

Supporting Information

Chloric Acid-Driven Nucleation Enhanced by Dimethylamine and Sulfuric acid in the Arctic: Mechanistic Study

Shengming Wang², Huidi Zhang¹, Xiangli Shi^{1,*}, Qingzhu Zhang²,
Wenxing Wang², Qiao Wang²

¹College of Geography and Environment, Shandong Normal
University, Jinan 250014, P. R. China

²Environment Research Institute, Shandong University,
Qingdao 266237, P. R. China

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*Corresponding authors. E-mail: shixl@sdnu.edu.cn

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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 ABCluster 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]. The structures of (SA)₁₋₄(DMA)₁₋₄, and (HIO₃)₁₋₃(DMA)₁₋₃ were obtained from previous studies^[7, 9] and were employed here.

Section S2. Atmospheric clusters dynamic simulations

Atmospheric Cluster Dynamics Code (ACDC)^[10] 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^[11].

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^[12] 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^[10]. Boundary conditions require that the growing clusters could be sufficiently stable and the clusters should be more likely to grow than evaporate. For $(CA)_m(DMA)_n$ ($m = 0-4$, $n = 0-4$) clusters, clusters with roughly equal numbers of CA and DMA molecules have lower evaporation rates and higher concentrations in the simulations. This allows us to select $(CA)_5(DMA)_4$ as the boundary clusters for chlorine oxoacid system in the 4×4 box simulation. For $(CA)_m(SA)_n$ ($m = 0-4$, $n = 0-4$) clusters, we select $(CA)_5(SA)_4$ cluster as the boundary clusters for chlorine oxoacid system in the 4×4 box simulation.

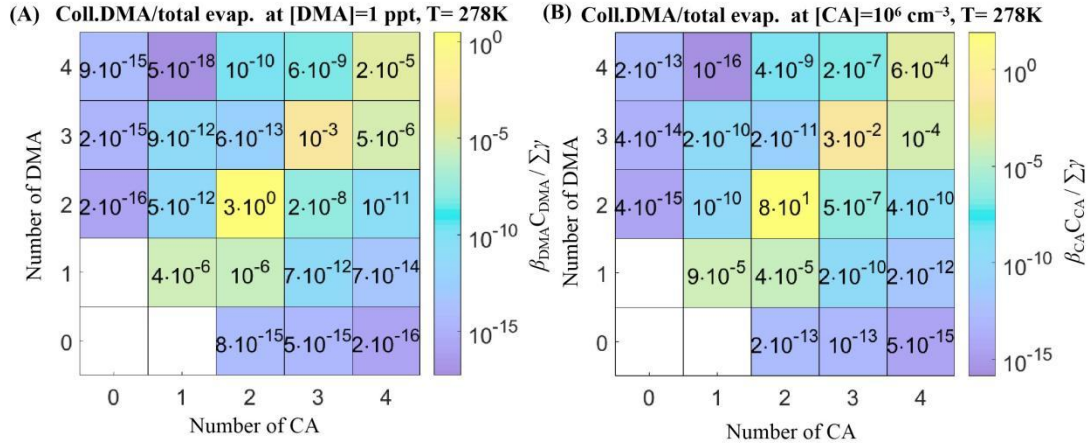


Figure S1. Ratios of collision frequencies with (A) DMA monomer or (B) CA monomer versus total evaporation rate coefficients ($\beta_{\text{DMA}} C_{\text{DMA}} / \Sigma \gamma$ or $\beta_{\text{CA}} C_{\text{CA}} / \Sigma \gamma$) of the corresponding clusters.

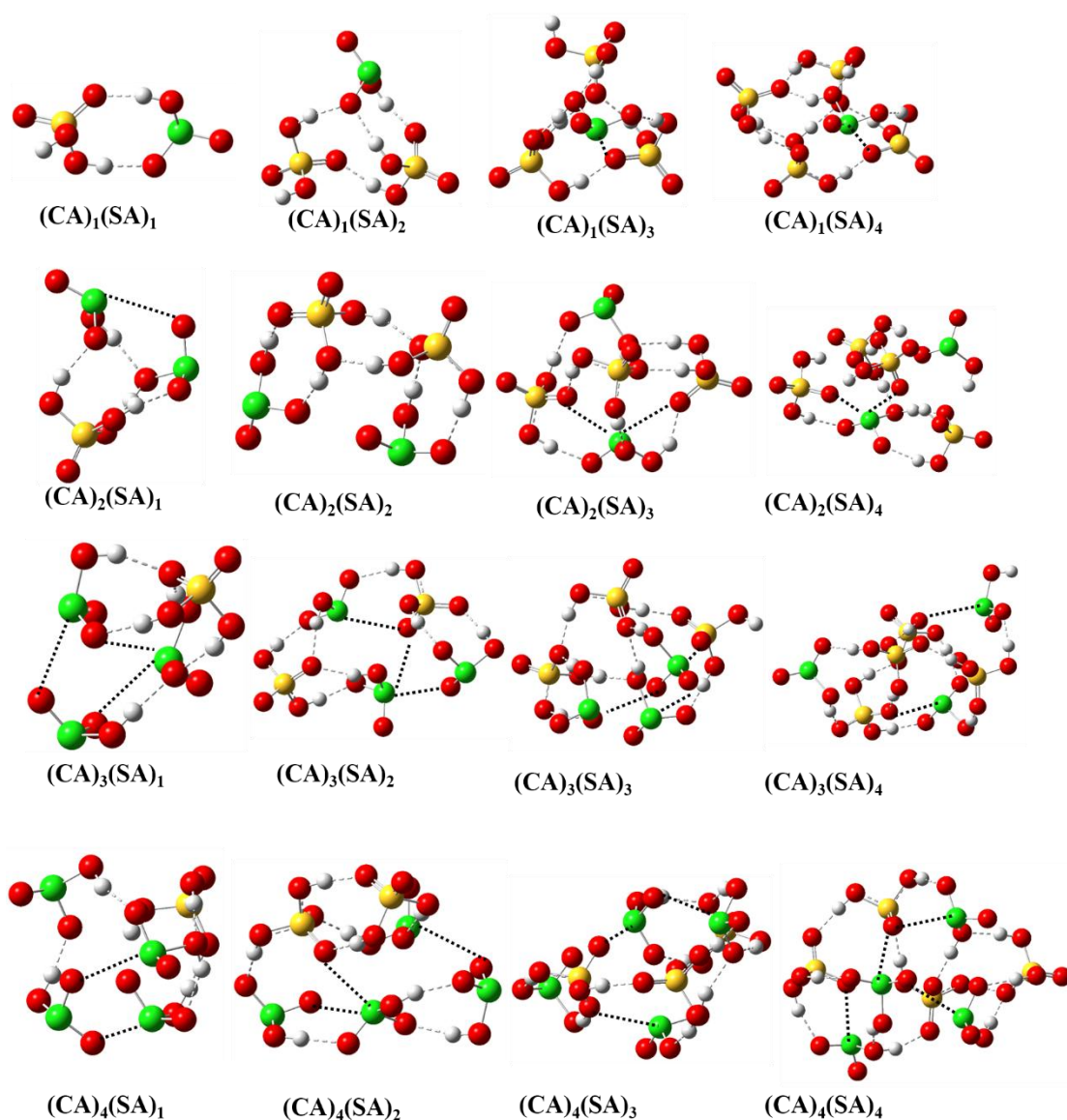


Figure S2. The most stable configurations of $(\text{CA})_m(\text{SA})_n$ ($m = 0-4$ and $n = 0-4$) clusters calculated at the DLPNO-CCSD(T)/aug-cc-pVTZ// ω B97X-D/6-31++G(d,p) level of theory. The dashed white lines indicate hydrogen bonds. The white, red, gray, yellow and green spheres denote the H, O, S, N and Cl atoms, respectively. The dashed black lines indicate halogen bonds.

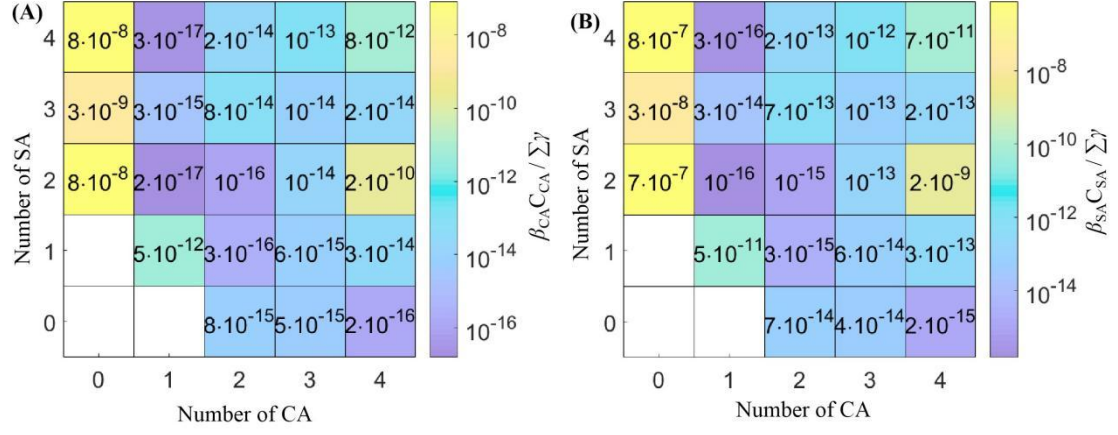


Figure S3. Ratios of collision frequencies with (A) CA monomer or (B) SA monomer versus total evaporation rate coefficients ($\beta_{CA}C_{CA}/\Sigma\gamma$ or $\beta_{SA}C_{SA}/\Sigma\gamma$) of the corresponding clusters.

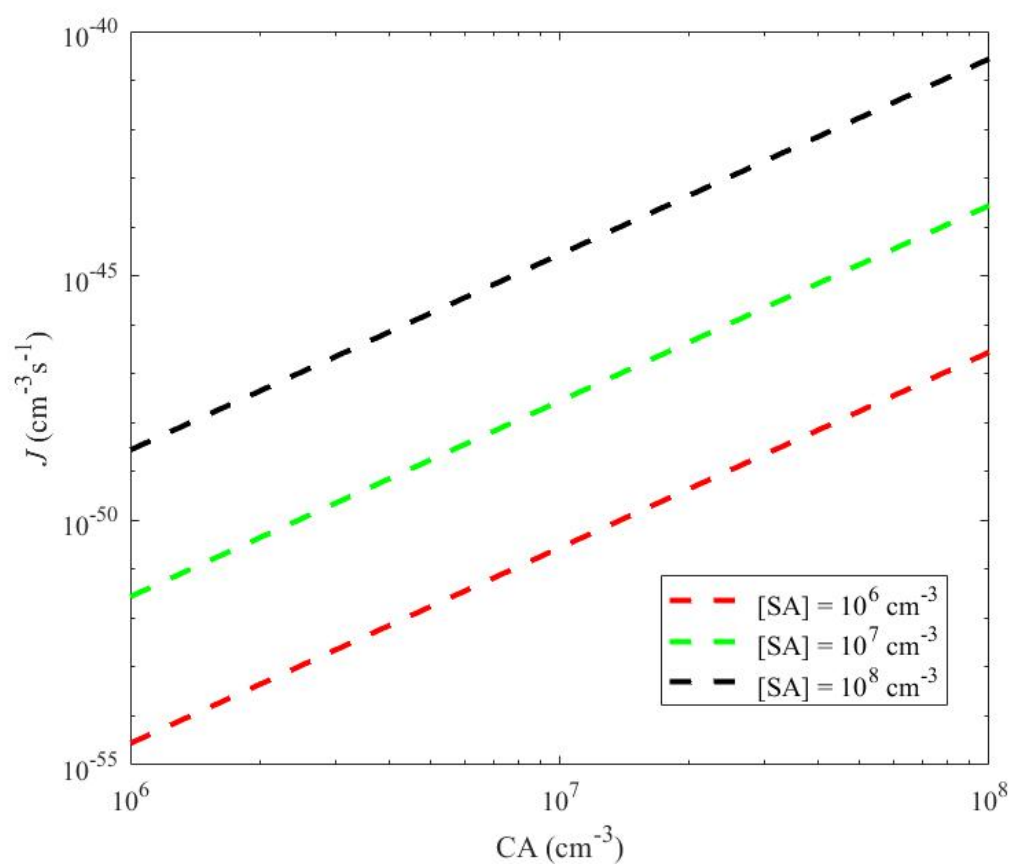


Figure S4. The simulated cluster formation rate J ($\text{cm}^{-3} \text{s}^{-1}$) of CA–SA system at 278 K with different [SA] (10^6 – 10^8 cm^{-3}), and $\text{CS} = 2 \times 10^{-3} \text{ s}^{-1}$.

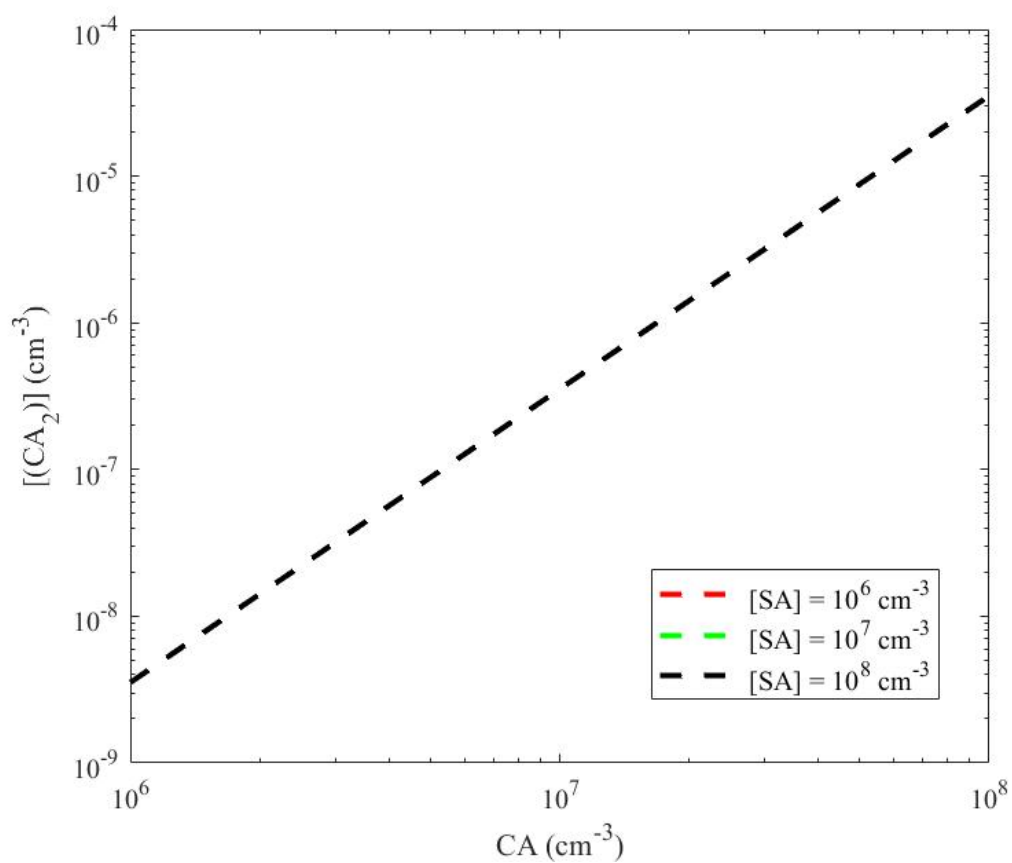


Figure S5. The simulated steady-state CA dimer concentration of CA–SA cluster system at 278 K with different [SA] (10^6 – 10^8 cm^{-3}), and $\text{CS} = 2 \times 10^{-3} \text{ s}^{-1}$.

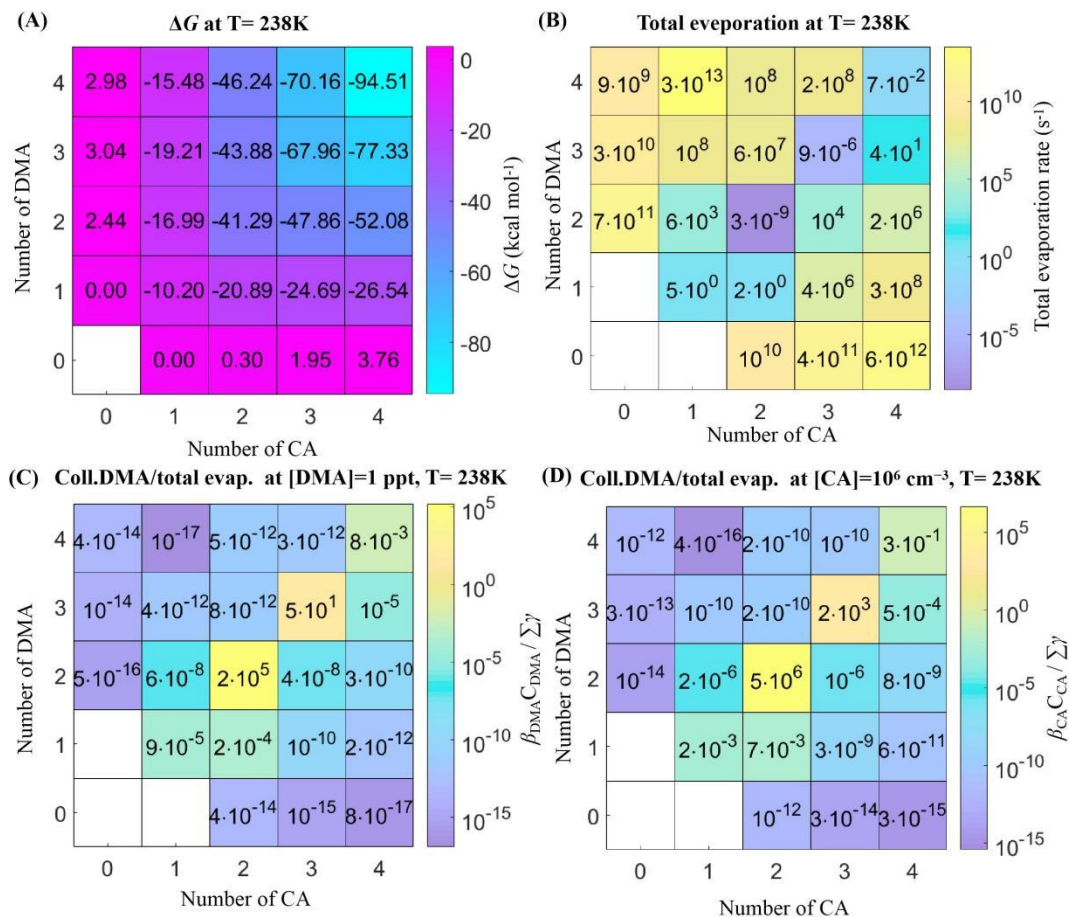


Figure S6. (A) Gibbs formation free energies (ΔG) of the $(\text{CA})_{1-4}(\text{DMA})_{1-4}$ clusters identified at the DLPNO-CCSD(T)/aug-cc-pVTZ// ω B97X-D/6-31++G(d,p) level of theory, $T = 238 \text{ K}$, $p = 1 \text{ atm}$. (B) Total evaporation rate coefficients ($\Sigma\gamma$ in s^{-1}) and the ratios of collision frequencies with (C) DMA monomer or (D) CA monomer versus total evaporation rate coefficients ($\beta_{\text{DMA}}C_{\text{DMA}}/\Sigma\gamma$ or $\beta_{\text{CA}}C_{\text{CA}}/\Sigma\gamma$) of the corresponding clusters.

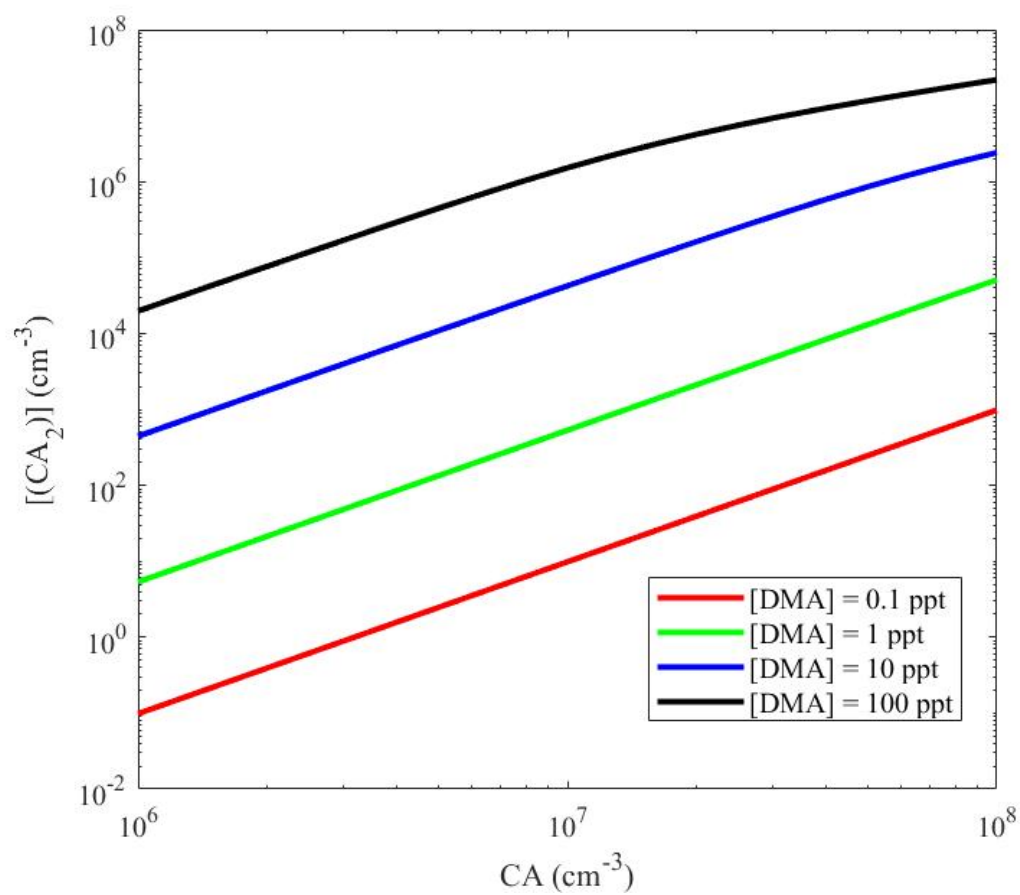


Figure S7. The simulated steady-state CA dimer concentration of CA–DMA cluster system at 238 K with different [DMA] (1 –100 ppt), and $CS = 2 \times 10^{-3} \text{ s}^{-1}$.

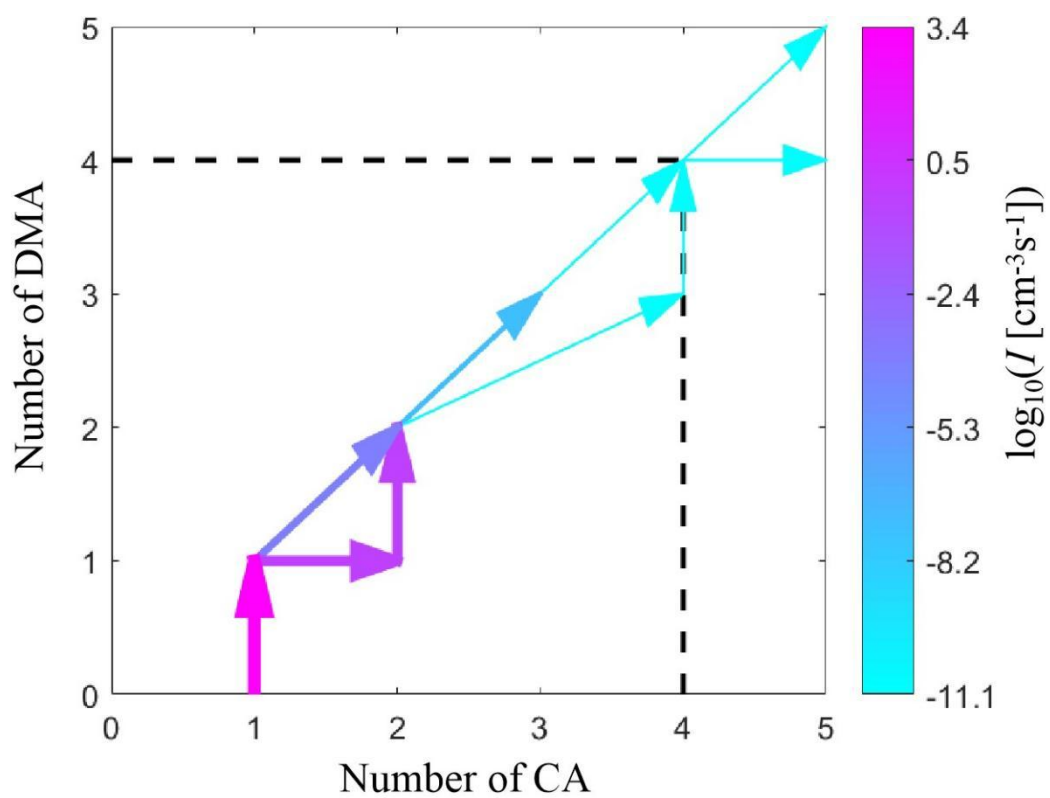


Figure S8. Main clustering pathways of $(\text{CA})_{1-4}(\text{DMA})_{1-4}$ clusters at 238 K, $[\text{CA}] = 10^6 \text{ cm}^{-3}$, and $[\text{DMA}] = 1 \text{ ppt}$.

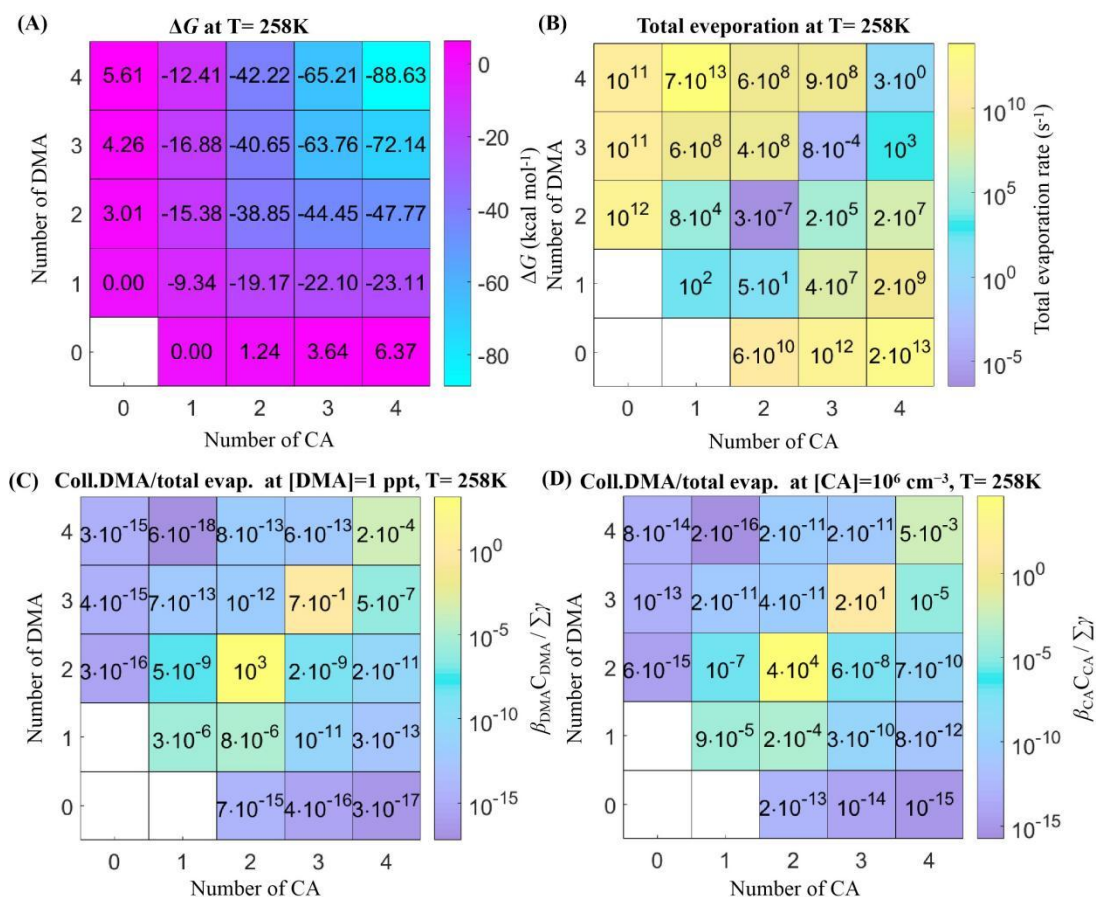


Figure S9. (A) Gibbs formation free energies (ΔG) of the $(\text{CA})_{1-4}(\text{DMA})_{1-4}$ clusters identified at the DLPNO-CCSD(T)/aug-cc-pVTZ// ω B97X-D/6-31++G(d,p) level of theory, $T = 258$ K, $p = 1$ atm. (B) Total evaporation rate coefficients ($\Sigma\gamma$ in s^{-1}) and the ratios of collision frequencies with (C) DMA monomer or (D) CA monomer versus total evaporation rate coefficients ($\beta_{\text{DMA}}C_{\text{DMA}}/\Sigma\gamma$ or $\beta_{\text{CA}}C_{\text{CA}}/\Sigma\gamma$) of the corresponding clusters.

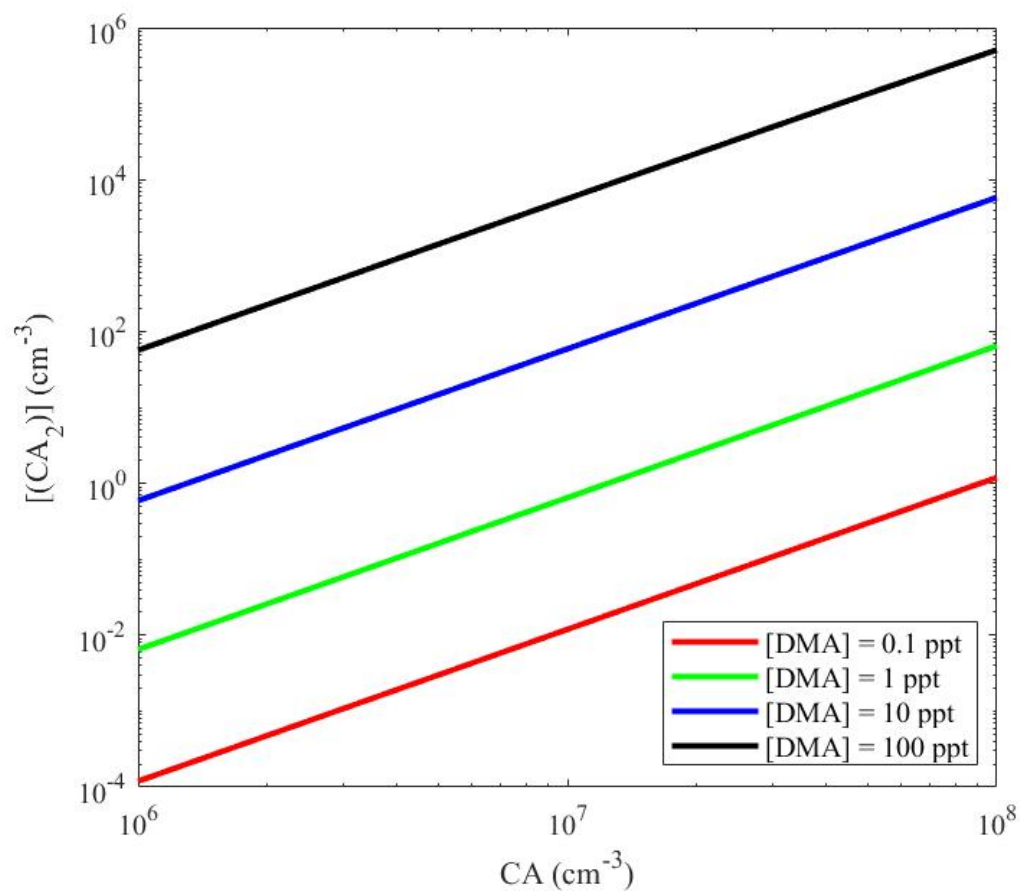


Figure S10. The simulated steady-state CA dimer concentration of CA–DMA cluster system at 258 K with different [DMA] (1 –100 ppt), and $CS = 2 \times 10^{-3} \text{ s}^{-1}$.

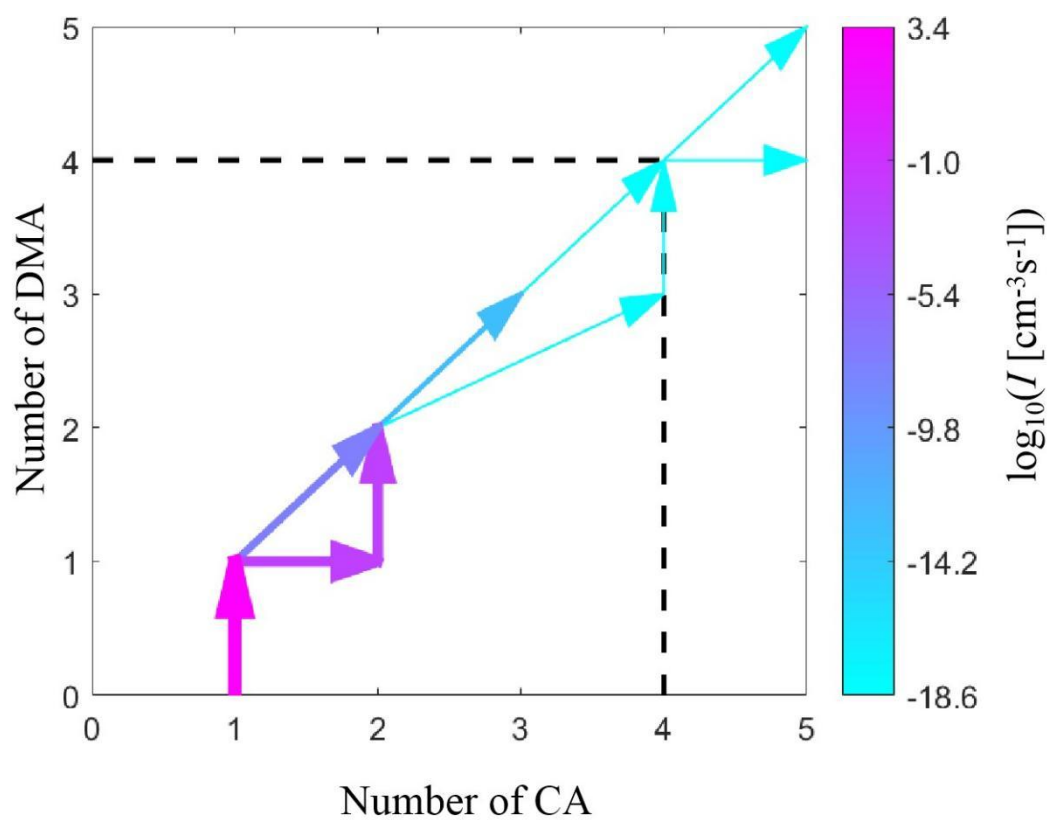


Figure S11. Main clustering pathways of $(\text{CA})_{1-4}(\text{DMA})_{1-4}$ clusters at 258 K, $[\text{CA}] = 10^6 \text{ cm}^{-3}$, and $[\text{DMA}] = 1 \text{ ppt}$.

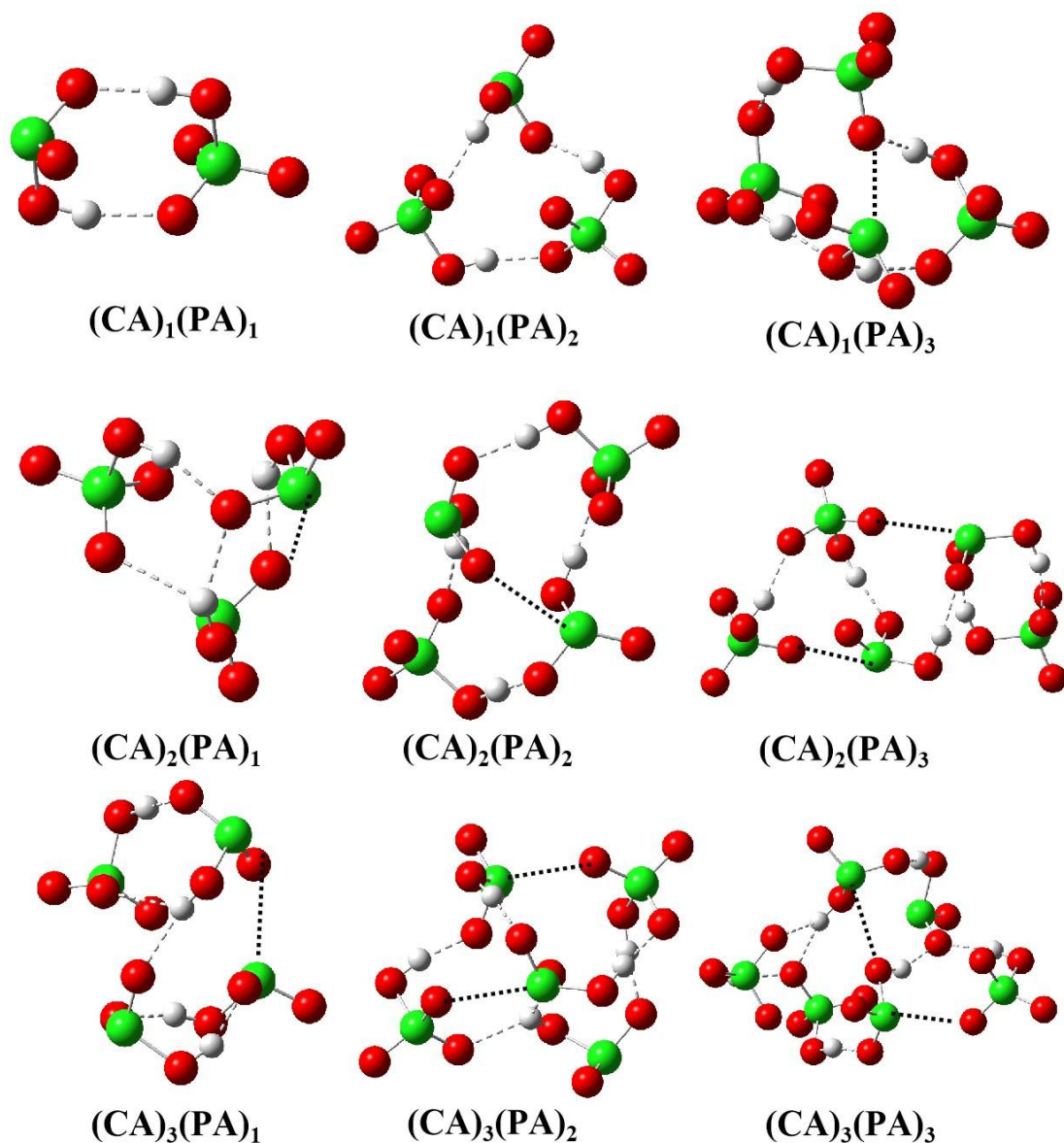


Figure S12. The most stable configurations of $(\text{CA})_m(\text{PA})_n$ ($m = 0-3$ and $n = 0-3$) clusters calculated at the DLPNO-CCSD(T)/aug-cc-pVTZ// ω B97X-D/6-31++G(d,p) level of theory. The dashed white lines indicate hydrogen bonds. The white, red, gray, and green spheres denote the H, O, C, and Cl atoms, respectively.

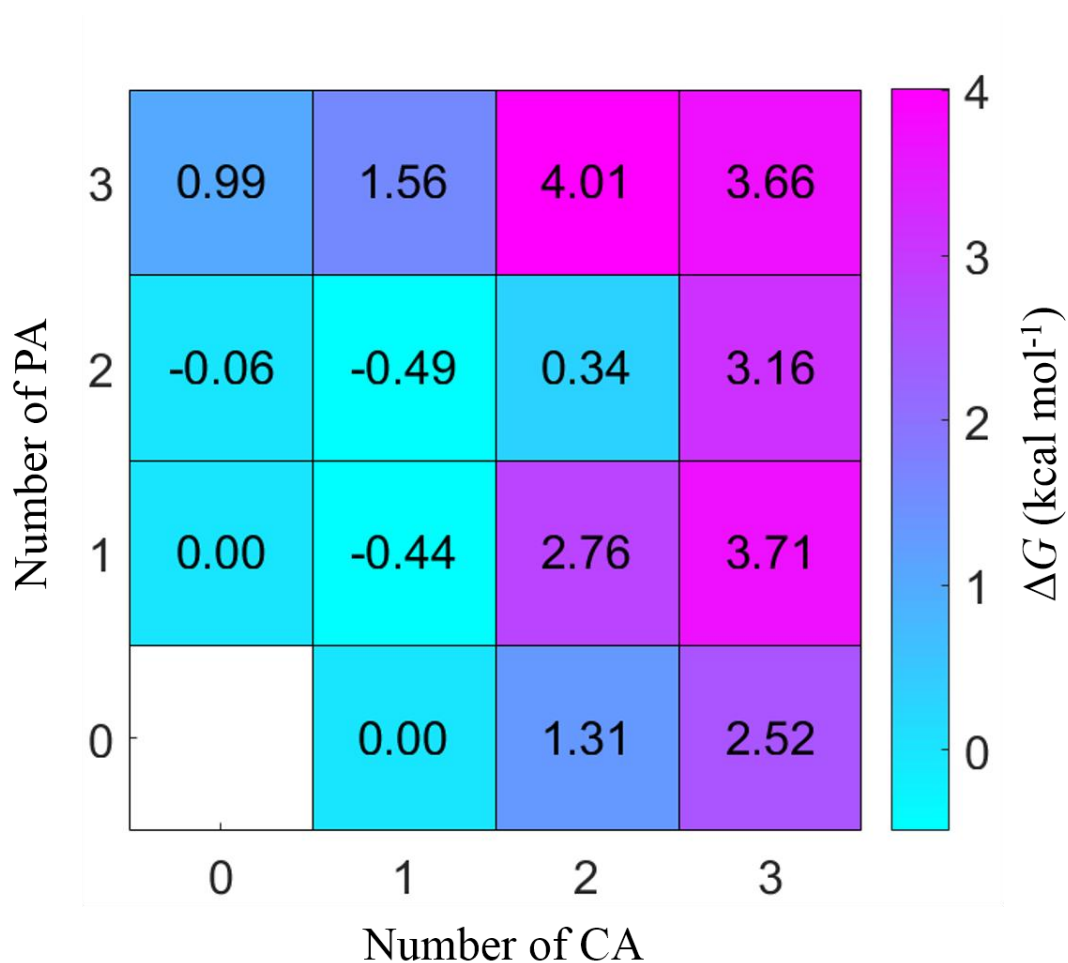


Figure S13. The formation free energy (ΔG) (in kcal mol⁻¹) of (CA)_m(PA)_n clusters ($m = 0-3$ and $n = 0-3$) calculated at the DLPNO-CCSD(T)/aug-cc-pVTZ// ω B97X-D/6-31++G(d,p) level of theory. The calculations are performed at 278 K and 1 atm.

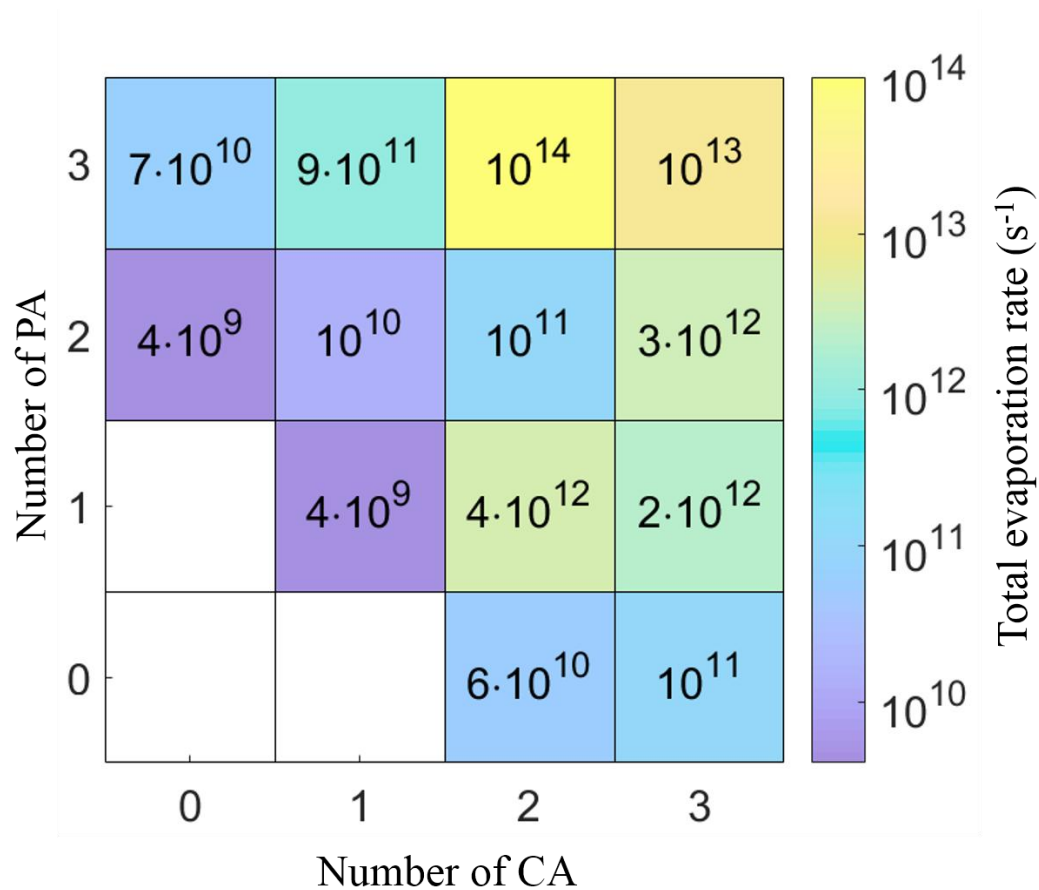


Figure S14. Evaporation rates for $(\text{CA})_m(\text{PA})_n$ clusters ($m = 0\text{--}3$ and $n = 0\text{--}3$), at 278 K and 1 atm.

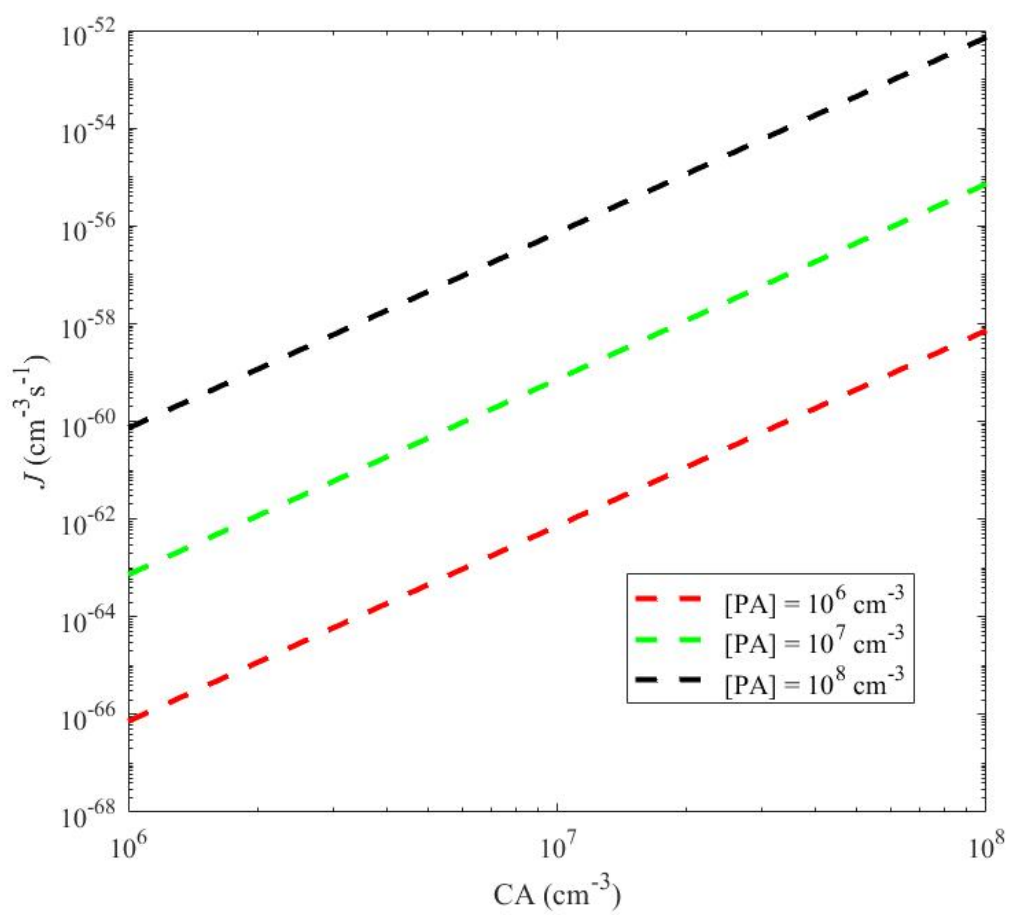


Figure S15. The simulated cluster formation rate J ($\text{cm}^{-3} \text{s}^{-1}$) of CA–PA system at 278 K with different $[\text{CA}]$ (10^6 – 10^8 cm^{-3}), and $\text{CS} = 2 \times 10^{-3} \text{ s}^{-1}$.

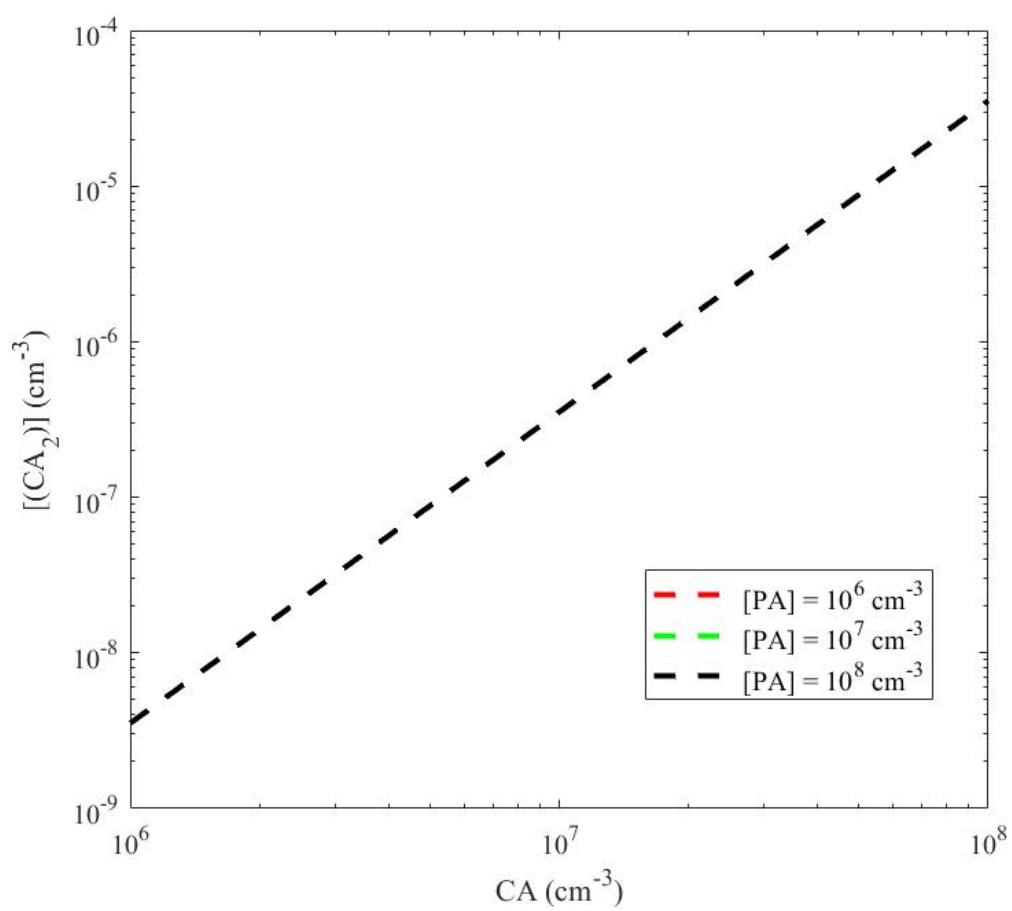


Figure S16. The simulated steady-state CA dimer concentration of CA-PA cluster system at 278 K with different [PA] (10^6 – 10^8 cm⁻³), and $CS = 2 \times 10^{-3}$ s⁻¹.

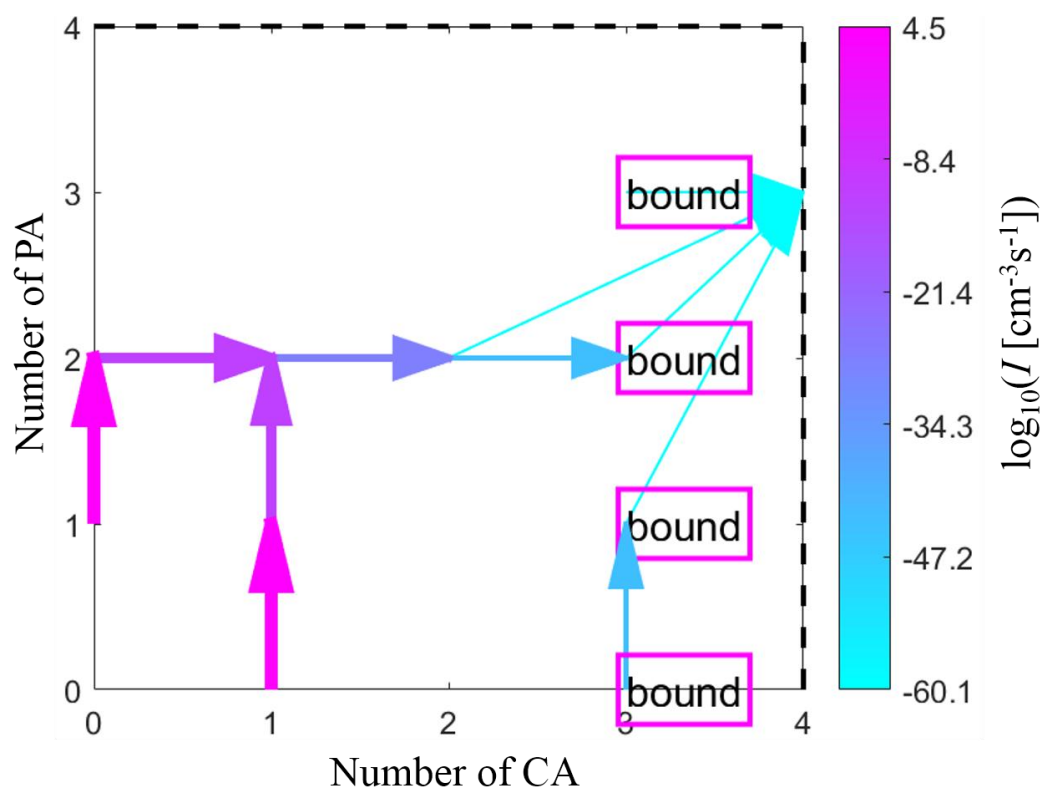


Figure S17. Main clustering pathways of $(\text{CA})_m(\text{PA})_n$ ($m = 0-3$ and $n = 0-3$) clusters at 278 K, $[\text{CA}] = 10^7 \text{ cm}^{-3}$, and $[\text{PA}] = 10^7 \text{ cm}^{-3}$.

Table S1. Coordinates of all optimized clusters

(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

(CA) ₄	x	y	z
O	0.07433600	-1.36450200	1.36098400
O	2.98472500	-1.93546300	-0.04041500
Cl	-0.18433700	-2.36896100	0.29195800
H	-0.68469400	-0.85950900	-1.17286100
O	-1.60133300	-2.76868000	0.27680700
O	2.36251000	0.27564800	1.00197800
O	0.61695200	1.62445700	-1.27068900
Cl	3.01355700	-0.51863900	-0.42642000
H	1.54731500	-0.22402500	1.24269600
O	4.34283100	0.08294100	-0.45219400
O	1.77508400	2.89936500	0.55151500
O	-0.41484200	1.82264200	0.94654500
Cl	0.31372700	2.52971700	-0.14804200
H	-2.17580900	1.47415600	0.99785100
O	0.06294600	-1.51244600	-1.12727800
O	-2.18109700	0.13285900	-1.04849000
O	-3.14032800	1.27747300	0.93523000
Cl	-3.27245500	-0.08636500	-0.05127500
H	2.13907300	2.01637400	0.83565500
O	-4.60645700	0.08652300	-0.61617900

(CA) ₅	x	y	z
O	-0.67184900	-0.83612800	-1.25903400
O	-2.07074500	-2.64796700	-0.53112500
Cl	-0.65148400	-2.51177200	-0.96051600
H	-2.69379700	-1.25523500	0.41499200
O	-0.39914500	-3.14573200	-2.25379600
O	-2.18375000	1.77522700	-0.18003300
O	-2.97052800	-0.37864100	0.78196400
Cl	-3.09188800	0.69345000	-0.59388900
H	0.25935700	-0.52123000	-1.24054000
O	-4.49995800	1.08360600	-0.57380300
O	2.07367300	2.95361600	0.33028700
O	0.77489500	0.38093400	1.48368400
Cl	0.60207700	2.58803100	-0.48162300
H	2.47700700	3.64980600	-0.21996400
O	0.31760000	3.82785000	-1.22029900
O	-1.32701800	0.33194400	2.84123300
O	3.47812000	-1.27740700	1.11095500
Cl	0.09540800	-0.45436000	2.50380700
H	-1.93981400	0.15134100	2.07402000

O	-0.30814600	-1.76316200	1.94463800
O	4.39143100	-0.27942400	-1.02217200
O	2.11468400	-1.25847700	-0.91769800
Cl	3.02201800	-0.48078900	-0.03216500
H	4.47740100	-1.12257000	-1.50506700
O	0.98430400	1.47710100	-1.37590200

(CA) ₆	x	y	z
O	-3.93046100	-1.75271300	0.35097800
O	-1.66151300	-2.80884500	0.25541400
Cl	-2.69275200	-2.24633100	-0.64971000
H	-3.63226000	-0.88800400	0.74011900
O	0.24232500	-2.47249600	-2.90297800
O	-0.64615000	-1.94467200	2.67343000
O	-0.16485900	0.22805300	1.58832000
Cl	0.48993100	-0.70836300	2.56100700
H	-0.89379900	-2.20962900	1.75311300
O	0.49845600	-0.20345900	3.92718800
O	-2.80817600	0.63982100	1.19746500
O	-4.15868900	1.86638600	-0.43489000
Cl	-2.73945500	1.76757100	-0.11492900
H	-1.87052000	0.51634600	1.50139000
O	-2.23876900	-1.00609900	-1.31835200
O	3.16440600	-1.91970100	0.18935500
O	2.67218300	0.43436200	0.81073200
Cl	3.81810000	-0.36160800	0.29283800
H	2.31319200	-1.80616500	-0.29958900
O	4.87706400	-0.56737600	1.27747500
O	0.73374600	-1.15226000	-0.88075300
O	0.23118200	1.58387500	-0.94777200
Cl	0.57919600	-1.07577000	-2.61826800
H	0.57489100	-0.23008200	-0.57043800
O	1.92676700	-0.68811400	-3.04989000
O	0.26202200	4.00622000	-0.42032200
O	-2.19432700	2.97819300	0.54186100
Cl	1.17333600	2.58836500	-0.35840200
H	-0.62000300	3.76969500	-0.05183100
O	2.28178800	2.92347900	-1.24474300

(CA) ₁ (DMA) ₁	x	y	z
C	-2.05160100	1.31109900	-0.02256300
H	-2.57068900	1.40140600	0.92765000

H	-1.26918000	2.06048600	-0.09827900
H	-2.75968300	1.41183300	-0.84093500
H	-0.81999300	-0.08411500	-0.92637500
C	-2.31493500	-1.17001400	-0.01246200
H	-3.01606500	-1.13898500	-0.84220500
H	-1.71338700	-2.07308400	-0.06038300
H	-2.85615900	-1.13260000	0.92873300
N	-1.40579100	-0.01264000	-0.08601300
O	1.16017600	1.26039300	-0.47526800
O	0.81084300	-0.23627300	1.33640400
Cl	1.59264500	-0.04049800	0.06545400
H	-0.65738800	-0.09068000	0.67233800
O	1.10739900	-1.07709800	-0.86876300

(CA) ₁ (DMA) ₂	x	y	z
C	-2.61715500	-1.50618900	-0.92179500
H	-3.54111000	-1.06292500	-0.53724900
H	-2.46485100	-1.15129400	-1.94348800
H	-2.75291900	-2.59619700	-0.95207100
H	-0.61360200	-1.43722000	-0.49724800
C	-1.57617400	-1.60997100	1.28019100
H	-0.64610300	-1.36833500	1.79785200
H	-2.41453300	-1.13506200	1.80039700
H	-1.72614500	-2.69773800	1.31507600
N	-1.49112500	-1.10476000	-0.08845600
C	-0.61493100	1.98490000	1.35980800
H	-1.62006800	1.97817700	1.78454400
H	0.03706000	1.30397100	1.90660500
H	-0.20530700	2.99533900	1.39752700
H	0.32016400	1.39990100	-0.38640600
C	-1.42925400	2.38416900	-0.95085800
H	-0.98140000	3.37810300	-0.98265400
H	-1.40725700	1.94736700	-1.94890700
H	-2.46240900	2.46068800	-0.60826800
N	-0.66610100	1.52101400	-0.03838500
O	1.87173700	0.92175700	-0.77889500
O	1.56039200	-0.37368300	1.26247000
Cl	2.12678800	-0.45239600	-0.13888400
H	-1.06922400	0.51991500	-0.05894500
O	1.30761800	-1.45747200	-0.91381600

(CA) ₁ (DMA) ₃	x	y	z
C	-3.31936200	0.24040300	-1.07151300
H	-4.07444300	0.85582700	-0.56773100
H	-2.83967200	0.85481900	-1.83903400
H	-3.84466700	-0.58703800	-1.57854500
H	-1.56193200	-0.66500500	-0.60904000
C	-2.87866800	-1.15523100	0.85171900
H	-3.41730600	-1.99379500	0.37886000
H	-2.06832900	-1.57836500	1.45132600
H	-3.58185700	-0.64077500	1.51895900
N	-2.32686700	-0.21290800	-0.11008400
C	-0.58645600	1.11122100	2.39779700
H	-0.37339500	2.15884900	2.62284400
H	-1.49329400	1.02872300	1.79418700
H	-0.69610700	0.55373800	3.33072800
H	0.32929100	-0.44215100	1.34542200
C	1.84755500	0.61659800	2.24615600
H	2.56194000	0.13077100	1.58011800
H	2.12176400	1.66234700	2.40194500
H	1.82011200	0.09672300	3.20621000
N	0.52168700	0.55095400	1.60481800
C	1.88504100	2.13047000	-1.32862000
H	2.25453400	2.95218400	-0.70488600
H	2.56636300	1.28113700	-1.24249100
H	1.87179500	2.47389900	-2.37345700
H	0.30127200	0.85696000	-1.35231400
C	-0.46605600	2.73358400	-1.03067700
H	-0.59180500	3.04249700	-2.07914700
H	-1.41616500	2.34311300	-0.65680900
H	-0.20050600	3.62245100	-0.44767200
N	0.56454700	1.71541900	-0.86198400
O	0.16725800	-1.16893900	-1.65674700
O	2.31005900	-1.09104600	-0.46693500
Cl	1.08218400	-1.93765000	-0.71389700
H	0.56452200	1.06164300	0.64684200
O	0.33440600	-2.04141500	0.62310400

(CA) ₁ (DMA) ₄	x	y	z
C	-4.66769900	0.08685400	0.63407400
H	-5.62586000	0.03108400	0.10399000
H	-4.71616500	-0.59796300	1.48523200
H	-4.56564200	1.11858100	1.02335600

H	-2.72923600	-0.43072500	0.26248300
C	-3.41148500	0.59623200	-1.37057600
H	-3.30767600	1.65628100	-1.06778800
H	-2.31559000	2.11142000	0.95367100
H	-4.27600200	0.53400100	-2.04216200
N	-3.59488000	-0.30941200	-0.25410100
C	-0.44234500	2.92606500	-0.78134700
H	-0.06060600	3.83831000	-0.30686700
H	0.16871000	2.72223300	-1.66531700
H	-1.47205500	3.12898900	-1.11994700
H	-0.53215400	0.93975900	-0.35034900
C	-1.27230400	1.93343000	1.26348700
H	-2.51949000	0.30783200	-1.93257900
H	-1.25214500	1.01450200	1.85666800
H	-0.96962700	2.76954900	1.90655000
N	-0.35020500	1.80989200	0.14595200
C	1.86184900	0.79377900	2.40050600
H	2.91966200	1.03266800	2.53218900
H	1.35731600	1.59134200	1.85127800
H	1.39690600	0.65068300	3.37850900
H	0.73958400	-0.67188800	1.42470100
C	2.41049700	-1.61981400	2.17104500
H	2.20839900	-2.46612200	1.51371100
H	3.48470600	-1.43128700	2.22980900
H	2.01778300	-1.82081800	3.17010000
N	1.74031500	-0.43709600	1.59985900
C	3.47474900	-0.91512100	-1.52144800
H	4.43046700	-0.89438700	-0.98590000
H	3.02471100	-1.90415400	-1.41166400
H	3.67573900	-0.72997700	-2.58671400
H	1.63997600	-0.05658400	-1.35611900
C	3.01055900	1.45302400	-1.12815900
H	3.13772500	1.72198400	-2.18728800
H	2.27715700	2.12510000	-0.67514300
H	3.97374500	1.59732300	-0.62629600
N	2.56783900	0.07502700	-0.94560000
O	-0.25122100	-0.83577400	-1.54751400
O	0.85387100	-2.70796400	-0.41090900
Cl	-0.46216400	-1.98609000	-0.57492800
H	2.13056200	-0.24627300	0.60231200
O	-0.77959600	-1.32914700	0.78323900

(CA)₂(DMA)₁

x

y

z

O	-1.22412300	-0.28365400	1.09466400
O	-1.60267500	1.16237500	-0.84473400
Cl	-2.10776700	-0.14120800	-0.31239100
H	-0.62754800	-1.11371900	0.98132800
O	-3.49972600	-0.03815000	0.13988200
C	0.76890500	2.55224300	1.27985100
H	0.27452000	3.46667600	0.94943800
H	0.11929800	2.00867300	1.96560000
H	1.71510500	2.79072100	1.76710300
H	1.47842100	0.79095300	0.41912500
C	1.88200700	2.28513500	-0.94048900
H	2.85301000	2.53645900	-0.51207000
H	2.00375100	1.54512900	-1.73142100
H	1.39949400	3.18186200	-1.33166400
N	1.03020600	1.68744600	0.11012500
O	2.26905900	-0.69844000	0.69565300
O	0.36580000	-2.25556200	0.68530800
Cl	1.53356900	-1.73113600	-0.15820600
H	0.12555300	1.41466100	-0.30944000
O	0.93375700	-0.97245300	-1.31954500

(CA) ₂ (DMA) ₂	x	y	z
C	0.49782300	-2.73107600	1.38173000
H	1.17509100	-3.56731000	1.20119100
H	1.01374000	-1.95302400	1.94413300
H	-0.38819800	-3.07084500	1.91962600
H	-0.55687100	-1.35551600	0.28504000
C	-0.56614300	-3.11173500	-0.83419800
H	-1.46408500	-3.50981900	-0.36239600
H	-0.85375800	-2.58361000	-1.74183600
H	0.13912200	-3.91177100	-1.06518600
N	0.08411900	-2.15410300	0.08485500
O	-2.92855500	1.23561900	-0.54259500
O	-2.92840500	-1.23594900	-0.54250700
Cl	-2.88793500	-0.00013100	0.30971700
H	0.93193600	-1.75304800	-0.37548500
O	-1.45926900	-0.00002900	0.95237100
C	-0.56650200	3.11167200	-0.83419000
H	0.13872700	3.91167600	-1.06540300
H	-0.85431200	2.58344500	-1.74170700
H	-1.46434600	3.50982800	-0.36225800
H	-0.55699500	1.35551400	0.28513800
C	0.49774400	2.73121400	1.38163700

H	-0.38823600	3.07094800	1.91962400
H	1.01379200	1.95323300	1.94401900
H	1.17492600	3.56748900	1.20096700
N	0.08392200	2.15413600	0.08484600
O	2.42887600	-1.22836000	-1.04669800
O	2.42868900	1.22850700	-1.04678200
Cl	2.94129700	0.00013700	-0.30355900
H	0.93171300	1.75310500	-0.37555900
O	2.26660000	0.00013000	1.05540500

(CA) ₂ (DMA) ₃	x	y	z
C	-1.54965300	-1.30046300	1.87611800
H	-0.76714800	-1.90476200	2.34912500
H	-1.11813500	-0.33793900	1.59177800
H	-2.34693400	-1.12175300	2.61099900
H	-2.66217700	-1.31655700	0.19291100
C	-2.73097700	-3.22041200	0.95510300
H	-3.57037500	-3.09027800	1.65402100
H	-3.11813400	-3.64538000	0.02541200
H	-2.03197600	-3.93955800	1.39681900
N	-2.03709100	-1.96955200	0.67102700
O	-3.45700800	0.34404800	-0.46598000
O	-1.10645100	0.76073200	-1.02679100
Cl	-2.50282500	1.42397400	-0.90157800
O	-2.35959100	2.45135800	0.19496000
C	0.45541800	2.29379000	1.79604300
H	-0.59667200	2.54026200	1.94500600
H	0.67845200	1.29410100	2.16922500
H	1.10101600	3.02316500	2.28847500
H	1.68659900	1.91450300	0.17529000
C	0.61708000	3.63757700	-0.28191200
H	1.34182800	4.31389700	0.17407500
H	0.82540600	3.54065400	-1.34774900
H	-0.40024600	4.00106400	-0.13340200
N	0.73492600	2.30402400	0.34365700
O	1.90335300	-0.47428000	0.99108500
O	3.25495000	-1.02289900	-0.96161200
Cl	3.26569000	-0.23041500	0.31693300
H	0.05922200	1.66122700	-0.12979300
O	3.29019300	1.25491900	-0.01891700
C	0.28284100	-1.77636800	-2.17744000
H	-0.22883900	-2.60129900	-2.67787100
H	-0.26358000	-0.84603000	-2.33104400

H	1.30682600	-1.68419900	-2.54321700
H	0.84954400	-1.29576200	-0.24263400
C	0.96599800	-3.32284100	-0.37060000
H	1.99530200	-3.31485100	-0.73227900
H	0.96360500	-3.42365700	0.71554300
H	0.40836600	-4.14655800	-0.82092900
N	0.32012000	-2.04493100	-0.72583000
H	-0.66658000	-2.02461100	-0.29365600

(CA) ₂ (DMA) ₄	x	y	z
C	1.77854400	2.90231600	0.61433500
H	1.89084000	3.78794800	-0.01286500
H	1.08210500	3.11717500	1.42576900
H	2.73737200	2.58273800	1.02330400
H	1.14969600	0.94393600	0.39280900
C	2.05287700	1.45889900	-1.38276300
H	3.02989900	1.11686000	-1.04029900
H	1.54154900	0.66824600	-1.93036200
H	2.14832100	2.34375200	-2.01454300
N	1.22721600	1.80044600	-0.20246600
O	1.28604000	-0.47478300	1.39777800
O	3.05793800	-1.52742000	0.08374100
Cl	2.78248000	-0.87602900	1.41894800
H	0.26728200	2.05467600	-0.51515900
O	3.56153200	0.40962500	1.50347600
C	-1.10656400	1.30665900	2.81032200
H	-1.32488500	0.52523600	3.54640300
H	-0.04563400	1.22145900	2.56269800
H	-1.30077800	2.28044700	3.28675600
H	-1.72659700	1.80287900	0.91795900
C	-3.35192700	1.10183100	1.89979000
H	-3.66892800	2.00594500	2.44187900
H	-3.89527800	1.05014700	0.95388200
H	-3.61553000	0.23326300	2.51609100
N	-1.91884600	1.08620000	1.61847000
C	-1.33552600	-2.21940100	1.73852300
H	-1.31829800	-3.29046300	1.52553800
H	-0.39034900	-1.90878200	2.18475800
H	-2.16522900	-1.99504200	2.41316700
H	-1.54024900	-0.44393800	0.73916500
C	-2.73722700	-1.82094300	-0.25655900
H	-2.80659300	-1.17902200	-1.13331400
H	-2.68690500	-2.87214200	-0.55091400

H	-3.60851200	-1.65723400	0.38104100
N	-1.50986400	-1.46825500	0.48183400
C	0.20722100	-2.41000900	-2.57747600
H	-0.71704400	-2.96336000	-2.77839500
H	0.03865100	-1.37030400	-2.86458700
H	1.00444000	-2.84294500	-3.20111800
H	1.35373600	-1.93860700	-0.94384500
C	0.74689700	-3.84327700	-0.69264200
H	1.51935600	-4.36265900	-1.27906900
H	1.06910000	-3.82519900	0.35157800
H	-0.18113100	-4.42347100	-0.76510600
N	0.51233500	-2.47784500	-1.15125300
O	-1.30082100	2.69442600	-0.93331900
O	-0.98388200	0.48478800	-1.88993300
Cl	-1.91970300	1.68456200	-1.92295600
H	-0.67985900	-1.67884700	-0.15274300
O	-3.24975600	1.26127500	-1.37048300

(CA) ₃ (DMA) ₁	x	y	z
O	-1.28944300	1.39703100	-1.92806600
O	0.13467300	1.78212800	0.08120000
Cl	-0.97902100	2.42248700	-0.69005400
H	-1.57154400	0.49886800	-1.52451800
O	-2.20317700	2.49515900	0.13367900
C	-1.86891200	0.07097900	2.42614100
H	-1.82759500	1.07644200	2.84551700
H	-2.53284700	0.05522600	1.56242000
H	-2.20681600	-0.64258300	3.17848300
H	-0.58645900	-1.23623700	1.48231600
C	0.50664300	-0.38138400	3.04207000
H	0.20148600	-1.12603500	3.77810000
H	1.46053000	-0.65381300	2.59349100
H	0.58475400	0.59975400	3.51158900
N	-0.51451000	-0.32082200	1.97097600
O	-1.10394800	-2.61875700	0.46134600
O	-2.07196400	-0.75389600	-0.75751300
Cl	-1.42754400	-2.14419700	-0.93885400
H	-0.20421400	0.34463400	1.24564500
O	-0.12881800	-1.93104400	-1.68861700
O	1.61026100	-0.99503400	0.11468400
O	3.08000900	0.74736300	0.90520900
Cl	2.69660500	0.20508200	-0.40960600
H	1.10952400	-1.35616700	-0.67058500

O	3.77268900	-0.52949300	-1.08798500
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(CA) ₃ (DMA) ₂	x	y	z
O	-3.16567500	-0.98048200	0.88207000
O	-2.66056500	0.03656800	3.02793200
Cl	-2.35600900	0.28501200	1.61436300
H	-2.91421200	-0.94532100	-0.09128000
O	-0.92669900	0.03442000	1.27846900
O	2.92159100	1.01464900	1.38625000
O	3.04294900	-0.12281400	-0.76703100
Cl	3.45060100	-0.23569600	0.69098400
O	2.70310100	-1.43384900	1.26159200
C	-0.39973500	-2.99801600	0.28129600
H	0.10915600	-3.92392400	0.55264000
H	-0.78949000	-2.50826100	1.17161100
H	-1.21435600	-3.20041300	-0.41499200
H	0.10838300	-1.22262300	-0.66900700
C	1.23126400	-2.66727500	-1.56421600
H	0.47090700	-2.88157600	-2.31601300
H	1.94394100	-1.93189900	-1.93609200
H	1.75221400	-3.58145300	-1.27632400
N	0.57345200	-2.09423600	-0.36835700
O	-2.33890800	-0.97984500	-1.63725700
O	-2.20320400	1.44888000	-1.28132300
Cl	-1.71936000	0.32033500	-2.15330100
H	1.31613000	-1.81270500	0.31284900
O	-0.21452400	0.17944200	-1.90619200
C	1.57050700	2.69502900	-1.29973800
H	2.22559800	3.49793400	-0.95879700
H	2.15639100	1.91220600	-1.77981700
H	0.81481100	3.08313900	-1.98355400
H	0.31408400	1.31836700	-0.47446400
C	0.06371500	3.04284700	0.64529200
H	-0.80471300	3.32069900	0.04652800
H	-0.25488900	2.55110100	1.56290600
H	0.66048700	3.92279500	0.88909000
N	0.89613500	2.09697900	-0.12600300
H	1.62444200	1.66785900	0.49373200

(CA) ₃ (DMA) ₃	x	y	z
O	0.03532100	2.08314000	0.96710300

O	1.99673200	2.35668900	-0.45791700
Cl	1.54685000	2.31972700	0.98367700
O	2.17444400	1.09329600	1.63552500
C	-1.93655900	0.58577600	3.05556000
H	-1.29607000	1.22531600	3.66428400
H	-2.59021100	1.18643500	2.42371800
H	-2.53356200	-0.06914200	3.69217000
H	-1.70506000	-0.78336500	1.52346800
C	-0.17038700	-1.15706600	2.88028800
H	-0.75178100	-1.79434800	3.54870900
H	0.34420200	-1.76711900	2.13774600
H	0.54767100	-0.56355100	3.44819000
N	-1.09115100	-0.24296000	2.17217400
O	-3.34115000	0.82472000	0.17754800
O	-2.78716400	-0.59720700	-1.72827000
Cl	-3.56703600	-0.55449000	-0.41835500
H	-0.54221000	0.38559300	1.56449000
O	-2.93659300	-1.55780700	0.53856100
C	0.12138400	1.21919900	-2.79480400
H	-0.40117400	1.21458600	-3.75284100
H	0.85131200	2.02837100	-2.75728900
H	0.61829300	0.26229300	-2.63384500
H	-1.53617100	0.61946800	-1.69485600
C	-1.62626300	2.68508000	-1.80925700
H	-2.14368500	2.71880400	-2.76935500
H	-2.35142700	2.69922200	-0.99625000
H	-0.93170000	3.52153700	-1.72183000
N	-0.86740600	1.42150300	-1.71571500
H	-0.38985800	1.39923600	-0.80190300
C	4.24567100	0.12224200	-0.91515600
H	4.82815500	-0.49552100	-1.60032400
H	3.73223800	0.92033300	-1.45002000
H	4.89654900	0.56150500	-0.15769700
H	2.62605000	-0.10691100	0.33524800
C	3.78432100	-1.78441900	0.61319900
H	4.31616000	-1.32485200	1.44764800
H	2.95256000	-2.39510500	0.96679200
H	4.46437300	-2.40237400	0.02493600
N	3.23023100	-0.71821100	-0.24953400
O	0.15195900	-0.74683600	-0.26252800
O	1.41244100	-1.99711900	-1.90271400
Cl	0.28051900	-2.14053000	-0.87125200
H	2.59956300	-1.15824700	-0.96254400
O	0.77457800	-3.04975600	0.22420000

(CA) ₃ (DMA) ₄	x	y	z
C	2.14557600	0.53565900	2.70890400
H	2.50425000	-0.23340900	-1.33660200
H	3.00134400	0.44707900	2.03667100
H	1.33589700	-0.42745200	4.49163400
H	1.06149700	1.22782800	1.11054700
C	-0.35641200	0.65870800	2.50767800
H	-0.30150500	1.54751300	3.13938900
H	-1.12853100	0.80103100	1.75013200
H	-0.57877000	-0.22545300	3.10366300
N	0.94529200	0.48177200	1.82846500
O	3.25317300	1.02507400	-0.34538200
O	1.94582000	2.20386300	-2.03628700
Cl	2.66871900	2.39624200	-0.73348400
H	0.95025600	-0.41863400	1.32341000
O	1.65519200	2.73459000	0.35552800
C	-1.83649600	3.25550100	0.81934800
H	-1.70327200	3.54245300	1.86930700
H	-0.88198600	2.86776600	0.45214800
H	-2.07558100	4.16972900	0.25131000
H	-2.89122200	1.88964600	-0.23822100
C	-4.18519600	2.73914500	1.08419000
H	-4.48993700	3.62834800	0.50643200
H	-4.94114900	1.96149600	0.93419300
H	-4.19281800	3.01323300	2.14532500
N	-2.87137100	2.23263400	0.71998900
O	-2.30484200	0.74466900	-1.94392000
O	-0.28474300	-0.12317700	-3.03776800
Cl	-0.77179500	0.85010800	-1.98490100
O	-0.30019500	0.30141100	-0.64529500
C	2.14766400	-0.55158100	3.76955500
H	2.16715000	1.53670500	3.14811200
H	2.06474900	-1.53861700	3.30741100
H	3.09063300	-0.50943700	4.32031400
H	1.69252800	-1.60063600	-0.90501100
C	3.00728600	-1.91052600	-2.49601100
H	3.84514600	-2.18344500	-1.85462900
H	2.50290400	-2.81112500	-2.84583400
H	3.36873400	-1.33284800	-3.34644900
N	2.05607300	-1.09024300	-1.72473800
O	-0.81828300	-2.35442800	1.56176400
O	-0.07527400	-3.49883400	-0.47694900
Cl	0.31530600	-3.16188800	0.93453200

H	1.24292000	-0.79083600	-2.29171700
O	1.50966300	-2.20058400	0.85511900
C	-3.06707500	-2.56788200	-1.05370200
H	-3.99405200	-2.38047100	-1.59756700
H	-2.24471100	-2.73465200	-1.74808400
H	-3.17195900	-3.43628000	-0.40251700
H	-1.84336600	-1.55386900	0.25130300
C	-3.75112300	-1.04121400	0.79339100
H	-3.80446600	-1.85131700	1.52213200
H	-3.44157700	-0.10856300	1.27133000
H	-4.72098800	-0.90498600	0.31127900
N	-2.74419300	-1.38238400	-0.23246300
H	-2.59386000	-0.56408300	-0.86565300

(CA) ₄ (DMA) ₁	x	y	z
O	-2.39124600	-1.71954600	-1.80944700
O	-1.54017600	-2.24241800	0.48311600
Cl	-1.41321400	-2.68327400	-0.92231900
H	-2.16970400	-0.73380700	-1.61000600
O	-0.03290400	-2.43793000	-1.44349000
C	1.00725100	2.90911600	-1.67377200
H	2.05577600	2.65977800	-1.83625200
H	0.38152100	2.38195000	-2.39323800
H	0.84953600	3.98534800	-1.75362300
H	-0.39924700	2.64497500	-0.19143000
C	1.38163500	3.09740100	0.78453700
H	1.22639500	4.17633400	0.74720900
H	1.01638700	2.69409200	1.72817200
H	2.43701400	2.85696700	0.65947300
N	0.61666200	2.46664500	-0.31573200
O	-2.16111700	2.85670300	-0.23436200
O	-1.85266200	0.74804400	-1.38219800
Cl	-2.82460500	1.51731800	-0.45362200
H	0.72188900	1.44275500	-0.26951700
O	-2.85157800	0.75928900	0.85486700
O	-0.30671500	0.50008600	1.55692200
O	1.43750500	-1.20242600	1.77040200
Cl	0.18140200	-0.84923000	2.46174600
H	-1.29745600	0.45543500	1.40662800
O	0.40777400	-0.30364300	3.80687200
O	1.39874200	-0.14814900	-1.17143600
O	3.61597000	-1.13973400	-1.84704400
Cl	2.99318600	-0.52823400	-0.66925900

H	0.87515200	-0.98905500	-1.22050000
O	3.45805400	0.84705800	-0.40472300

(CA) ₄ (DMA) ₂	x	y	z
O	-1.85353800	-2.91785500	-0.42439300
O	-2.77673600	-0.92650200	-1.54115200
Cl	-2.91857000	-1.84052200	-0.32942300
H	-0.46222700	-2.76853000	-1.31603100
O	-2.60197400	-0.98760300	0.89164300
C	-0.11433100	-2.45758400	2.35724800
H	-0.95376500	-2.64267000	3.02835600
H	-0.29442700	-2.96249400	1.40879500
H	0.82139000	-2.79602500	2.80267500
H	0.83331800	-0.84821600	1.52839500
C	0.09834900	-0.18202500	3.32618000
H	0.94470700	-0.54710700	3.90873800
H	0.27458800	0.85131600	3.03494400
H	-0.82699000	-0.26643200	3.89694100
N	-0.01439200	-1.00267600	2.10146900
O	0.43789400	-0.65376000	-0.73762500
O	0.44319700	-2.92635800	-1.72171800
Cl	1.32272700	-1.52064600	-1.57770800
H	-0.83730900	-0.71632900	1.54668600
O	1.43027300	-0.99486800	-2.94780600
O	-1.74298500	1.43250500	-1.10196400
O	-1.35952200	1.69512600	1.33528700
Cl	-2.45534500	1.89548000	0.35554700
H	-2.04161100	0.47738300	-1.27704200
O	-2.71593200	3.32411200	0.11665600
C	0.76968800	3.60310300	-0.28527600
H	0.11135800	4.13193700	-0.97548900
H	0.27467800	3.48501900	0.67729500
H	1.70707300	4.14580000	-0.15975800
H	1.60906100	1.73502000	-0.10027200
C	1.82851600	2.28696700	-2.10205400
H	2.80009000	2.74626100	-1.92067700
H	1.96911100	1.26733000	-2.45486000
H	1.26223300	2.86561200	-2.83344200
N	1.07297700	2.25933300	-0.82844500
O	2.67532200	-1.19183800	1.39088900
O	3.49448200	0.14817700	-0.50072500
Cl	3.36560700	0.10550200	1.00210300
H	0.19575600	1.73764000	-0.96031300

O	2.38523100	1.22864500	1.37939300
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(CA) ₄ (DMA) ₃	x	y	z
O	-1.28554000	-1.45918700	-2.32401100
O	0.60849100	-0.20891000	-3.14453900
Cl	0.28436700	-1.03996300	-1.97036000
H	-1.64834900	-1.99713600	-1.53564100
O	0.15080200	-0.20427100	-0.74010300
O	1.26081100	2.27549400	1.66805400
O	-1.07745600	1.56953100	1.61503000
Cl	-0.16707900	2.78699000	1.50296100
O	-0.30616900	3.31316600	0.09289100
C	-2.17533600	1.89680800	-2.09487300
H	-1.67250100	2.84037400	-1.88263200
H	-1.50011100	1.21946500	-2.61530900
H	-3.06962100	2.06022100	-2.69808900
H	-2.97699000	0.33963400	-0.94854700
C	-3.57310100	2.07384200	-0.05104400
H	-4.49230000	2.13072400	-0.63551100
H	-3.75394700	1.56357900	0.89359500
H	-3.16768900	3.06946600	0.12904000
N	-2.57435300	1.28627100	-0.80877900
O	-4.02947700	-1.09341400	-0.62995300
O	-2.24993100	-2.73913300	-0.28744300
Cl	-3.33872300	-1.92985600	0.43416400
H	-1.75057700	1.16469500	-0.19665700
O	-2.64351800	-0.97148300	1.37440300
C	0.61801900	-0.41571700	3.46582800
H	1.40670100	-1.02121000	3.91409500
H	0.96425400	0.60743600	3.32949600
H	-0.27917800	-0.43685300	4.08522700
H	-0.46476600	-0.42791900	1.71156200
C	-0.06934800	-2.41347400	2.17671700
H	-0.91310100	-2.53742700	2.85557300
H	-0.35017800	-2.73460300	1.17650000
H	0.79816600	-2.97859100	2.51715600
N	0.29505100	-0.97900700	2.13625100
H	1.13427500	-0.86865000	1.53578800
C	3.97325100	1.98892800	-0.06009000
H	3.91031800	3.01602100	0.30124300
H	4.20293300	1.31320300	0.76355700
H	4.73253200	1.90353700	-0.83880900
H	2.72070100	0.59083600	-0.89070600

C	2.20821900	2.41608400	-1.75656200
H	2.94263300	2.34479200	-2.56013900
H	1.24873400	2.03213200	-2.09796400
H	2.09298000	3.44803900	-1.42434900
N	2.66226600	1.59304800	-0.61660100
O	2.93557600	-0.90195900	1.14915200
O	2.04859100	-2.85228900	-0.03031900
Cl	3.20428500	-1.89568200	0.01103500
H	1.96944000	1.66309100	0.15399800
O	3.17323800	-1.05870700	-1.27193200

(CA) ₄ (DMA) ₄	x	y	z
O	3.04217200	2.05576500	-0.20840600
O	1.00069600	2.66080400	0.95858800
Cl	1.90610300	3.07646500	-0.19647700
O	1.12047300	2.90643400	-1.47397800
C	4.39867200	0.10596900	-2.43620800
H	4.53073300	1.11716600	-2.82322500
H	5.03135600	-0.05409500	-1.56342300
H	4.63247000	-0.62956300	-3.20759400
H	2.89464900	-0.99779000	-1.55707100
C	2.00208400	0.08538900	-3.09780300
H	2.23180800	-0.62753600	-3.89140100
H	1.01498300	-0.11472900	-2.68462300
H	2.04611900	1.10835300	-3.47369300
N	2.99357900	-0.06719800	-2.01273200
O	4.53081700	-1.17688000	0.53878300
O	2.70135700	-2.37725800	1.62569500
Cl	3.77227800	-2.48836100	0.54292600
H	2.79903600	0.63235700	-1.27129500
O	3.05569400	-2.59358600	-0.79888800
C	0.93378100	0.33289600	3.08613000
H	1.15226900	-0.18953100	4.01876700
H	0.69723600	1.37931300	3.28154200
H	0.10135300	-0.15134900	2.57293300
H	2.33828800	-0.72068600	1.97238900
C	3.33716900	0.90311800	2.77926200
H	3.57491900	0.42073300	3.72871900
H	4.15193300	0.75950600	2.07096000
H	3.14182300	1.96552300	2.92725300
N	2.12691400	0.27272200	2.21410900
H	1.89552000	0.73284800	1.32467400

C	-1.87846000	3.09570100	0.09038500
H	-2.94016400	3.22940900	-0.11948600
H	-1.66688700	3.29328900	1.13971000
H	-1.26604000	3.74164000	-0.53815800
H	-0.53951800	1.52036300	0.03136900
C	-1.75677400	1.32440400	-1.62160100
H	-1.11040700	1.95022200	-2.23771600
H	-1.49598900	0.27467400	-1.75950900
H	-2.80982600	1.49591300	-1.84755800
N	-1.52871800	1.68744200	-0.20475000
O	0.74496100	-0.29573500	-0.25405700
O	-1.06040200	-1.40762500	0.92563800
Cl	0.04132500	-1.64152300	-0.11620100
H	-2.10475700	1.08478500	0.41534300
O	-0.65854200	-1.92253600	-1.42869500
C	-3.46092300	-3.52867500	0.24353300
H	-2.64767100	-3.92344300	-0.36713200
H	-3.23383500	-3.68003800	1.29850600
H	-4.40008300	-4.02113100	-0.01298300
H	-4.33525400	-1.64547600	0.56605400
C	-3.84585000	-1.73464900	-1.42755100
H	-4.72128500	-2.29012000	-1.76776500
H	-4.05645200	-0.66520500	-1.47941500
H	-2.96475800	-1.98961600	-2.01672300
N	-3.58187200	-2.07926500	-0.01178200
O	-5.49929500	-0.49917600	1.18603600
O	-3.37435100	0.61493600	1.63020900
Cl	-4.81754800	0.86412100	1.18648800
H	-2.69046600	-1.63646000	0.30034900
O	-4.74252700	1.35742000	-0.24203600

(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

(CA) ₁ (SA) ₁	x	y	z
O	-1.35199400	1.09195100	0.47515700
O	-1.71461100	-1.36561900	0.16706200

Cl	-2.22495500	0.16359200	-0.30556400
H	0.33703400	1.36726000	0.20919000
O	-3.60411800	0.16723900	0.17090300
S	1.86367300	-0.07603600	-0.13366600
O	1.31148400	1.39087100	0.03534800
O	0.83250800	-0.90657800	-0.73132300
O	3.17722300	0.02423800	-0.69889700
O	1.95926000	-0.60885800	1.37423600
H	-0.76002700	-1.40804600	-0.08607300
H	2.74942600	-0.24521300	1.80158700

(CA) ₁ (SA) ₂	x	y	z
S	-2.29595900	-0.89765200	-0.15463900
O	-2.55636400	0.55277400	0.39610500
O	-3.52877700	-1.37834100	-0.70452600
O	-1.05754900	-0.89647100	-0.91452700
O	-1.92653400	-1.72889900	1.16691200
H	-1.70172500	0.98873200	0.63941200
H	-2.73809400	-2.00491200	1.61943600
O	-0.05759600	1.46678000	1.01085600
O	0.34267600	1.98634800	-1.38853200
Cl	0.57173800	2.54598800	0.15590400
H	0.92318600	-0.08975500	1.32945300
O	-0.22656700	3.76670000	0.15883900
S	2.18561500	-1.16351100	-0.01995000
O	1.49537100	-0.88347600	1.38693700
O	2.08708400	0.07783600	-0.79214300
O	3.45840800	-1.76820300	0.21182700
O	1.25934400	-2.25331300	-0.67874600
H	0.88969800	1.15675300	-1.43068100
H	0.35690900	-1.88788800	-0.83859100

(CA) ₁ (SA) ₃	x	y	z
S	-0.34412600	-2.75861300	0.34993600
O	-1.35956800	-2.03586300	1.29086400
O	-0.94678200	-3.97156100	-0.11135300
O	0.20529700	-1.78522400	-0.59857200
O	0.90959000	-3.05756300	1.29000800
H	-1.02309200	-1.13759700	1.57380400

H	0.74657400	-3.84853100	1.82758000
O	-0.29437900	0.28261700	2.00595900
O	-2.45709800	1.27039200	1.37716300
Cl	-1.13896100	1.77414900	1.84406000
H	0.62628800	0.43307500	1.62571100
O	-1.20473700	2.29977400	3.20126700
S	-1.39373500	0.84538100	-1.97833900
O	2.07166200	0.72112300	1.07277100
O	-2.60901900	0.23720400	-1.16784800
O	-1.82215400	1.77777600	-2.97350000
O	-0.86622700	-0.43628500	-2.71798300
H	-2.64658100	0.63398300	-0.26607400
H	-0.52851600	-1.08617400	-2.06089600
S	2.87352800	0.74621800	-0.15572900
O	2.71563200	-0.66287700	-0.86187000
O	-0.40744100	1.26894200	-0.96981200
O	4.26672100	1.04750000	-0.08575600
O	2.21232000	1.76096900	-1.16144000
H	1.84409800	-1.07393800	-0.67523300
H	1.22718700	1.66293000	-1.17226900

(CA) ₁ (SA) ₄	x	y	z
S	-3.59186900	0.23087000	0.24798900
O	-3.46856900	-1.03837100	1.16373700
O	-4.78676200	0.92811500	0.58566600
O	-2.28135300	0.91957400	0.30621200
O	-3.74278600	-0.32219200	-1.22300800
H	-2.57374000	-1.45361900	1.07707800
H	-2.87787800	-0.61846400	-1.58351900
S	0.31228900	2.45498300	-1.32499400
O	0.71277800	2.90955500	0.12266900
O	0.93246000	3.31736700	-2.27524300
O	0.58621400	0.99418200	-1.40513900
O	-1.23906900	2.64748700	-1.40574800
H	0.55327500	2.19429100	0.79049600
H	-1.72491800	2.06632200	-0.76047600
O	-0.01403400	0.93218100	1.79134900
O	2.10233700	0.42948200	2.88011500
Cl	0.85615800	-0.32741900	2.62827400
H	-0.85168300	0.56519300	1.42693500
O	0.07528300	-0.55761000	3.83634400

S	3.47175000	-0.41608800	-0.27736100
O	-0.90171500	-1.78532500	0.62125500
O	3.55035000	0.92819500	0.55275600
O	4.72859200	-1.09147900	-0.33712500
O	3.13499700	0.12741700	-1.70565500
H	3.17017200	0.79155600	1.45030600
H	2.22772100	0.52344200	-1.71506600
S	-0.77352300	-2.31753400	-0.74434500
O	-1.06514100	-1.09098200	-1.74064100
O	2.29367800	-1.13281800	0.25391100
O	-1.64038900	-3.37087700	-1.16853200
O	0.70603500	-2.69201200	-1.01595300
H	-0.46512600	-0.31239200	-1.58653800
H	1.36437300	-2.12517800	-0.50199900

(CA) ₂ (SA) ₁	x	y	z
O	2.15234000	-1.00248200	1.32382400
O	2.39749600	-2.81243500	-0.28611900
Cl	2.12042000	-1.38017200	-0.31930000
H	1.72201100	-0.11844600	1.40707600
O	0.71582000	-1.05526100	-0.71073800
O	-0.15708700	2.17618200	-0.93200600
O	0.62386900	1.36333100	1.31350500
Cl	0.97331500	2.37993500	0.00254900
H	-1.36219200	0.80290800	-1.28261800
O	2.24541900	1.81789300	-0.46503100
S	-2.45704400	-0.40234700	0.10804300
O	-2.12929100	0.19499400	-1.32592300
O	-1.76575200	0.43300200	1.09660700
O	-3.86466900	-0.60615500	0.22256500
O	-1.77940000	-1.82523700	0.06930200
H	-0.33151300	1.03513100	1.21962900
H	-0.81905700	-1.74866400	-0.13590600

(CA) ₂ (SA) ₂	x	y	z
O	0.42834200	1.82133400	-1.10992100
O	0.52336100	1.95027200	1.39287500
Cl	0.87611600	2.72334300	-0.03404100
H	-1.00995800	-0.15161400	-0.86247300
O	2.36379500	2.85178100	-0.02725800

S	-0.81298500	-2.16405800	-0.08619800
O	-0.38858100	-0.91180500	-0.99857700
O	-2.25954400	-2.27169900	-0.09555000
O	0.03130700	-3.24144800	-0.50704700
O	-0.45118500	-1.66788100	1.36975100
H	1.03298100	1.09710000	1.36443900
H	0.50000600	-1.40861400	1.40654800
O	-2.30627400	0.92467800	-0.39934200
O	-3.93026000	-0.37814400	0.99456700
Cl	-3.76799800	0.61704800	-0.34815100
H	1.39143300	-0.64968900	-1.32194900
O	-4.55966100	1.77531300	0.05547100
S	3.01143800	-0.65054100	0.07801300
O	2.37467900	-0.63051600	-1.36570800
O	1.90599500	-0.38973600	1.03044100
O	3.82778800	-1.80311200	0.27664500
O	3.94420300	0.60764500	0.04696800
H	-3.38494100	-1.17759700	0.79350000
H	3.42548200	1.44389000	-0.05836500

(CA) ₂ (SA) ₃	x	y	z
S	0.14232600	-0.14588200	2.71756500
O	-0.14922200	-1.68584000	2.74779300
O	0.72663100	0.26272400	3.95330300
O	0.87812400	0.12236000	1.45461100
O	-1.26190800	0.53301400	2.58190700
H	-0.10565200	-2.08636500	1.84214800
H	-1.71921600	0.22287300	1.75162700
O	0.05059300	-2.87588100	0.32329000
O	1.05285300	-2.87272800	-1.94485300
Cl	-0.13745300	-2.22230700	-0.99801000
H	2.36549600	1.70806200	-1.08779700
O	-1.33489100	-2.74850100	-1.69918100
S	3.56940900	-0.00089600	-0.70177900
O	3.32858000	1.52072700	-1.07483200
O	2.38634800	-0.73080100	-1.16666100
O	4.88327500	-0.35986700	-1.12861400
O	3.54684800	-0.01758300	0.87617200
H	1.82044500	-2.26401300	-1.79546200
H	2.61824200	-0.01710500	1.20876400
O	-1.67754100	2.76012300	-0.26784100
O	0.55171500	1.69747300	-0.65847100
Cl	-0.25345000	3.16441500	-0.27353400

H	-2.45687500	1.56892700	-1.43076400
O	0.13096600	3.97753200	-1.42080700
S	-3.27548500	-0.15001600	-0.49979700
O	-2.85179000	0.72675700	-1.74891400
O	-2.04559000	-0.42721700	0.26858000
O	-4.39759300	0.40449000	0.19413100
O	-3.70315600	-1.45986300	-1.23222900
H	0.47555400	1.09171800	0.12913800
H	-2.90605000	-1.99108000	-1.47798900

(CA) ₂ (SA) ₄	x	y	z
O	1.64158700	1.76165300	0.04337700
O	4.09177800	1.38732000	-0.13685700
Cl	2.83440800	1.62930200	0.94351200
H	1.73832100	-2.12245500	0.95607400
O	3.21113300	2.89644300	1.55901200
S	3.21114400	-2.31698300	-0.59524900
O	2.48774600	-2.74205600	0.72540100
O	2.80441100	-0.92005600	-0.88154600
O	4.60356900	-2.61778400	-0.52220400
O	2.58151600	-3.24102600	-1.70626300
H	3.88634400	0.52082400	-0.56280400
H	1.61474700	-3.09830400	-1.77850100
S	-1.22720700	2.81468700	-1.05658400
O	-0.43264400	2.39929200	-2.34542400
O	-2.33374600	3.64352800	-1.40637700
O	-1.50215900	1.55928000	-0.30525800
O	-0.21004600	3.66856800	-0.22759000
H	-0.03244400	1.49890100	-2.25761000
H	0.61085100	3.14802600	-0.03958300
O	0.50134500	-0.14509300	-2.06547000
O	-1.78131900	-0.91574300	-2.36511700
Cl	-0.70494400	-1.15285200	-1.38700200
H	1.34122100	-0.32848700	-1.55991100
O	-0.12119600	-2.50404100	-1.50639000
S	-4.08576800	-0.69720000	0.33819200
O	0.54522400	-1.01682600	1.14969200
O	-4.37913300	-0.98541700	-1.18808800
O	-5.19239600	-1.17022900	1.10283800
O	-4.04755800	0.87295600	0.44317600
H	-3.55190100	-0.95170100	-1.71242500
H	-3.17654300	1.22424300	0.14024200

S	0.01056400	-0.51803300	2.43150400
O	-0.53827500	0.93439500	2.15890800
O	-2.72044000	-1.18953800	0.59952300
O	0.87881300	-0.46936200	3.56606900
O	-1.25408800	-1.35778400	2.81187700
H	-0.80901000	1.08275900	1.22023700
H	-1.89889700	-1.39312000	2.05616900

(CA) ₃ (SA) ₁	x	y	z
O	0.74147100	1.99203300	1.60375000
O	-0.99557000	3.39812800	0.65138500
Cl	-0.69293500	1.97697100	0.74112900
H	1.19392900	1.12676500	1.44019800
O	-0.24519100	1.39632500	-0.58639600
O	-0.01284600	-1.92184600	-0.47305900
O	1.24020500	-2.48592200	1.61881700
Cl	-0.24707800	-2.05536100	0.99279700
H	1.41327000	-1.33445100	-1.23213600
O	-0.56325800	-0.75990400	1.62230500
S	2.91201800	0.06565000	-0.62902800
O	2.28313500	-1.01964000	-1.58291900
O	2.28573700	-0.12661400	0.69851500
O	4.33207600	0.03275300	-0.75854100
O	2.40624000	1.43803100	-1.20424800
H	1.82772300	-1.71040300	1.42243700
H	1.43416100	1.55424000	-1.06328900
O	-2.20395000	-0.14452100	-2.00275200
O	-3.02709600	-1.67273100	-0.16845400
Cl	-3.40502700	-0.42481500	-0.85442400
H	-1.48304400	0.32782500	-1.52164100
O	-3.31993700	0.75908900	0.03075400

(CA) ₃ (SA) ₂	x	y	z
O	-0.27208000	-3.08665600	-1.08302700
O	-1.20189000	-0.88443300	-1.60917700
Cl	-0.01439700	-1.64461700	-1.08621200
H	4.64178600	-0.11290200	-0.16697900
O	0.04191200	-1.18224300	0.53212500
O	3.09241100	-1.02778900	1.75110000
O	2.88443500	-2.07567300	-0.45453300

Cl	3.75697700	-1.87209700	0.71620900
H	1.18706400	3.37759300	-0.54255400
O	5.03491100	-0.96048400	0.17733500
S	2.30298600	1.59816800	-0.41043600
O	2.14346200	3.15740100	-0.47594400
O	1.89043800	1.35439700	1.09811400
O	1.33704000	0.96510200	-1.28330800
O	3.71395300	1.30777400	-0.58512100
H	2.17999200	0.45337400	1.38375100
H	-0.89836100	-1.14918100	0.83706700
O	-2.69551400	1.97635600	-0.96544700
O	-1.67238300	2.07601000	1.31806000
Cl	-1.35496800	1.98527300	-0.32826900
H	-4.07447300	1.02043400	-0.28278900
O	-0.67584400	3.28138500	-0.52981100
S	-3.89233000	-0.91885700	0.60006800
O	-4.66354800	0.39696500	0.19932900
O	-2.57002500	-0.50578300	1.12311600
O	-4.76597700	-1.70179800	1.41033200
O	-3.63649800	-1.66240200	-0.75832700
H	-2.04298700	1.18841200	1.54261100
H	-2.76351900	-1.40752000	-1.16009700

(CA) ₃ (SA) ₃	x	y	z
O	-2.21105000	1.50267800	1.12082500
O	-2.29375900	1.40425600	-1.35347200
Cl	-2.51086200	2.40826300	-0.05112600
H	1.42338100	-2.55128500	-0.60707800
O	-3.91872400	2.80815700	-0.05656400
S	0.25043100	-1.68330800	-2.17382300
O	0.50731100	-2.66796100	-0.96889400
O	0.17403300	-0.32304400	-1.60716500
O	1.14312900	-1.90262800	-3.27264100
O	-1.18715800	-2.14383600	-2.58097000
H	-2.47684100	0.47900300	-1.03948900
H	-1.83476300	-1.91522200	-1.86657500
O	0.49509700	2.24461600	-0.11698500
O	0.68331600	2.16090300	-2.59239500
Cl	1.44622000	2.66780700	-1.18884700
H	-0.99455300	-1.52790400	1.35275600
O	1.46440900	4.11787600	-1.37863500

S	-3.03498700	-1.81021100	0.73350400
O	-1.71202600	-2.19359700	1.48802400
O	-2.64295900	-1.17892000	-0.54940200
O	-3.88927000	-2.95162600	0.71911800
O	-3.70351200	-0.69255700	1.60936500
H	0.43750400	1.21566600	-2.42453700
H	-3.23937900	0.17763400	1.50705100
O	1.82908800	1.03101600	2.56738400
O	0.27582000	-0.33089700	1.13838200
Cl	0.36792100	0.91385400	2.34281300
H	3.00010200	-0.16706800	2.18697500
O	-0.32507400	0.24662600	3.44139800
S	3.59086400	-0.96740500	0.30073500
O	3.71674300	-0.76696700	1.85931800
O	2.95529100	-2.23438900	0.00625800
O	3.08896900	0.24458400	-0.30606100
O	5.11459600	-1.20315300	-0.06124100
H	0.31778500	0.08629500	0.24124300
H	5.62414900	-0.38718700	0.05910700

(CA) ₃ (SA) ₄	x	y	z
O	-4.70339600	-1.90303900	-0.23979900
O	-5.03564200	-1.63651200	-2.70874100
Cl	-4.14624300	-1.03675500	-1.35048300
H	-4.38936200	-1.36819700	1.40097200
O	-4.51946800	0.38417400	-1.19197600
S	-2.47420100	-0.84275100	2.16785700
O	-4.05139100	-0.97519300	2.24814000
O	-2.05027300	-0.53881100	0.79695100
O	-2.09759800	0.09970500	3.22141000
O	-2.00129200	-2.29911600	2.56090400
H	-5.94316900	-1.75770500	-2.35877100
H	-1.26927400	-2.60201100	1.94569100
S	2.81454500	1.92669900	0.56310900
O	2.45287200	3.45780300	0.63245800
O	4.19964400	1.76954200	0.98256700
O	1.75330400	1.18426500	1.27312500
O	2.78273100	1.53909400	-0.97163300
H	1.46379000	3.57393200	0.75512900
H	1.83345100	1.50171800	-1.30968300
O	-0.20563100	3.73871000	0.86691300
O	-1.68465800	2.69456600	2.52443400

Cl	-1.07991200	2.51701000	0.96079500
H	3.00597000	-2.90995100	-0.12360700
O	-2.28369200	2.64261700	0.07771100
S	1.04197500	-2.29232400	0.51314900
O	2.24844100	-3.29640700	0.40172400
O	0.99402500	-1.44793500	-0.69093700
O	-0.11554300	-3.10756700	0.87107000
O	1.37189900	-1.38400900	1.76600100
H	-1.88619400	1.76145300	2.82938700
H	1.59648900	-0.44374900	1.50439700
O	4.18449400	-2.34029800	-1.20883400
O	4.53762800	-0.94547300	0.77499900
Cl	5.06192000	-1.16751400	-0.86018700
H	-0.34512200	-0.87551500	-1.53806200
O	6.49789400	-1.50101600	-0.79178200
S	-0.62570300	0.98265000	-2.59454800
O	-1.06801100	-0.46801500	-2.09302800
O	0.24249600	1.56699200	-1.54156100
O	-0.15963000	0.95204900	-3.95700000
O	-2.01594200	1.73733000	-2.55241800
H	4.66293200	0.02046300	0.96589900
H	-2.22943700	2.00692600	-1.62212600

(CA) ₄ (SA) ₁	x	y	z
O	-0.86946600	1.74113900	-1.13354200
O	-2.62248400	3.17671600	-0.20529400
Cl	-1.18470200	3.04521000	-0.46290100
H	-2.10771600	0.50822200	-1.57290600
O	-0.42053000	2.92147900	1.00646200
O	1.19666400	-1.05149000	2.01828000
O	-0.96996100	-1.75117600	3.13464800
Cl	-0.54095700	-0.87287200	2.05501700
H	1.35536400	-1.79203300	1.38977400
O	-0.60444600	0.55774200	2.42481500
O	0.13794400	-0.72588100	-1.05634200
O	1.90438900	-2.09616300	-2.15354300
Cl	0.47593000	-2.15417300	-1.33879400
H	1.23138800	0.84463600	-1.10203000
O	0.75696200	-2.87184700	-0.06814500
S	3.17843900	0.81092100	-0.18744100
O	2.03043900	1.41338200	-1.09771500
O	3.17458100	-0.64917100	-0.35804400
O	4.35579700	1.57700600	-0.44294500

O	2.69936600	1.10025300	1.28486500
H	2.52710800	-1.56615400	-1.56884300
H	2.14930500	0.35391900	1.62829900
O	-2.82879300	-0.06828600	-1.93509200
O	-2.38213000	-2.32594600	-0.92295600
Cl	-3.24650700	-1.14382900	-0.72429300
H	-0.64015400	2.03944500	1.39977100
O	-2.92960200	-0.42343800	0.53099300

(CA) ₄ (SA) ₂	x	y	z
O	-0.26663900	-2.82560500	1.25421500
O	0.93116500	-0.84714300	1.89655400
Cl	0.46126800	-1.73422100	0.56666500
H	-1.95267800	-3.10183900	0.87455600
O	1.73309300	-2.21292700	-0.03496500
S	-2.63446600	0.84306500	-0.31475100
O	-1.71576600	0.34623000	0.71007600
O	-2.19859700	0.65514200	-1.69349200
O	-4.05697600	0.22137900	-0.12859200
O	-3.02344000	2.31568800	-0.02347900
H	1.71203600	-0.30003500	1.62430500
H	-2.20051400	2.84543100	0.22081200
O	0.12889800	-0.36137000	-2.54022200
O	1.11482000	1.94954400	-2.80193200
Cl	1.33120900	0.68246100	-2.09710700
H	-0.74031000	0.02603900	-2.22634400
O	1.08766200	0.84488600	-0.61808900
O	-2.89486700	-3.27671200	0.61058000
O	-4.11160200	-2.26495000	-1.25490100
Cl	-2.95206300	-3.16770500	-1.05857000
H	-0.73409600	1.30038900	1.81692700
O	-1.66805900	-2.54646100	-1.43597200
S	0.14916400	3.26203800	1.66767900
O	-0.24060400	1.91929300	2.40648100
O	-0.80005600	3.46267800	0.56642400
O	0.34300500	4.27623000	2.65439700
O	1.55820900	2.95083600	1.03221300
H	-4.10841400	-0.66550500	-0.56571600
H	1.47199100	2.29111000	0.30591700
O	4.38622600	-1.81417500	0.71604700
O	4.11192300	0.08413200	-0.91560200
Cl	4.42344400	-0.15519800	0.50424400
H	3.46618900	-2.10049000	0.49229700

O	3.35934800	0.36470500	1.40496700
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(CA) ₄ (SA) ₃	x	y	z
O	-1.04263200	2.03526000	2.71074100
O	0.89294300	0.46770400	2.43126400
Cl	-0.77306400	0.66014200	2.18932100
H	-0.47867200	3.49683300	1.93699800
O	-1.30864700	-0.36504400	3.08270100
S	-0.30561000	3.52294600	-0.15497800
O	-0.16133400	4.16431300	1.27396600
O	0.19808600	2.15731200	-0.10371200
O	-1.63681900	3.74298100	-0.67891500
O	0.66435600	4.43247400	-0.98539200
H	1.33195200	0.84487300	1.63750700
H	1.57207800	4.05654700	-0.98328000
O	0.41590500	-1.12395500	-0.05656600
O	0.98040300	-0.50909300	-2.35450900
Cl	0.20523200	-1.43395500	-1.50791600
H	-2.99253600	-1.56481500	1.36287200
O	0.94739000	-2.91659400	-1.71874700
O	-4.58466300	-2.67515700	-0.40218300
O	-2.18636300	-3.09833700	-0.66275200
Cl	-3.37319800	-3.32579900	0.18335300
H	-2.91620800	2.60091100	-0.86516200
O	-3.09231800	-2.52372000	1.60250000
S	-3.12422700	0.48307800	-0.86487100
O	-3.66412900	1.95264800	-0.86993800
O	-4.37611900	-0.19361400	-1.52414800
O	-1.94815300	0.37797400	-1.69908400
O	-3.00166600	0.00101100	0.51228000
H	-4.49851900	-1.10377300	-1.15316800
H	1.90861000	-2.73523200	-1.56914200
O	2.87373000	0.98058700	0.50138000
O	3.92788200	0.66250800	-1.71612400
Cl	2.67248800	1.40280000	-0.92547100
H	4.12601500	-0.21428500	1.02480200
O	3.02648800	2.82284700	-1.11744200
S	3.75428000	-2.26013800	0.54626900
O	4.59017600	-1.07117500	1.15436400
O	3.37011800	-1.88289800	-0.83466400
O	4.49057000	-3.46092400	0.76990700
O	2.43097800	-2.28522500	1.39402800
H	3.76979800	-0.31195800	-1.59539700

H	1.68988600	-1.81644300	0.93549700
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(CA) ₄ (SA) ₄	x	y	z
O	-4.68411400	-2.57737100	-0.20495200
O	-2.30387800	-3.01621600	0.06181600
Cl	-3.53170100	-2.79992500	-1.11486900
H	-5.40875700	-0.94910100	-0.19011300
O	-3.59722500	-4.07875600	-1.81467600
S	-4.28979400	0.77803500	0.27130700
O	-5.53885400	0.02538600	-0.29350000
O	-3.07342200	0.01521900	0.02696900
O	-4.36386400	2.12846800	-0.25213500
O	-4.59659100	0.76821000	1.81215500
H	-1.46158100	-3.10006100	-0.45457300
H	-3.73901100	0.74655800	2.31452700
O	3.02464400	-0.49851600	1.54060200
O	2.76875000	-2.86010200	0.79283500
Cl	2.28700900	-1.74114000	1.95870200
H	-1.11527700	0.45239200	-2.05568300
O	2.81476500	-2.32957300	3.18203800
S	0.17135200	-1.21487600	-1.58820600
O	-1.09792700	-0.54803500	-2.17547800
O	0.58960600	-0.55453500	-0.34755900
O	-0.10716000	-2.63608500	-1.49405200
O	1.23158100	-0.92148600	-2.70057400
H	2.97485100	-2.35166000	-0.02892800
H	2.15129100	-1.09021900	-2.34667200
O	0.25529400	0.29935500	2.68753500
O	-1.22108000	-1.56978900	2.17547600
Cl	-1.05449300	0.10455200	2.05199500
H	3.62256500	1.24943200	-1.28479900
O	-2.14532900	0.63499100	2.91987100
S	4.75608500	-0.56205800	-1.41817100
O	4.40452300	0.92171700	-1.79658100
O	3.47428600	-1.31396900	-1.39581500
O	5.81189500	-0.99992700	-2.26951700
O	5.27316800	-0.51085100	0.05990600
H	-1.83363900	-1.85558800	1.45684200
H	4.52828700	-0.48136600	0.71669000
O	2.03555400	3.86091200	0.64882300
O	2.18446800	1.63048000	-0.40641200
Cl	2.38467500	2.49195800	1.09341800
H	0.72831900	4.10258700	-0.55796500

O	3.81201100	2.35830900	1.36631900
S	-1.00680100	2.93042500	-0.82129900
O	-0.00874700	4.06976000	-1.21249100
O	-1.15345200	2.03044600	-1.96159300
O	-0.61241700	2.34196600	0.44490700
O	-2.30475400	3.78849400	-0.67812400
H	1.61422900	0.83689600	-0.22787300
H	-3.09984200	3.20354200	-0.55863800

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