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The Effect of Atmospherically Relevant Aminium Salts on Water Uptake

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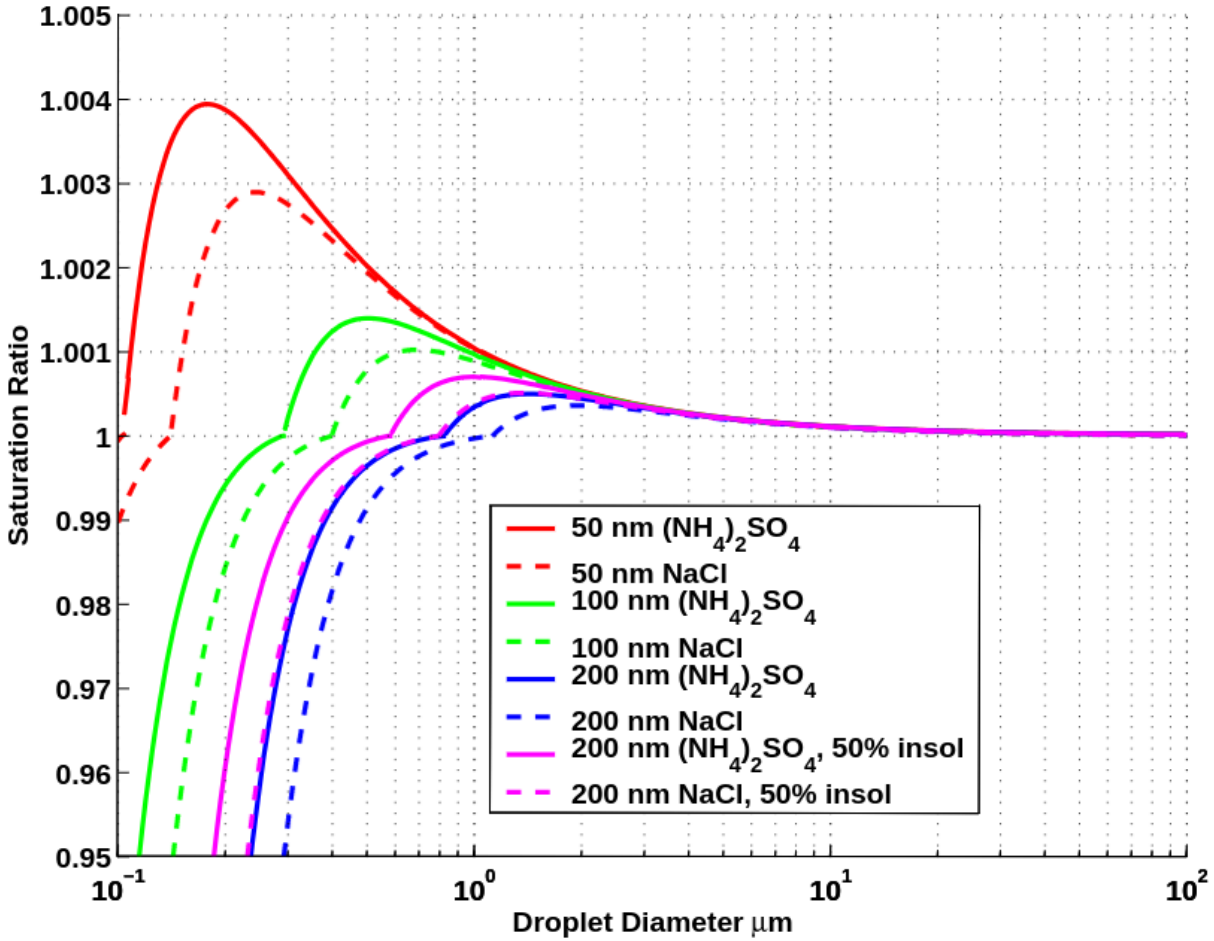
Introduction

- Salts increase water uptake of aerosol particles compared to purely organic particles
- Even small amounts of salt dominate the hygroscopic behavior of particles
- Some salts can reduce the critical supersaturation of cloud activation

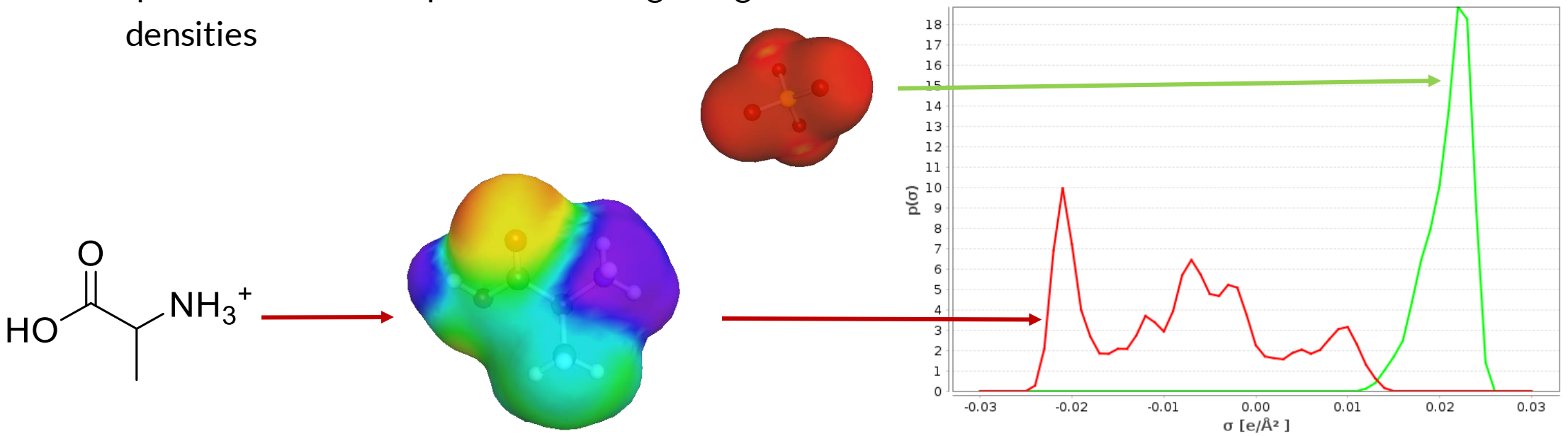
McFiggans et al. 2006



Computational methods

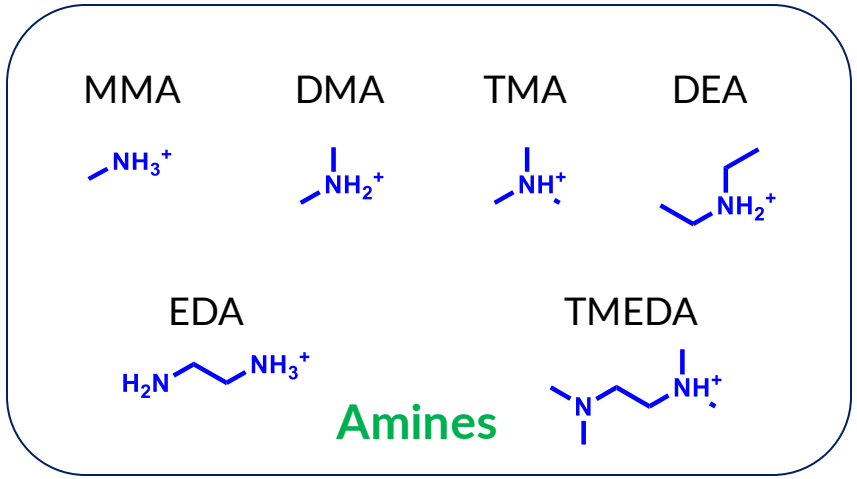
- Water activity coefficients were calculated using the conductor-like screening model for real solvents (COSMO-RS) in COSMO*therm*
- Thermodynamic properties are calculated from quantum chemical input of screening charge densities

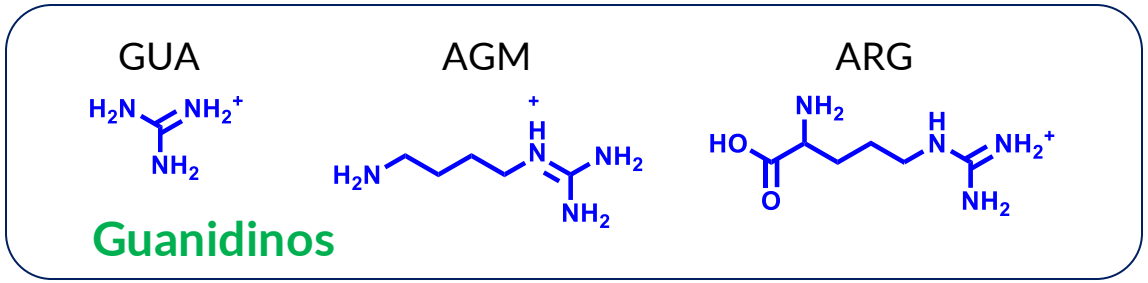
- Activity (a) = activity coefficient * mole fraction
- At equilibrium: a(water) = RH/100%

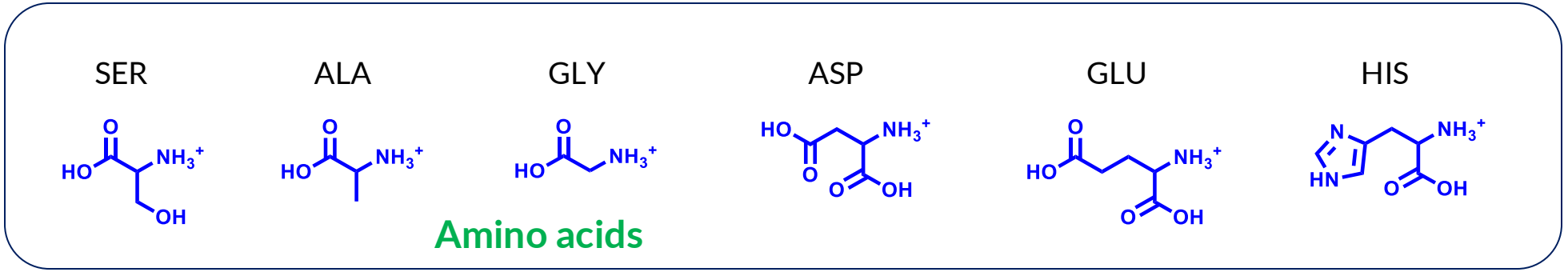


Aminium salts

- Amines and strong acids (sulfuric, nitric, iodic) take part in cluster formation
- Many amines that have been measured in aerosol particles







Water activity, pure aminium salts, mole fractions

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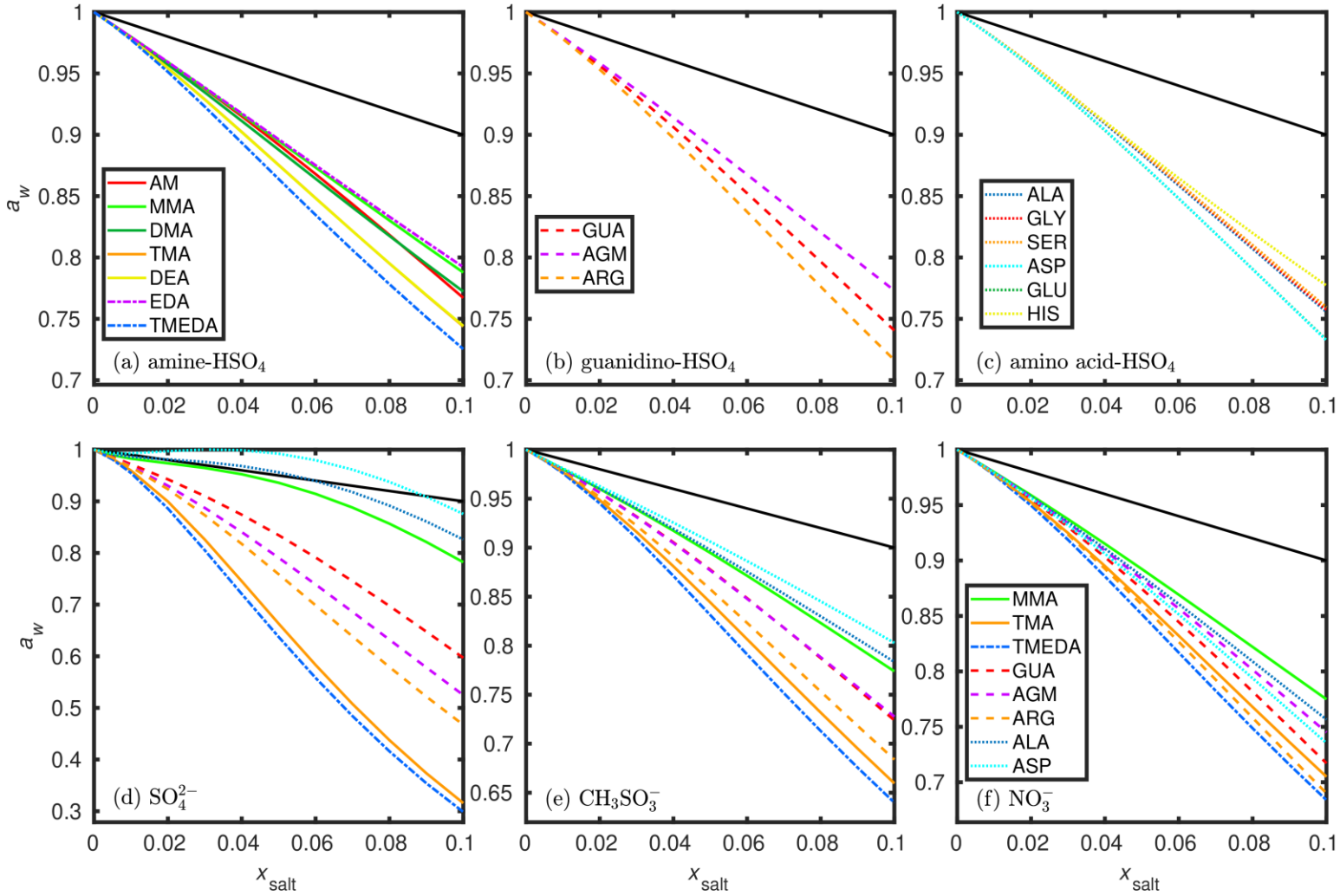
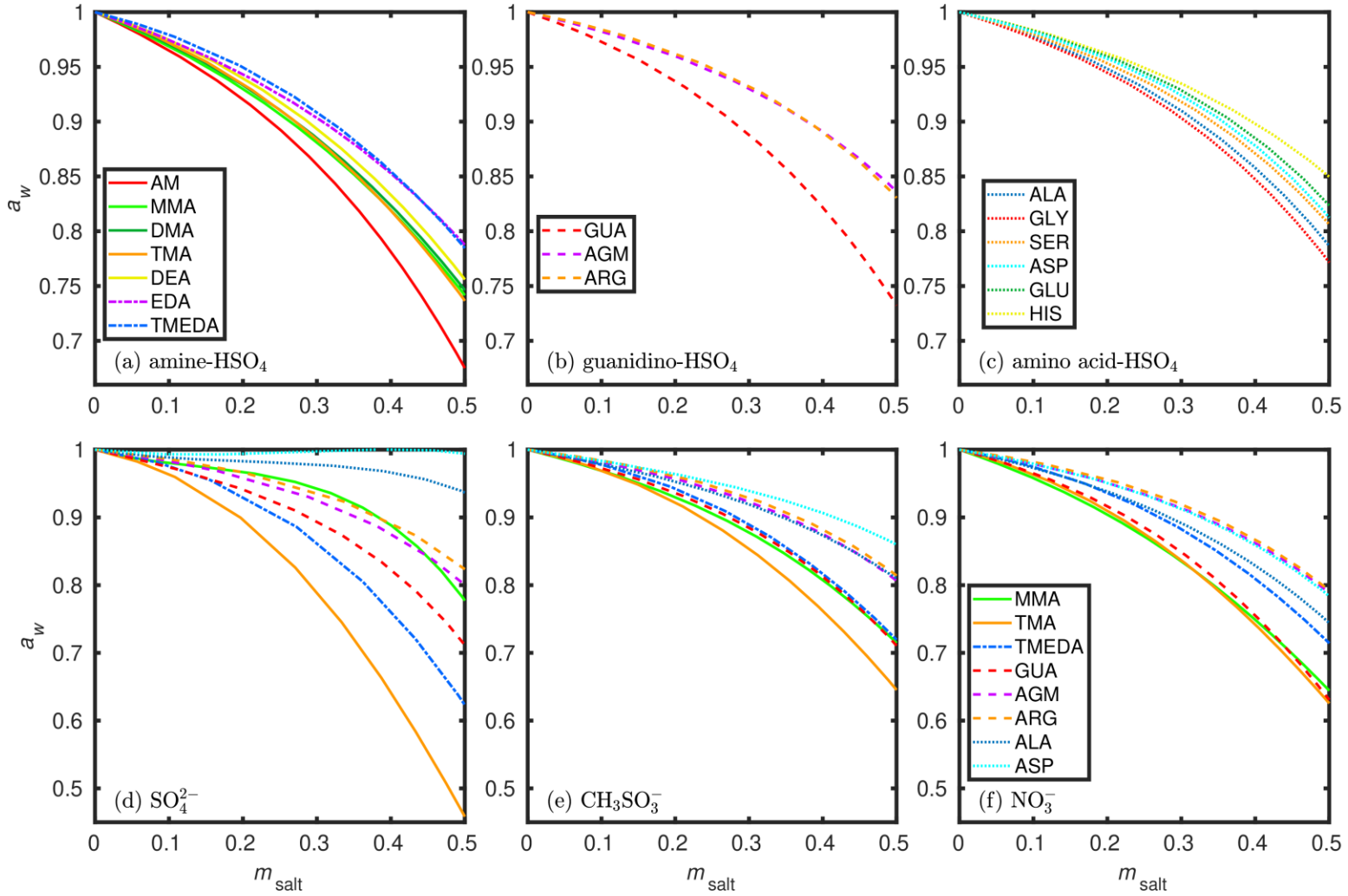
- At equilibrium, the highest water content (mole fraction) in tetramethyl ethylene diamine
- Strongest water uptake in sulfate solutions



Water activity, pure aminium salts, mass fractions

- In mass fraction, water uptake is strongest for smallest amines



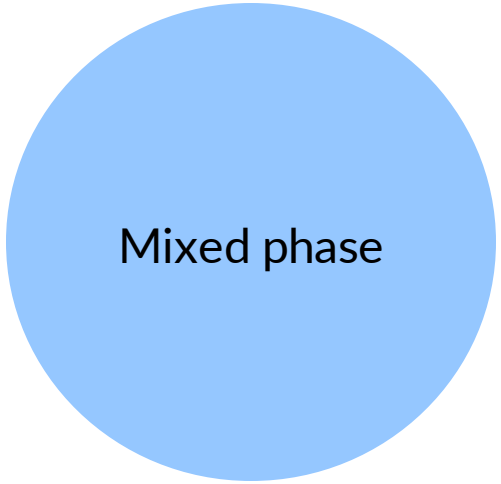
Salt-organic mixtures

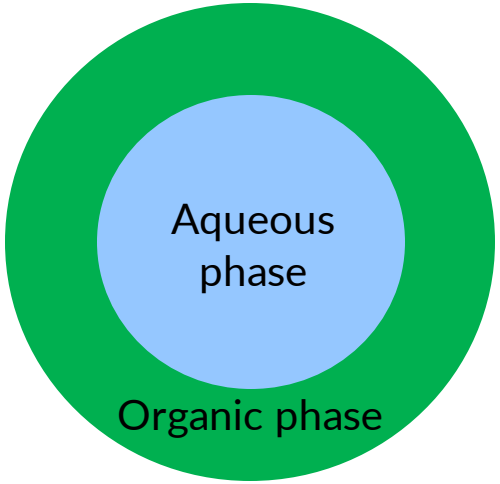
Hydrophilic organic

- Miscible with water
- No phase separation
- Organic can affect water activity

Hydrophobic organic

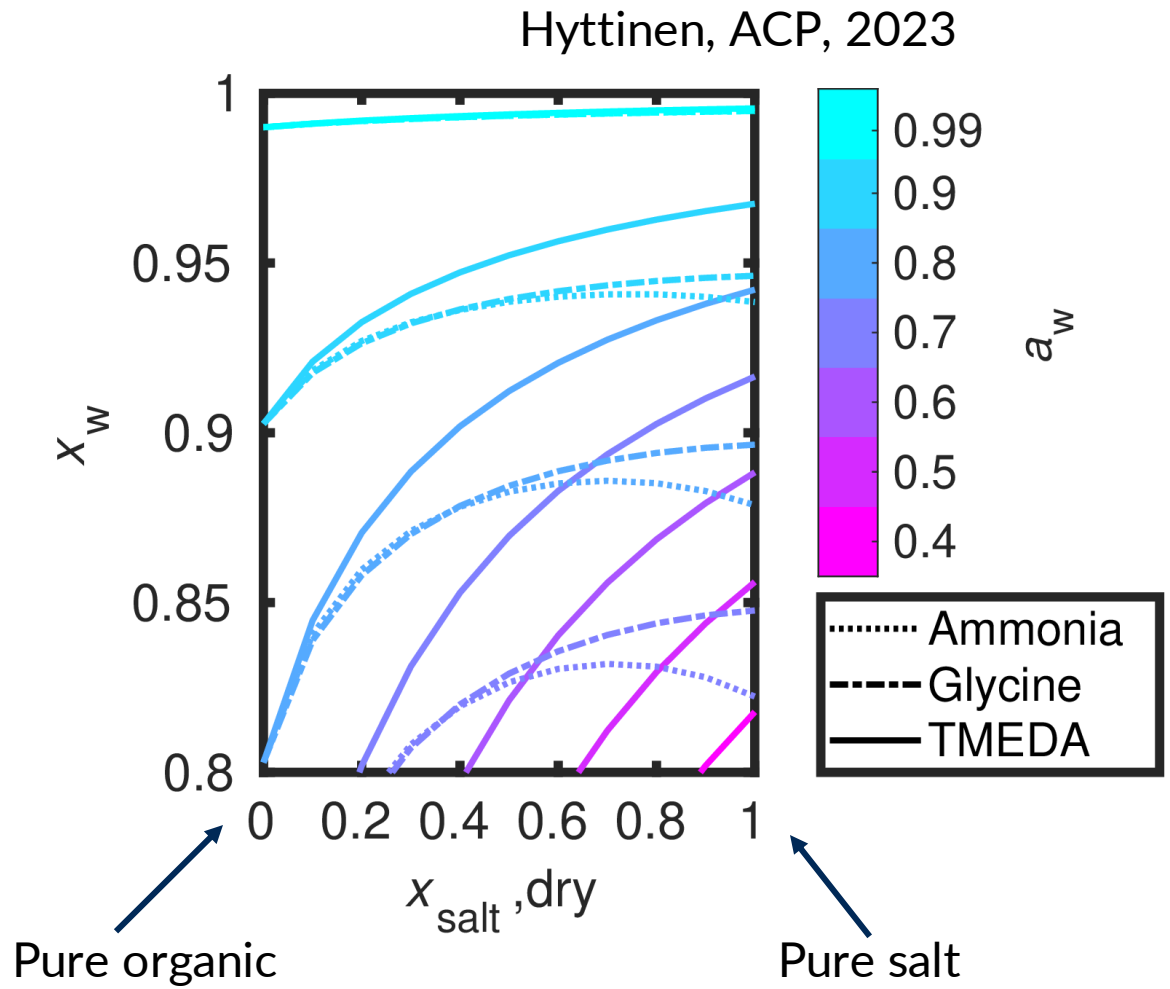
- Phase separates with water
- Aqueous phase has only small amounts of organic
- Smaller effect on water activity





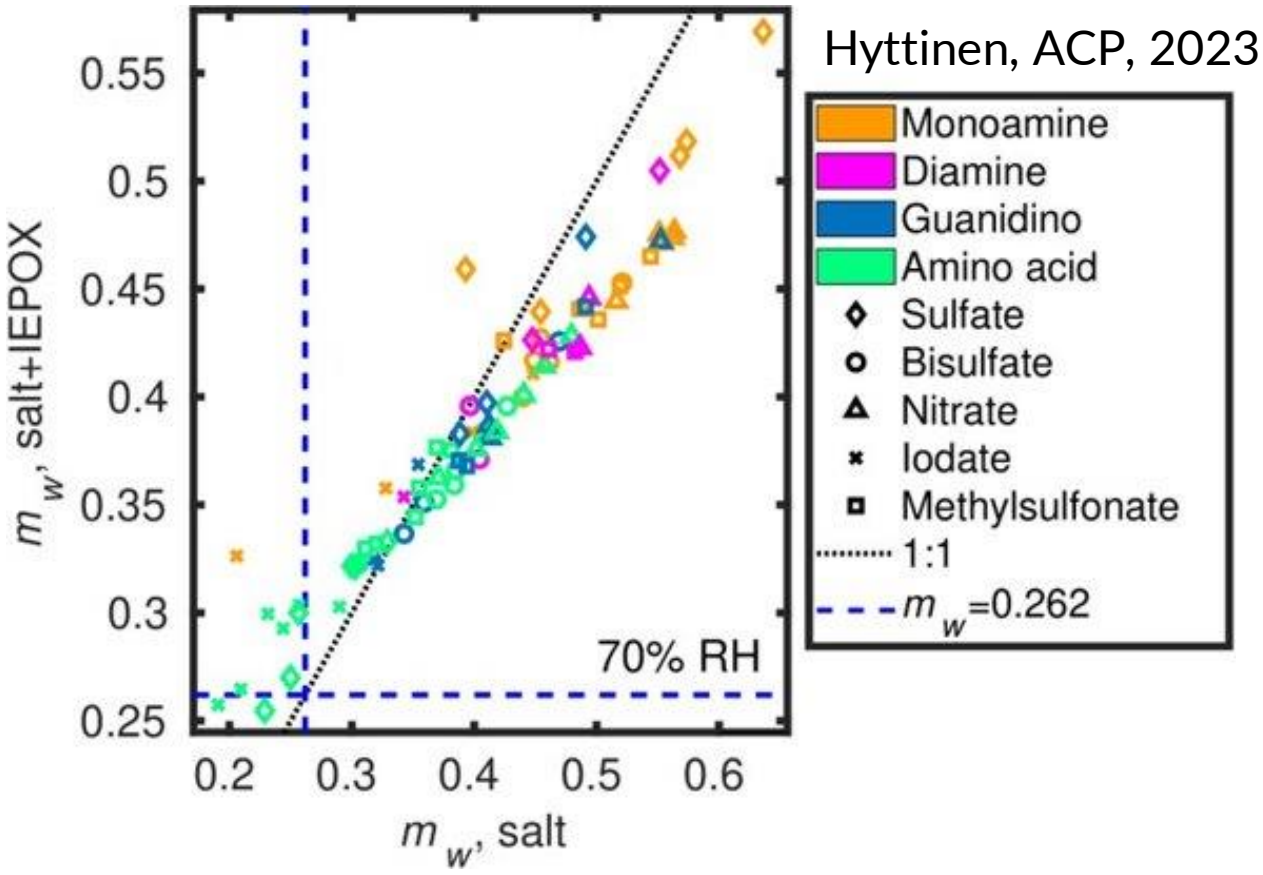
Hydrophilic organic

- The organic compound is isoprene-derived epoxydiol (IEPOX)
- IEPOX-water mixtures are close to ideal solution
- Hydrophilic organic increases water activity in a particle –> decreased water uptake compared to pure salt



1:1 ratio of hydrophilic organic and salt

- Equilibrium water content at 70% RH in IEPOX is 0.262 mass fraction
- Most salts have higher water uptake than IEPOX (x axis)



Conclusions

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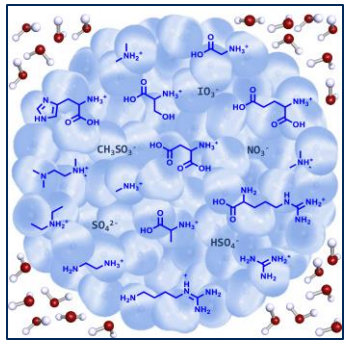
- Aminium salts take up more water than pure organic
- Smaller aminium salts lead to higher water uptake in mass fraction
- The effect of organics depend on the solubility of the organic



The effect of atmospherically relevant aminium salts on water uptake

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Abstract. Atmospheric new particle formation is initiated by clustering of gaseous precursors, such as small acids and bases. The hygroscopic properties of those precursors therefore affect the hygroscopic properties of aerosol particles. In this work, the water uptake of different salts consisting of atmospheric small acids and amines was studied computationally using the conductor-like screening model for real solvents (COSMO-RS). This method allows for the prediction of water activities in atmospherically relevant salts that have not been included in other thermodynamics models. Water activities are reported here for binary aqueous salt solutions, as well as ternary solutions containing proxies for organic aerosol constituents. The order of the studied cation species regarding water activities is similar in sulfate, iodate, and methylsulfonate, as well as in bisulfate and nitrate. Predicted water uptake strengths (in mole fraction) conform to the following orders: tertiary > secondary > primary amines and guanidinos > amino acids. The addition of water-soluble organic to the studied salts generally leads to weaker water uptake compared to pure salts. On the other hand, water-insoluble organic likely phase separates with aqueous salt solutions, leading to minimal effects on water uptake.