THERMOPHORESIS AS A PROMISING TOOL TO STUDY ION SPECIFICITY

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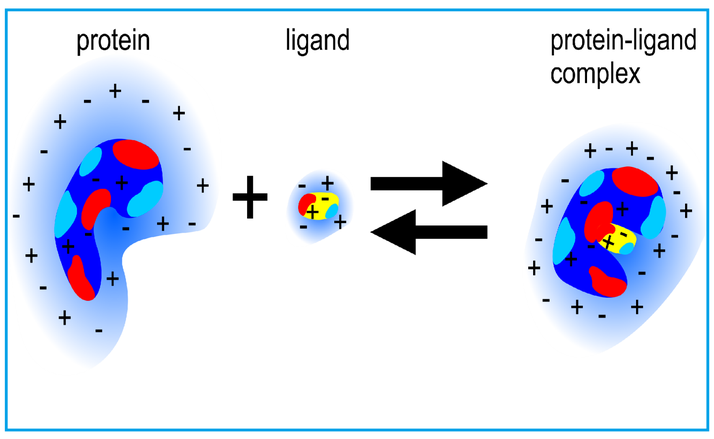
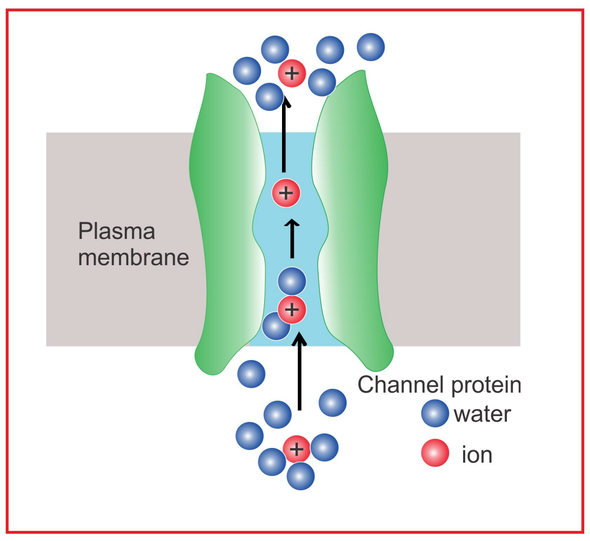
Motivation [1], [2], [7]

- Thermophoresis is used to monitor protein-ligand binding

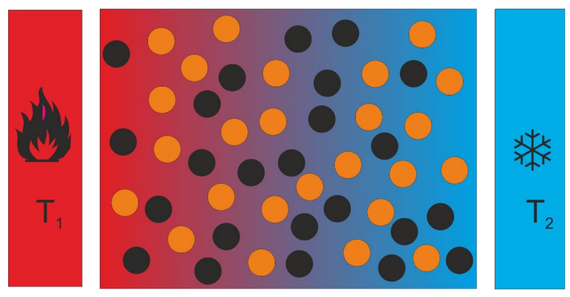


Protein ligand binding



Movements of ions through ion channels

Thermophoresis [3]

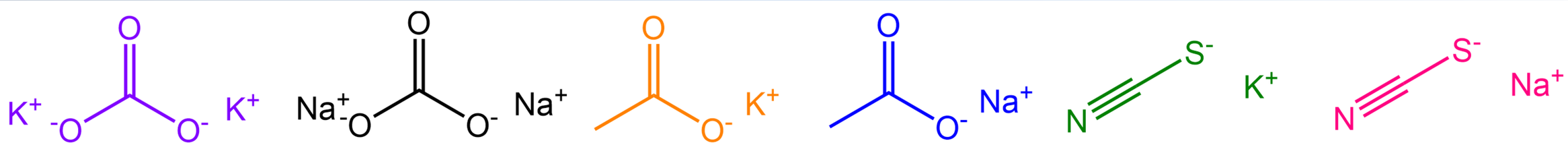


Flux, $\vec{j} = -D\vec{\nabla}c - c(1-c)D_T\vec{\nabla}T$

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

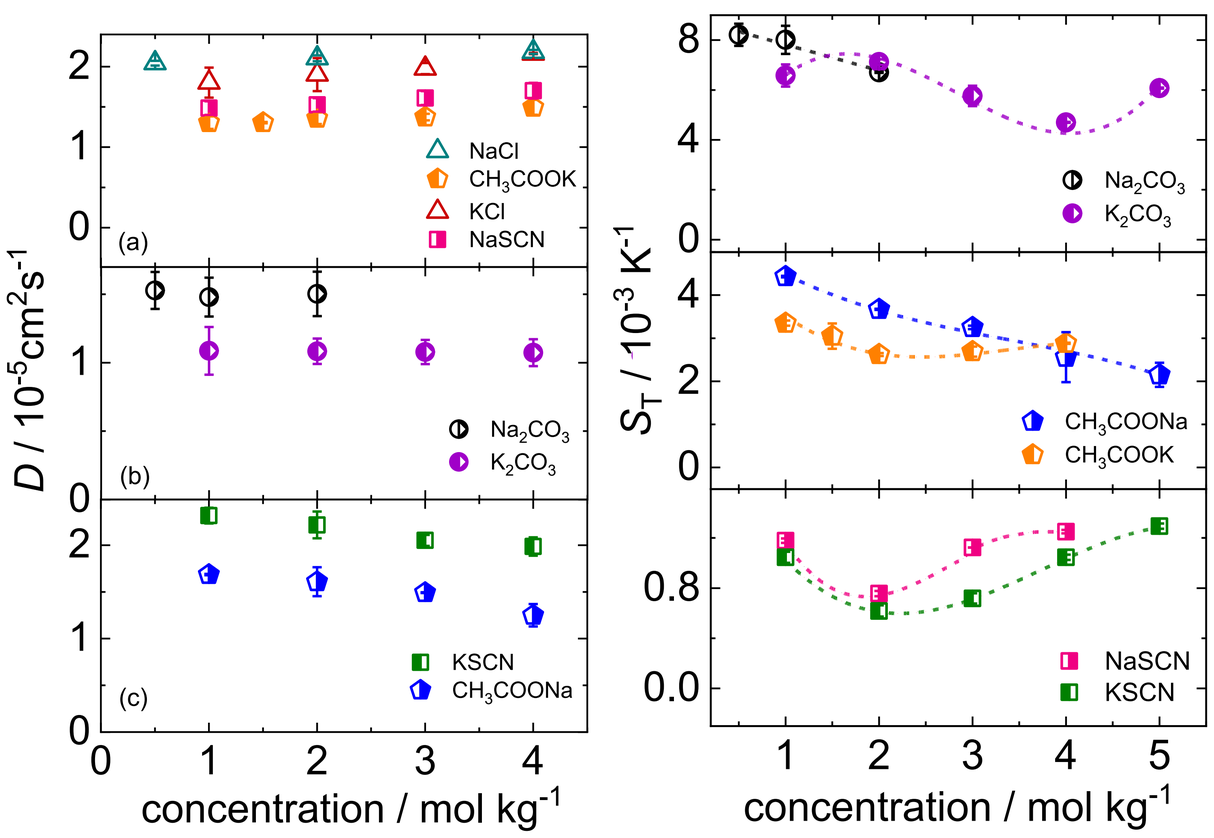
$$S_T = \frac{\text{Thermodiffusion}}{\text{Diffusion}} = \frac{D_T}{D} = -\frac{1}{c(1-c)}\frac{\Delta c}{\Delta T}$$

Systems [7]



Results and Discussion [4], [5], [6], [7]

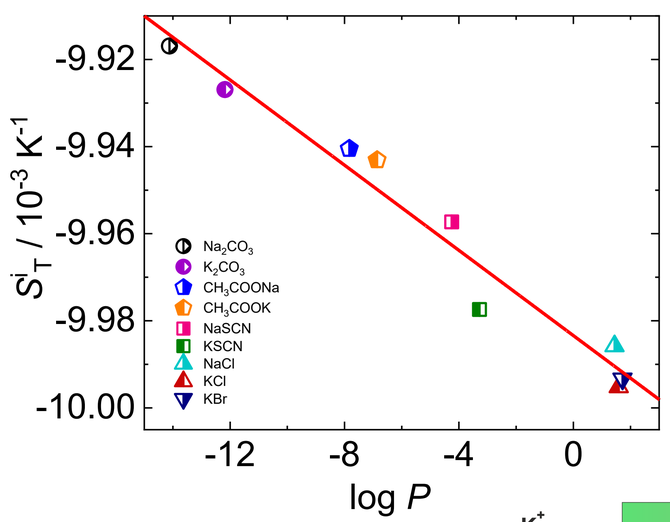
1. Concentration dependence of *D* and S_T

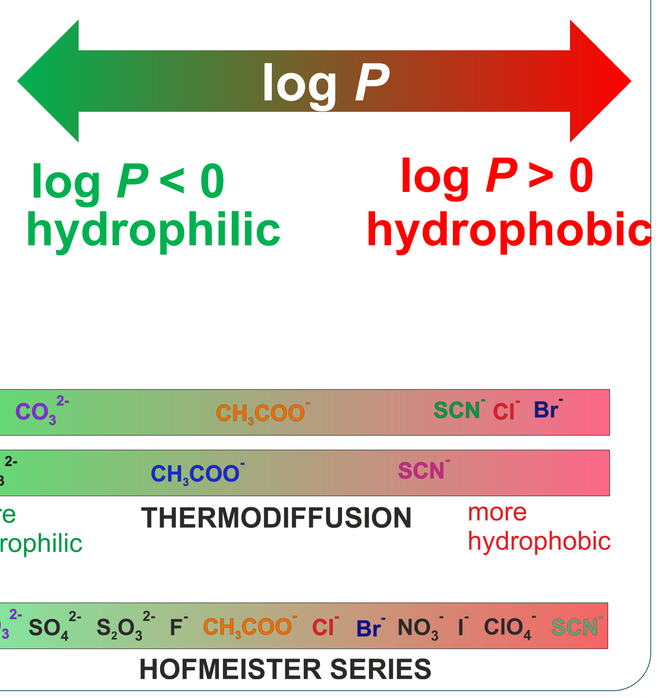


$$S_T(m,T) = \alpha(m)\beta(T) + S_T^i$$

$$\alpha(m) = a_1 m + a_2 m^2 + \ldots,$$

$$\beta(T) = 1 + b_1(T - T_0) + b_2(T - T_0)^2 + \cdots,$$





- We define a new hydrophilic-hydrophobic scale for anions based on our experimental observations

Conclusion [7]

- Thermophoretic behavior of salts are majorly influenced by changes in anion while diffusive behavior can be influenced by both cation and anion changes
- Thermophoretic behavior of salts in water shows a strong correlation with the log *P* values, which provides us with a new hydrophilicity scale for ions in aqueous salt systems.

References

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[4] Virginia et al, *Chem. Sci.*, ***10*** (2017), 7052
[5] Choi et al., *J. Chem. Phys.* 147 (15), 154107
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