2.76844200	-2.87067300
Cl	0.21773800	-2.62107000	-2.20598300
O	0.14222900	-1.25236600	-1.58125400
O	0.08719800	-3.61015500	-1.10008300
C	-3.02536700	-2.47315600	-0.65971300
H	-2.78011300	-3.11160700	-1.50743900
H	-2.42925600	-2.75934400	0.20453800
H	-4.08610500	-2.53709700	-0.41641200
H	-2.96158700	-0.46794000	-0.22343800
C	-3.37766700	-0.61950900	-2.26464300
H	-4.45031200	-0.79214700	-2.16593000
H	-3.18628600	0.44199900	-2.41194100
H	-2.97337800	-1.20179100	-3.09263800
N	-2.70774900	-1.06725800	-1.01950500
H	-1.68366300	-0.95601900	-1.12165500
O	-0.87573400	3.80544900	-1.01584000

O	-2.80413300	2.67904700	-1.96467400
Cl	-1.36845000	2.58424600	-1.68529900
O	-0.60389400	2.33405600	-2.93000800
O	-1.11444000	1.41820400	-0.76520200
C	-2.23726900	2.91645400	1.89310300
H	-2.33683300	3.67787800	1.11960600
H	-2.91405300	2.08445700	1.70189100
H	-2.43915400	3.33786000	2.87834400
H	-0.77101700	1.64469500	2.56125900
C	0.17720700	3.45370900	2.11525600
H	-0.00714100	3.90033700	3.09333400
H	1.16820600	3.00242300	2.08880800
H	0.08188600	4.20657900	1.33269600
N	-0.84218700	2.40631600	1.87107600
H	-0.68249400	1.96042500	0.95089500
O	-2.21096500	-2.13587800	2.96523800
O	-3.30001500	-0.32597600	1.76067900
Cl	-2.03851200	-0.79570200	2.39794800
O	-1.62771000	0.16779300	3.44861600
O	-0.98924200	-0.82087500	1.33985900
C	2.28022100	2.53540700	-1.61307800
H	2.37337800	3.05987500	-2.56408100
H	1.54041900	3.04001000	-0.99304800
H	3.23922200	2.48745100	-1.09791000
H	1.64238900	0.68994200	-0.96961600
C	2.77525600	0.35119000	-2.68095500
H	3.70977000	0.28253100	-2.12459200
H	2.35719200	-0.64069400	-2.84804000
H	2.93554600	0.85753200	-3.63377100
N	1.81821000	1.14952500	-1.87776800
H	0.90569900	1.19837400	-2.35122400
O	3.26303800	-0.18057700	2.56904100
O	1.64716200	0.57576900	0.94184000
Cl	3.06067900	0.76900600	1.46529200
O	3.20316500	2.15886500	1.91531100
O	3.98598500	0.48236500	0.34995000

(PA) ₄ (DMA) ₄	x	y	z
C	1.24478000	-2.85396300	2.49600400
H	1.97414800	-2.34889200	3.12887100
H	0.23332300	-2.65724100	2.84898700
H	1.43200200	-3.92845800	2.47821300

H	0.64577400	-2.71089000	0.51029200
C	2.69082300	-2.63465400	0.48836700
H	2.77217500	-3.71499100	0.36843600
H	2.72857200	-2.15824800	-0.49045000
H	3.48655900	-2.24792300	1.12350500
N	1.38291200	-2.32565700	1.11777900
H	1.23469600	-1.30288200	1.12493400
O	-0.89689200	-2.77439200	-3.14981100
O	1.51834600	-2.76844200	-2.87067300
Cl	0.21773800	-2.62107000	-2.20598300
O	0.14222900	-1.25236600	-1.58125400
O	0.08719800	-3.61015500	-1.10008300
C	-3.02536700	-2.47315600	-0.65971300
H	-2.78011300	-3.11160700	-1.50743900
H	-2.42925600	-2.75934400	0.20453800
H	-4.08610500	-2.53709700	-0.41641200
H	-2.96158700	-0.46794000	-0.22343800
C	-3.37766700	-0.61950900	-2.26464300
H	-4.45031200	-0.79214700	-2.16593000
H	-3.18628600	0.44199900	-2.41194100
H	-2.97337800	-1.20179100	-3.09263800
N	-2.70774900	-1.06725800	-1.01950500
H	-1.68366300	-0.95601900	-1.12165500
O	-0.87573400	3.80544900	-1.01584000
O	-2.80413300	2.67904700	-1.96467400
Cl	-1.36845000	2.58424600	-1.68529900
O	-0.60389400	2.33405600	-2.93000800
O	-1.11444000	1.41820400	-0.76520200
C	-2.23726900	2.91645400	1.89310300
H	-2.33683300	3.67787800	1.11960600
H	-2.91405300	2.08445700	1.70189100
H	-2.43915400	3.33786000	2.87834400
H	-0.77101700	1.64469500	2.56125900
C	0.17720700	3.45370900	2.11525600
H	-0.00714100	3.90033700	3.09333400
H	1.16820600	3.00242300	2.08880800
H	0.08188600	4.20657900	1.33269600
N	-0.84218700	2.40631600	1.87107600
H	-0.68249400	1.96042500	0.95089500
O	-2.21096500	-2.13587800	2.96523800
O	-3.30001500	-0.32597600	1.76067900
Cl	-2.03851200	-0.79570200	2.39794800
O	-1.62771000	0.16779300	3.44861600
O	-0.98924200	-0.82087500	1.33985900

C	2.28022100	2.53540700	-1.61307800
H	2.37337800	3.05987500	-2.56408100
H	1.54041900	3.04001000	-0.99304800
H	3.23922200	2.48745100	-1.09791000
H	1.64238900	0.68994200	-0.96961600
C	2.77525600	0.35119000	-2.68095500
H	3.70977000	0.28253100	-2.12459200
H	2.35719200	-0.64069400	-2.84804000
H	2.93554600	0.85753200	-3.63377100
N	1.81821000	1.14952500	-1.87776800
H	0.90569900	1.19837400	-2.35122400
O	3.26303800	-0.18057700	2.56904100
O	1.64716200	0.57576900	0.94184000
Cl	3.06067900	0.76900600	1.46529200
O	3.20316500	2.15886500	1.91531100
O	3.98598500	0.48236500	0.34995000

(PA) ₁ (SA) ₁	x	y	z
O	-1.47196000	1.35544100	-0.43719200
O	-3.37380900	0.26732000	0.53876800
Cl	-2.07934000	-0.08357400	0.02299300
H	-0.51646100	1.18689600	-0.67723500
O	-2.08060900	-0.93442400	-1.14618900
O	-1.15831600	-0.57405000	1.06255200
S	2.05077700	0.00217200	-0.13756600
O	2.20472300	0.95146500	1.14355800
O	1.05034200	0.67265000	-0.94882400
O	3.34049400	-0.33155600	-0.66232100
O	1.43614800	-1.32070500	0.46686000
H	2.98837700	0.69228600	1.65185900
H	0.48832400	-1.18229700	0.69785600

(PA) ₁ (SA) ₃	x	y	z
S	3.54771300	0.52176700	-0.35507400
O	3.28342900	2.07589900	-0.21937500
O	4.88529300	0.36190400	-0.82454400
O	3.10043000	-0.10387500	0.89551800
O	2.54276100	0.07139200	-1.49165700
H	2.39440900	2.23327700	0.15428700
H	1.73394800	-0.33569000	-1.10586700
O	-1.87262200	2.33338400	0.25002000

O	0.52602400	1.85782200	0.50193700
Cl	-0.45985700	2.35449700	-0.50015100
H	-2.18004600	1.35375000	0.30035200
O	-0.55135300	1.45610700	-1.62939400
O	-0.23935000	3.73883000	-0.80714000
S	-3.09151100	-1.11249500	-0.42599000
O	-2.06500100	-1.42369700	-1.58458400
O	-2.45161000	-0.12076300	0.46041700
O	-4.36781500	-0.85364300	-1.00666200
O	-3.18007000	-2.44764600	0.39860800
H	-1.14125100	-1.31817700	-1.26220400
H	-2.34434100	-2.60379800	0.89677200
S	0.36844400	-1.66719800	1.11621900
O	0.20437800	-0.42035900	2.05746600
O	-0.62566900	-2.65345200	1.46039900
O	0.39038900	-1.18609400	-0.27640300
O	1.75559000	-2.25837600	1.49518400
H	0.30364300	0.41659500	1.54949000
H	2.45930000	-1.57360900	1.31103900

(PA) ₁ (SA) ₄	x	y	z
S	4.30541100	-0.89840200	-0.21390300
O	4.72387600	0.36646700	0.37983700
O	5.27200900	-1.90810700	-0.51732700
O	1.67709900	1.21808800	-0.61366600
O	3.48362600	-0.62443700	-1.53560000
H	3.83089800	1.64258200	0.81583000
H	2.79864300	0.06282200	-1.36257300
S	1.74428000	1.97694200	0.63233200
O	3.18951800	-1.42018400	0.79423300
O	3.19354200	2.40462700	0.97362400
O	0.93584100	3.18363000	0.70074900
O	1.38146400	1.01885600	1.82209300
H	2.72136100	-2.20902200	0.44834600
H	0.92736700	0.20277100	1.49827400
O	-1.29351500	-2.79286200	-0.22657500
O	0.11249100	-1.14947000	-1.32421800
Cl	0.00805000	-2.03423200	-0.14480900
H	-2.41641600	-1.98450600	-0.46227400
O	-0.00919800	-1.23868900	1.10003200
O	1.09713000	-3.00864800	-0.13741000
S	-4.17485000	-0.98474800	0.46772100
O	-3.28248500	-0.46854200	1.62759400

O	-3.22441400	-1.32799100	-0.68327300
O	-5.05004100	-2.00052000	0.93493200
O	-4.96273900	0.21422100	-0.10084400
H	-2.56030900	0.15026100	1.30241800
H	-4.37366200	0.91106500	-0.52810900
S	-1.87239700	1.86821100	-0.72006900
O	-1.11271500	1.20242600	-1.91096500
O	-3.27982300	1.98286300	-1.06615100
O	-1.54320400	1.13367200	0.50626200
O	-1.31064200	3.30711600	-0.64909400
H	-0.59891700	0.40538200	-1.61764200
H	-0.42732000	3.32469300	-0.16550800

(PA) ₂ (SA) ₁	x	y	z
O	3.84216500	1.06455500	-0.27766100
O	3.10287800	-1.11302000	-1.18450000
Cl	3.73890000	-0.54348800	-0.01695200
H	2.90372200	1.38617800	-0.34876800
O	5.10794500	-0.91786900	0.19673500
O	2.90476200	-0.68440400	1.18700500
S	-0.00041400	0.96070200	0.00649500
O	-0.22677400	0.00978000	-1.22475400
O	1.21391000	1.69555000	-0.27945400
O	-1.21515900	1.69060000	0.30308200
O	0.22630600	-0.00785000	1.22379800
H	-1.14856400	-0.34100700	-1.23246700
H	1.14802100	-0.35893900	1.22618800
O	-3.84334500	1.05955300	0.29288900
O	-3.10346100	-1.13103800	1.16737200
Cl	-3.73958800	-0.54448300	0.00836600
H	-2.90501200	1.38033600	0.36882300
O	-5.10852700	-0.91601700	-0.21092200
O	-2.90538600	-0.66734100	-1.19750300

(PA) ₂ (SA) ₂	x	y	z
O	-3.88368800	1.48169100	-0.62453600
O	-4.80561300	-0.73073300	-0.74706900
Cl	-3.66937000	-0.06536800	-0.17069400
H	-3.05371800	1.96150000	-0.35078700
O	-2.38471500	-0.44011100	-0.78514900
O	-3.60394000	-0.07932000	1.27316300
S	-0.26313900	2.11097200	0.37558700

O	0.28269900	1.73480400	-1.03904000
O	-1.59624600	2.64008600	0.15075500
O	-0.03781900	1.06226200	1.33812200
O	0.66853400	3.30361100	0.85819700
H	1.20427900	1.36590400	-0.99897200
H	0.45379400	4.11558700	0.37276400
O	3.27038300	0.17742800	1.10274900
O	2.89443200	1.16981100	-1.07203700
Cl	3.72019700	0.24568500	-0.27075100
H	-0.19779800	-0.66714800	1.48819600
O	5.12660600	0.46915000	-0.45894100
O	3.48687900	-1.21462300	-0.92464000
S	0.25100100	-2.41073400	0.33165300
O	-1.07559700	-2.85509000	-0.39535400
O	-0.26828800	-1.64282000	1.60446700
O	0.93717800	-3.60037000	0.72555200
O	0.92829200	-1.42289600	-0.52463200
H	-1.60935000	-2.07269100	-0.65054600
H	2.50643300	-1.41984100	-0.79514400

(PA) ₂ (SA) ₃	x	y	z
O	-3.68652000	-1.25281700	-1.24745400
O	-4.97226700	0.71040400	-0.69376900
Cl	-3.78517300	-0.05171600	-0.41022600
H	-0.90080300	-0.56200600	1.92277100
O	-3.54297700	-0.31167800	0.99522800
O	-2.52618400	0.83451300	-0.93642400
S	-0.55140600	1.50283800	2.31265500
O	0.98675000	1.32440800	1.84651000
O	-0.88785100	0.02694300	2.71506300
O	-0.60601900	2.30031000	3.49477800
O	-1.28050400	1.90994800	1.11671200
H	1.14159100	1.78179600	0.98883300
H	-2.06567800	1.21671800	-0.13031800
O	2.65487900	1.24537500	-2.22465900
O	0.21446800	1.19982900	-1.87087300
Cl	1.35340000	2.11893700	-1.84929600
H	2.73000600	0.53388200	-1.50468100
O	1.58327100	2.64682800	-0.50346600
O	1.31490400	3.12551700	-2.86826900
S	3.23196200	-1.13495600	0.67790300
O	2.40838400	-1.04938100	2.02412000
O	2.40112500	-0.46801200	-0.34518200

O	4.58904800	-0.71209100	0.83696500
O	3.20993300	-2.67345500	0.42415900
H	1.92280700	-0.19463500	2.07187200
H	2.29374900	-2.96808000	0.18670900
S	-0.35433300	-2.22150500	-0.59099100
O	-0.03439900	-1.58706200	-1.99698600
O	0.65281100	-3.20046000	-0.25002100
O	-0.62935400	-1.12813000	0.32961000
O	-1.65045000	-3.04238000	-0.87696100
H	0.10263100	-0.61789300	-1.91709000
H	-2.42027200	-2.43884700	-1.02632600

(PA) ₂ (SA) ₄	x	y	z
O	3.77769400	-0.66768100	-1.29655900
O	5.42693800	-1.46297400	0.31329300
Cl	4.03599200	-1.24185500	0.03363200
H	2.96973600	0.96076100	-1.42337800
O	3.30163200	-0.54649500	1.06807800
O	3.44944800	-2.75625600	-0.03772600
S	0.05003300	-1.92464000	-1.59361300
O	-0.25673100	-1.92154400	-3.15554700
O	0.66983700	-0.52253700	-1.31223800
O	-1.24119000	-2.06574800	-0.96385400
O	1.10640400	-2.88379900	-1.33526100
H	0.56500000	-2.01118700	-3.66310400
H	2.53638900	-2.72089800	-0.43699400
S	-4.43965500	-0.88117700	0.07640400
O	-3.70835500	-1.79089700	1.14831300
O	-5.83791200	-1.16919100	0.09185400
O	-3.97001100	0.48892800	0.30698000
O	-3.86863200	-1.39585500	-1.30178900
H	-2.86327600	-1.37849300	1.42203900
H	-2.89182200	-1.50955700	-1.27731000
O	0.76149100	0.47241000	2.70066700
O	-1.33635900	-0.32432800	1.70896700
Cl	-0.13324300	-0.82709600	2.42397400
H	1.00496600	0.91621000	1.81284600
O	0.62218400	-1.73280800	1.59062900
O	-0.44074700	-1.31163600	3.74034100
S	2.23051800	2.47262400	-0.10260200
O	2.54428500	1.84301100	-1.52010800
O	1.13316500	1.68129500	0.48308200
O	3.42098300	2.67716300	0.66571800

O	1.64524800	3.84504900	-0.55330500
H	-0.03564500	0.18621600	-1.21881600
H	0.68272900	3.77194900	-0.78459900
S	-1.73364500	2.36758800	-0.66810500
O	-1.69306200	2.32937500	0.90431400
O	-0.98584200	3.52882500	-1.09474900
O	-1.36613600	1.05545400	-1.19368800
O	-3.22913800	2.64341800	-1.01360400
H	-1.72698200	1.40553300	1.23473800
H	-3.76650400	1.88174400	-0.66666800

(PA) ₃ (SA) ₁	x	y	z
O	1.70307200	2.78355000	-0.30570100
O	-0.27405300	3.90339200	0.45766400
Cl	0.13286400	2.57212800	0.10939300
H	2.07244600	1.87743000	-0.45626700
O	-0.52075600	2.00041800	-1.04671500
O	0.16317100	1.65345500	1.25281000
O	-2.93920400	0.17323600	-1.57261400
O	-2.72710400	0.67572400	0.83535700
Cl	-3.61157000	0.00633000	-0.09773900
H	-2.01693700	-0.18667300	-1.48501700
O	-4.90655900	0.59925200	-0.26908900
O	-3.66412200	-1.44187200	0.14760100
S	-0.18621200	-1.92091600	0.11575500
O	-0.04105200	-1.06788500	1.42604700
O	-0.58773500	-1.05207900	-0.97943300
O	0.98878100	-2.75084700	-0.04844300
O	-1.33338700	-2.91786500	0.49197200
H	-0.02160800	-0.09855000	1.24087000
H	-2.20423700	-2.45719400	0.47842800
O	3.46891100	-2.04786300	-0.65395100
O	4.83041900	-0.07175800	-0.61406900
Cl	3.60247300	-0.55460300	-0.04260700
H	2.54207700	-2.35987800	-0.43143900
O	2.40322100	0.14251200	-0.54843200
O	3.58943800	-0.67111200	1.39709300

(PA) ₃ (SA) ₂	x	y	z
O	1.14482100	2.40908400	-0.85724700
O	-0.10994800	4.44233600	-0.65240000
Cl	-0.34364700	3.02652700	-0.58118300

H	1.02887100	1.42370600	-0.85965600
O	-1.21390500	2.48151300	-1.59696800
O	-0.69836500	2.58622900	0.77474300
S	0.12565900	-0.57129600	2.39124700
O	0.04984100	-0.72384600	3.96554900
O	1.33438300	0.18101000	2.11408400
O	-0.04532400	-1.89859400	1.82398700
O	-1.12883800	0.30375400	2.11094900
H	-0.55520000	-1.44360200	4.20428300
H	-0.97360400	1.03237500	1.45399100
O	3.75745600	-0.57560800	1.37160800
O	3.38310800	0.58075100	-0.77941900
Cl	3.89937400	-0.66227200	-0.24017200
H	2.81738900	-0.31094700	1.59420600
O	5.30768600	-0.87591900	-0.42069700
O	3.07871900	-1.81447300	-0.64373200
S	-0.09322700	-1.19869000	-1.59439500
O	-1.23396800	-0.98668200	-2.45185400
O	0.29056700	-0.14801800	-0.65181100
O	-0.24223100	-2.52913300	-0.78259300
O	1.10036100	-1.52040600	-2.55899400
H	-2.92136100	-0.71065800	-2.08280300
H	1.91557800	-1.67223300	-2.02919600
O	-2.87604500	-1.51225900	0.31116700
O	-5.13028600	-0.58537800	0.26948800
Cl	-3.75658900	-0.44295100	-0.13855000
H	-0.23803400	-2.33909300	0.19135200
O	-3.19361700	0.87473500	0.08888700
O	-3.85638700	-0.62032100	-1.76488400

(PA) ₃ (SA) ₃	x	y	z
O	-2.69128100	2.06098700	-2.20591100
O	-2.39883100	2.84094800	0.06756000
Cl	-3.32468600	2.24388300	-0.91687700
H	-0.13753800	-1.99100400	-2.35087500
O	-4.59898500	2.90742500	-0.93022600
O	-3.67568500	0.78226100	-0.34225100
S	-2.18017400	-2.15355700	-1.77210200
O	-2.12841300	-3.43305300	-0.85572100
O	-0.95360000	-2.34142800	-2.76067100
O	-3.38877600	-2.20639200	-2.52910200
O	-1.86318000	-0.98237000	-0.94114000

H	-1.31835500	-3.42464500	-0.29966700
H	-2.92122000	0.14690400	-0.56952900
O	3.98177000	1.11759700	-1.46927600
O	5.80467600	1.40043300	0.17584000
Cl	5.02286400	0.37301400	-0.46494300
H	3.39147400	1.70355900	-0.91175900
O	4.17230500	-0.34425400	0.50190900
O	5.73940500	-0.50498400	-1.35177100
S	0.86757900	2.27075100	0.08574600
O	0.54079600	2.08614600	1.60610800
O	2.28563900	2.54008400	-0.01327800
O	0.29612600	1.15854200	-0.66877200
O	0.14291400	3.58691200	-0.33568100
H	-0.26657500	1.53134100	1.74071900
H	-0.83840600	3.44650000	-0.33064900
O	-2.10659000	-1.88158700	2.07425200
O	-1.62729700	0.47220200	1.85692200
Cl	-1.81879700	-0.65452100	2.78094400
H	0.79342000	-0.31097500	-0.89584500
O	-2.68724900	-0.35147000	3.88291300
O	-0.37119300	-0.85615600	3.51014400
S	1.27992000	-2.06638500	0.26402700
O	2.73638000	-2.61292800	0.14486000
O	1.10994800	-1.25024000	-1.08215600
O	0.41226600	-3.21839400	0.23147800
O	1.18548900	-1.11410600	1.36335600
H	3.38762500	-1.87246100	0.23003900
H	0.27602200	-1.05443300	2.77921000

(PA) ₃ (SA) ₄	x	y	z
O	5.13708800	2.05632800	-0.91806300
O	5.80942100	-0.17167800	-1.50629000
Cl	4.86117500	0.46834400	-0.64025000
H	4.40173200	2.53877900	-0.45998300
O	5.04816500	0.25084800	0.77529400
O	3.46332400	0.25649800	-1.05528600
S	1.54281500	2.66323500	0.31957500
O	1.07924700	2.91492100	-1.15993200
O	2.93980400	3.02715800	0.37928100
O	0.60563400	3.24348400	1.25703600
O	1.38140000	1.09250700	0.50018900
H	0.11401700	2.70156200	-1.23009100
H	2.10318300	0.59698400	0.03679100

O	2.95298800	-2.72890600	-0.85747300
O	3.13578600	-3.73789900	1.30929100
Cl	2.21832800	-2.89578400	0.59426500
H	0.12638700	0.27698600	1.66239900
O	2.08735100	-1.54721700	1.13030600
O	0.92162700	-3.49666200	0.31475000
S	-1.46327000	-0.78666700	2.69687900
O	-2.51109800	-0.28189800	1.77299000
O	-0.22660400	0.17119500	2.57209000
O	-1.77466900	-0.93183500	4.07910000
O	-0.98728300	-2.17620200	2.14070800
H	-3.49969400	-1.27295800	0.95878300
H	-0.78841600	-2.12861600	1.17802100
O	-3.75295500	0.01004500	-1.02072600
O	-3.66436800	-2.24991500	-1.90346700
Cl	-4.35636300	-1.31192000	-1.01635800
H	-2.70824600	1.29986900	1.28100400
O	-4.11742000	-1.90399000	0.47599600
O	-5.77991700	-1.33934600	-1.20158500
S	-2.49197500	2.94010500	-0.14533300
O	-1.78716600	4.25283400	0.34915700
O	-2.88392500	2.27613000	1.21572400
O	-3.62904900	3.30865100	-0.92505700
O	-1.44853900	2.08989100	-0.77542000
H	-0.95975600	4.03475900	0.83911300
H	-1.39820500	0.78237200	-1.85043000
S	-0.36213600	-1.08005700	-1.71832400
O	-0.96025800	-2.31712000	-2.46633800
O	-1.00666600	0.12534000	-2.48392200
O	-0.82628400	-1.04058000	-0.33779200
O	1.06242800	-1.10301300	-1.96961200
H	-1.93173800	-2.36844400	-2.30790200
H	2.34743300	-2.15515200	-1.39479400

(PA) ₄ (SA) ₁	x	y	z
O	0.16225000	1.28974300	-1.78160800
O	0.59731100	2.76285900	0.09882900
Cl	0.71229300	2.55618800	-1.34849900
H	0.43653100	-1.71057700	-0.81605900
O	2.32136700	2.48198700	-1.63643200
O	0.31434200	3.69757300	-2.12225100
O	-1.91815700	-0.99262000	-1.82888200
O	-1.76942100	-3.29124100	-2.56781000
Cl	-1.46656700	-2.35642100	-1.52122100

H	-1.99754400	0.36893200	-0.73576400
O	0.16515400	-2.30072800	-1.56432300
O	-1.83263300	-2.76916000	-0.18251500
O	3.14710700	0.67633800	0.25037400
O	2.92450300	-1.58098900	-0.59748000
Cl	3.76909000	-0.65415300	0.12668700
H	2.68444200	1.78819500	-1.03041400
O	5.13920800	-0.61627200	-0.30258400
O	3.87073000	-1.18457300	1.65156400
S	0.25986700	-0.39697000	1.94620800
O	-0.93859600	-1.08753300	2.66259200
O	0.21553600	-0.57548600	0.50414000
O	-0.01593700	1.12177600	2.24367700
O	1.44099900	-0.84660700	2.65672300
H	-1.79966500	-0.85475900	2.23612600
H	2.95727900	-1.08231800	2.05545800
O	-3.63354800	1.97049000	1.56740400
O	-4.59601000	0.69760900	-0.28008000
Cl	-3.54417900	0.82927900	0.69666200
H	0.13919900	1.66312800	1.43445300
O	-2.15807200	1.13572600	-0.12287000
O	-3.28806500	-0.43497800	1.40125000

(PA) ₄ (SA) ₂	x	y	z
O	2.36643600	-0.40096200	2.06516500
O	0.00243200	-0.79904600	2.39109600
Cl	1.23238100	-0.20798400	2.94520400
H	0.46724000	0.50294700	-1.66638200
O	1.45138300	-0.53713800	4.32579900
O	0.94223500	1.38795100	2.99959700
S	1.29647000	2.25035600	-0.76206400
O	0.74994400	3.65220400	-1.18672400
O	0.90801100	1.34087900	-1.97143500
O	2.73627600	2.40290400	-0.70264000
O	0.58274700	1.77723100	0.41686800
H	-0.22903800	3.68452900	-1.06826600
H	0.79998800	1.66972700	2.05257800
O	-2.17073500	1.26094000	-0.79898100
O	-1.99190700	3.63654600	-0.73291400
Cl	-2.68925700	2.58717200	0.00995000
H	-2.35048800	0.46663000	-0.23057400
O	-4.12034400	2.64717400	-0.15095700
O	-2.24516000	2.43741700	1.37773700

O	4.60221300	0.56214600	-0.27862400
O	4.43603100	-0.18106600	-2.63090400
Cl	4.25611500	-0.66050800	-1.27975500
H	3.91135800	1.27115400	-0.43332100
O	5.16640300	-1.69229600	-0.86301500
O	2.84379400	-0.97386500	-0.99248100
S	-0.18855500	-2.28047400	-1.00049600
O	-1.32390500	-3.07407200	-1.42409500
O	-0.30237800	-0.83120100	-1.09698600
O	0.21506600	-2.66607400	0.46141500
O	1.02447200	-2.81008100	-1.83273900
H	-2.93312900	-2.63723300	-1.19998500
H	1.83212200	-2.28536600	-1.62002700
O	-3.74470300	-3.03469100	1.34027600
O	-5.08111900	-1.10061300	0.67857100
Cl	-3.84805900	-1.82880500	0.55654500
H	0.09869400	-1.91926800	1.10323600
O	-2.64758600	-0.98396800	0.71206200
O	-3.84340000	-2.26804400	-1.01223600

(PA) ₄ (SA) ₃	x	y	z
O	-4.07936200	2.72335700	-1.01707300
O	-3.16363300	3.48408400	-3.09127400
Cl	-2.77746400	3.38286500	-1.71185700
H	-3.81701900	2.47023900	-0.07966700
O	-2.51016700	4.63754300	-1.04354400
O	-1.69297300	2.40645100	-1.47504400
S	-2.40110600	0.84578700	1.58221200
O	-2.41358600	0.52785000	3.11848500
O	-3.24533700	2.00762300	1.37789300
O	-1.02218900	0.87956100	1.12771600
O	-3.18257700	-0.33844700	0.91983500
H	-1.52002100	0.22162000	3.40598500
H	-2.70032200	-1.20158300	0.93411400
O	1.69688700	0.84269300	2.47468800
O	2.36314700	-1.07471900	3.81506800
Cl	1.24067300	-0.61868700	3.04248200
H	1.51550800	0.83912800	1.49790700
O	0.07550800	-0.33863300	3.88626800
O	0.91808600	-1.41374500	1.87354100
S	0.26104600	-1.73828500	-1.80721700
O	-0.48207500	-2.90016200	-2.23981700
O	1.46507500	-2.24356400	-0.94138700

O	0.74884800	-0.81118500	-2.81908700
O	-0.69165100	-1.00870700	-0.79806300
H	-1.23366200	-3.98557800	-1.20063300
H	-0.28268200	-0.24041700	-0.33870400
O	3.72939700	-0.75645400	-1.37981200
O	4.14874100	-0.29465600	0.95598200
Cl	4.74062500	-0.43262400	-0.35734500
H	2.25255300	-1.65284000	-1.01228600
O	5.91499000	-1.25513200	-0.42603000
O	5.29879000	1.03037400	-0.78722100
S	1.73510300	2.03036800	-1.05789100
O	0.78962200	3.22620700	-0.74554200
O	1.37208800	0.85474100	-0.25550200
O	1.43981800	1.70571100	-2.55283800
O	3.07900600	2.54155700	-0.89632500
H	-0.15838200	2.99093800	-0.91801200
H	4.50643400	1.63657700	-0.83021800
O	-3.71773800	-3.32200600	-0.71743300
O	-1.63749200	-4.64973200	-0.57184200
Cl	-2.81714200	-3.90112800	0.25641900
H	1.18198600	0.74669600	-2.68358500
O	-2.13509000	-2.86824300	1.05318700
O	-3.35878500	-4.96617800	1.05392300

(PA) ₄ (SA) ₄	x	y	z
O	3.45943000	-2.38205600	-1.28444800
O	5.55143400	-3.54964100	-1.16938300
Cl	4.86903600	-2.50009900	-0.46748700
H	2.90920600	-1.72336600	-0.78303300
O	5.49109200	-1.19621000	-0.51807900
O	4.48660800	-2.88047100	0.90364100
S	1.95778900	-0.72826900	1.80547400
O	1.07642900	-2.00757200	2.04883700
O	2.25506700	-0.60121100	0.38130300
O	1.37260000	0.42049700	2.46238500
O	3.24855600	-1.12115000	2.58529700
H	0.13483200	-1.82678300	1.80622800
H	3.80381600	-1.74005100	2.05018300
O	-0.51619500	-3.47759900	0.22611400
O	-1.30223900	-2.96168900	-2.00421200
Cl	-1.65569900	-3.48296600	-0.67515700
H	-0.16976000	0.54093100	3.20045200
O	-2.38922600	-4.71394800	-0.75257200

O	-2.72561500	-2.43092000	-0.06634700
S	-2.04758500	-0.49761500	3.02448800
O	-3.30600500	0.37795800	2.74029400
O	-1.04846100	0.53447900	3.65974700
O	-2.42398900	-1.52359400	3.94550800
O	-1.44138300	-0.92294400	1.73284400
H	-3.11187000	1.22436800	2.26019000
H	-2.23644800	-1.79501800	0.53773300
O	2.57393300	2.24675400	-0.07110600
O	3.31283400	3.93072600	-1.72405200
Cl	2.49830300	3.80546100	-0.54023200
H	2.20223200	1.69425000	-0.81019400
O	1.07753500	4.05971600	-0.83094700
O	2.97372800	4.49992100	0.62743600
S	0.28502800	-0.01209000	-2.04801400
O	-0.67877000	0.27796200	-3.24531500
O	1.37340000	0.93188100	-2.11402100
O	-0.51496200	-0.12048800	-0.82725900
O	0.90660400	-1.41734100	-2.36384100
H	-1.61905900	0.09492600	-2.99466200
H	0.21911500	-2.11933600	-2.25868700
O	-3.60413700	0.24463100	-0.27006800
O	-3.24772700	-0.27622800	-2.61086100
Cl	-4.14185500	0.32761800	-1.61452400
H	-0.58767700	1.06894900	0.25097600
O	-5.50031000	-0.10553700	-1.76890900
O	-4.20338900	1.90920700	-1.97530800
S	-1.71061600	2.87465900	0.54186600
O	-1.01607200	4.22221500	0.90732800
O	-0.58382100	1.84391600	0.88314000
O	-2.82435400	2.71935200	1.45441100
O	-1.98159300	2.81271200	-0.89450700
H	-0.20502000	4.33966100	0.35496500
H	-3.38032500	2.32293900	-1.57310800

(PA) ₁ (AM) ₁	x	y	z
I	1.51854900	-2.35425000	0.08061000
O	0.27514400	-2.06442000	-2.28338500
O	3.09798100	-2.48130600	-0.99074600
H	3.19925600	-1.63577100	-1.45422600
O	2.40932700	-2.51576900	1.74299400

O	1.91933500	-0.35757900	-2.55902300
Cl	0.71909300	-0.96155400	-3.21166700
H	2.58795600	-1.61770800	2.10688000
O	-0.33903600	0.03198600	-3.21662400
I	-0.89820500	0.55327600	2.43645500
O	3.06935600	0.84927500	0.76974100
O	0.01503900	-0.27744000	3.87609700
H	0.97584600	-0.21977700	3.67613900
O	-0.87880900	2.29103400	3.20542700
O	2.57038200	-0.07065900	2.89509900
Cl	3.00016200	1.19320700	2.21434800
H	-0.05193000	2.71289500	2.92174000
O	1.92596000	2.16528600	2.40366600
I	-2.97824000	-0.78288300	-1.16467100
O	-1.46086600	2.53405500	-1.65490100
O	-3.23412200	0.49298000	-2.55178600
H	-2.44402800	1.06300800	-2.59012100
O	-2.50652100	-2.26347600	-2.24086000
O	-0.64334700	3.43935500	0.39225100
Cl	-1.85165500	2.96142000	-0.28992000
H	-1.52509700	-2.29018100	-2.30120600
O	-2.28846500	1.72120900	0.42399000
I	1.90251400	2.01014200	-1.28930000
O	-0.73269000	-1.86435300	1.40400100
O	1.07904500	2.75365800	-2.82965000
H	0.11683000	2.72251700	-2.66191100
O	2.04452200	3.65438900	-0.35002900
O	-1.36181800	-4.02523200	0.65820900
Cl	-1.81606700	-2.94536300	1.49857000
H	1.19035800	3.78055800	0.10392100
O	-3.01203700	-2.30566700	0.89784900

(PA) ₁ (AM) ₂	x	y	z
O	-0.26683700	-0.24318100	1.24193000
O	-0.40068100	1.46744700	-0.45864100
Cl	-0.93557300	0.15393500	-0.02865200
H	1.57102100	-1.78424700	0.90562800
O	-0.55253100	-0.87542900	-1.06520400
O	-2.38303800	0.19355000	0.11645800
N	1.86721000	-1.52377100	-0.03421500
H	2.50864800	-2.20771800	-0.42384900
H	2.28584100	-0.52632800	0.00747700
H	0.98148300	-1.43710600	-0.59532100

N	2.54011300	1.13320200	0.06748400
H	1.59990900	1.47500200	-0.15884200
H	3.19411400	1.56957700	-0.57476900
H	2.75560000	1.47248200	1.00044800

(PA) ₁ (AM) ₃	x	y	z
O	0.14934700	-0.37714300	-1.02128800
O	1.51659800	1.27647700	0.07857300
Cl	1.19593600	-0.16764400	0.02365300
H	-2.36449300	-0.48067300	0.50293700
O	0.60305500	-0.57872600	1.34130500
O	2.38181900	-0.96791100	-0.25694600
N	-2.01207500	0.32442500	1.08715300
H	-2.62936400	0.52371500	1.86786800
H	-1.86482800	1.18215100	0.47591100
H	-1.06842900	0.03385600	1.41661900
N	-1.22281400	2.43308300	-0.58364400
H	-0.22276600	2.33443300	-0.39212800
H	-1.46545700	3.41593800	-0.51546000
H	-1.34700000	2.14917300	-1.55111100
N	-2.36381900	-1.92041600	-0.57711300
H	-2.35714100	-2.83025200	-0.12692700
H	-1.41739600	-1.73824000	-0.91847900
H	-2.97920900	-1.98371700	-1.38140200

(PA) ₁ (AM) ₄	x	y	z
O	0.70680000	0.98914500	0.99234500
O	0.77017900	-1.35489700	0.40473400
Cl	1.22675200	0.00939900	-0.00255200
H	-2.10188600	1.00293900	-0.31714700
O	0.63435600	0.32216300	-1.32968300
O	2.68550900	0.05951100	-0.05977500
N	-2.47746600	0.05000600	-0.05521400
H	-3.49311200	0.06645500	-0.07424600
H	-2.14459800	-0.20220200	0.91661400
H	-2.12115900	-0.67949800	-0.73278600
N	-1.29736900	-1.90660500	-1.73727100
H	-0.84072200	-1.40230400	-2.49208900
H	-1.68387300	-2.76532100	-2.11399800
H	-0.54750400	-2.14002800	-1.08510000
N	-1.25772800	2.53521600	-0.67713500
H	-0.75685600	2.36276700	-1.54478800

H	-0.54490700	2.47884400	0.05046600
H	-1.63067800	3.47795400	-0.70148000
N	-1.33710700	-0.66007500	2.44292400
H	-0.58546600	-1.22553300	2.04628400
H	-1.74018600	-1.15516800	3.23101500
H	-0.87654800	0.17634500	2.79115300

(PA) ₂ (AM) ₁	x	y	z
O	2.09088500	0.66272300	1.18188900
O	1.24524900	-1.44817600	0.24269400
Cl	2.21767800	-0.19876200	0.00783300
H	0.14867900	2.08500300	0.91262600
O	1.72746400	0.49742500	-1.19084200
O	3.51263700	-0.79771700	-0.16248600
N	-0.12998300	2.39242000	-0.02217200
H	-0.08623700	3.40515500	-0.10167400
H	-1.10374000	2.01866700	-0.20352600
H	0.51975900	1.93993000	-0.68058700
O	-0.89929100	-0.22034200	0.80587700
O	-1.91702700	-1.06965300	-1.22453800
Cl	-2.18486800	-0.29040800	-0.02175500
H	0.30582700	-1.06201900	0.42953400
O	-3.25395100	-0.83490900	0.79171000
O	-2.48007100	1.13989300	-0.37730300

(PA) ₂ (AM) ₂	x	y	z
O	2.34604400	-1.21326900	-0.86620800
O	2.34601400	1.21337800	-0.86635500
Cl	2.60052200	0.00010700	-0.03521200
H	0.86051900	-2.03386300	-0.35798500
O	1.60528600	0.00009600	1.08294100
O	3.96149600	0.00015700	0.47137200
N	0.00057100	-2.24802500	0.18745400
H	-0.86004700	-2.03294300	-0.35672200
H	0.00162500	-1.59367400	0.97790600
H	0.00031200	-3.21052700	0.51367500
O	-2.34449900	1.21303200	-0.86705600
O	-2.34482700	-1.21363700	-0.86611900
Cl	-2.59959700	0.00006200	-0.03558800
H	-0.85988700	2.03308400	-0.35774200
O	-1.60491300	0.00047800	1.08296500
O	-3.96084900	0.00051000	0.47021800

N	0.00038700	2.24826300	0.18690600
H	0.86066600	2.03439200	-0.35813000
H	0.00114300	1.59376200	0.97725100
H	-0.00030700	3.21070200	0.51331200

(PA) ₂ (AM) ₃	x	y	z
O	-2.62400100	0.70499200	1.27503400
O	-3.95885100	0.10809700	-0.65646500
Cl	-2.71661100	-0.14292100	0.05672500
H	-0.95312800	1.47737400	1.43987800
O	-1.52956700	0.14906100	-0.80204000
O	-2.62562100	-1.58175600	0.46297800
N	0.03921800	1.73462600	1.31333200
H	0.32903300	2.43576000	1.98875300
H	0.17960300	2.08929000	0.30095100
H	0.61919000	0.88841200	1.42364100
N	0.36600900	2.36827500	-1.33820800
H	1.01664800	1.63761900	-1.62503200
H	0.71351500	3.25285000	-1.69279900
H	-0.52786600	2.16543500	-1.77755600
O	2.00026400	-0.36137700	-1.27407900
O	2.95587900	1.20032800	0.31446700
Cl	2.66241900	-0.21366700	0.05049600
H	-0.01021200	-1.67164000	-1.19944600
O	1.64300400	-0.66715500	1.09326900
O	3.84295700	-1.06033200	0.14009600
N	-0.07905200	-2.25396200	-0.36157500
H	0.19987800	-3.21021200	-0.56291400
H	-1.06078300	-2.18981000	-0.01361900
H	0.57022600	-1.81251200	0.32625200

(PA) ₂ (AM) ₄	x	y	z
O	2.70819600	1.06414300	-1.14557600
O	1.41623200	0.01386800	0.59854000
Cl	2.69203100	-0.06799000	-0.17478500
H	-0.55559700	-1.42214700	-1.15483800
O	2.69002900	-1.35019500	-0.93094600
O	3.84340400	0.00315400	0.71634500
N	-0.01129900	-2.24570800	-0.84657900
H	-0.33471700	-3.07468600	-1.33589400
H	-0.16042200	-2.33350300	0.21593600
H	0.99178500	-2.06697000	-1.01715200

N	-0.34421600	-2.09962600	1.87639000
H	0.52049500	-1.65044300	2.16661600
H	-0.56757600	-2.83981000	2.53252000
H	-1.07984300	-1.39437400	1.91947100
N	-0.03333700	2.42164300	1.77687900
H	-0.02478100	3.18838900	2.44011700
H	0.72834800	1.78416300	1.99898300
H	-0.90092000	1.89847400	1.88546900
O	-3.76207200	0.87029100	-0.60482400
O	-3.08033700	-1.44815600	-0.26849200
Cl	-2.67568000	-0.03635100	-0.25204300
H	-0.02233700	3.13136300	-1.52975200
O	-1.55739500	0.11876900	-1.27215000
O	-2.11697700	0.30903600	1.08109800
N	0.17211400	2.31409900	-0.95914500
H	0.10163800	2.53096100	0.08913200
H	1.12296200	1.94857000	-1.14522800
H	-0.51428900	1.56202300	-1.15662200

(PA) ₃ (AM) ₁	x	y	z
O	0.59947200	0.53050300	-0.89774000
O	-1.32717300	1.99078900	-0.87170900
Cl	-0.02956500	1.71310000	-0.20051500
H	-0.23571800	-2.04557800	1.93037900
O	-0.29710700	1.29527800	1.19984000
O	0.84380700	2.86584800	-0.27346600
N	-0.01223900	-1.48646300	1.11035200
H	-0.05234900	-0.47287100	1.34094600
H	-0.71447300	-1.64555200	0.37503800
H	0.92695400	-1.71173100	0.74902200
O	-3.57044300	0.72854900	-0.44640600
O	-2.94057200	-0.63065700	1.51986000
Cl	-3.37829900	-0.75864300	0.13717400
H	-2.65999800	1.16519000	-0.54320400
O	-4.68065300	-1.34292900	-0.02896400
O	-2.32982800	-1.38385600	-0.68099100
O	3.18018800	0.23037100	-1.16308600
O	3.07646200	0.07030600	1.29637500
Cl	3.47193600	-0.69640900	0.12833600
H	2.19928200	0.47152500	-1.12098300
O	2.62091000	-1.88756400	-0.03118400
O	4.87548400	-0.98064500	0.01621400

(PA) ₃ (AM) ₂	x	y	z
O	-0.98379700	1.44608200	-1.18973700
O	-3.09193100	1.22847600	0.06099900
Cl	-1.72932000	2.08549800	-0.11748900
H	-0.18965100	-1.03044400	-1.99264500
O	-1.03142400	2.00349000	1.16481400
O	-2.21225200	3.40269000	-0.42917700
N	0.76397000	-0.66192800	-2.15378100
H	0.86747000	-0.32140300	-3.10641400
H	1.47089700	-1.37488100	-1.95234400
H	0.96602000	0.10609800	-1.47802600
O	-2.14291100	-1.04134700	0.92566000
O	-2.28512700	-3.37826700	0.29256200
Cl	-1.60895800	-2.12651600	0.02540200
H	-2.80672900	0.29497100	0.32287300
O	-1.78088200	-1.69684700	-1.38461400
O	-0.14460300	-2.22140200	0.30652400
O	3.28415700	-0.10834100	1.47506200
O	3.27720300	-0.91851000	-0.81671400
Cl	3.20476400	0.28780900	0.03856600
H	1.64884600	-0.15927100	2.10468300
O	1.84141700	0.90738600	-0.16125100
O	4.25060800	1.23981400	-0.29200400
N	0.61310000	-0.24563200	2.18783100
H	0.17598100	0.59887900	1.79924900
H	0.31703600	-0.38231300	3.15076800
H	0.31312200	-1.04833500	1.60561700

(PA) ₃ (AM) ₃	x	y	z
O	-2.15254300	-1.29349800	-1.20474600
O	-0.44140000	-2.40231600	0.08017600
Cl	-1.90580200	-2.20983500	-0.02051700
H	-3.28052600	0.06313200	-0.72976500
O	-2.39219200	-1.51436800	1.20049900
O	-2.60375700	-3.46620400	-0.22499200
N	-3.72223000	0.68807600	-0.02937300
H	-4.73232500	0.71442900	-0.13932500
H	-3.29416200	1.63862900	-0.09426900
H	-3.45876900	0.25943600	0.86421600
O	3.06510900	0.88413000	-0.83722800
O	3.28596500	0.06602800	1.44294300
Cl	3.39325300	-0.28739700	-0.00723200

H	1.17032200	-0.70336100	-1.34142200
O	2.32922000	-1.33376300	-0.26533100
O	4.71156100	-0.82252300	-0.30214100
N	0.47434100	-0.22803500	-1.96491000
H	0.45317100	0.77905800	-1.73955200
H	-0.46129200	-0.62901700	-1.80077700
H	0.75504900	-0.35335000	-2.93416600
O	-0.13063100	3.38134600	0.95720300
O	-0.18027600	2.50918500	-1.31192200
Cl	-0.84565500	2.54905700	0.00643600
H	1.68716000	-0.32961500	1.96197800
O	-0.94321800	1.13128900	0.51331500
O	-2.25216800	3.02365700	-0.16562100
N	0.67137100	-0.56925900	2.03287200
H	0.48267200	-1.38456700	1.43057600
H	0.11381900	0.21429300	1.65260000
H	0.39597600	-0.76797400	2.99060100

(PA) ₃ (AM) ₄	x	y	z
O	-1.33517600	1.12811400	0.54910400
O	-0.58356200	3.45887200	0.81508400
Cl	-0.97040700	2.41356400	-0.15427900
H	-0.04610900	0.03333500	1.73892300
O	0.16525700	2.13214100	-1.09787400
O	-2.18065900	2.84990400	-0.94588100
N	0.93058600	-0.04706100	2.03813800
H	0.97929500	-0.25677800	3.03223500
H	1.46283400	0.89786700	1.78143900
H	1.36844600	-0.81234800	1.49421600
N	2.20618100	2.16974700	1.19888500
H	3.12976600	2.28615000	1.60646600
H	1.68936100	3.04449100	1.24639100
H	2.34975100	1.94613800	0.21379800
O	2.94189200	0.31090700	-1.18492900
O	3.90754500	-0.21616000	1.00899300
Cl	3.41762000	-0.78744800	-0.27315100
H	0.32913600	0.34642000	-1.48812700
O	2.17181100	-1.64751400	0.05737600
O	4.42425800	-1.63048300	-0.93642400
N	0.29786500	-0.66326700	-1.71568300
H	0.66756100	-0.79557600	-2.65506500
H	-0.67481800	-1.01013300	-1.62498300
H	0.92314200	-1.16402800	-1.04040300

O	-2.37677700	-1.43382000	-1.13592900
O	-0.84638100	-1.94431000	0.70272300
Cl	-2.26356600	-2.09449300	0.26790400
H	-3.44005600	-0.05928400	-1.01231800
O	-3.17550700	-1.34281100	1.18823200
O	-2.65858700	-3.50479600	0.15880500
N	-3.91930300	0.73255000	-0.52162300
H	-4.90922200	0.77981600	-0.75272900
H	-3.41302600	1.62202600	-0.72489500
H	-3.77828300	0.48017900	0.46472900

(PA) ₄ (AM) ₁	x	y	z
O	-1.13058500	-1.05925600	0.99573700
O	1.03282100	-0.96029100	2.03366900
Cl	-0.27703100	-0.26755000	1.93967500
H	-0.25811200	0.52980800	-2.50213900
O	-0.05922300	1.06755500	1.29566200
O	-0.90890500	-0.12352900	3.23354200
N	-0.09093100	0.28892500	-1.52721000
H	0.90399800	0.41975600	-1.29290900
H	-0.35618700	-0.69295500	-1.36577700
H	-0.66300100	0.89015500	-0.92146600
O	1.46881600	-3.23520000	0.68101100
O	2.24573400	-1.66549300	-1.05602500
Cl	1.45996500	-2.88308500	-0.90305500
H	1.25234800	-2.39477800	1.18160700
O	2.03176600	-4.06267100	-1.49013600
O	0.06295800	-2.65482400	-1.27318000
O	-3.71778900	-0.65492000	0.54417800
O	-2.73854800	1.30289600	-0.59431900
Cl	-3.55029200	0.11967200	-0.87386100
H	-2.78771400	-0.84303600	0.86382400
O	-2.84924800	-0.79931300	-1.76326000
O	-4.90881900	0.40082100	-1.24556700
O	2.09033700	2.62426000	1.33222000
O	3.39263800	3.58035300	-0.43411100
Cl	2.27889400	2.68731100	-0.28010100
H	1.31035400	2.01875100	1.49438200
O	2.54771700	1.31198800	-0.70833000
O	1.01686800	3.16618700	-0.82604900

(PA) ₄ (AM) ₂	x	y	z
O	2.77147900	0.23356800	-2.44779700
O	3.03809900	-1.88505800	-1.21911000
Cl	2.00555400	-0.93985900	-2.02383100
H	0.35076800	-1.15945600	1.62207200
O	0.96599200	-0.56326200	-1.07203500
O	1.56221400	-1.77599800	-3.10303800
N	-0.56723200	-0.77545800	1.34314400
H	-0.85496600	-1.15444200	0.43697500
H	-0.49025800	0.25419900	1.24687400
H	-1.29740900	-0.98979300	2.02240500
O	3.67313500	-0.19034200	0.64747300
O	2.12411100	-1.48533700	1.99149100
Cl	2.90927800	-0.22650800	1.94918500
H	3.34541000	-1.33614400	-0.42346000
O	3.82450400	-0.12370600	3.06563500
O	1.95265500	0.91966600	1.92184300
O	-4.27756700	-0.15169300	-0.65196300
O	-2.80115200	-2.08676600	-0.25739100
Cl	-3.92003900	-1.37095700	0.34996100
H	-3.42033900	0.36160400	-0.79011600
O	-3.52668300	-0.76140300	1.61873100
O	-5.14886600	-2.11411600	0.40503100
O	-1.87622700	0.85305900	-0.91655700
O	-0.62952300	2.00468400	0.79439200
Cl	-1.41330000	2.20761900	-0.46031300
H	1.18383900	2.58016600	-0.89680700
O	-0.48698300	2.75467600	-1.48277800
O	-2.55045600	3.08397000	-0.24761500
N	2.11955600	2.36227300	-0.49920600
H	2.65845700	3.21504800	-0.36903800
H	2.61039000	1.72350300	-1.13516700
H	1.99393500	1.88553100	0.41580400

(PA) ₄ (AM) ₃	x	y	z
O	-1.13821600	3.52846100	-0.38980800
O	-0.95303900	1.33218000	-1.28690100
Cl	-2.01396500	2.43314800	-0.77674300
H	1.74660600	-3.44795200	0.30082500
O	-2.71329900	1.84589300	0.36499100
O	-2.89430800	2.74558900	-1.87543400
N	1.70548200	-2.43208400	0.30624400
H	2.62554100	-2.02051500	0.03989800

H	1.44161900	-2.09386600	1.24456700
H	0.99952800	-2.11611100	-0.37851100
O	-2.34788900	-0.81882500	-1.25739100
O	-2.44146400	-3.02159500	-2.25683000
Cl	-1.71190500	-2.19297600	-1.31870300
H	-1.43367800	0.42859800	-1.34263700
O	-0.29833300	-2.02836500	-1.70449400
O	-1.78302400	-2.75737500	0.06308700
O	-1.06277300	-0.26588800	3.53496400
O	1.02011800	-1.32142700	2.88948400
Cl	0.14851300	-0.14448300	2.68621200
H	-2.47263400	-0.61058900	2.46346600
O	-0.26457400	-0.09018800	1.25876800
O	0.87510300	1.09602100	3.02749300
N	-3.05340100	-0.80663100	1.62715700
H	-2.99320200	0.00331000	0.99889300
H	-4.02161600	-0.99091000	1.87640600
H	-2.64116000	-1.61496000	1.11872500
O	3.98391200	1.34061400	-0.37594900
O	4.01981600	-1.08554300	-0.45391500
Cl	3.54443500	0.15203200	-1.14185500
H	2.42540300	2.61799300	0.34737000
O	2.03870700	0.10952000	-1.11241600
O	4.02580600	0.19575500	-2.51282900
N	1.46325700	2.29514700	0.47575600
H	0.77151500	2.99373300	0.19862400
H	1.30820900	2.00696100	1.45429700
H	1.37882000	1.45199700	-0.12959700

(PA) ₄ (AM) ₄	x	y	z
O	-1.62739300	2.33048000	-0.92471300
O	-2.94231500	0.44656100	-1.65245100
Cl	-2.98811600	1.67424000	-0.83180400
H	-0.79638100	2.70544600	0.62473800
O	-3.19677400	1.29319300	0.59484700
O	-4.00977500	2.60285100	-1.28014100
N	0.00232300	2.90310000	1.25525700
H	-0.05135000	3.85694100	1.60279000
H	0.85170400	2.77948100	0.67543800
H	0.00643900	2.22873900	2.04235900
O	1.24841400	-2.32511900	-1.50033500
O	-0.02454100	-3.28053600	0.32806200
Cl	-0.00381400	-3.05096300	-1.12546900

H	-0.50478800	-0.51308400	-2.00890800
O	-1.14948500	-2.12217000	-1.47537300
O	-0.13006400	-4.28383000	-1.88275500
N	-0.03346200	0.36166100	-2.30215400
H	0.97752700	0.30548700	-2.08811200
H	-0.46063300	1.15749600	-1.80170000
H	-0.16844600	0.49034700	-3.30195800
O	-1.20246800	-1.13208200	3.03221700
O	1.21309300	-1.13523500	3.02313400
Cl	0.00470300	-0.38118600	2.62876800
H	-2.19710900	-1.65265700	1.58108300
O	-0.00027100	-0.17666100	1.15544200
O	0.00894800	0.94480500	3.29330700
N	-2.77387500	-1.52392800	0.73436600
H	-2.20137600	-1.74562500	-0.10358000
H	-3.05078100	-0.52726700	0.69493900
H	-3.59574200	-2.12128200	0.75895600
O	3.23000100	1.26278700	0.59240600
O	4.14204800	2.41008000	-1.34403100
Cl	3.00020000	1.68327300	-0.81993800
H	3.05307800	-0.54817100	0.66669500
O	2.73193800	0.45243300	-1.62327400
O	1.76851100	2.52891700	-0.86111400
N	2.78291600	-1.54588000	0.72897600
H	2.19187200	-1.65388200	1.56925500
H	3.60930200	-2.13429600	0.79158400
H	2.23257200	-1.80182800	-0.11285500

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