Physical Principles in Biology
Biology 3550
Spring 2024

Lecture 30

More on Water

Friday, 29 March

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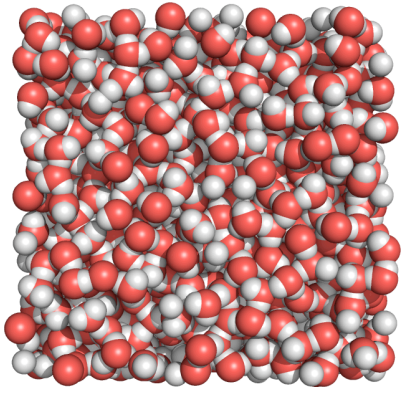
Announcements

- Problem Set 4:
  - Due Monday, 1 April at 11:59 PM
  - Submit pdf file on Gradescope
- No class on Monday, 8 April

Hydrogen Bonds in Liquid Water



Picture from simulation by
Prof. Valeria Molinero
U of U Chemistry Department.

- On average, each water molecule forms 3 hydrogen bonds at any instant.
- Explains high boiling point of water.
- Hydrogen bonds break and form constantly, giving water liquid properties.

A Simulation of 1,000 Water Molecules

(Water Movie)

- 4.5×10^{-12} s (4.5 ps) total time.
- 0.5 ps/frame

Simulation courtesy of Prof. Valeria Molinero, University of Utah

Ionization of Water

- A second consequence of polarity of water:

  Covalent O-H bonds break relatively easily

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

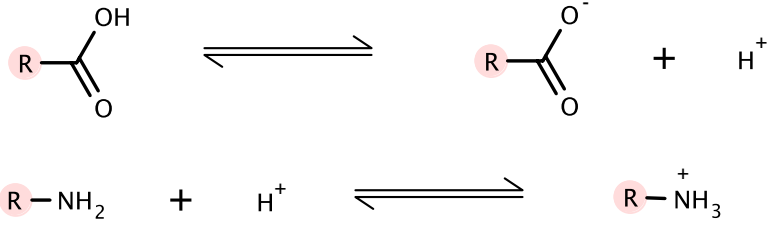
- This is very unfavorable in vacuum or non-polar liquids.
- Interactions between H^+ or OH^- with polar water molecules stabilize the ions.
- H^+ or OH^- are in complexes with clusters of water molecules.
- Equilibrium constant for ionization:

$$K_{eq} = \frac{[H^+]_{eq}[OH^-]_{eq}}{[H_2O]_{eq}} = 1.8 \times 10^{-16}\,M$$

- By most standards, not a very favorable reaction at all, but H^+ and OH^- 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_a) and H^+ concentration (pH)

Dynamics of H^+ Ion Diffusion in Water

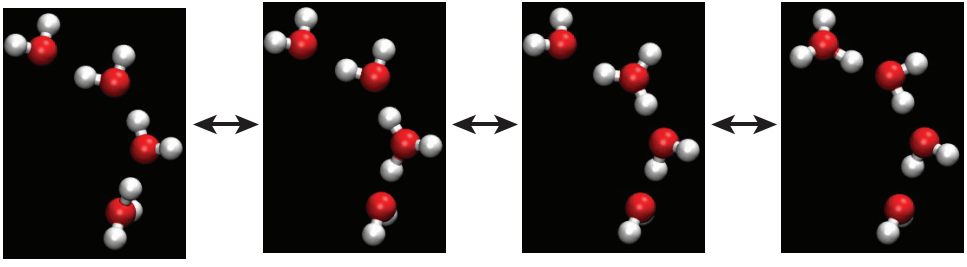
- H^+ ions diffuse through water much more rapidly than other ions, and much more rapidly than predicted by Stokes–Einstein equation.
  - Relay mechanism proposed by Theodor Grotthaus in 1806.
  - Basic mechanism is still thought to be correct, but details are still being studied and debated.

(Grotthuss Movie)

  - H^+ exchange reactions require only about 1 microsecond.
  - Mechanism may play a role in some H^+ pores in membrane proteins.

Animation by Matt K. Petersen, https://en.wikipedia.org/wiki/Grotthuss_mechanism

Dynamics of H^+ Ion Diffusion in Water



Animation by Matt K. Petersen, https://en.wikipedia.org/wiki/Grotthuss_mechanism

The Hydrophobic Effect

- The basic observation: Water and oil don’t mix!
- A confusing and still controversial subject, partly because of terminology.
- Non-polar molecules are poorly soluble in water.
- Are non-polar molecules afraid of water?
- What happens when a non-polar molecule does dissolve in water?

Clicker Question #1

Why don't oil and water mix?

A) Water and oil molecules repel one another.

B) Oil molecules stick together very tightly.

C) Water molecules stick together very tightly.

D) All of the above.

E) None of the above.

All answers count for now!