Ions in the atmosphere

High-energy cosmic ray, radon decay, ...

Cascade of ion production reactions until energy is dissipated

The charges go to molecules that are abundant and can accommodate the charge

$\text{H}_3\text{O}^+$, $\text{O}_2^-$

$\text{HSO}_4^-$, $\text{NO}_3^-$, $\text{NH}_4^+$, $\text{HPy}^+$

Negative charges end up on acid molecules, positive charges on base molecules

Molecular ions can participate in particle formation

Lost by recombination and onto surfaces
Ions in ACDC (1)

- Positive molecular ions: $1N1P = N$ molecule with an extra proton

- Negative molecular ions: either freely choosable name, e.g. $1B$, or $1A1RP = A$ molecule with a removed proton

- When using the P/RP notation, P and/or RP need to be included as molecule types with mass +1 and -1 in the cluster set file
Ions in ACDC (2)

- Generic charger ions $O_2^-$ and $H_3O^+$ used by default when there are ions.

- Charge transfer between ion/molecule types works automatically with the P/RP notation.

- Charging and neutralization require “corresponding neutral molecule” etc.
Ions in ACDC (3)

- Ion-neutral collision rates require dipole moment and polarizability of the neutral species
  → --dip_file_name dip_pol.txt

- Recombination collision rate $1.6 \times 10^{-6} \text{ cm}^{-3}\text{s}^{-1}$

- By default, wall loss coefficients have an ion enhancement

- Two ions of the same polarity cannot collide
Ions in ACDC (4)

- Each charging state requires its own nucleation criterion: out neutral/negative/positive

- Formation rates for each charging state + recombination separately (does not follow the whole formation pathway, just the last step)

- Separate coagulation clusters for each charging state → collisions between these allowed
Different uses for ACDC simulations

- Explaining an individual experiment
  - using theoretical cluster properties and seeing if the simulation results match the experiment
  - finding rate constants that produce a good fit
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• Evaluating data analysis methods
  – in a simulation, we know exactly what happened
Flux growth rate

- Net forward flux (assuming only 1-mer collisions)
  \[ I_{n,n+1} = \beta_{n,1} C_n C_1 - \gamma_{n+1} C_{n+1} \]

- Growth frequency (1/s) from \( n \) to \( n+1 \)
  \[ f_{n,n+1} = I_{n,n+1} / C_n = \beta_{n,1} C_1 - \gamma_{n+1} C_{n+1} / C_n \]

- Diameter growth rate (nm/h)
  \[ \frac{dd}{dt} = (d_{n+1} - d_n) \times f_{n,n+1} \]
“Banana plot”

“Concentration density” $c(d,t)$: concentration of clusters in the diameter range $d...d+\delta d$ divided by $\delta d$

Notation when using logarithmic size bins: $dC/d(\log d)$
GR from maximum concentration method

GR = slope of the line fitted to the points
GR = slope of the line fitted to the points
GR from time delay method

\[ GR = \frac{(3 \text{ nm} - d_{\text{monomer}})}{\Delta t} \]