

Supporting Information

Perchloric acid (HClO₄) Drives Atmospheric New Particle Formation Enhanced by Dimethylamine, ammonia and Sulfuric Acid: Mechanisms and Implications

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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 [SA] (10^6 – 10^8 cm^{-3}), and $\text{CS} = 2 \times 10^{-3} \text{ s}^{-1}$.

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Figure S14. The formation free energy (ΔG) (in kcal mol^{-1}) of $(\text{CA})_m(\text{PA})_n$ 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 [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 $\text{CS} = 2 \times 10^{-3} \text{ s}^{-1}$.

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 $g_{(i+j) \rightarrow i}$ is given as follows:

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

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 $(\text{PA})_m(\text{DMA})_n$ ($m = 0-4$, $n = 0-4$) 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 $(\text{PA})_5(\text{DMA})_4$ and $(\text{PA})_4(\text{DMA})_5$ as the boundary clusters for chlorine oxoacid system in the 4×4 box simulation.

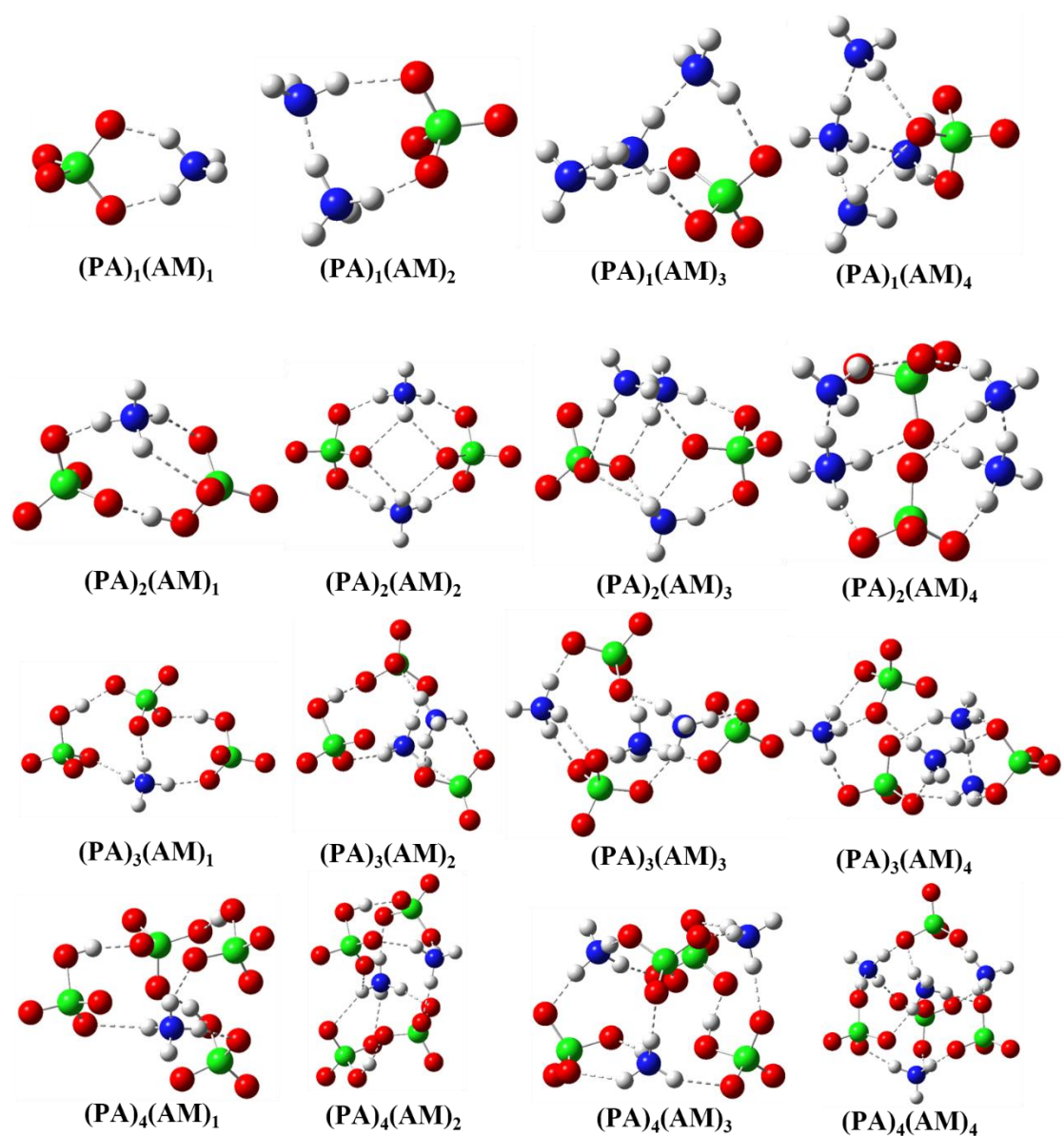


Figure S1. The most stable configurations of $(PA)_m(AM)_n$ ($m = 0-4$ and $n = 0-4$) clusters calculated at the DLPNO-CCSD(T)/aug-cc-pVTZ// ω B97X-D/6-31++G(d,p) level of theory. The dashed white lines indicate hydrogen bonds. The white, red, gray, blue and green spheres denote the H, O, C, N and Cl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

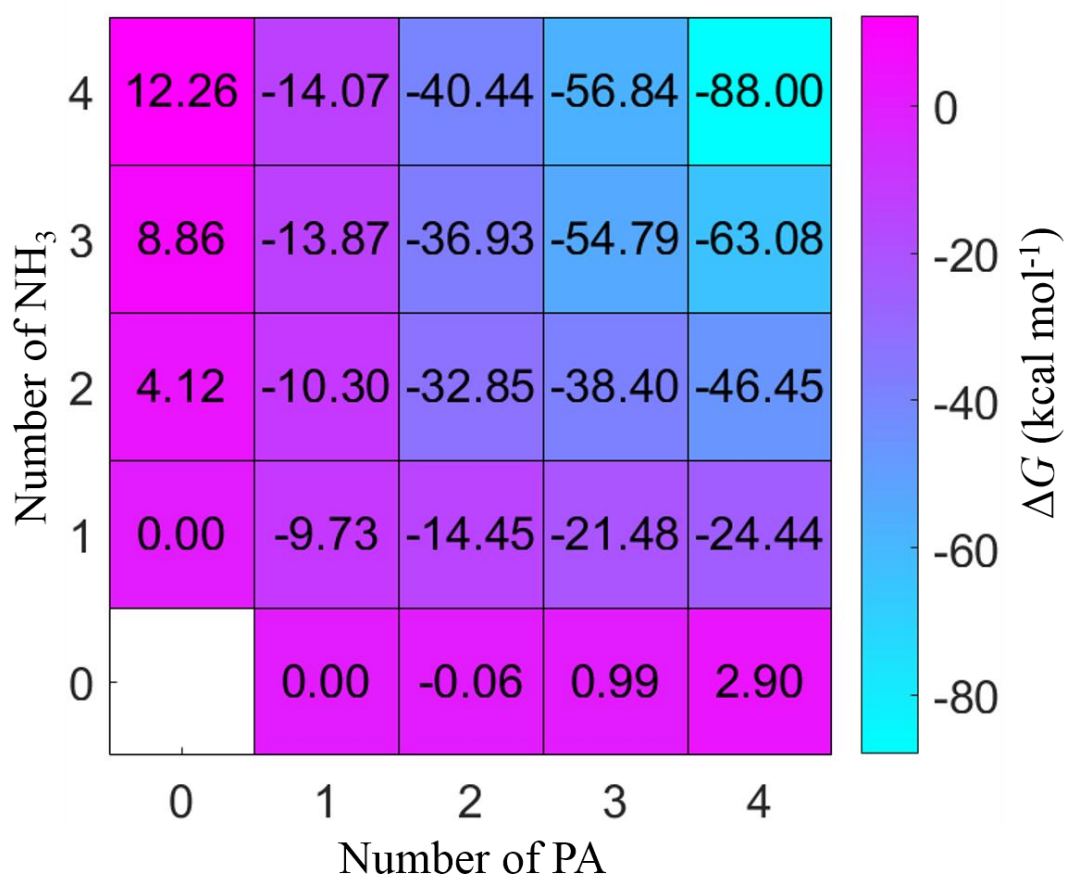


Figure S2. The formation free energy (ΔG) (in kcal mol⁻¹) of (PA)_m(NH₃)_n clusters (m = 0–4 and n = 0–4) calculated at the DLPNO-CCSD(T)/aug-cc-pVTZ// ω B97X-D/6-31++G(d,p) level of theory. The calculations are performed at 278 K and 1 atm.

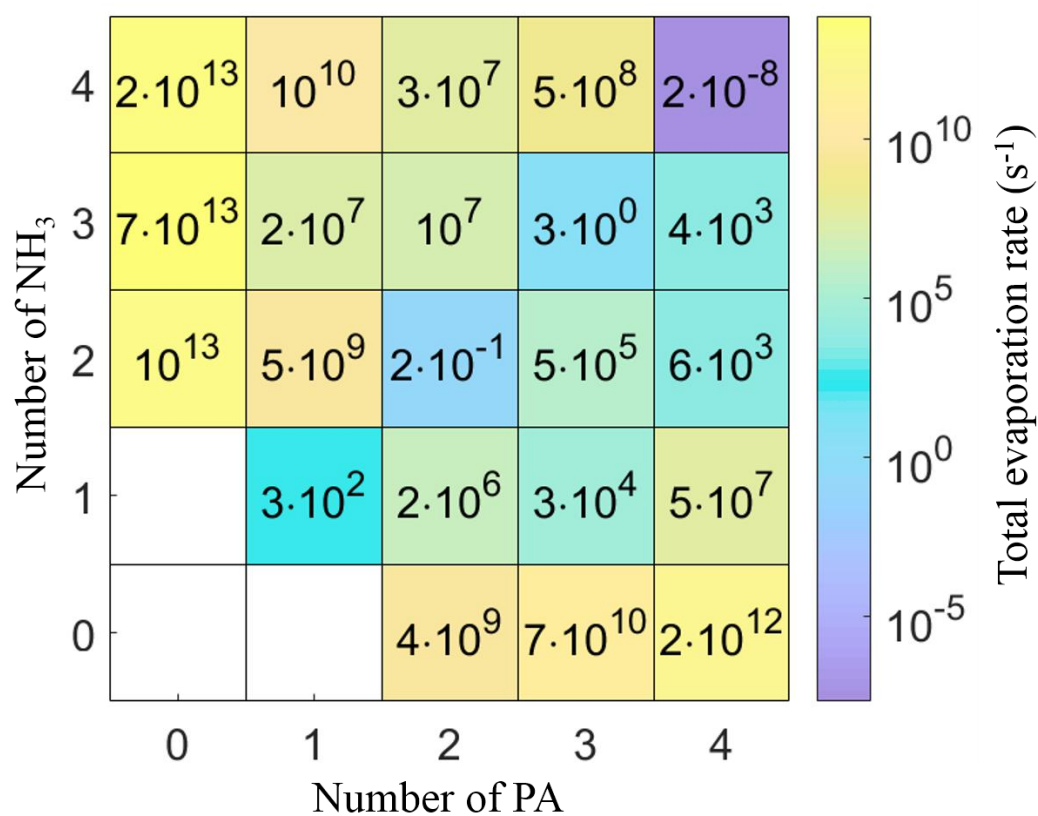


Figure S3. Evaporation rates for $(\text{PA})_m(\text{NH}_3)_n$ clusters ($m = 0-4$ and $n = 0-4$), at 278 K and 1 atm.

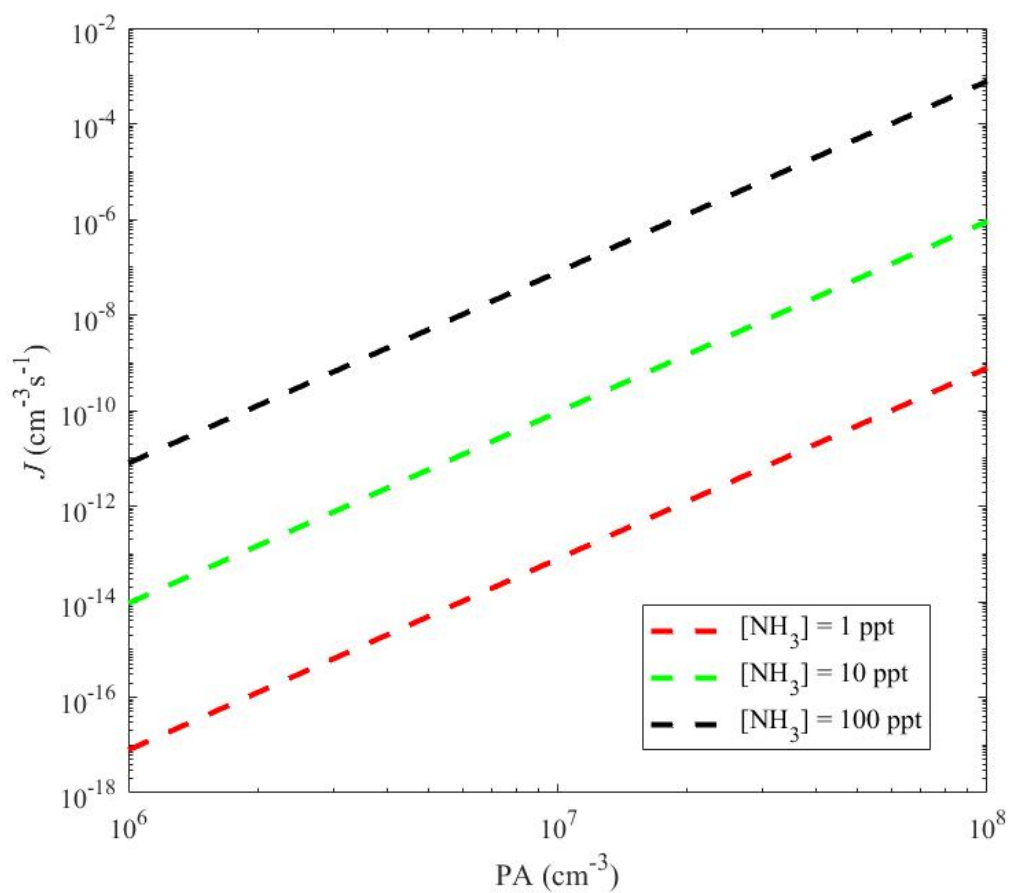


Figure S4. The simulated cluster formation rate J ($\text{cm}^{-3} \text{s}^{-1}$) of PA–NH₃ system at 278 K with different [DMA] (0.1–10 ppt), and $\text{CS} = 2 \times 10^{-3} \text{s}^{-1}$.

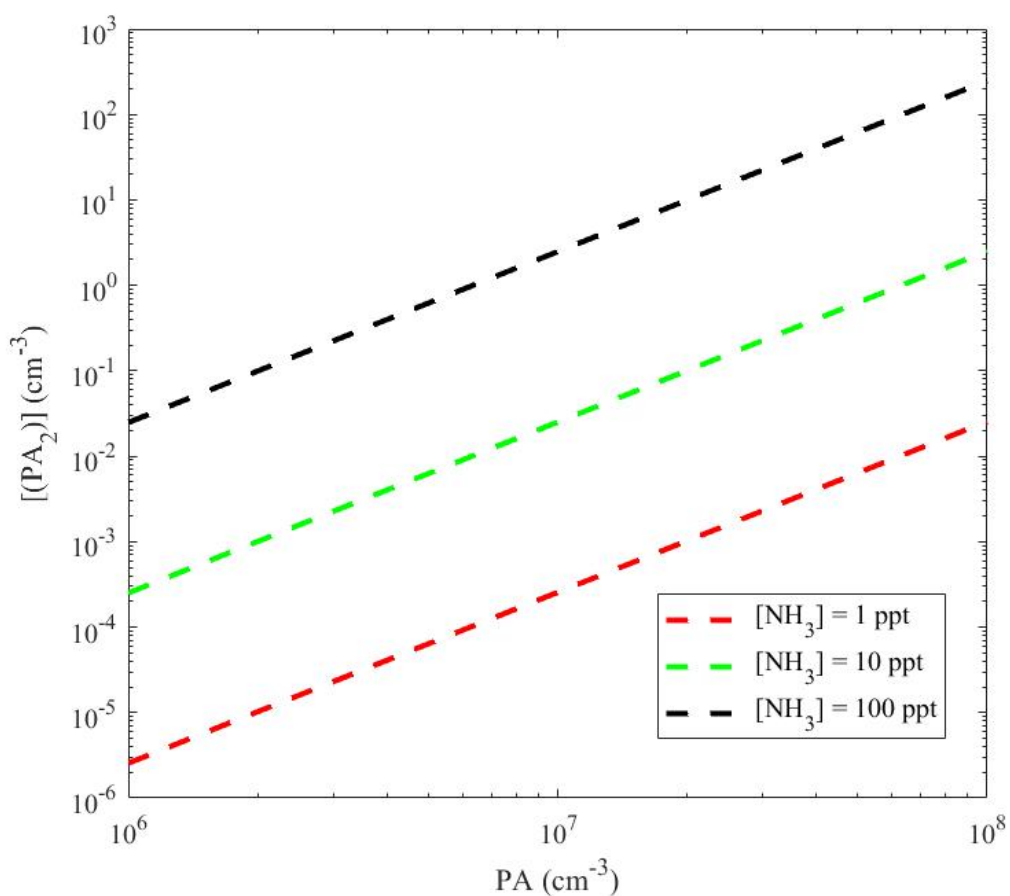


Figure S5. The simulated steady-state PA dimer concentration of PA–NH₃ cluster system at 278 K with different [NH₃] (0.1 –10 ppt), and CS = 2 × 10⁻³ s⁻¹.

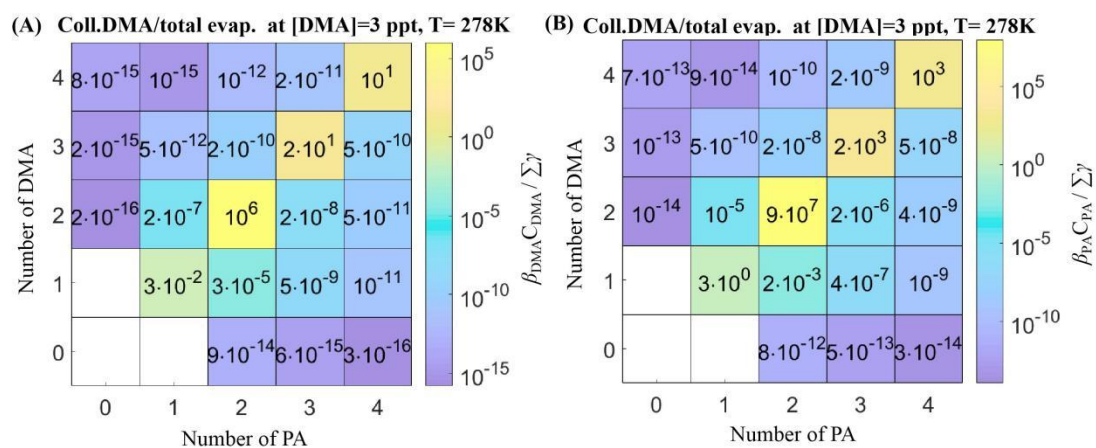


Figure S6. Ratios of collision frequencies with (A) DMA monomer or (B) PA

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.

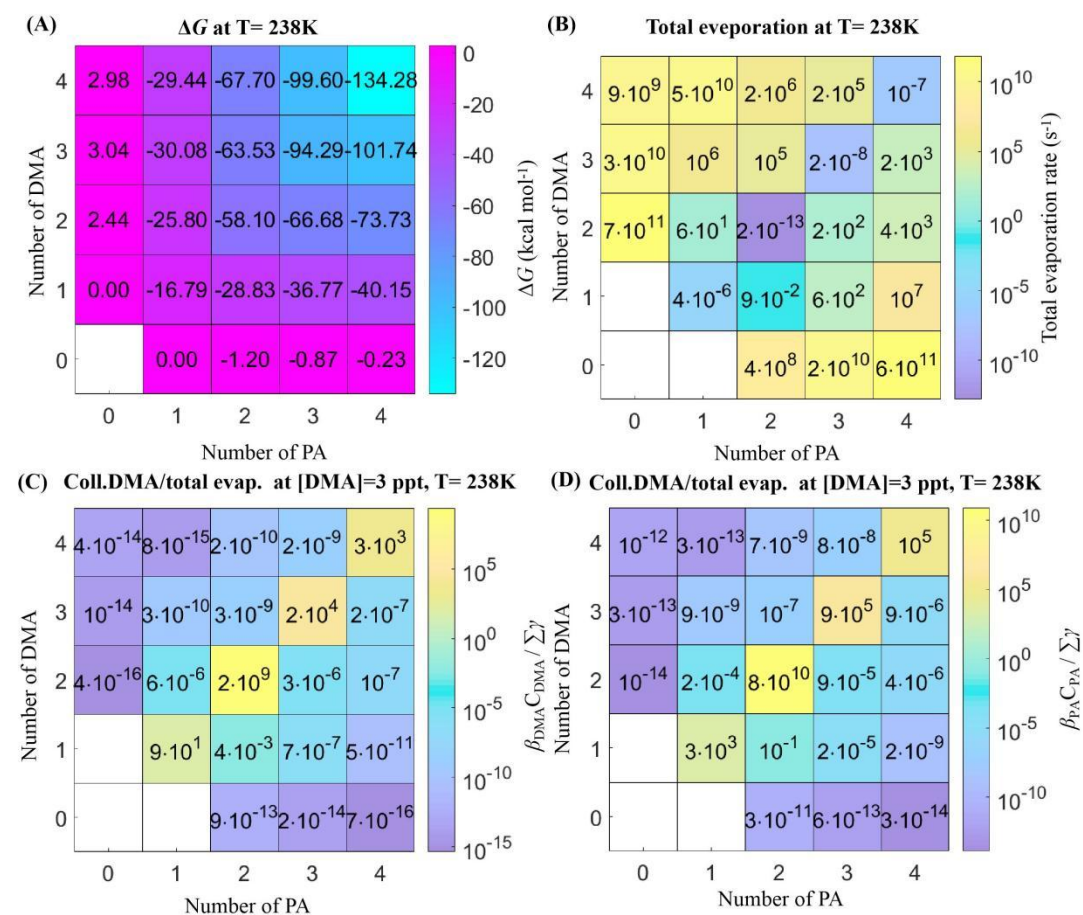


Figure S7. (A) Gibbs formation free energies (ΔG) of the $(\text{PA})_{1-4}(\text{DMA})_{1-4}$ clusters identified at the DLPNO-CCSD(T)/aug-cc-pVTZ// ω B97X-D/6-31++G(d,p) level of theory, T = 238 K, p = 1 atm. (B) Total evaporation rate coefficients ($\Sigma\gamma$ in s^{-1}) and the ratios of collision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

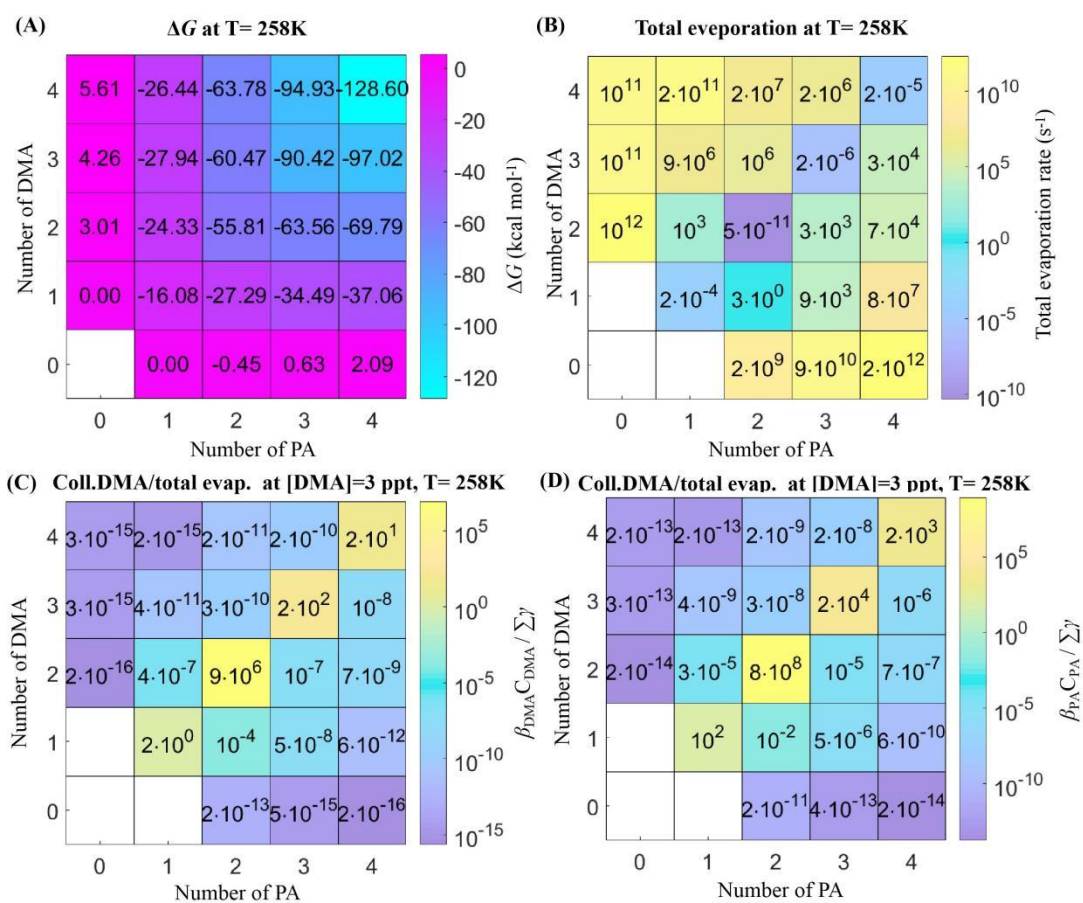


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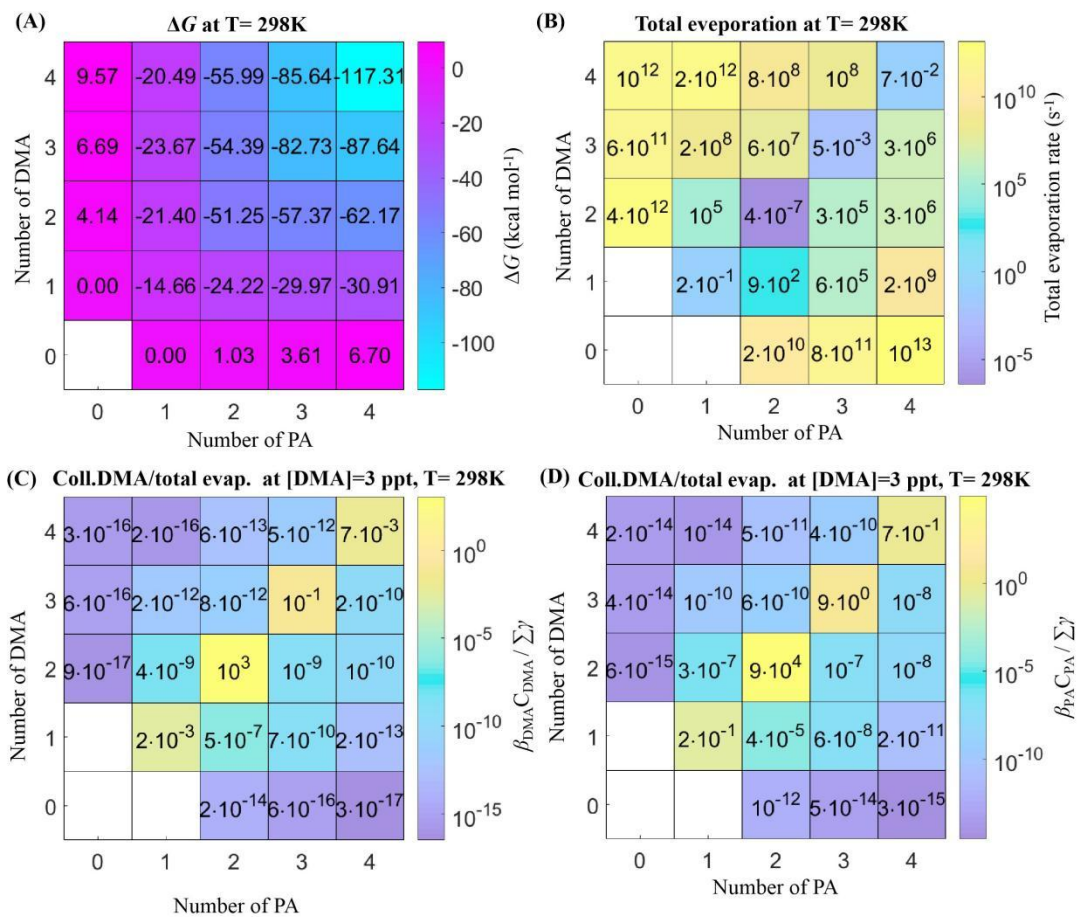


Figure S9. (A) Gibbs formation free energies (ΔG) of the $(\text{PA})_{1-4}(\text{DMA})_{1-4}$ clusters identified at the DLPNO-CCSD(T)/aug-cc-pVTZ// ω B97X-D/6-31++G(d,p) level of theory, $T = 298 \text{ K}$, $p = 1 \text{ atm}$. (B) Total evaporation rate coefficients ($\Sigma\gamma$ in s^{-1}) and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

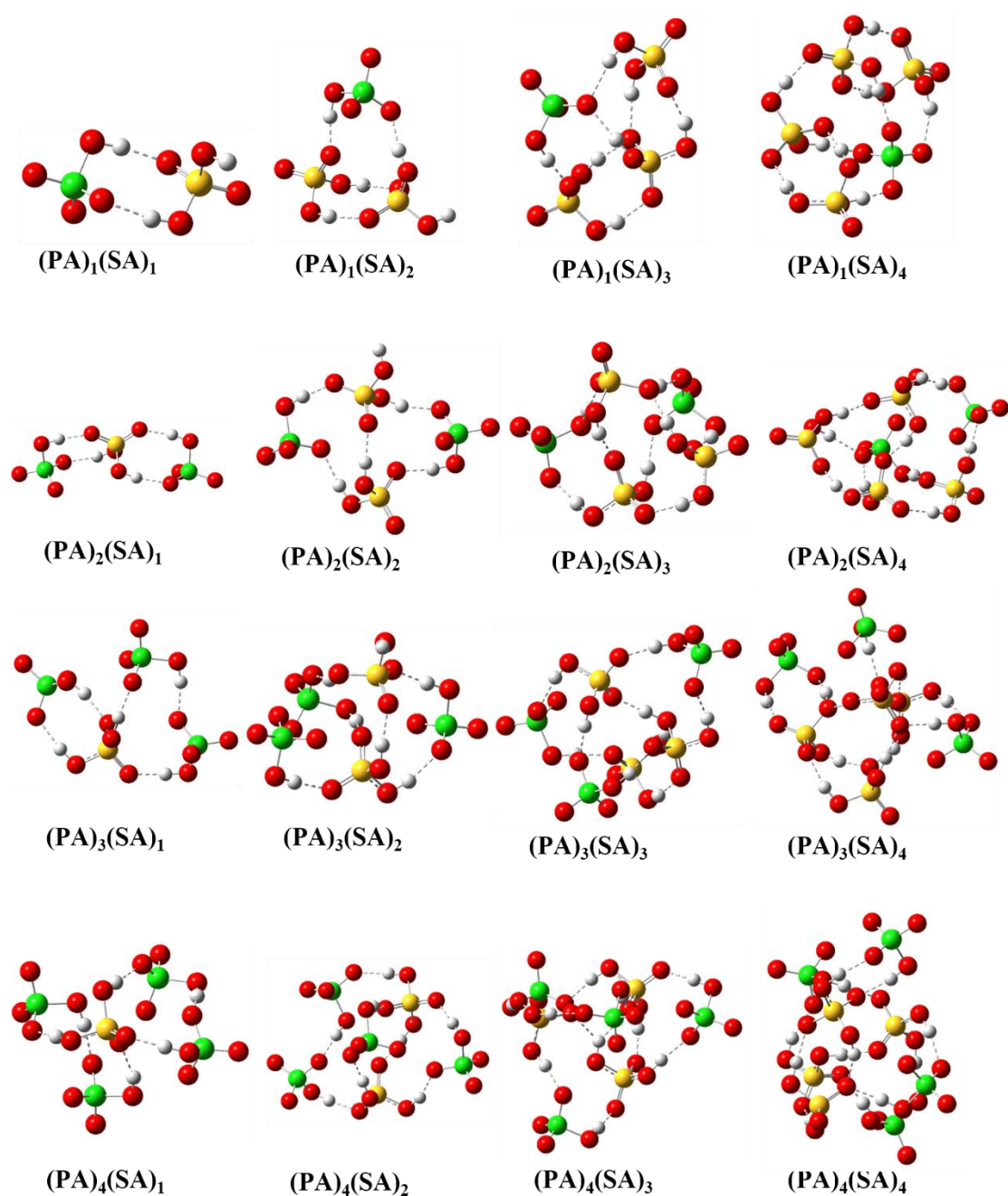


Figure S10. The most stable configurations of $(PA)_m(SA)_n$ ($m = 0-4$ and $n = 0-4$) clusters calculated at the DLPNO-CCSD(T)/aug-cc-pVTZ// ω B97X-D/6-31++G(d,p) level of theory. The dashed white lines indicate hydrogen bonds. The white, red, gray, yellow and green spheres denote the H, O, S, N and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

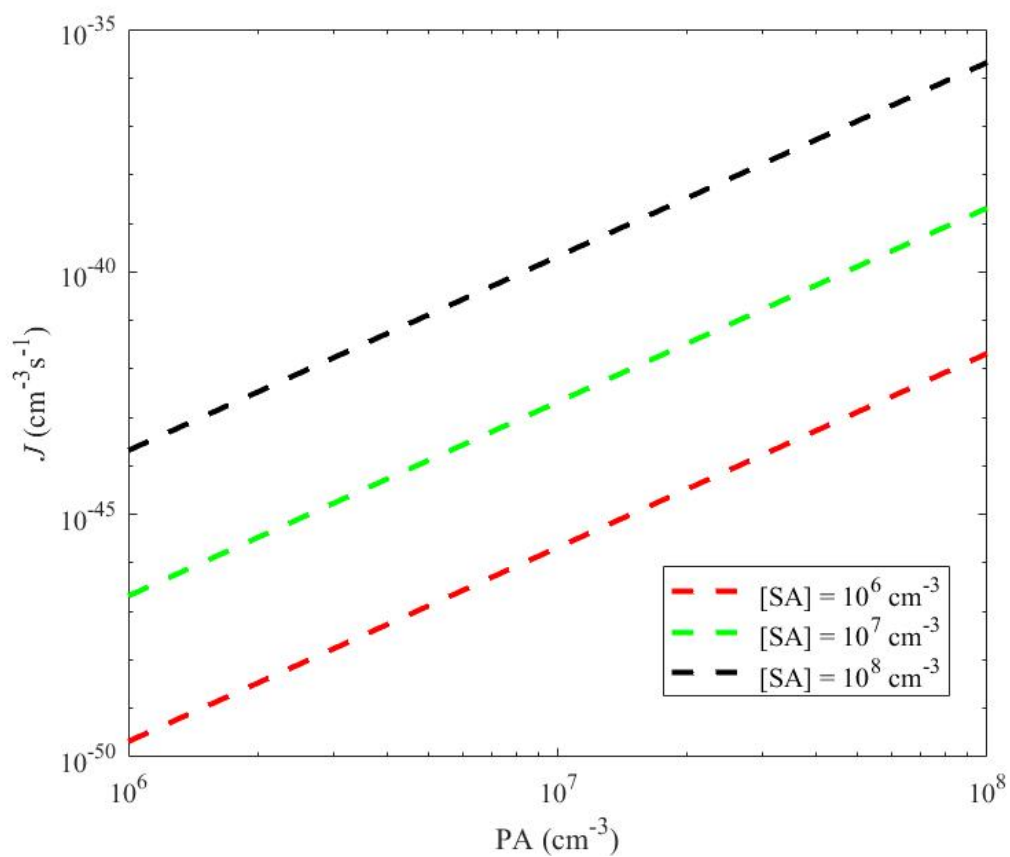


Figure S11. The simulated cluster formation rate J ($\text{cm}^{-3} \text{s}^{-1}$) of PA–SA system at 278 K with different [SA] (10^6 – 10^8 cm^{-3}), and $\text{CS} = 2 \times 10^{-3} \text{ s}^{-1}$.

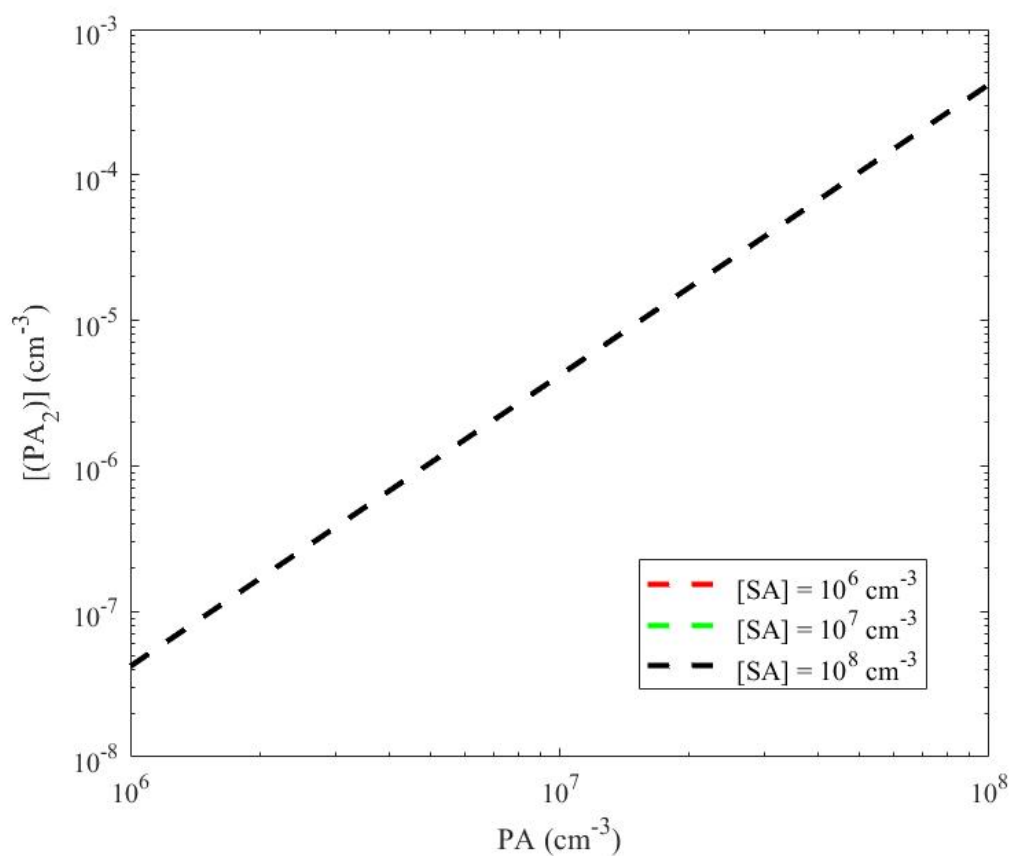


Figure S12. The simulated steady-state PA dimer concentration of PA–SA cluster system at 278 K with different $[SA]$ (10^6 – $10^8 cm^{-3}$), and $CS = 2 \times 10^{-3} s^{-1}$.

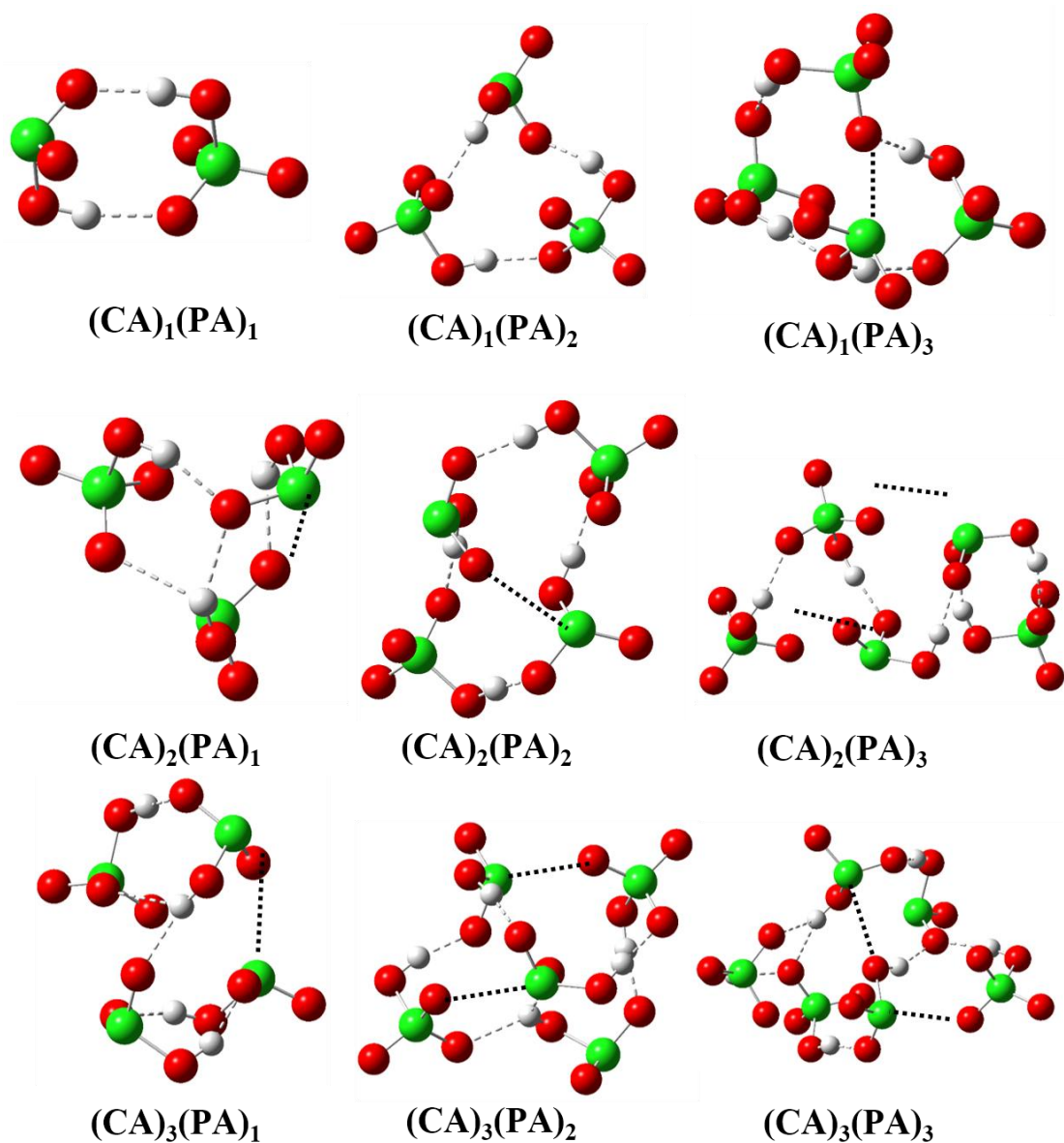


Figure S13. The most stable configurations of $(\text{CA})_m(\text{PA})_n$ ($m = 0-3$ and $n = 0-3$) clusters calculated at the DLPNO-CCSD(T)/aug-cc-pVTZ// ω B97X-D/6-31++G(d,p) level of theory. The dashed white lines indicate hydrogen bonds. The white, red, gray, and green spheres denote the H, O, C,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

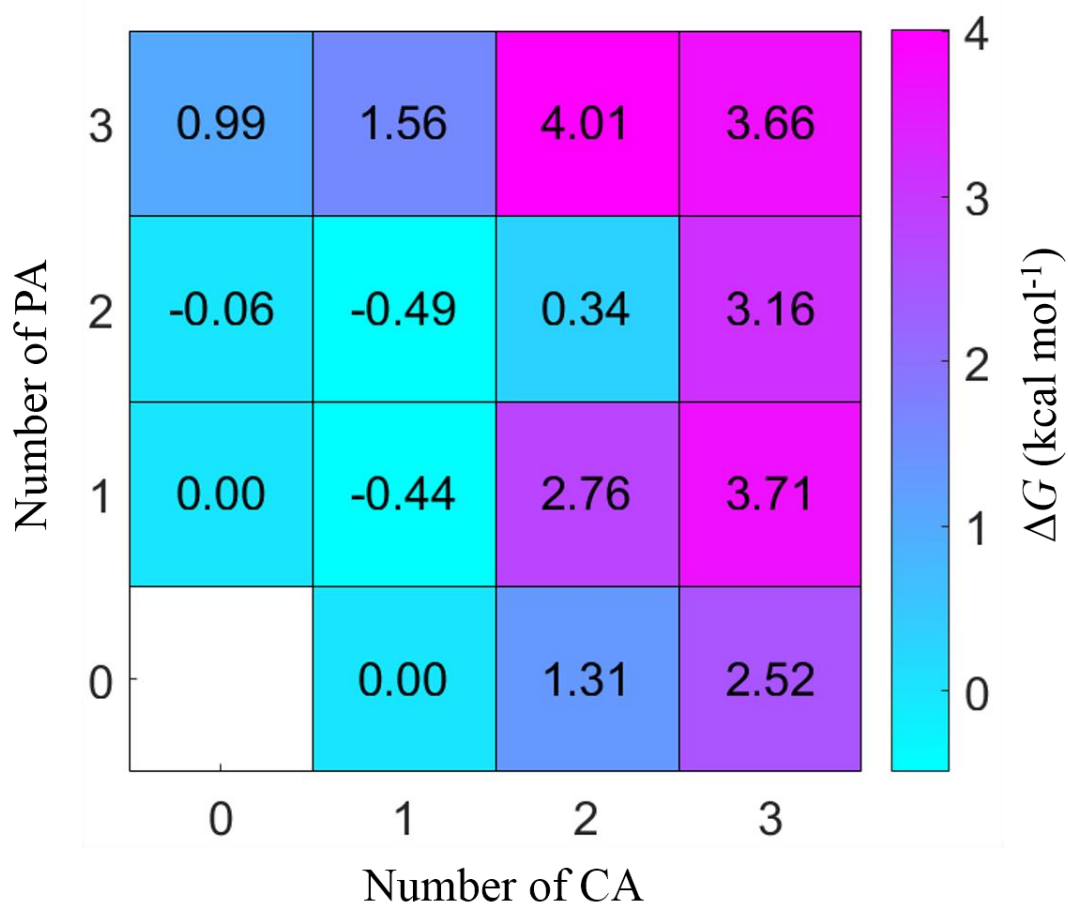


Figure S14. The formation free energy (ΔG) (in kcal mol⁻¹) of (CA)_m(PA)_n clusters (m = 0–3 and n = 0–3) calculated at the DLPNO-CCSD(T)/aug-cc-pVTZ// ω B97X-D/6-31++G(d,p) level of theory. The calculations are performed at 278 K and 1 atm.

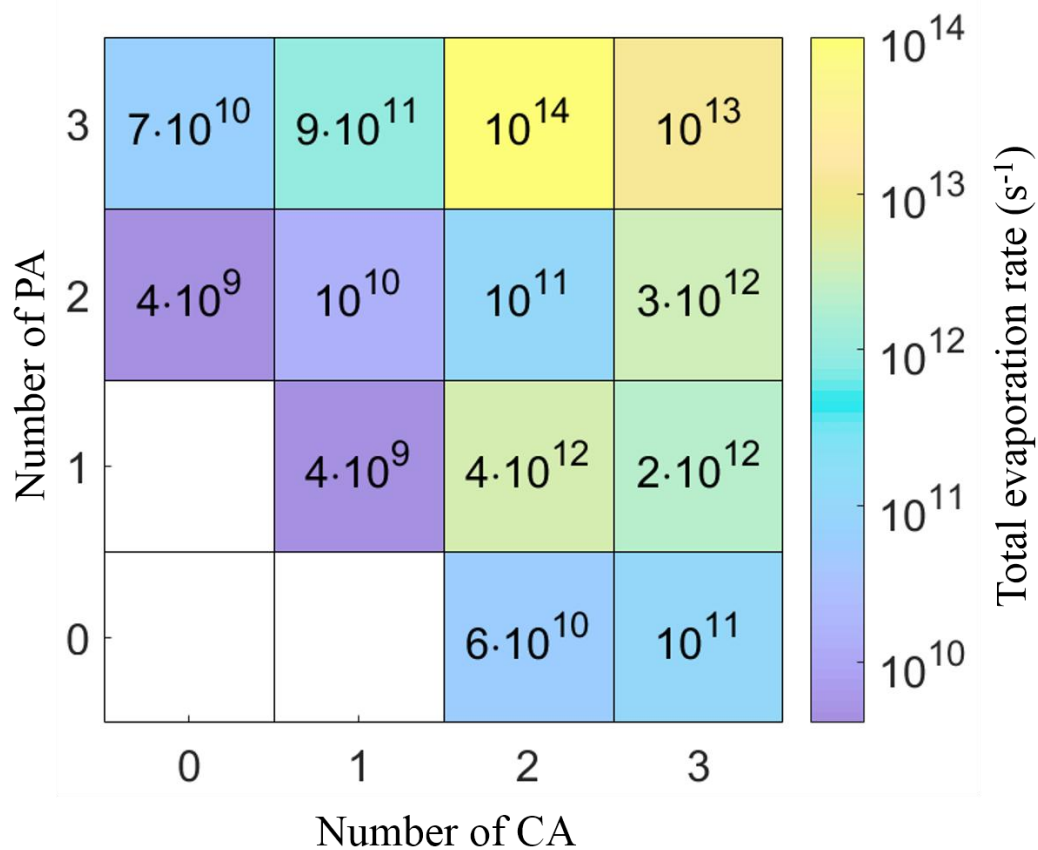


Figure S15. Evaporation rates for $(CA)_m(PA)_n$ clusters ($m = 0-3$ and $n = 0-3$), at 278 K and 1 atm.

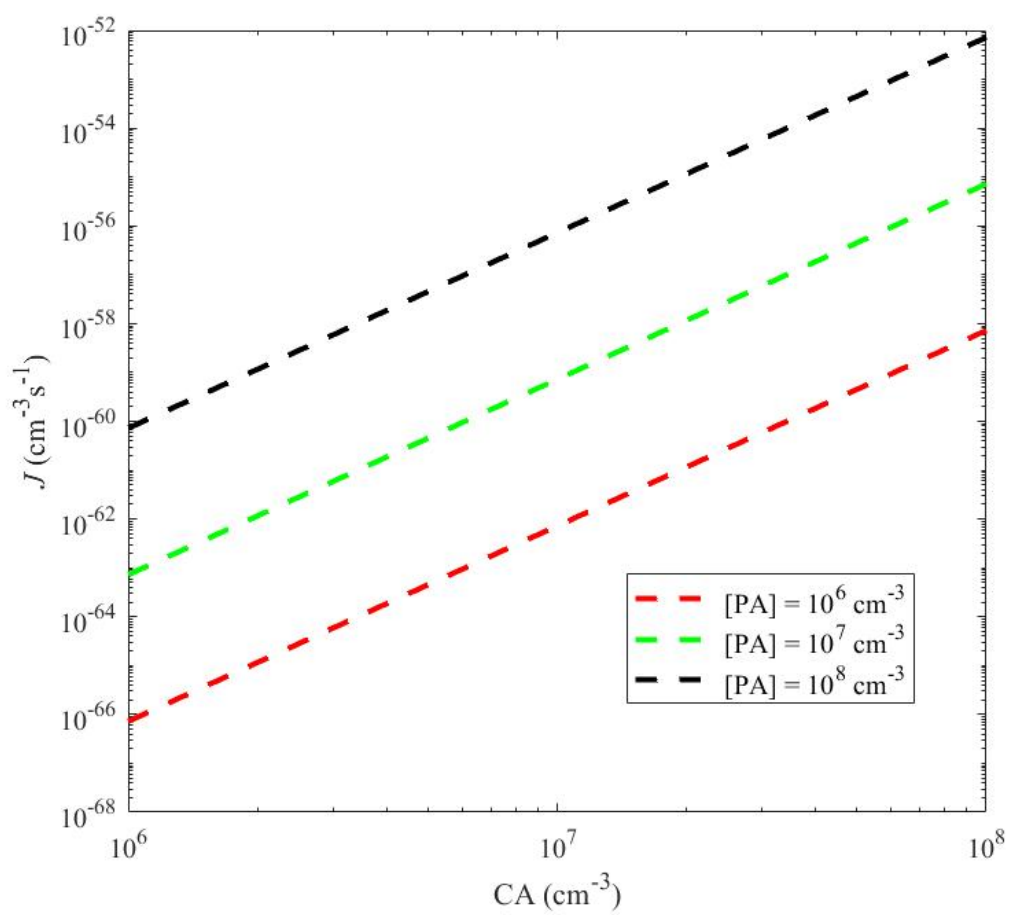


Figure S16. The simulated cluster formation rate J ($\text{cm}^{-3} \text{s}^{-1}$) of CA–PA system at 278 K with different $[\text{CA}]$ (10^6 – 10^8 cm^{-3}), and $\text{CS} = 2 \times 10^{-3} \text{ s}^{-1}$.

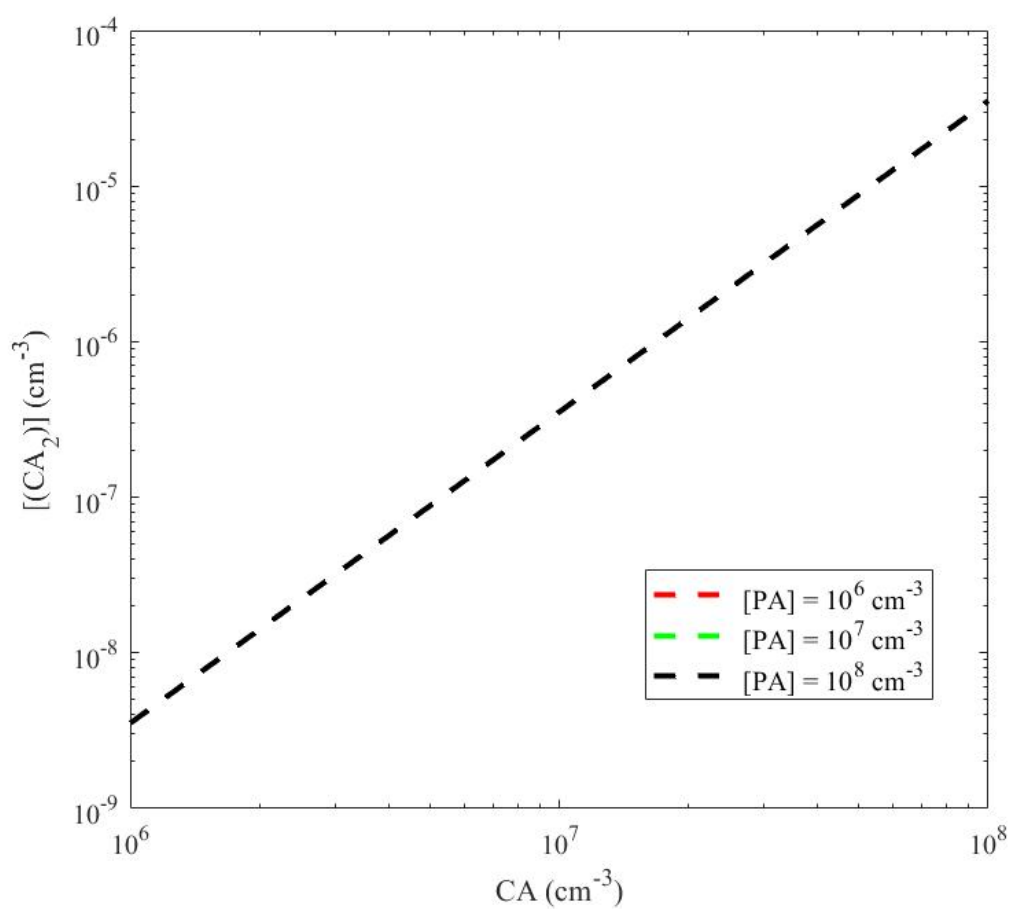


Figure S17. The simulated steady-state CA dimer concentration of CA–PA cluster system at 278 K with different $[PA]$ (10^6 – $10^8 cm^{-3}$), and $CS = 2 \times 10^{-3} s^{-1}$.

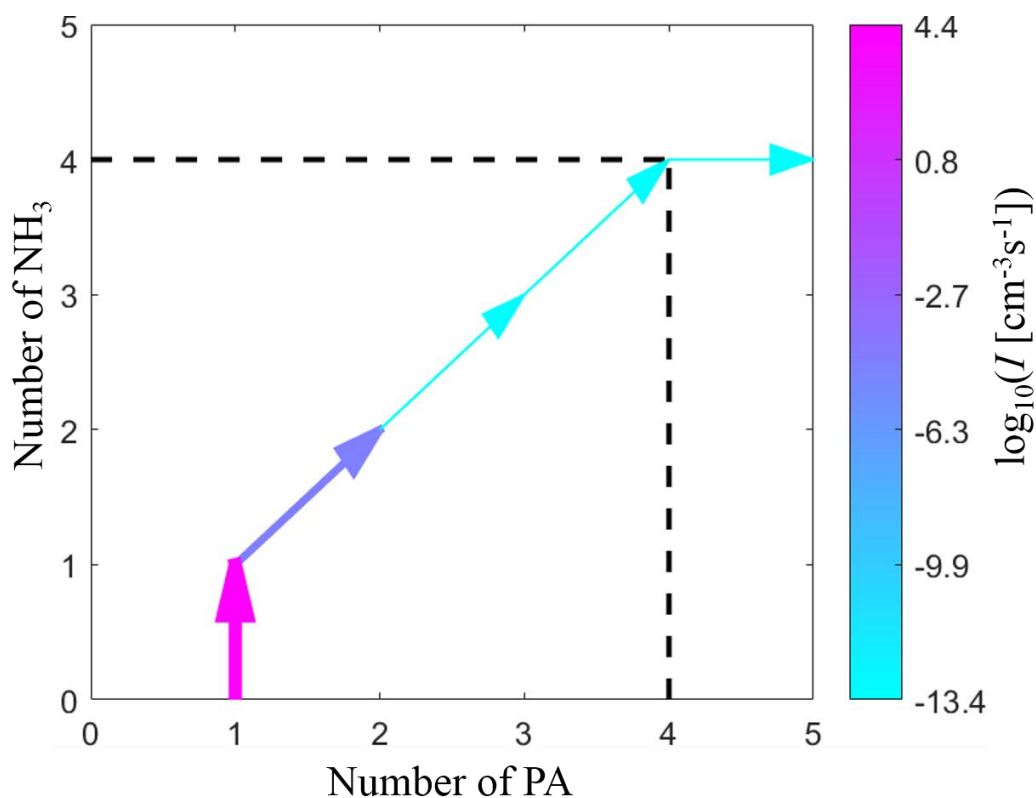


Figure S18. Main clustering pathways of $(\text{CA})_m(\text{PA})_n$ ($m = 0-3$ and $n = 0-3$) clusters at 278 K, $[\text{CA}] = 10^7 \text{ cm}^{-3}$, and $[\text{PA}] = 10^7 \text{ cm}^{-3}$.

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) _i (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) _i (SA) _i	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) _i (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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