

HYDROPHILICITY CONTROLS THERMODIFFUSION IN ALKYLAMMONIUM CHLORIDES

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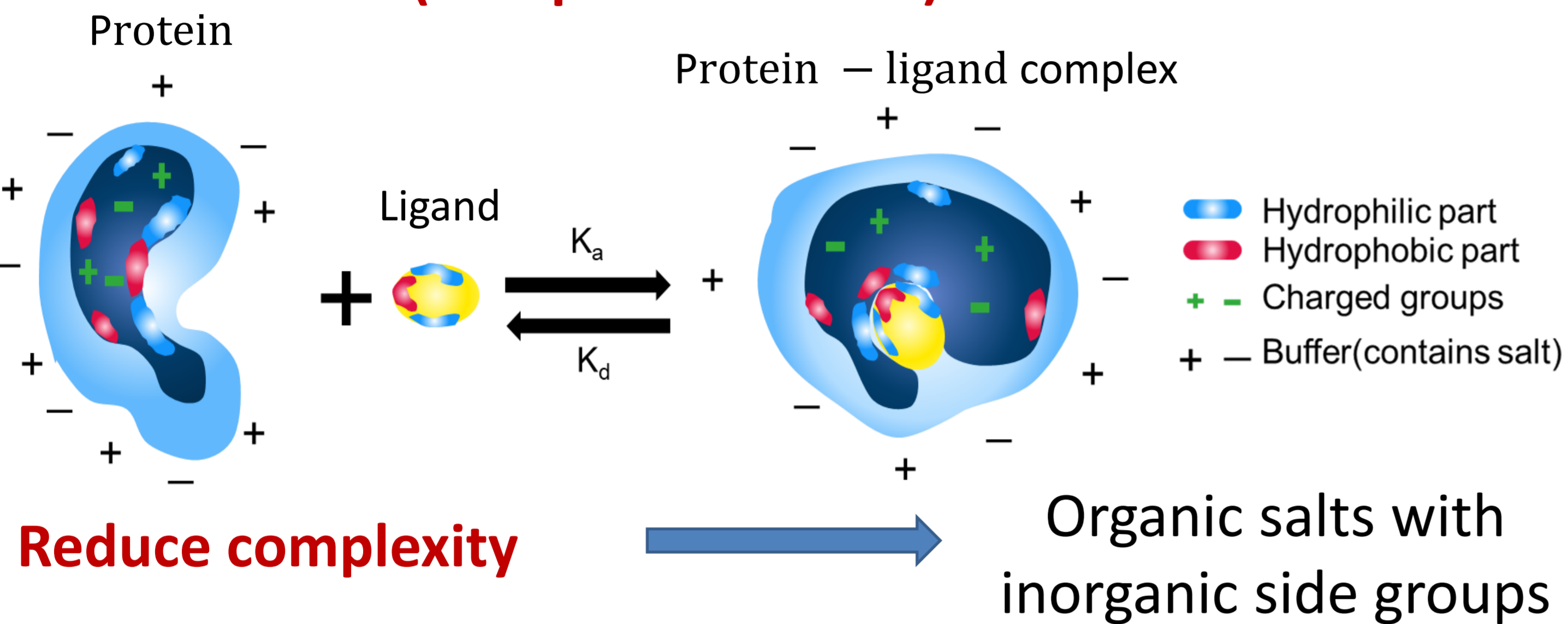
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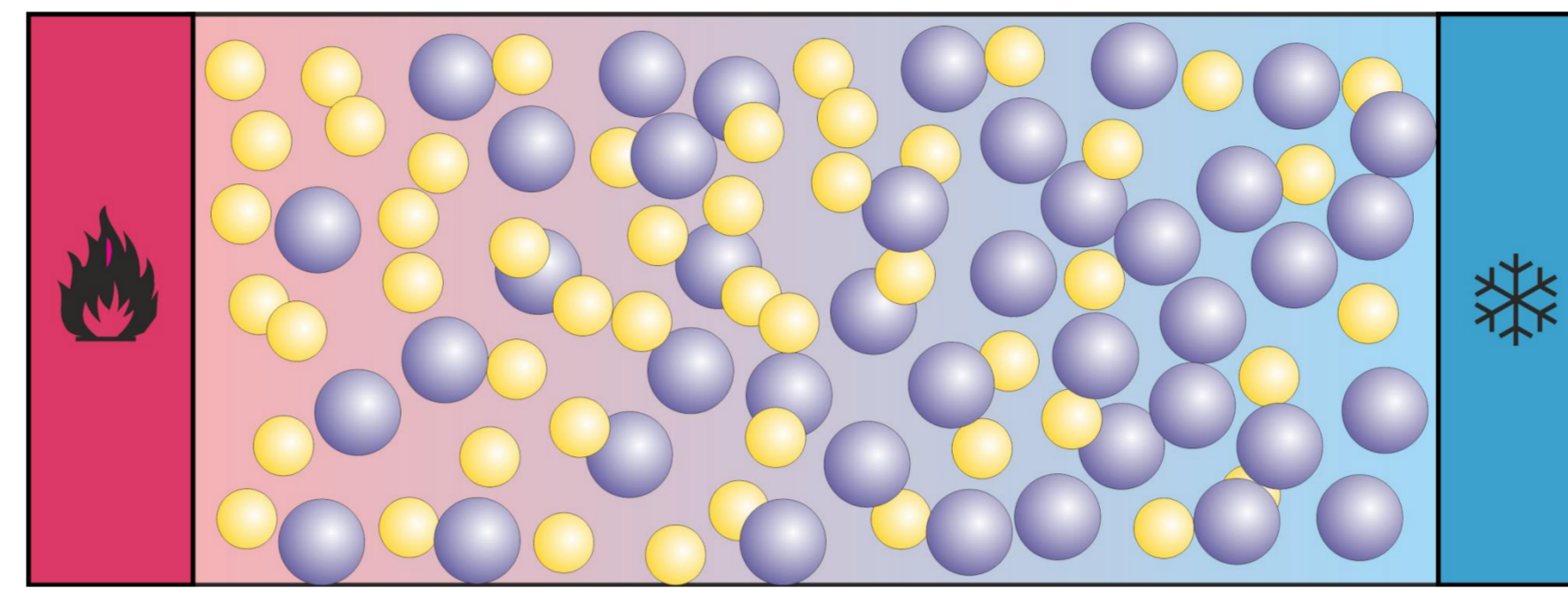
Motivation

- Thermophoresis is used to monitor protein-ligand binding

(Complex Problem!)



Thermodiffusion



\vec{j} - mass flux
 ρ - mass density
 c - mass fraction
 T - temperature

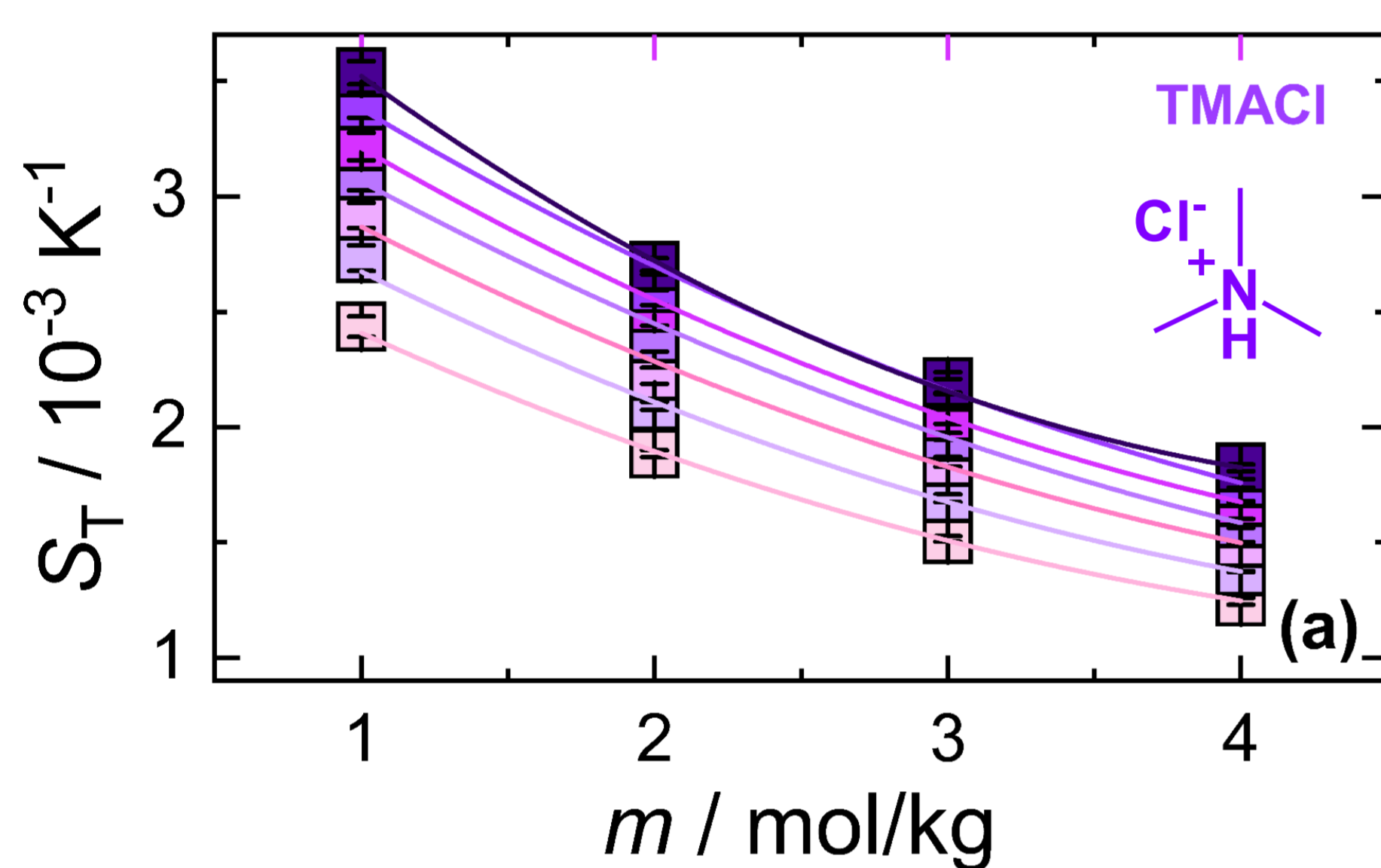
$$\text{Flux, } \vec{j} = -\rho D \vec{\nabla} c - \rho c(1-c) D_T \vec{\nabla} T$$

Steady state ($\vec{j}=0$) defines the Soret coefficient S_T :

$$S_T = \frac{\text{Thermodiffusion}}{\text{Diffusion}} = \frac{D_T}{D} = -\frac{1}{c(1-c)} \frac{\Delta c}{\Delta T}$$

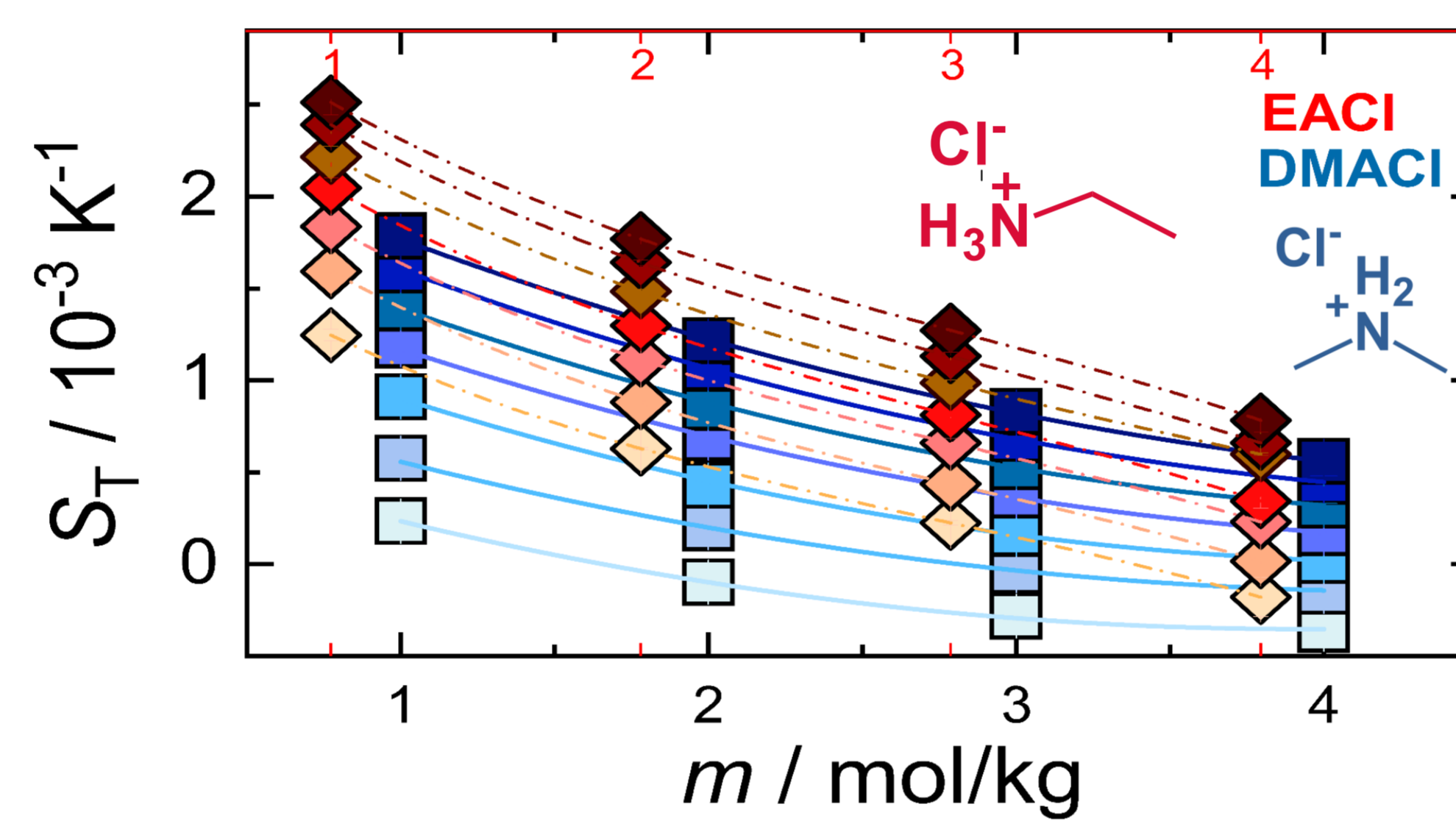
Results and Discussion

Trimethylammonium chloride



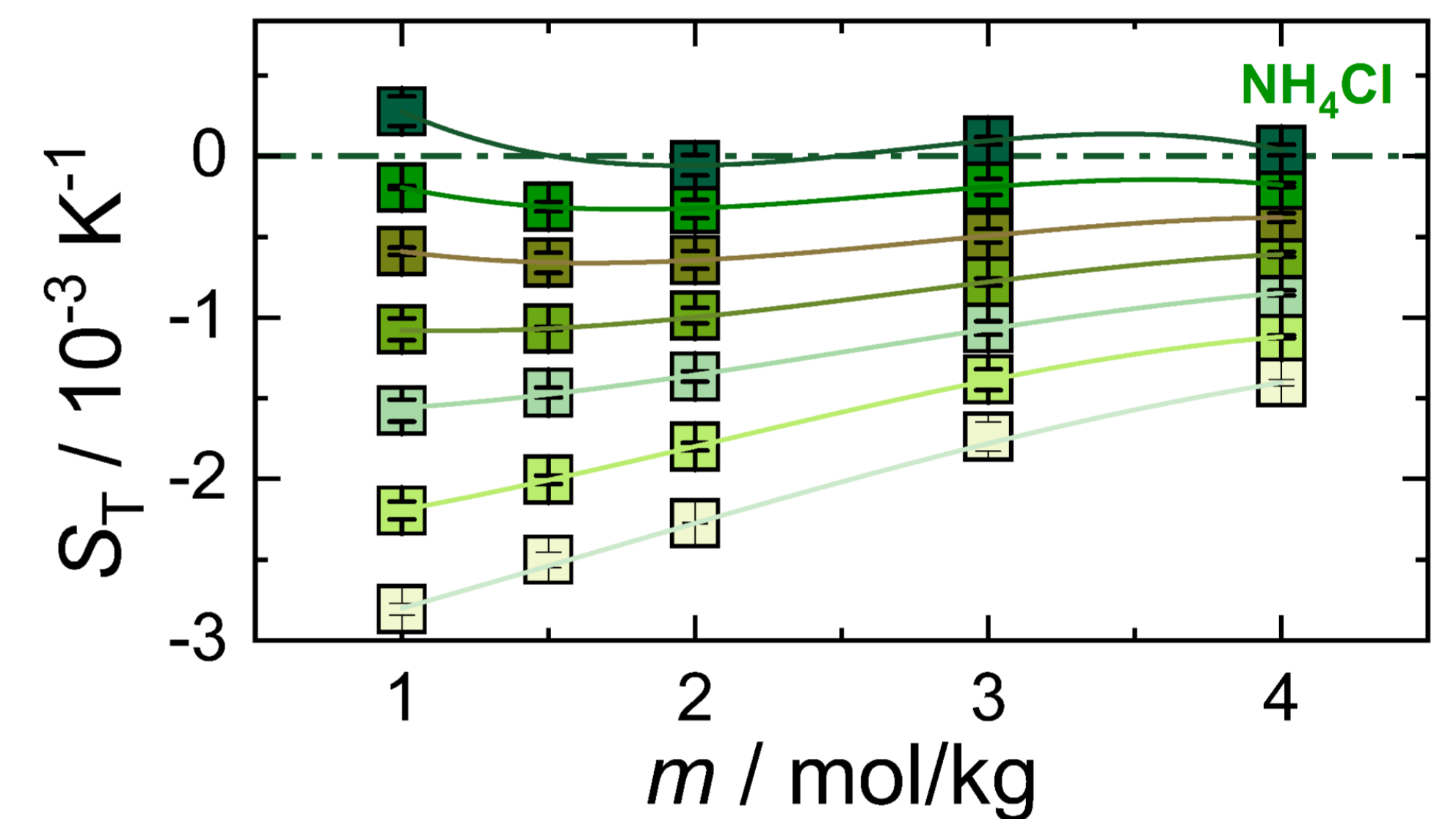
- S_T increases with temperature and decreases with increase in concentration; Thermophobic behaviour

Ethyl- and di-methylammonium chloride



- S_T behaves similarly to TMACl; Thermophobic behaviour at most concentrations.

Ammonium chloride

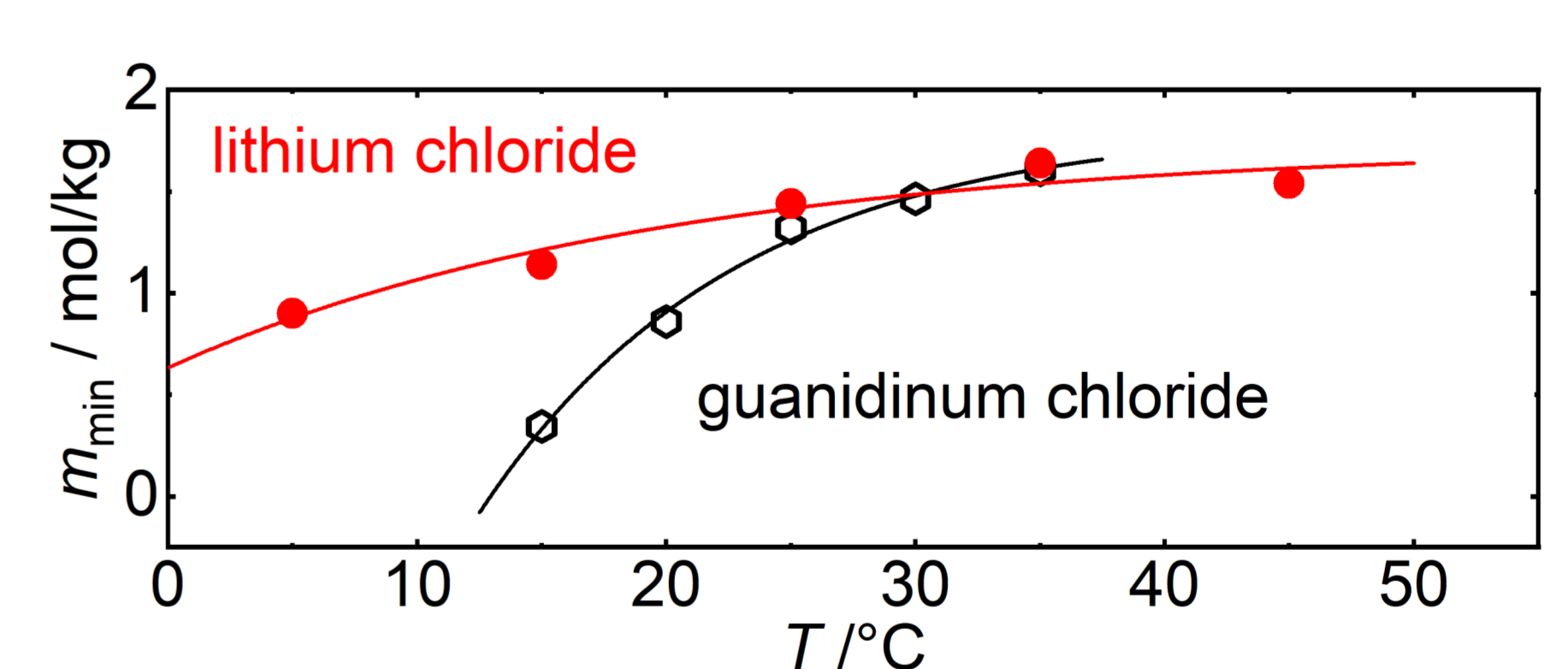
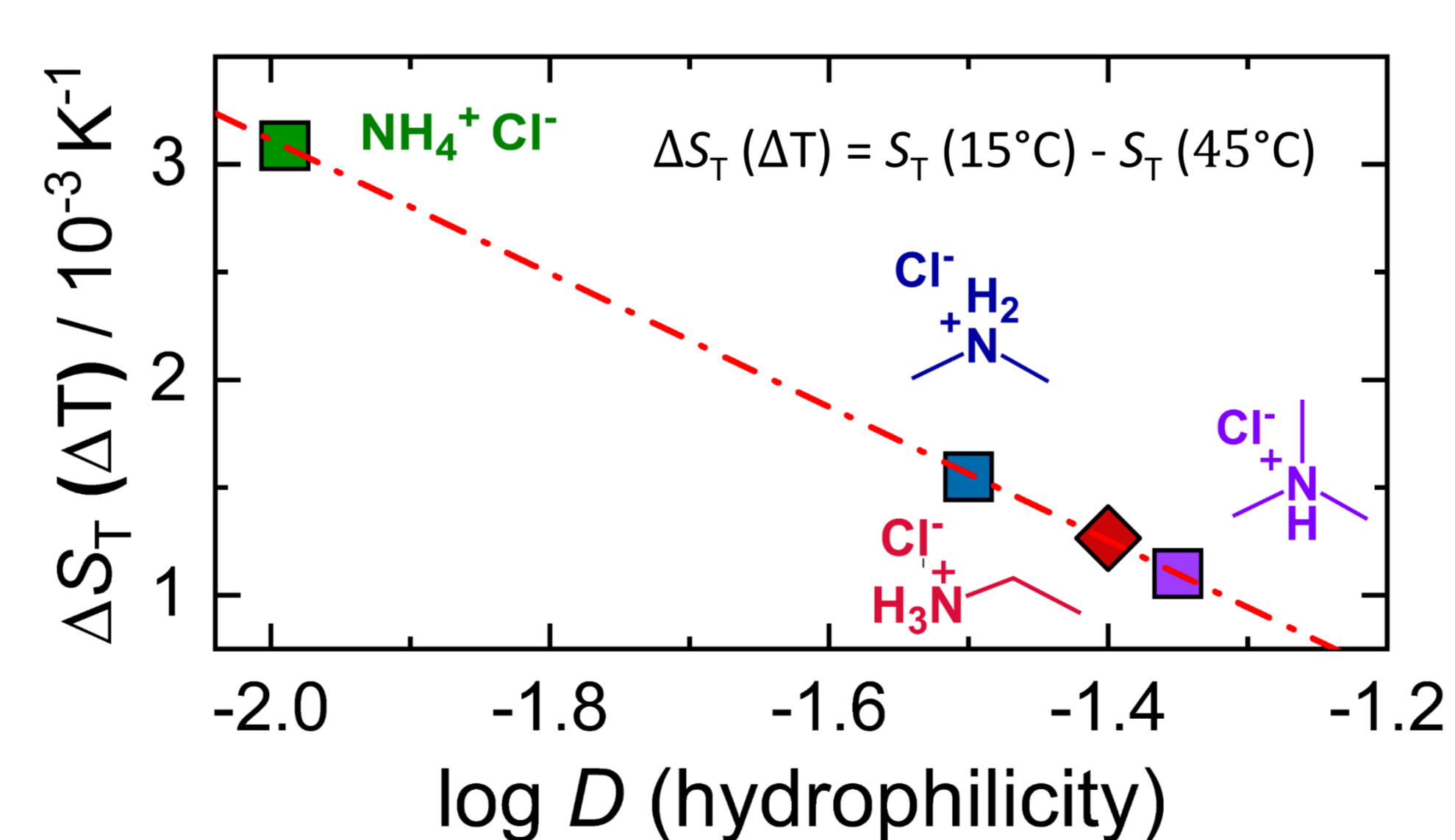
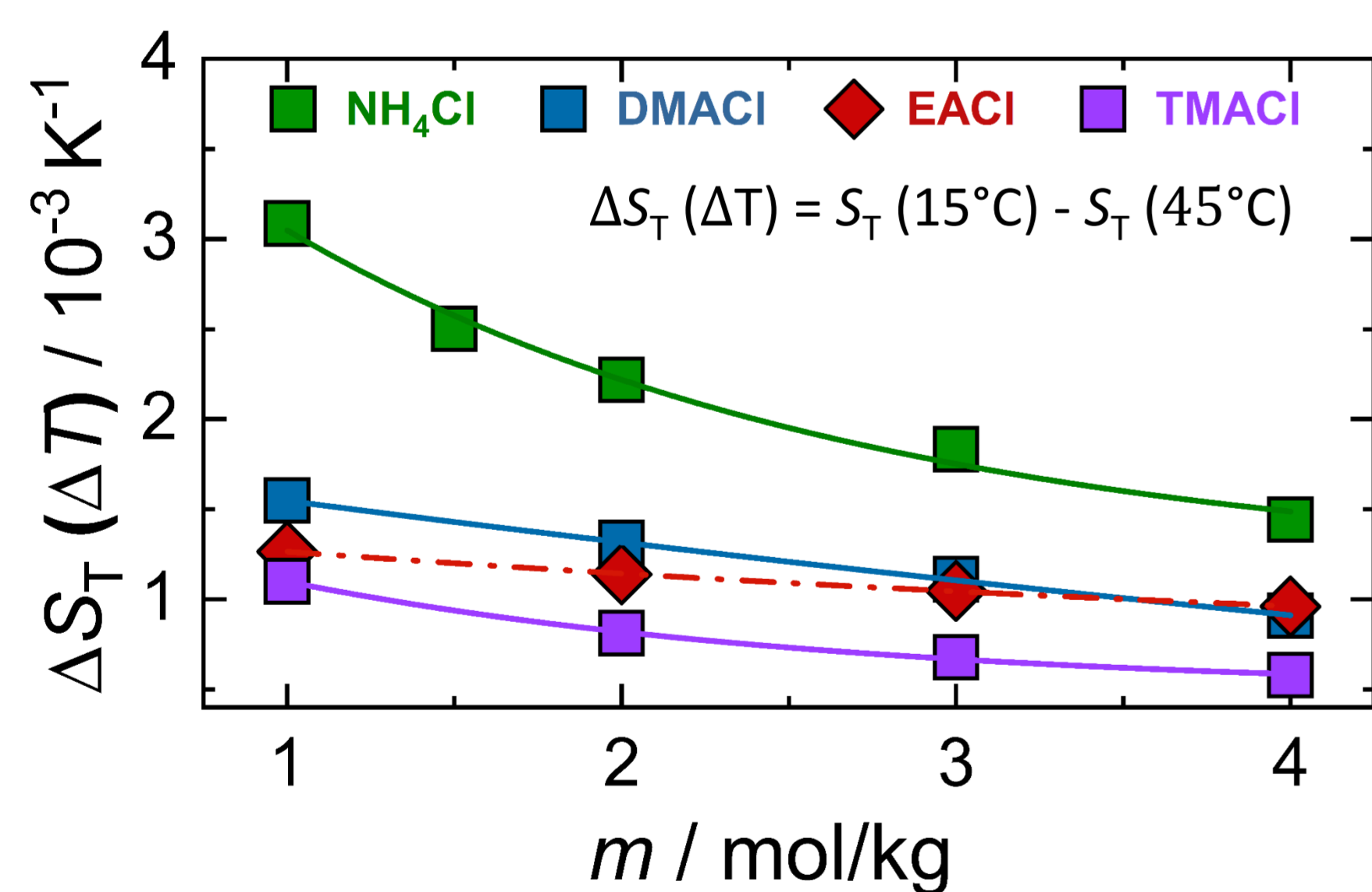


- Minimum in S_T occurs at higher temperatures and shifts toward higher concentrations as the temperature increases; thermophilic behavior.

Thermophobicity of S_T : **TMACl** > **EACl** > **DMACl** > **NH₄Cl**

Shift of minimum in S_T also observed for other salts

KEY FINDINGS: Thermodiffusion is strongly correlated with hydrophilicity



Conclusion

- With increasing salt concentration, hydrogen bonding decreases, leading to a decrease in $\Delta S_T(\Delta T)$.

- At a given concentration, $\Delta S_T(\Delta T)$ correlates with $\log D$.

Order $\{\Delta S_T(\Delta T)\}$: **NH₄Cl** > **DMACl** > **EACl** > **TMACl**

- $\Delta S_T(\Delta T)$ decreases as the degree of alkyl substitution increases, or equivalently, as the hydrophilicity of the salts decreases.

- It is assumed that the hydration layer shrinks with increase in temperature. So, a higher salt concentration is required to reach the minimum in S_T , which has been mapped to random closed packing of hydrated spheres.

References

The results presented in this poster have been published in Rudani, B. et al., *Eur. Phys. J. E.*, **49** (2026), 17

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