Physical Principles in Biology Biology 3550 Spring 2025

Lecture 30

More on Water

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#### REVIEW





International Society of Sports Nutrition position stand: safety and efficacy of creatine supplementation in exercise, sport, and medicine

Kreider, R. B., Kalman, D. S., Antonio, J., Ziegenfuss, T. N., Wildman, R., Collins, R., Candow, D. G., Kleiner, S. M., Almada, A. L. & Lopez, H. L. (2017). *Journal of the International Society of Sports Nutrition*, 14. https://doi.org/10.1186/s12970-017-0173-z

# Ionization of Water

A second consequence of polarity of water:

Covalent O-H bonds break relatively easily

 $H_2O \Longrightarrow H^+ + OH^-$ 

This is very unfavorable in vacuum or non-polar liquids.

- Interactions between H<sup>+</sup> or OH<sup>-</sup> with polar water molecules stabilize the ions.
- H<sup>+</sup> or OH<sup>-</sup> are in complexes with clusters of water molecules.
- Equilibrium constant for ionization:

$$K_{
m eq} = rac{[{
m H}^+]_{
m eq}[{
m O}{
m H}^-]_{
m eq}}{[{
m H}_2{
m O}]_{
m eq}} = 1.8 imes 10^{-16} \, {
m M}$$

By most standards, not a very favorable reaction at all, but H<sup>+</sup> and OH<sup>-</sup> are potent!

### Ionization of Other Molecules

Other polar groups can ionize in water.



- Ionized groups are stabilized by interactions with water.
- Electric charge has huge effect on chemical and physical properties of molecules.
- Extent of ionization is determined by thermodynamics!
   Ionization equilibrium constants (pK<sub>a</sub>) and H<sup>+</sup> concentration (pH)

Crraig, S. L. (2025). John Brauman (1937–2024): Physical organic chemist, sage and servant of science. *Proc. Natl. Acad. Sci., USA*, 12, e2502896122. https://doi.org/10.1073/pnas.2502896122

# Dynamics of H<sup>+</sup> Ion Diffusion in Water

- H<sup>+</sup> ions diffuse through water much more rapidly than other ions, and much more rapidly than predicted by Stokes–Einstein equation.
  - Relay mechanism proposed by Theodor Grotthaus in 1806.
  - Basic mechanism is still thought to be correct, but details are still being studied and debated.
  - H<sup>+</sup> exchange reactions require only about 1 microsecond.
    - Mechanism may play a role in some H<sup>+</sup> pores in membrane proteins.

(Grotthuss Movie)

# Dynamics of H<sup>+</sup> Ion Diffusion in Water



Animation by Matt K. Petersen, https://en.wikipedia.org/wiki/Grotthuss\_mechanism