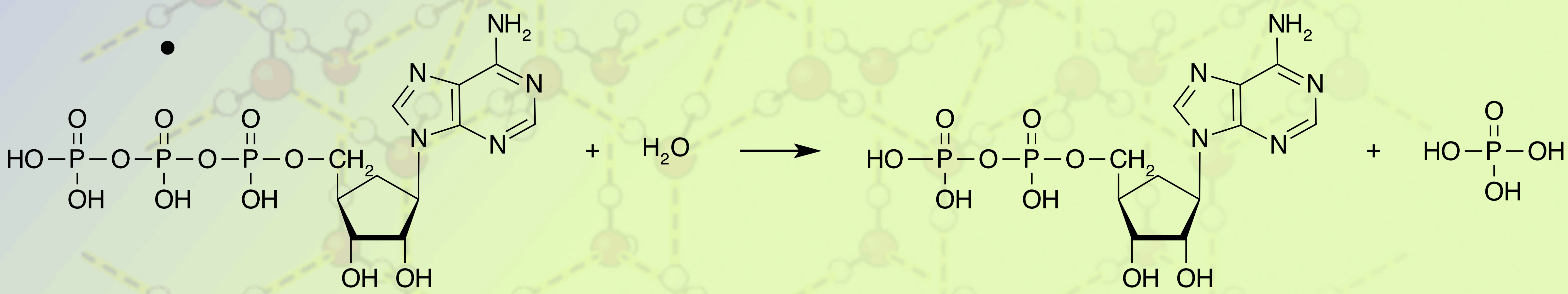
Chem 352 - Lecture 2
Water

Question for the Day: What physical characteristics of a water molecule allows a groundhog to walk across Halfmoon Lake on Groundhog day?

Question for the Day: How does the pH of a solution influence charge/charge interactions between biological molecules?

Review

- The chemical reaction equation for the hydrolysis of ATP is,
- 

adenosine triphosphate — adenosine diphosphate — inorganic phosphate

$$ATP + H_2O \longrightarrow ADP + P_i$$

Review

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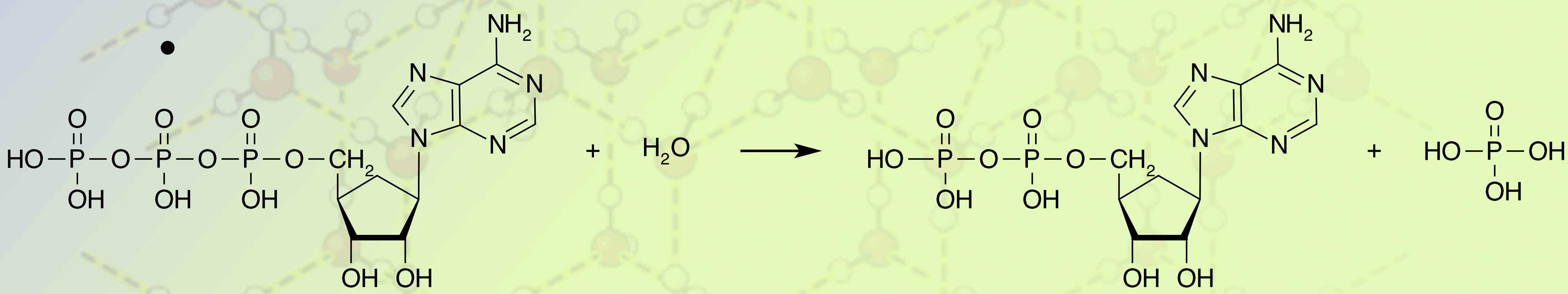


adenosine triphosphate　　　　adenosine diphosphate　　　　inorganic phosphate

$$ATP + H_2O \longrightarrow ADP + P_i$$

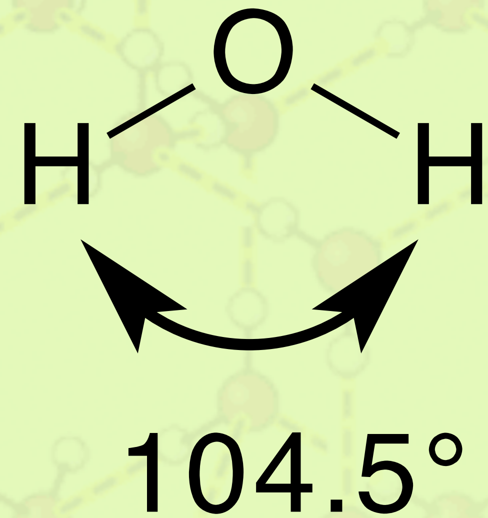
$$K_{eq} = e^{-\frac{\Delta G^o}{RT}} = e^{-\left(\frac{(-30.5)}{(8.314x10^{-3})(273+37)}\right)} = 1.4x10^5$$

Water

- Water makes up 60% to 90% of the mass of living cells.
  - Since the other components of the cell have no choice but to interact with water, a deeper understanding of the physical and chemical properties of water is key to understanding the structures and functions of all the other molecules that make up a living cell.
- In this lecture we will also consider non-covalent interactions.

Physical Properties of Water

- The unusual physical properties of water are determined largely by the high polarity and geometry of the water molecule.



Physical Properties of Water

Question:

Explain why the H-O-H bond angle for water is 104.5°

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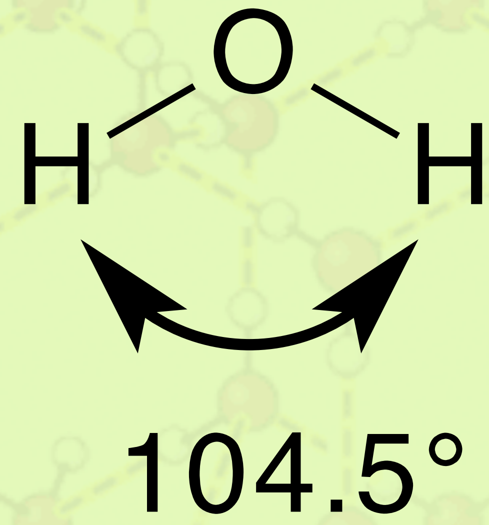
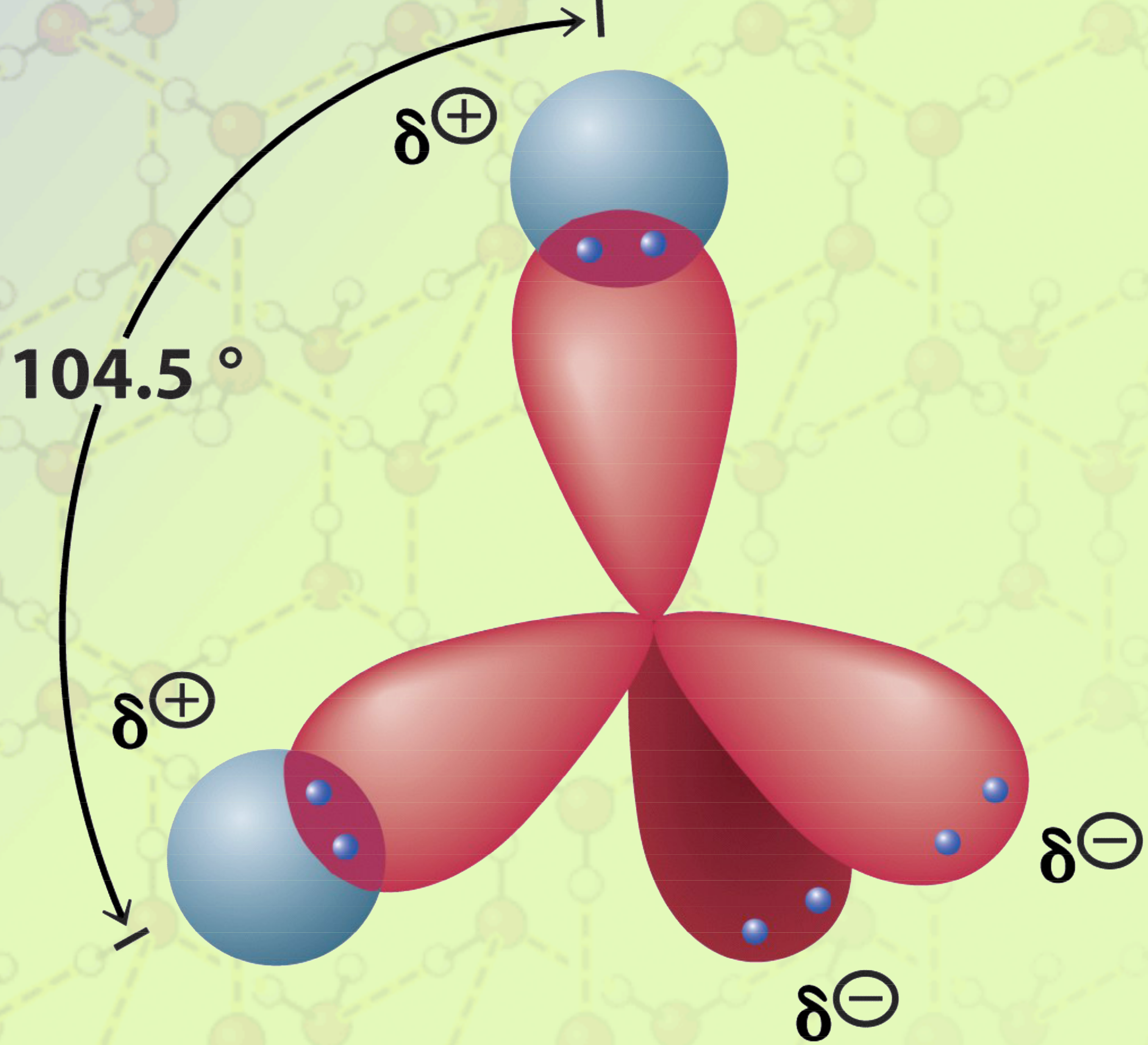


Physical Properties of Water



Physical Properties of Water

Question:

List the physical interactions that one water molecule can have with another.

Physical Properties of Water

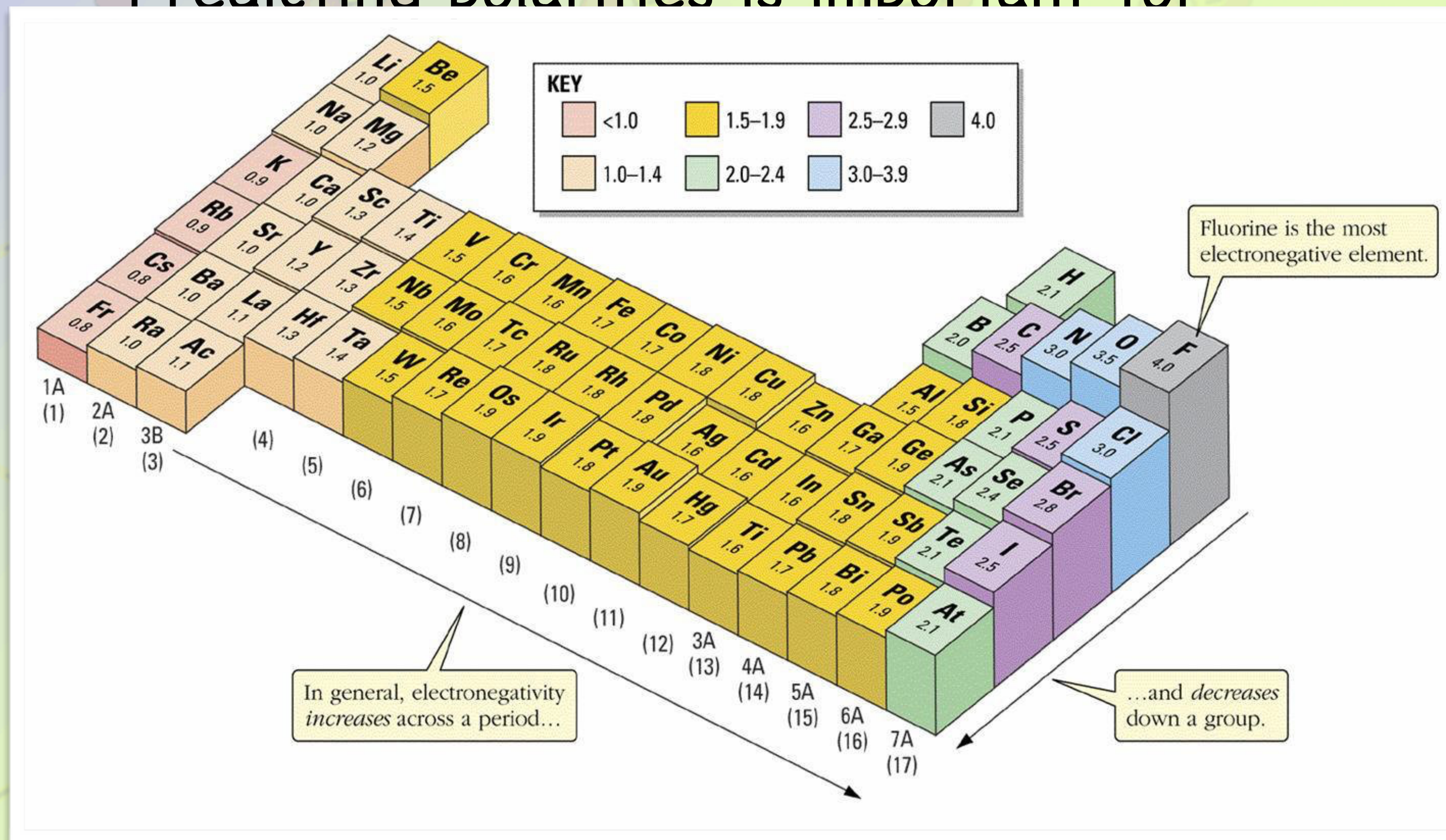
- Predicting polarities is important for predicting what molecules will dissolve in water.

"Like dissolves like"

- Having polar bonds is required, but not sufficient, for a molecule to be polar.
    - A molecule's geometry is also important.

Physical Properties of Water

- Predicting polarities is important for



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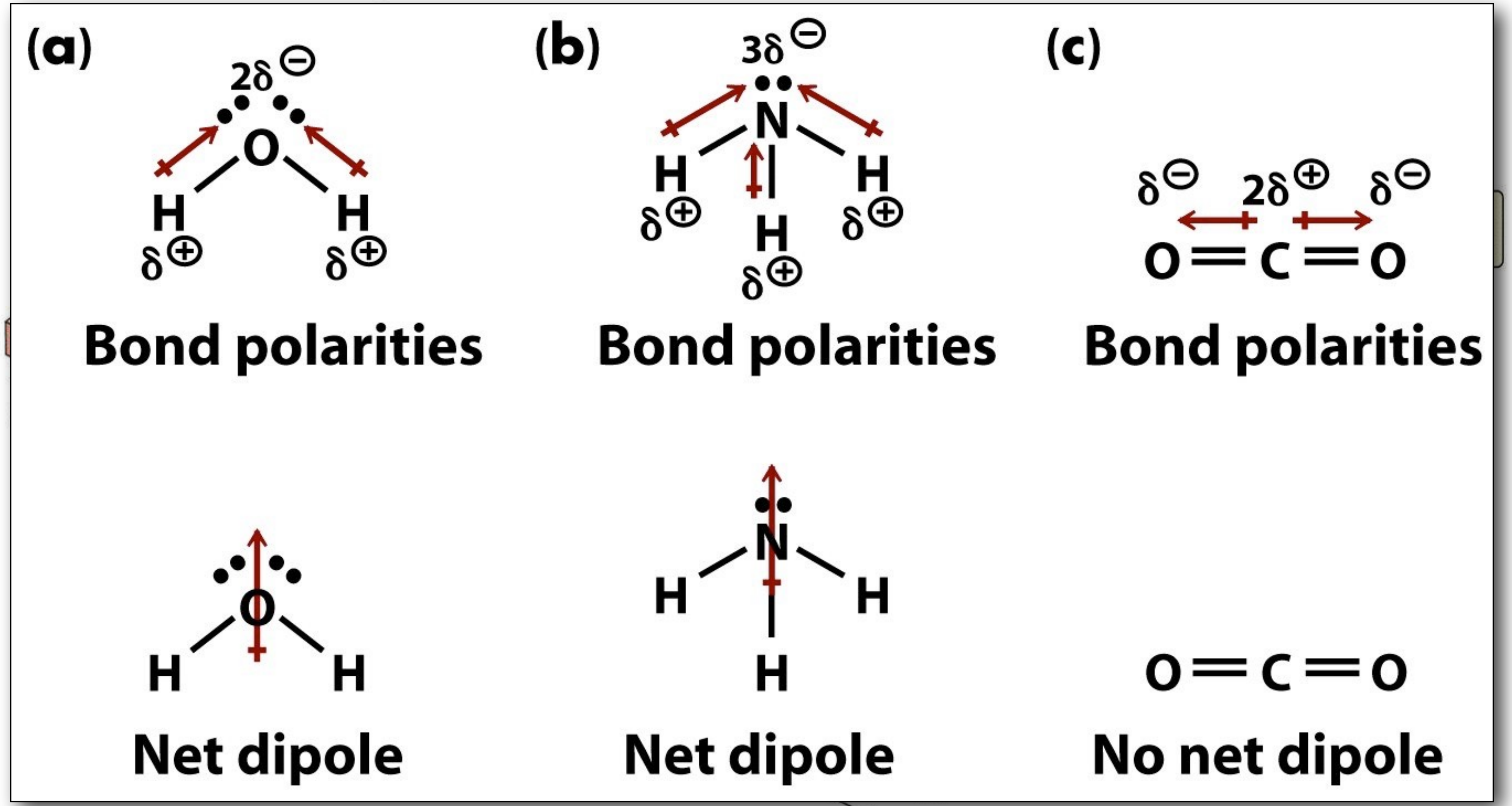

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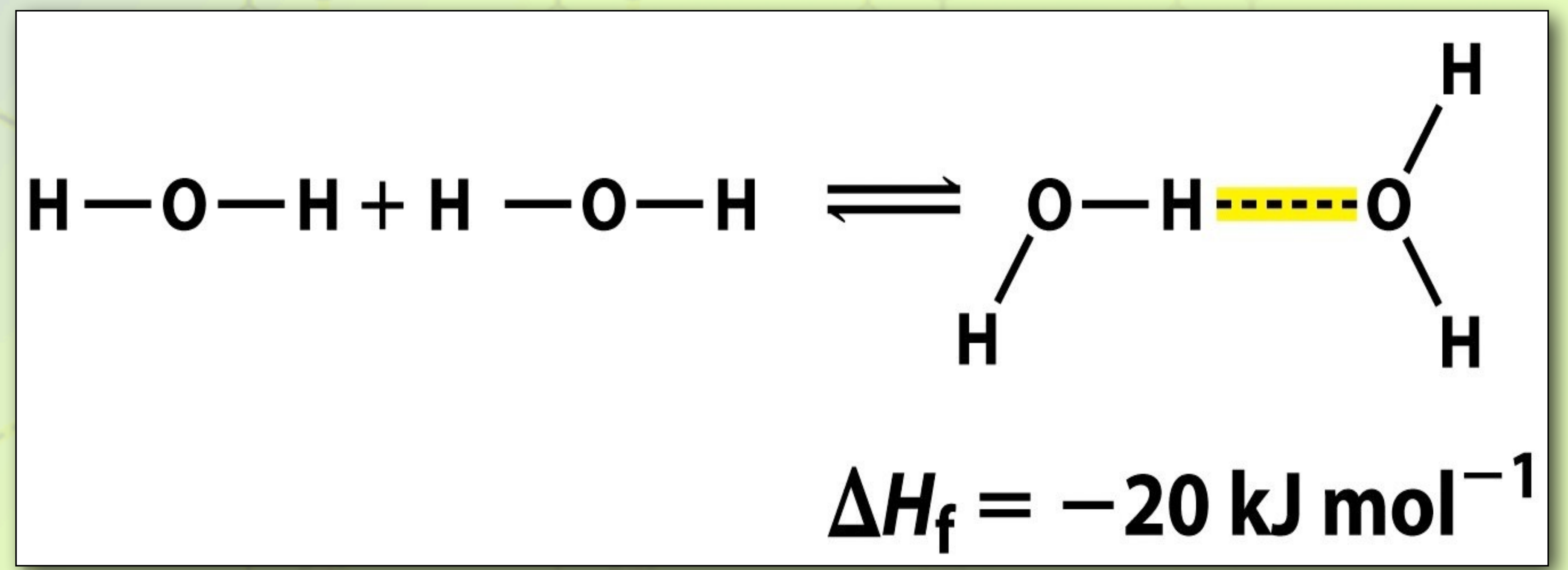
Physical Properties of Water

- Hydrogen bonding
  - In addition to dipole/dipole interactions, water can also interact with itself, and other molecules, through hydrogen bonding.



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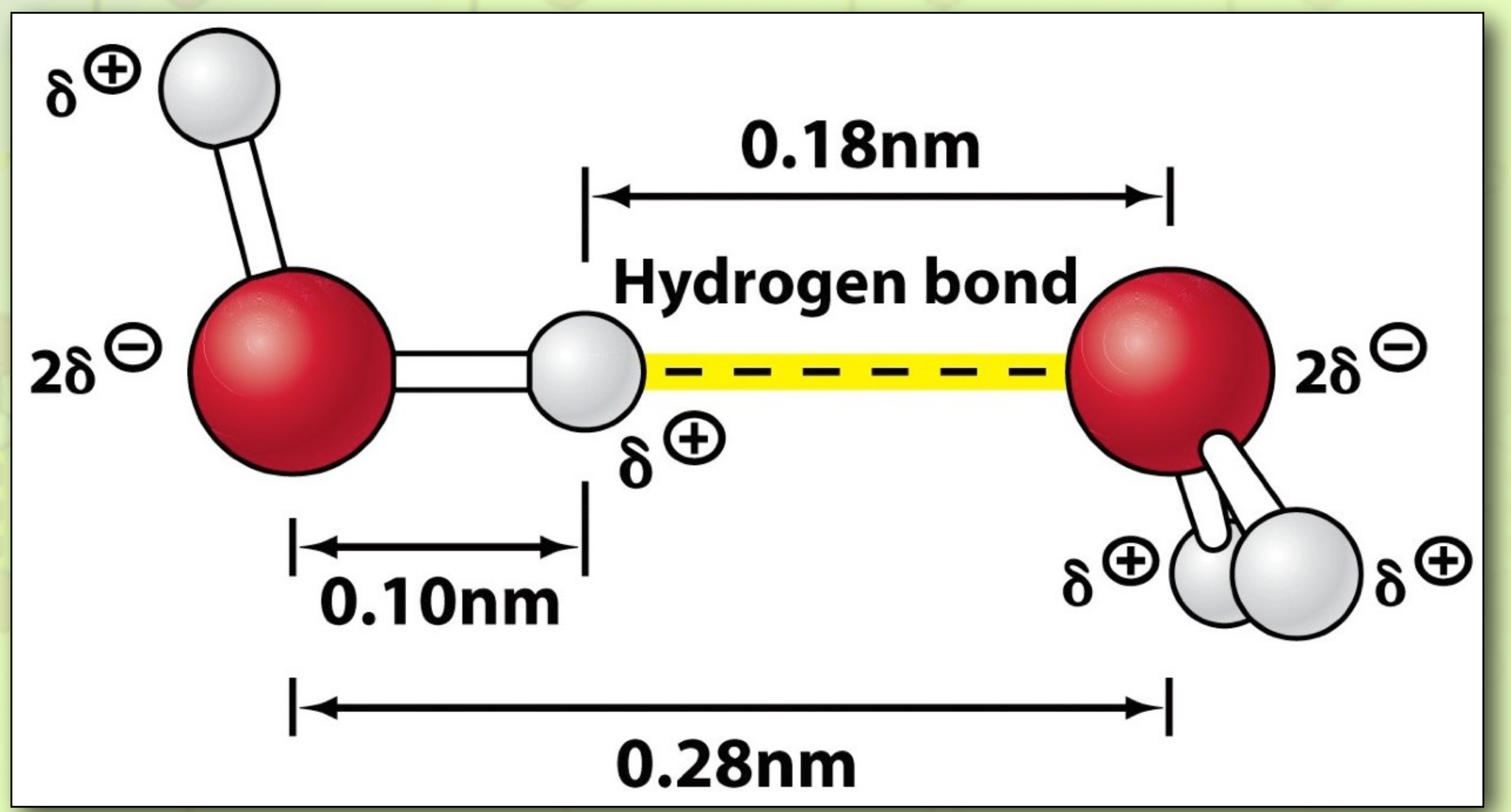

Physical P … Water

- Hydrogen
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Element	radius (Å)
Hydrogen	1.2
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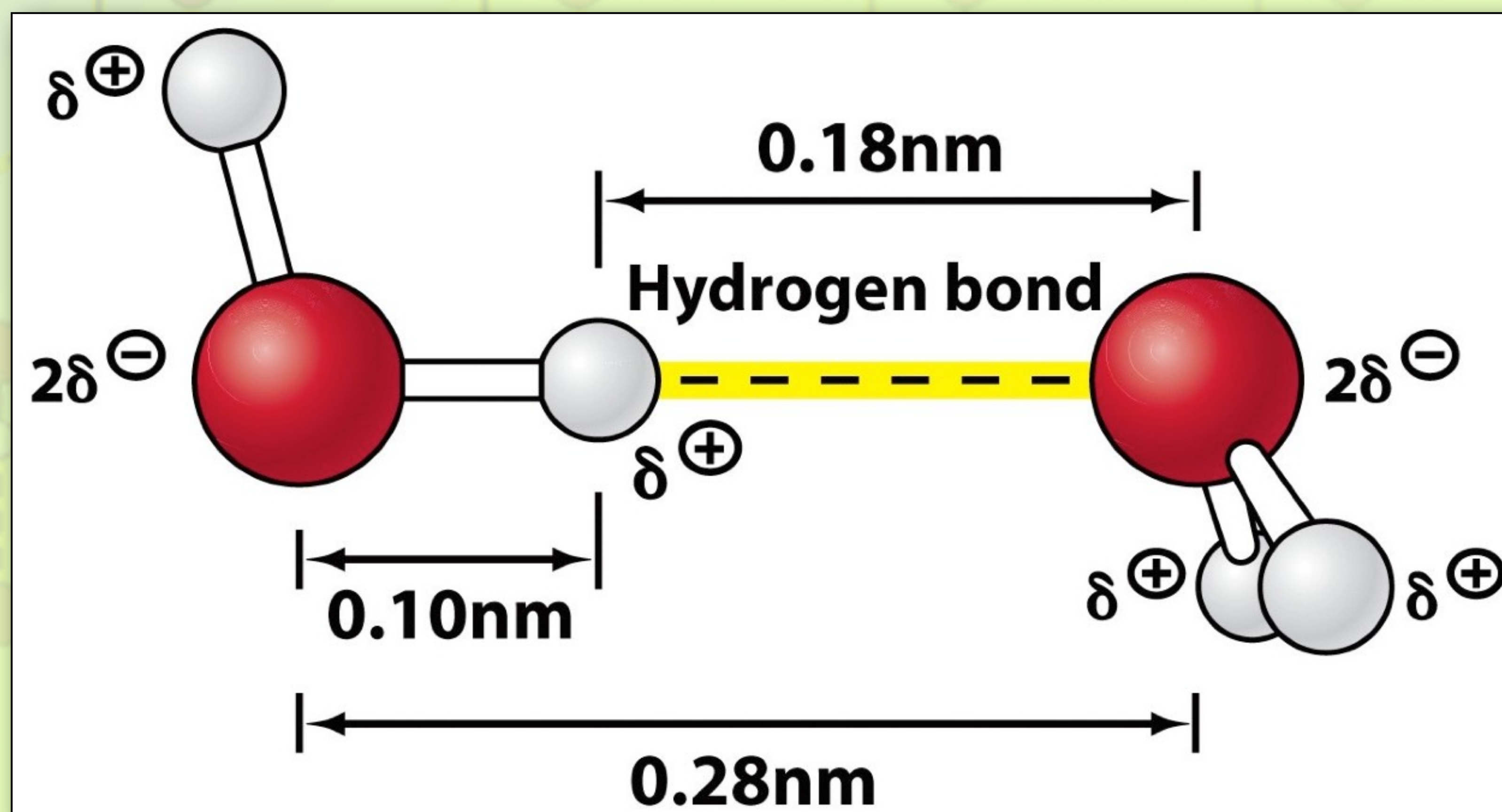
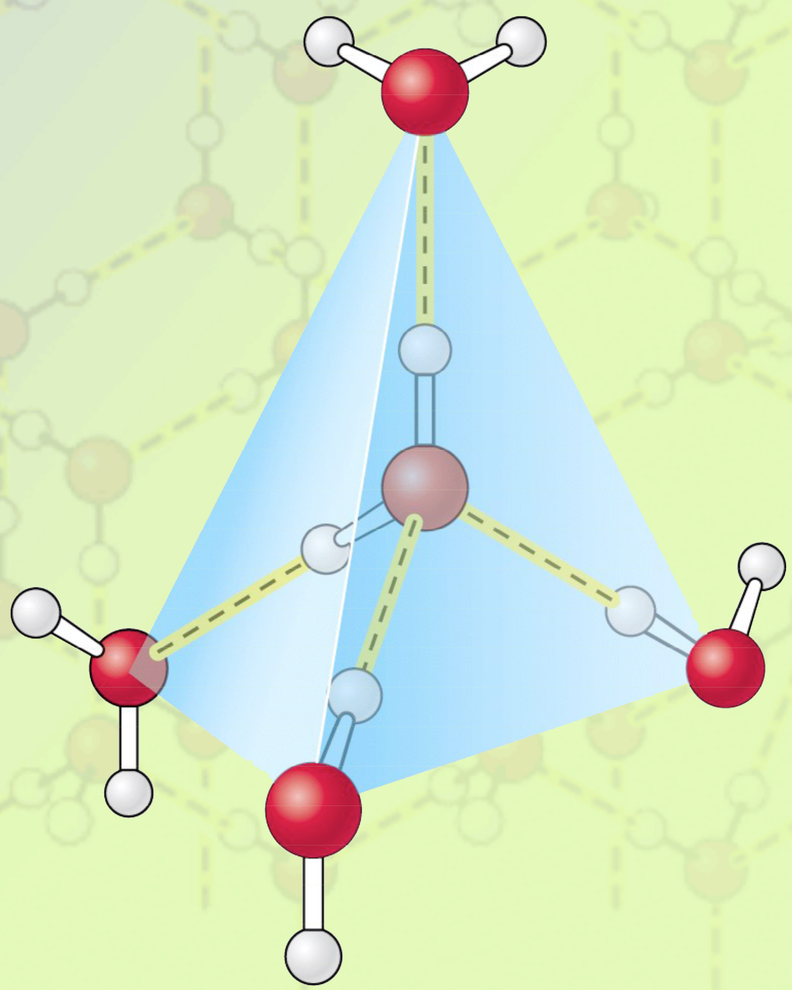


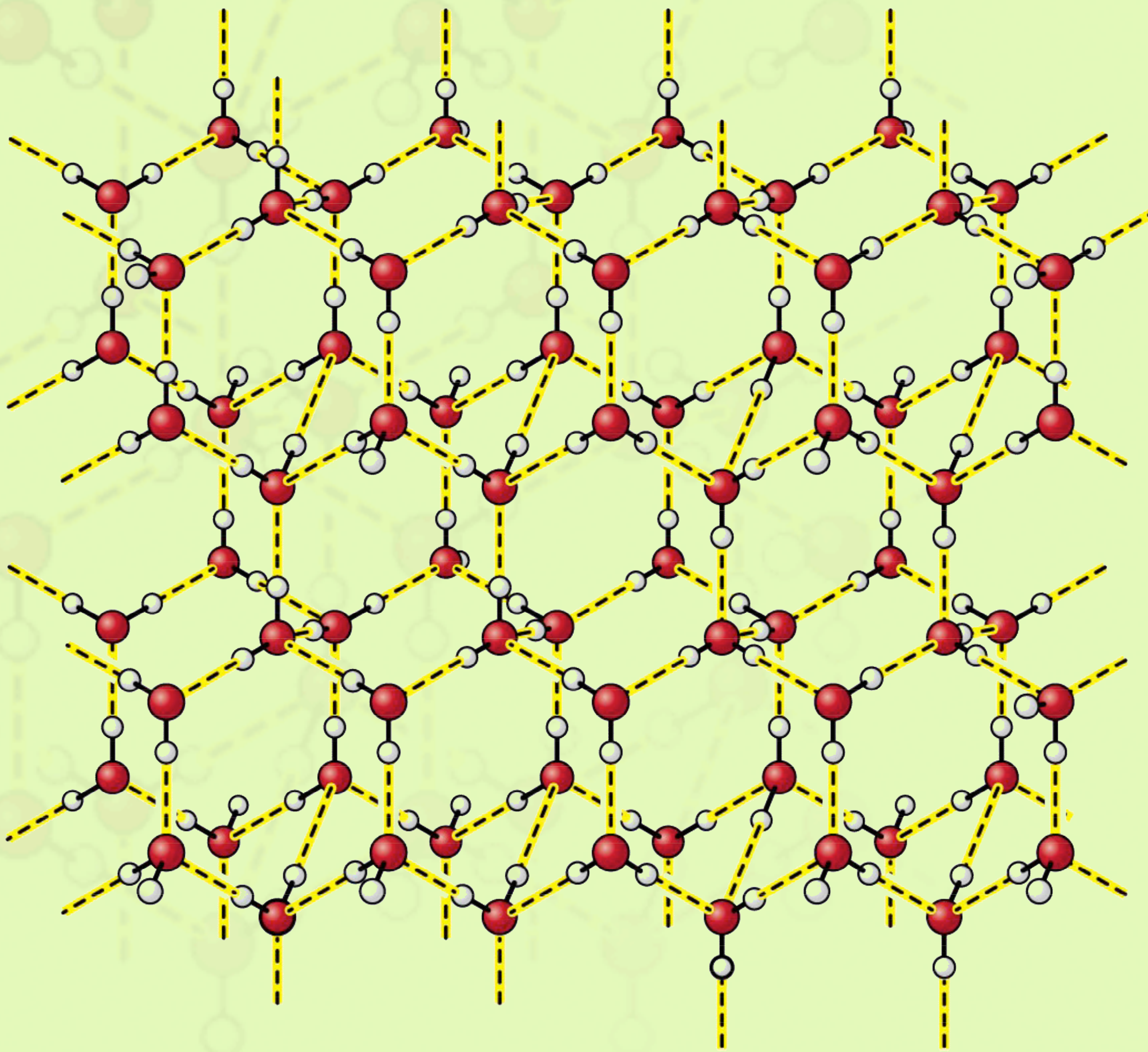
Physical Properties of Water

- Hydrogen bonding has a big effect on the structure physical properties of water.
  - Studying the 3-dimensional structure of water is very difficult.
  - One of our chemistry department graduates, Prof. Rich Saykally, has made a distinguished career of it.

Physical Properties of Water

- Much of our basic understanding of liquid water is inferred from what we know about solid water (ice).





Physical Properties of Water

- Water has unusual physical properties for a molecule of its size and mass.

Physical Properties of Water

Property	Value
Molar mass	18.015
Molar Volume	55.5 moles/liter
Boiling Point (BP)	100°C at 1 atm
Freezing point (FP)	0°C at 1 atm
Triple point	273.16 K at 4.6 torr
Surface Tension	73 dynes/cm at 20°C
Vapor pressure	0.0212 atm at 20°C
Heat of vaporization	40.63 kJ/mol
Heat of Fusion	6.013 kJ/mol
Heat Capacity (cp)	4.22 kJ/kg.K
Dielectric Constant	78.54 at 25°C
Viscosity	1.002 centipoise at 20°C
Density	1 g/cc
Density maxima	4°C
Specific heat	4180 J kg-1 K-1 (T=293...373 K)

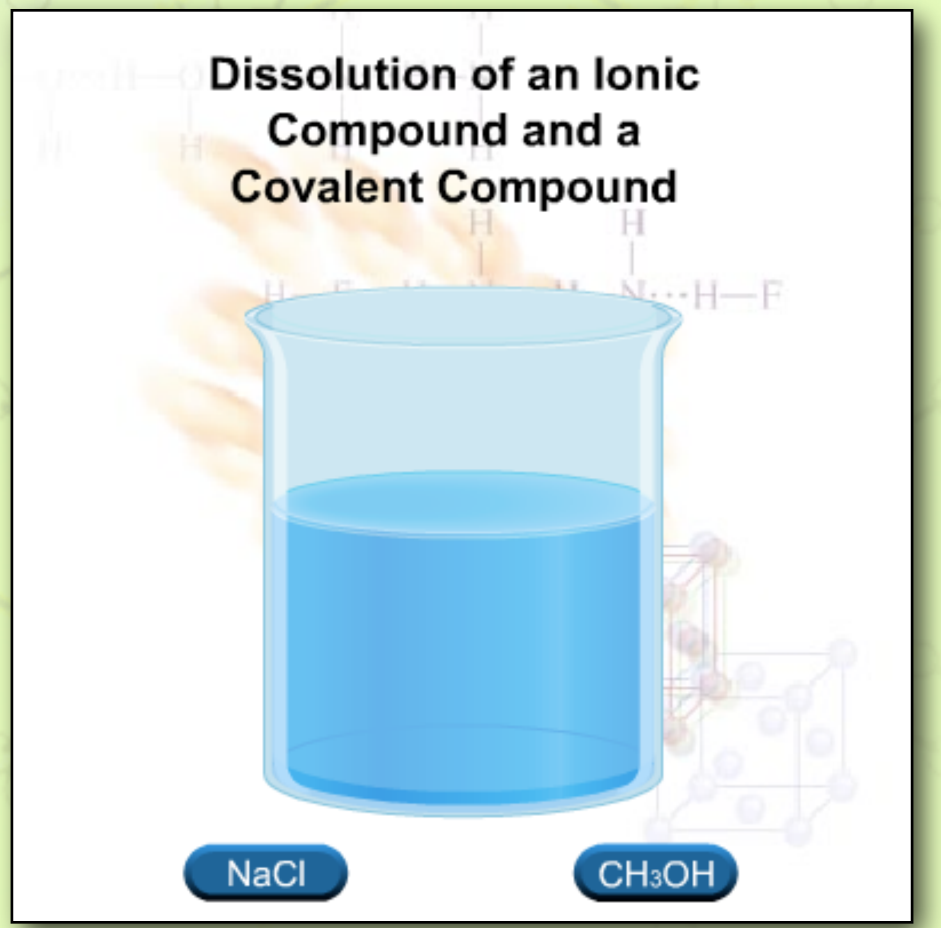
Physical Properties of Water

- Water has unusual physical properties for a molecule of its size and mass.

Name	Formula	Mw (daltons)	Melting Point (°C)	Heat of Fusion (J/g)	Boiling Point (°C)
Water	H_2O	18	0	335	100
Hydrogen Sulfide	H_2S	34	-85.5	69.9	-60.7
Hydrogen Selenide	H_2Se	81	-50.4	31	-41.5

Physical Properties of Water

- Water is a good solvent for solutes that share water's physical properties.
  - "Like dissolves like"



Physical Properties of Water

- The water-like hydroxyl groups make organic molecules more soluble

TABLE 2.1 Solubilities of short-chain alcohols in water

Alcohol	Structure	Solubility in water (mol/100 g H_2O at 20°C)[a]
Methanol	CH_3OH	∞
Ethanol	CH_3CH_2OH	∞
Propanol	$CH_3(CH_2)_2OH$	∞
Butanol	$CH_3(CH_2)_3OH$	0.11
Pentanol	$CH_3(CH_2)_4OH$	0.030
Hexanol	$CH_3(CH_2)_5OH$	0.0058
Heptanol	$CH_3(CH_2)_6OH$	0.0008

[a]Infinity (∞) indicates that there is no limit to the solubility of the alcohol in water.

Physical Properties of Water

- Osmotic pressure

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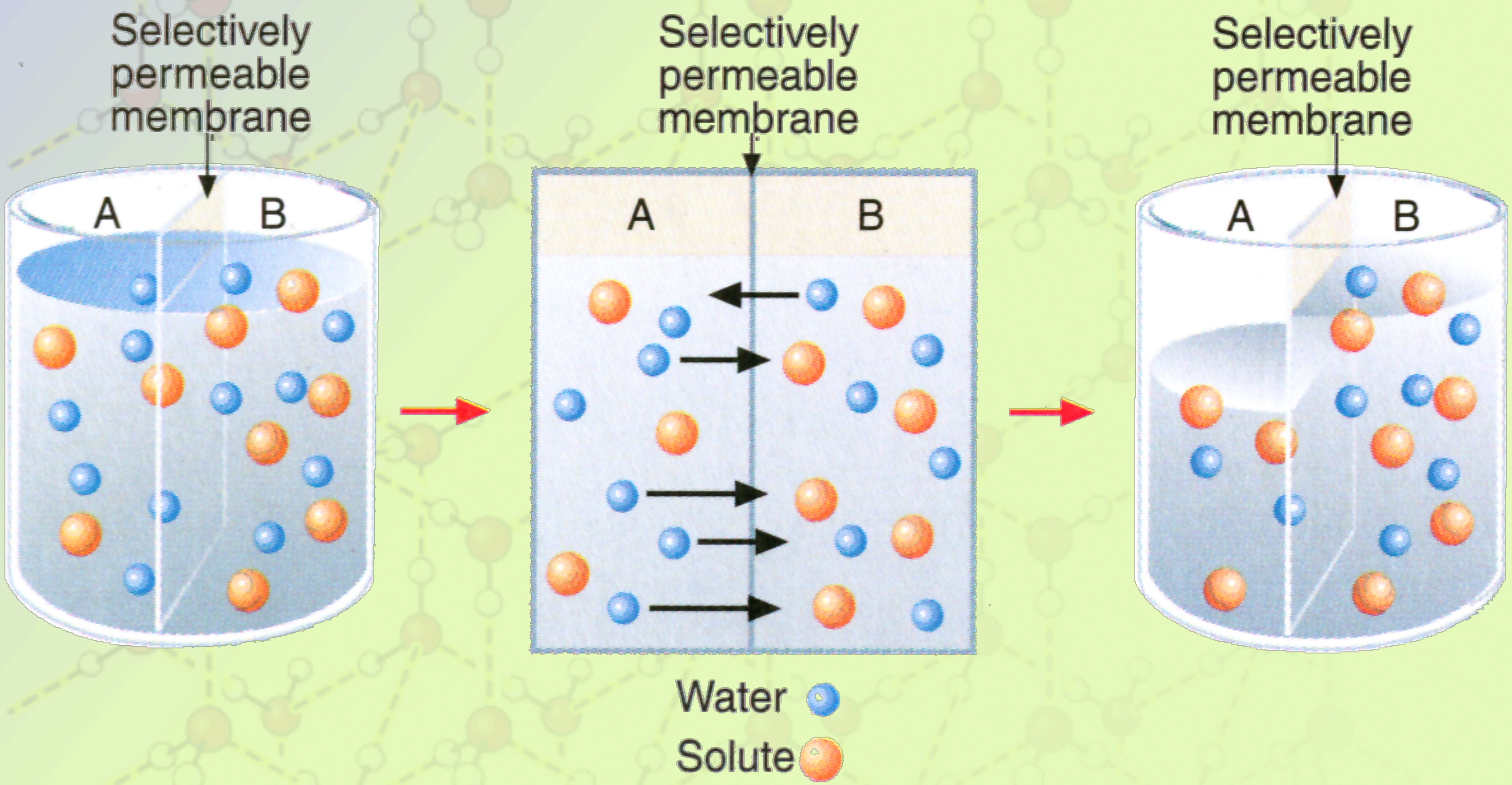

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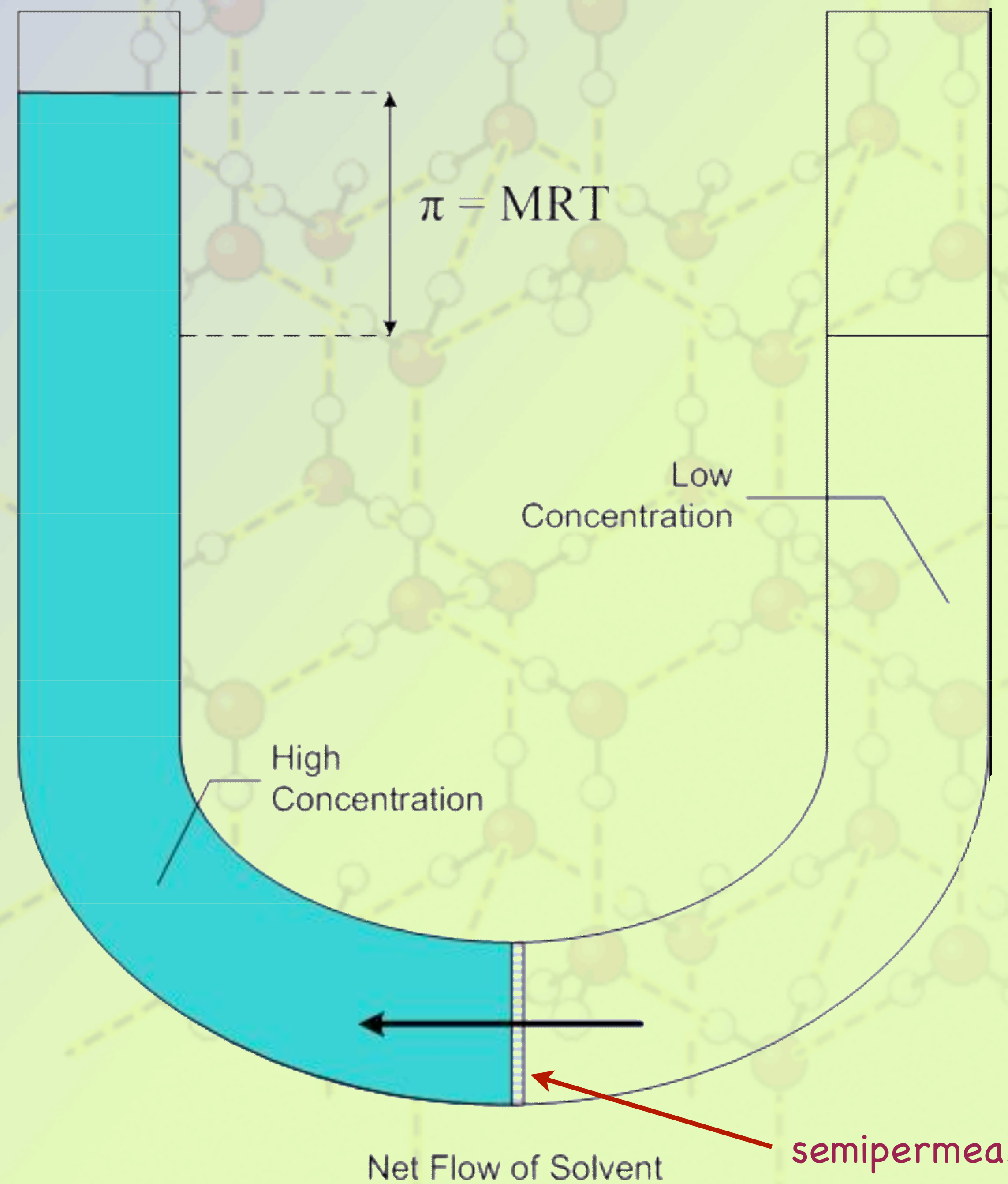

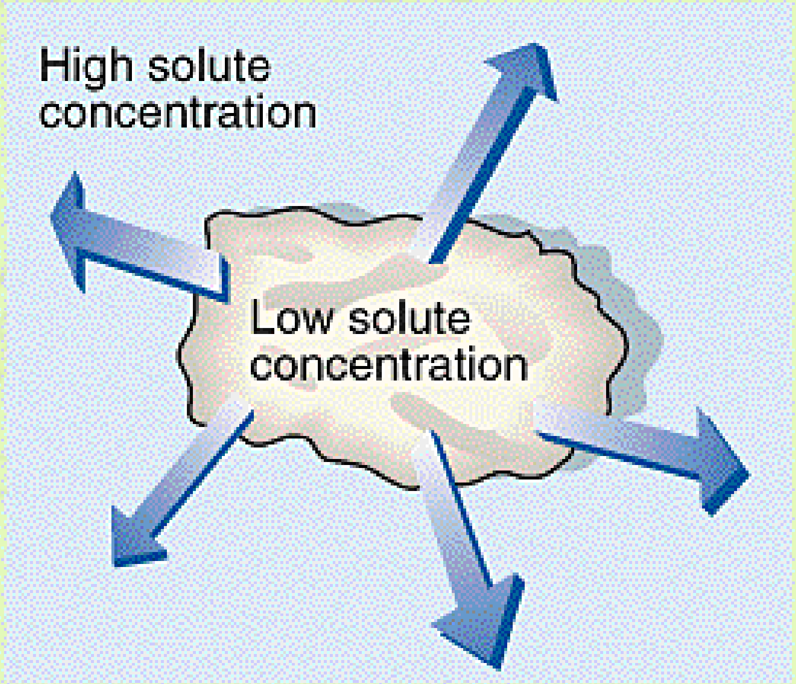

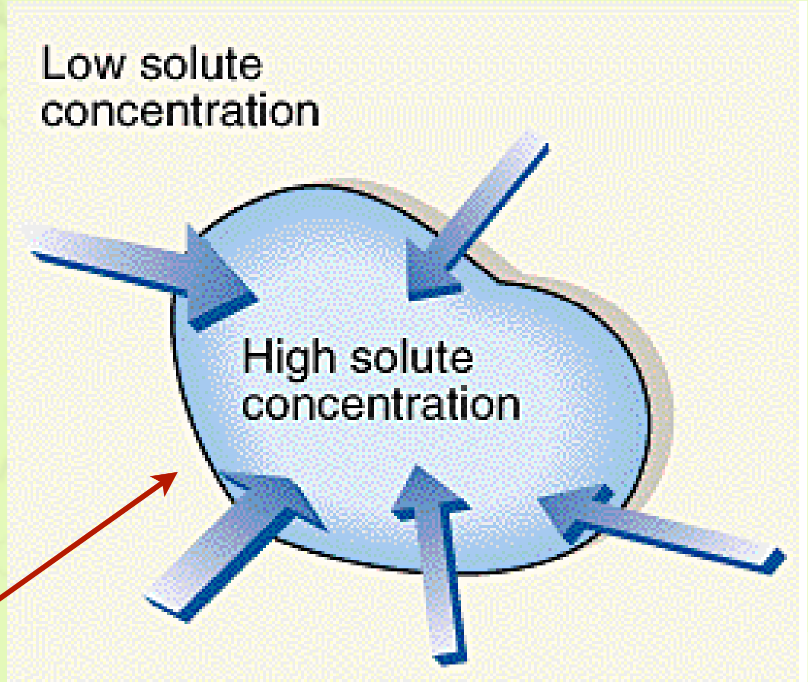

semipermeable
membrane

Physical Properties of Water

- Water is not a good solvent for all substances.
  - Substances with non-polar molecules are generally not soluble in water
    - These molecules are said to be **hydrophobic**.
  - When placed in water, hydrophobic molecules will be pushed aside in ways that minimize their contact with water.

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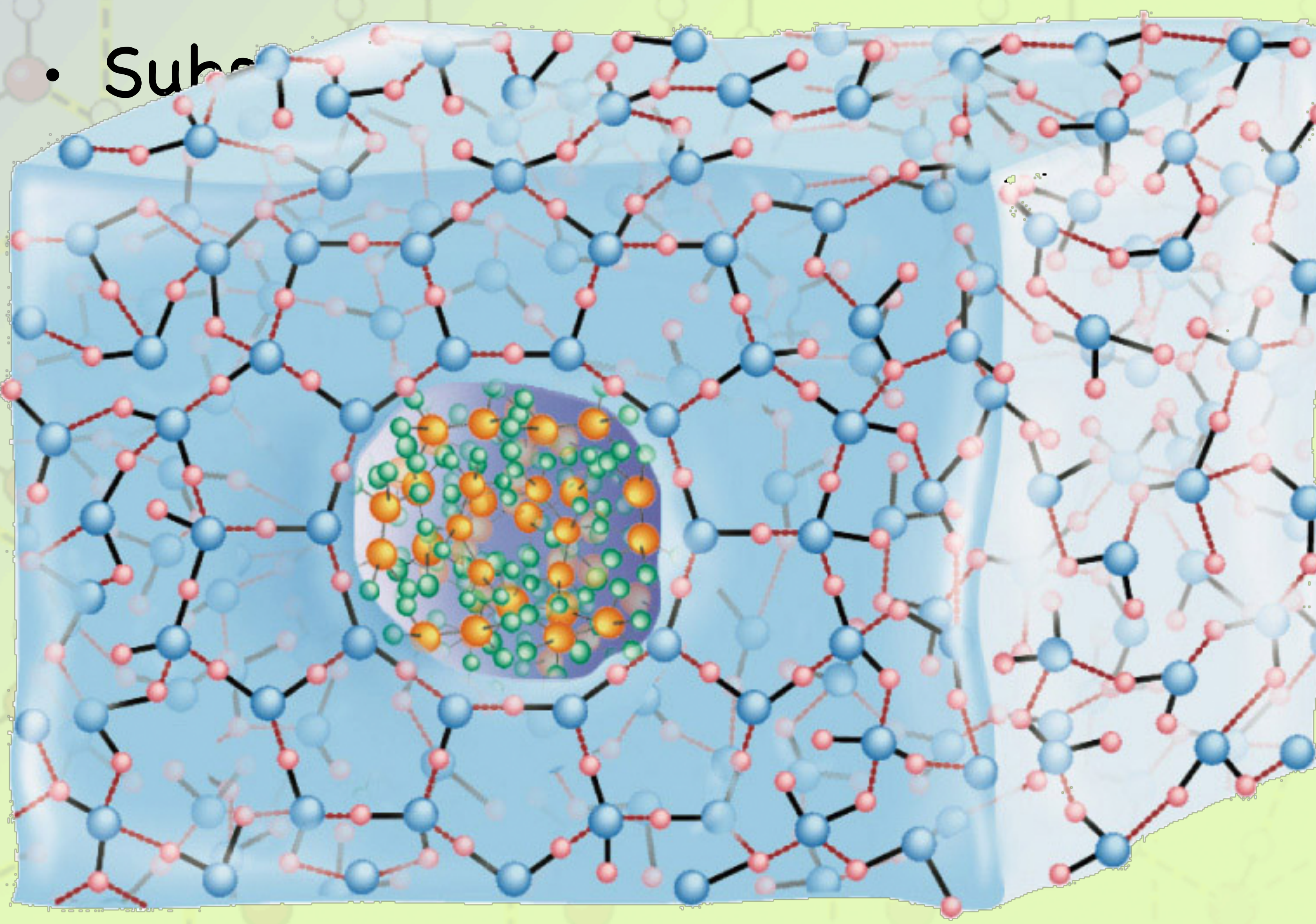

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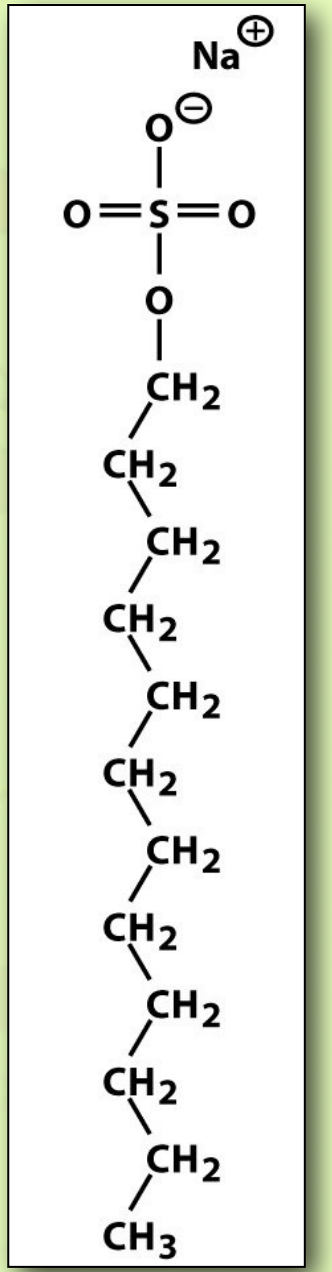
Physical Properties of Water

- Molecules that contain both a hydrophobic and a hydrophilic component, are said to be **amphipathic**.
  - Amphiphathic molecules are conflicted when placed in water and produce some interesting structures in response.



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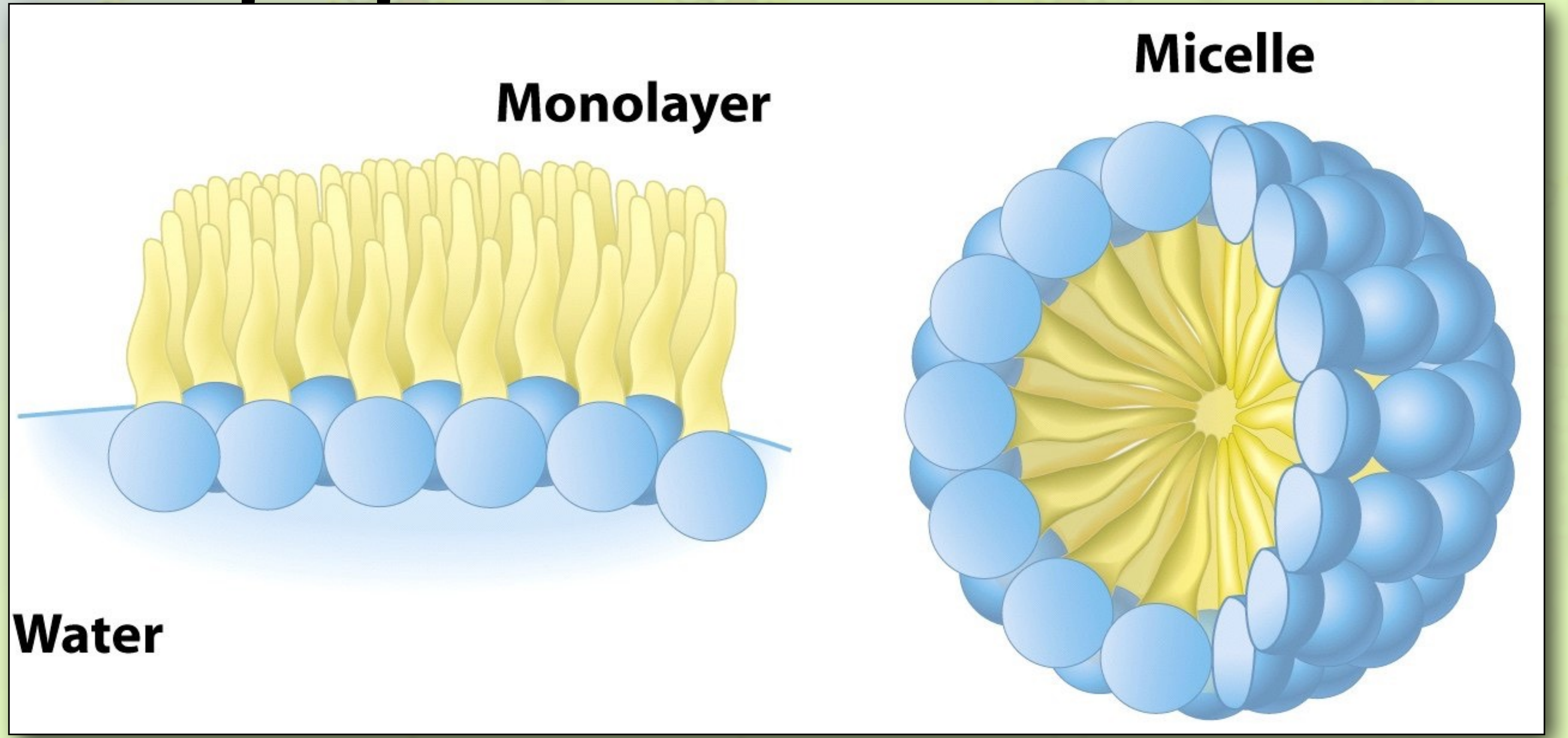

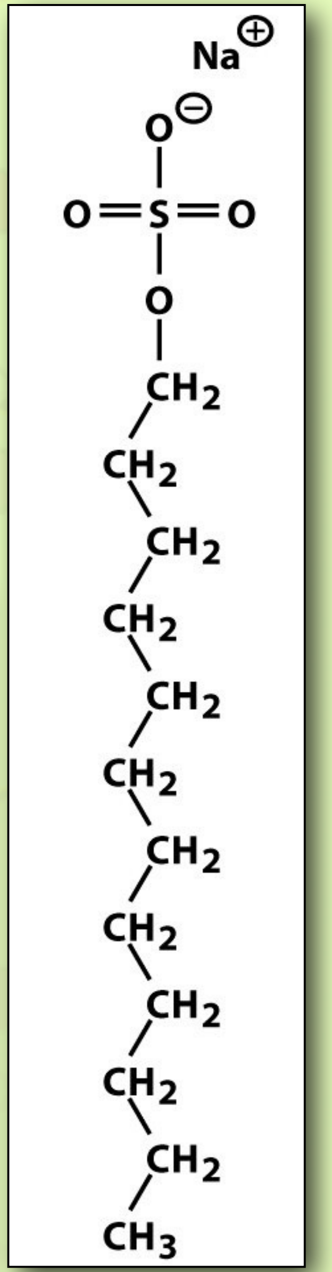

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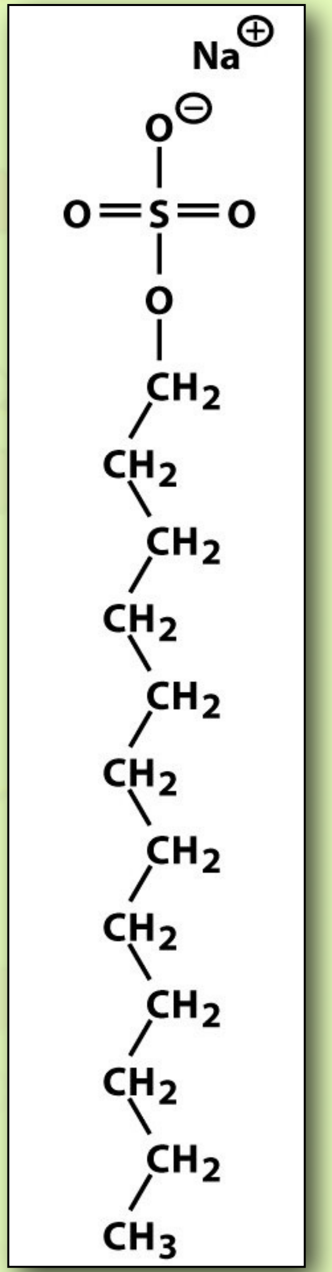

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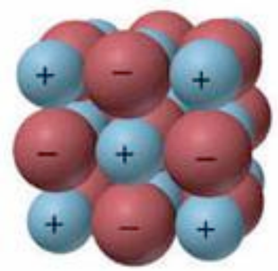
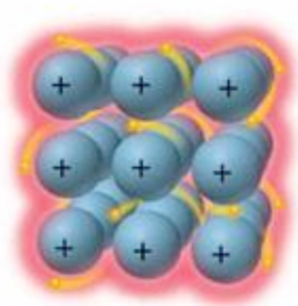
Noncovalent Interactions

- Summary of intermolecular interactions:
  - Bonding Interactions

Force	Model	Basis of Attraction	Energy (kJ/mol)	Example
Bonding				
Ionic		Cation–anion	400–4000	NaCl
Covalent		Nuclei–shared e^- pair	150–1100	H—H
Metallic		Cations–delocalized electrons	75–1000	Fe

metals bonding to nonmetals

nonmetals bonding to nonmetals

metals bonding to metals

Noncovalent Interactions

- Noncovalent (Nonbonding) can be broadly catalogued into 4 types that are based on electrostatics,
  - **Charge-Charge**
  - **Hydrogen bonding**
  - **Dipole/Dipole**
  - **vander Waals**
- These help to stabilize the structures after they form form.

Noncovalent Interactions

- And **hydrophobic interactions**, which drives structure formation in the presence of water,
  - **hydrophobic interactions** drive such processes as,
    - Protein foldings
    - DNA double helix formation
    - Membrane assembly

Noncovalent Interactions

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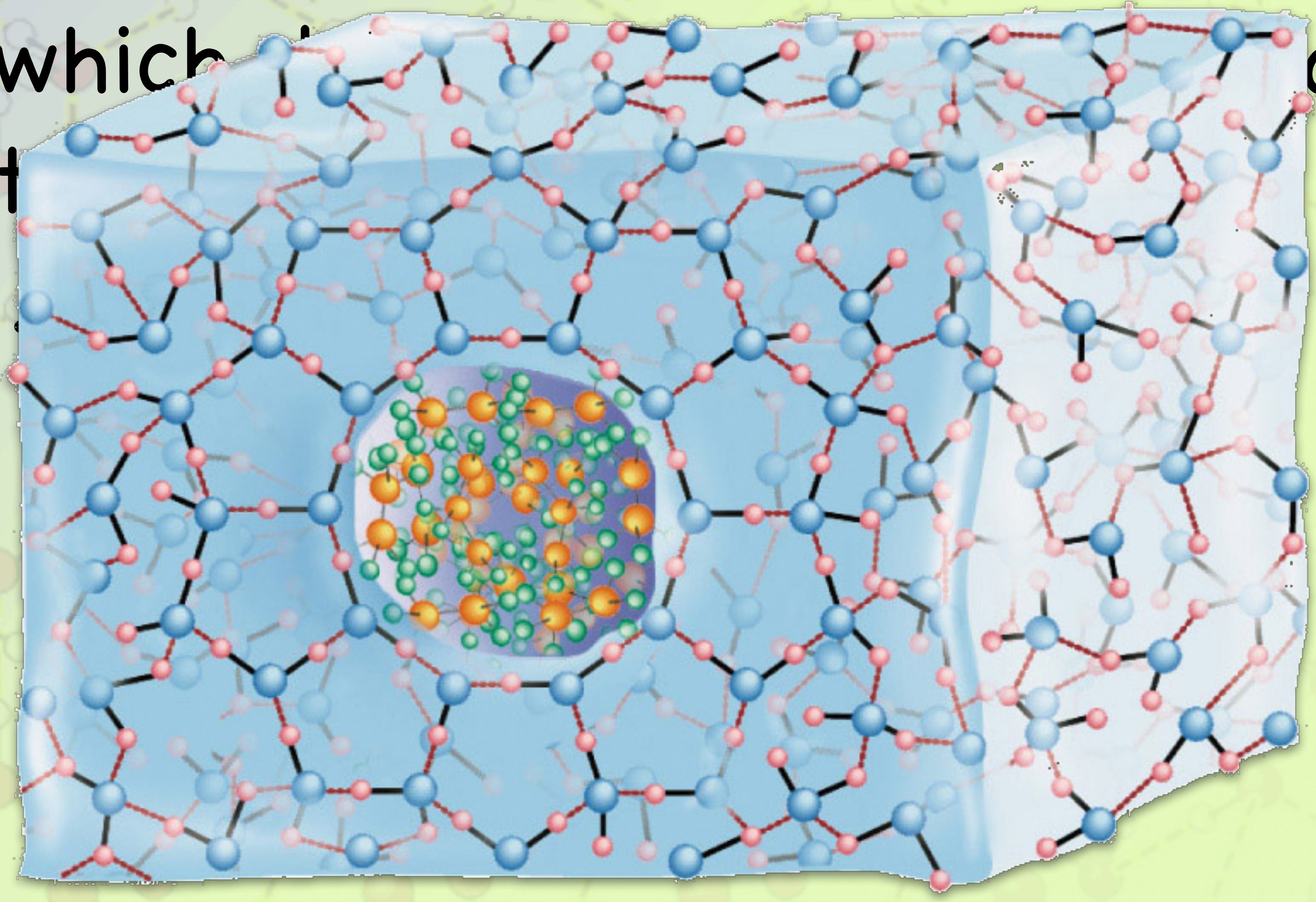

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Noncovalent Interactions

The stabilizing noncovalent interactions are electrostatic in nature,

Including:

- Charge/charge

r

q+ ⟷ q-

$$F = \frac{(q+)(q-)}{Dr^2}$$

(Force)

Coulomb's Law

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Water has a huge, mitigating effect on electrostatic interactions

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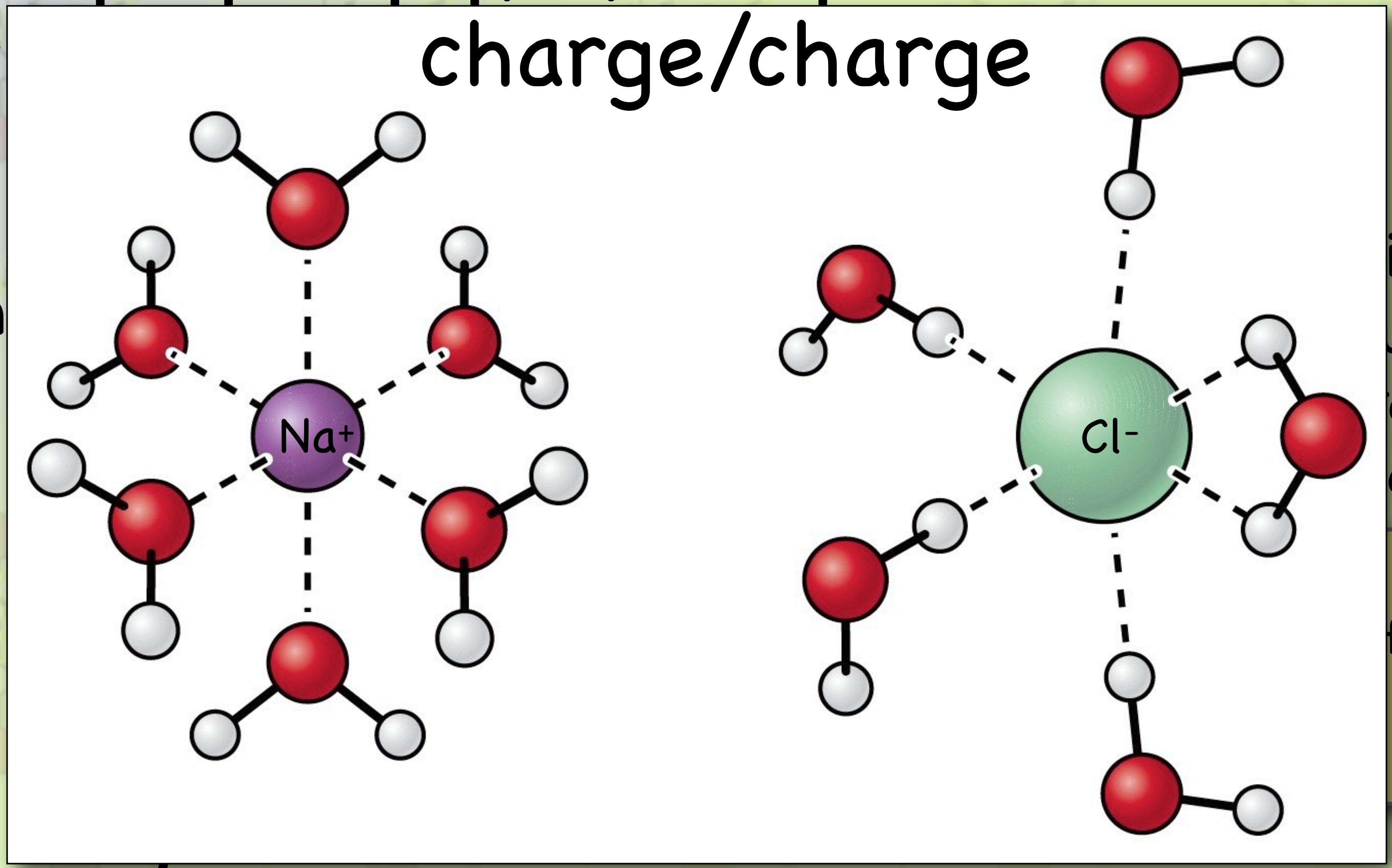

(Force)

Dr^2

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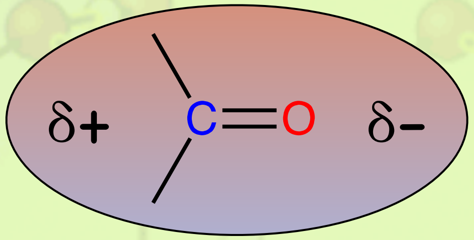

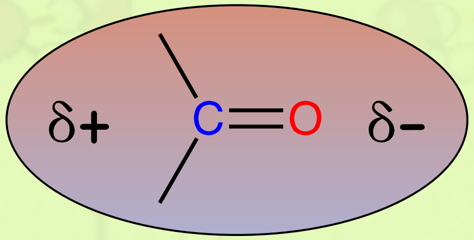

Noncovalent Interactions

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While dipole/dipole interactions can be either attractive or repulsive, they will tend to arrange themselves to produce an attractive interaction.

Noncovalent Interactions

The stabilizing noncovalent interactions are electrostatic in nature,

Including:

- Charge/charge
- Dipole/dipole
- Hydrogen bonding

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Hydrogen bonding can be thought of as a special case of dipole/dipole interaction.

Noncovalent Interactions

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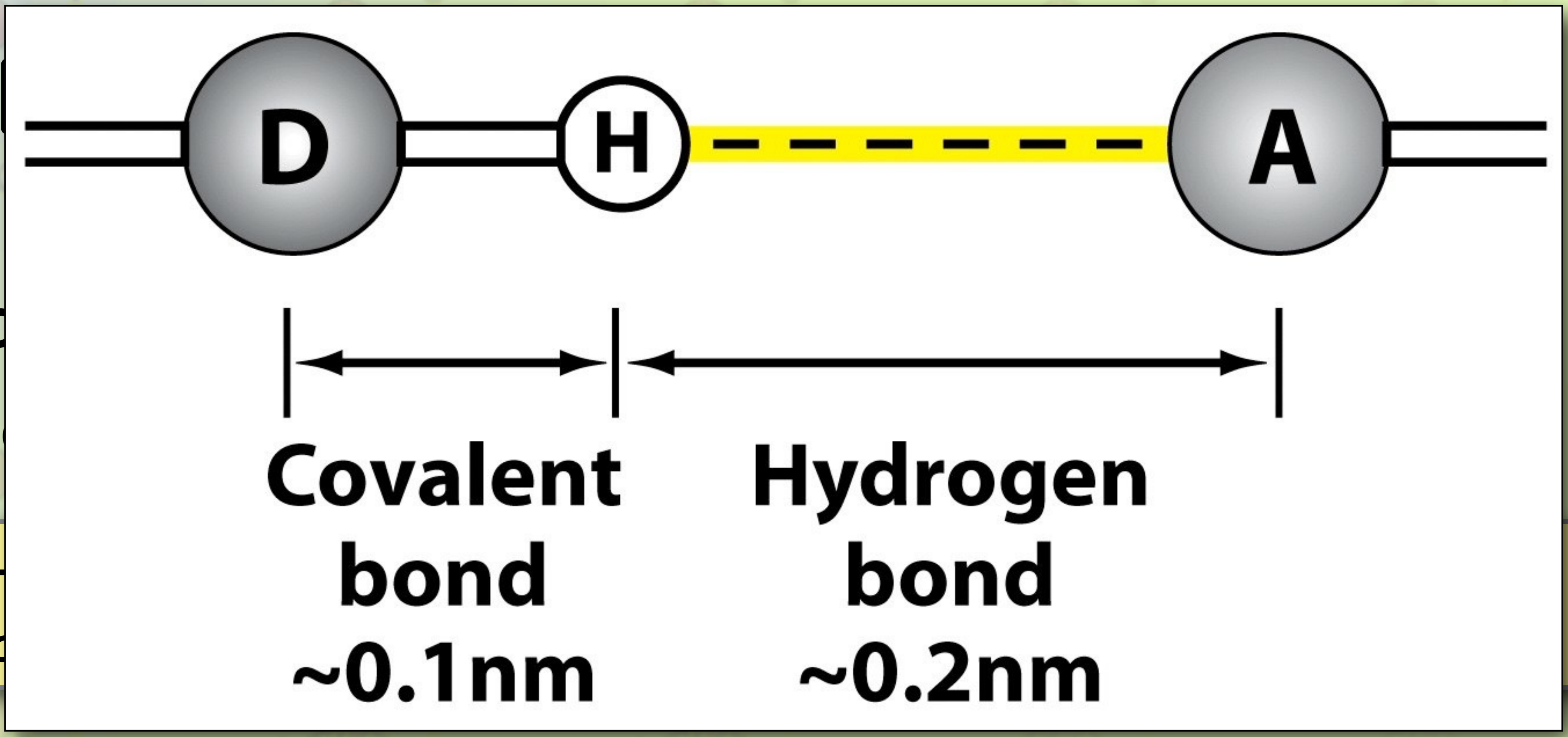

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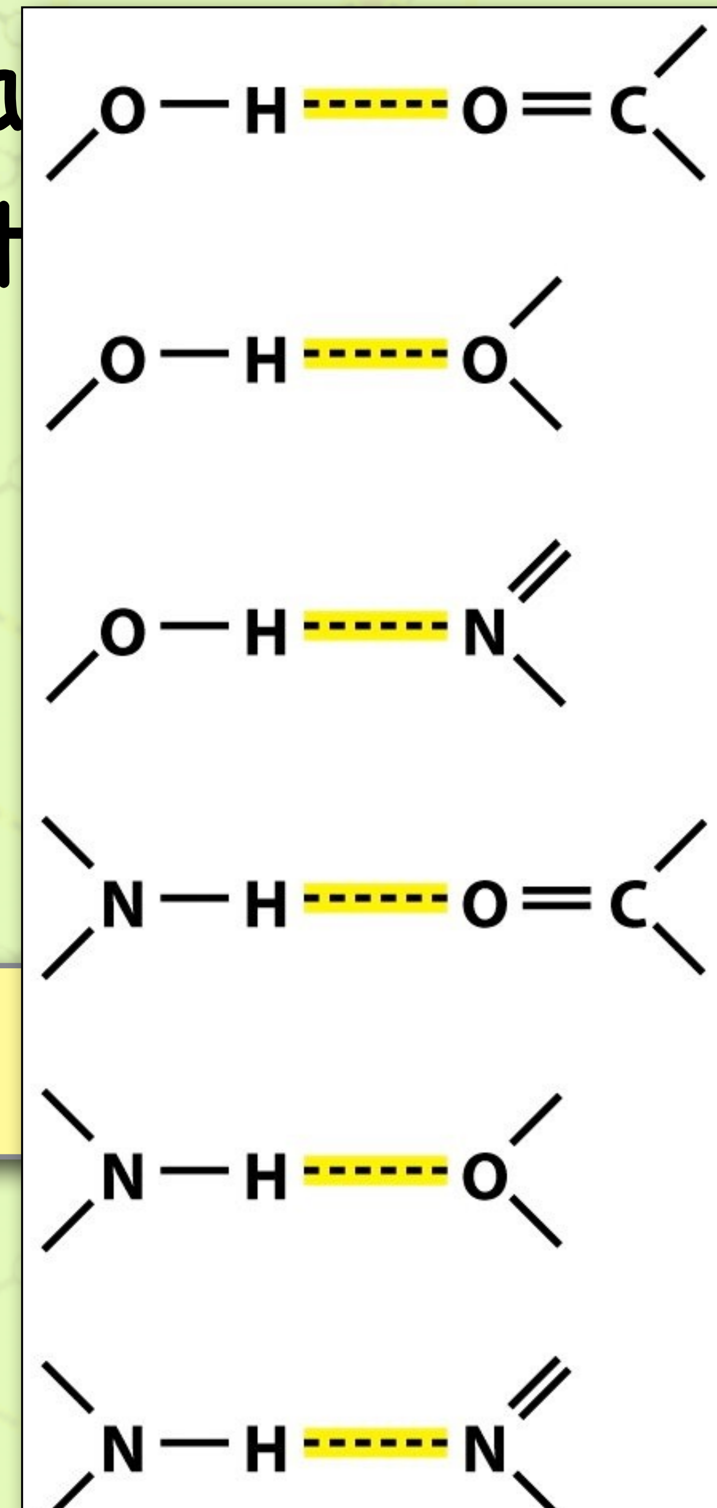

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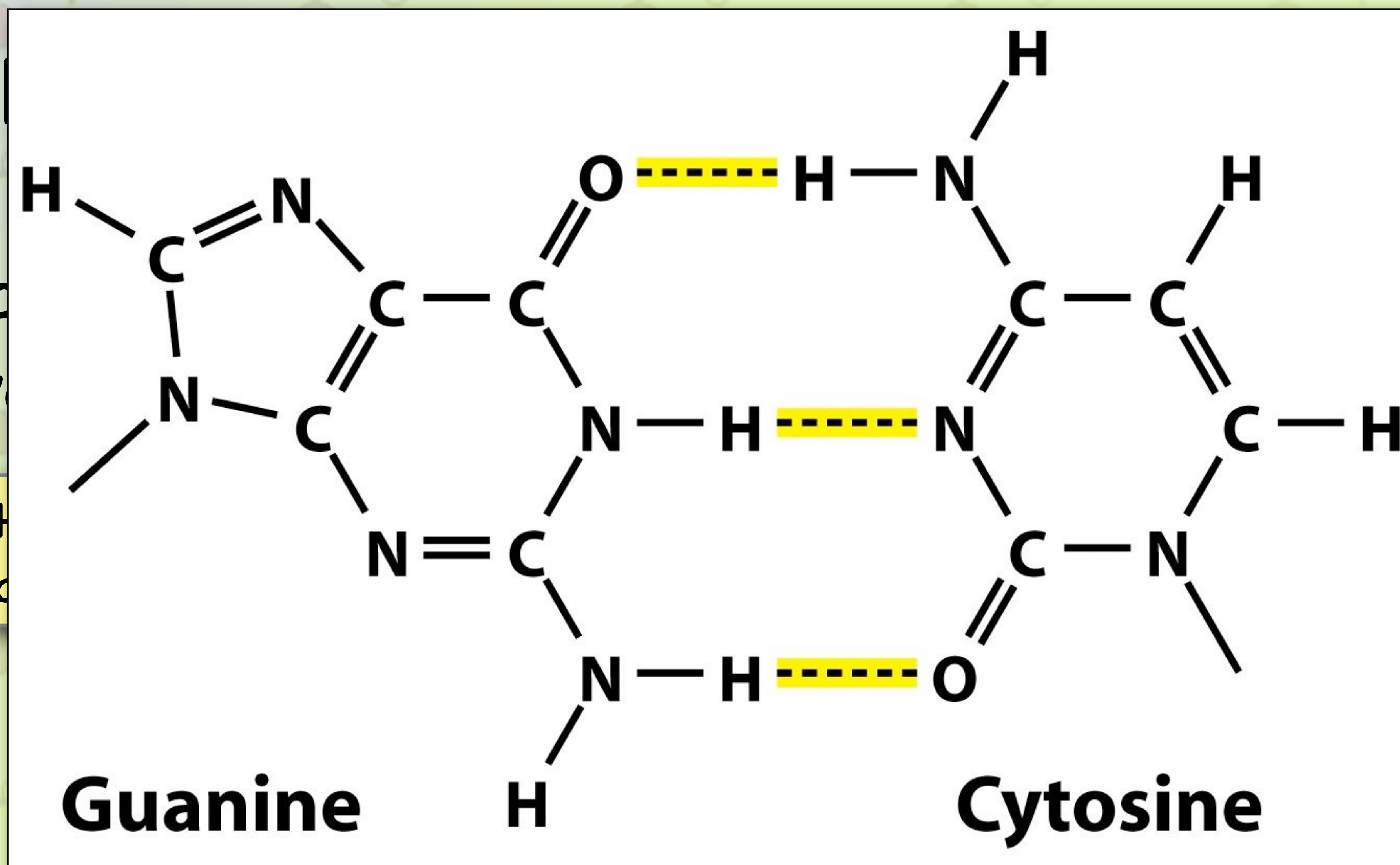

Noncovalent Interactions

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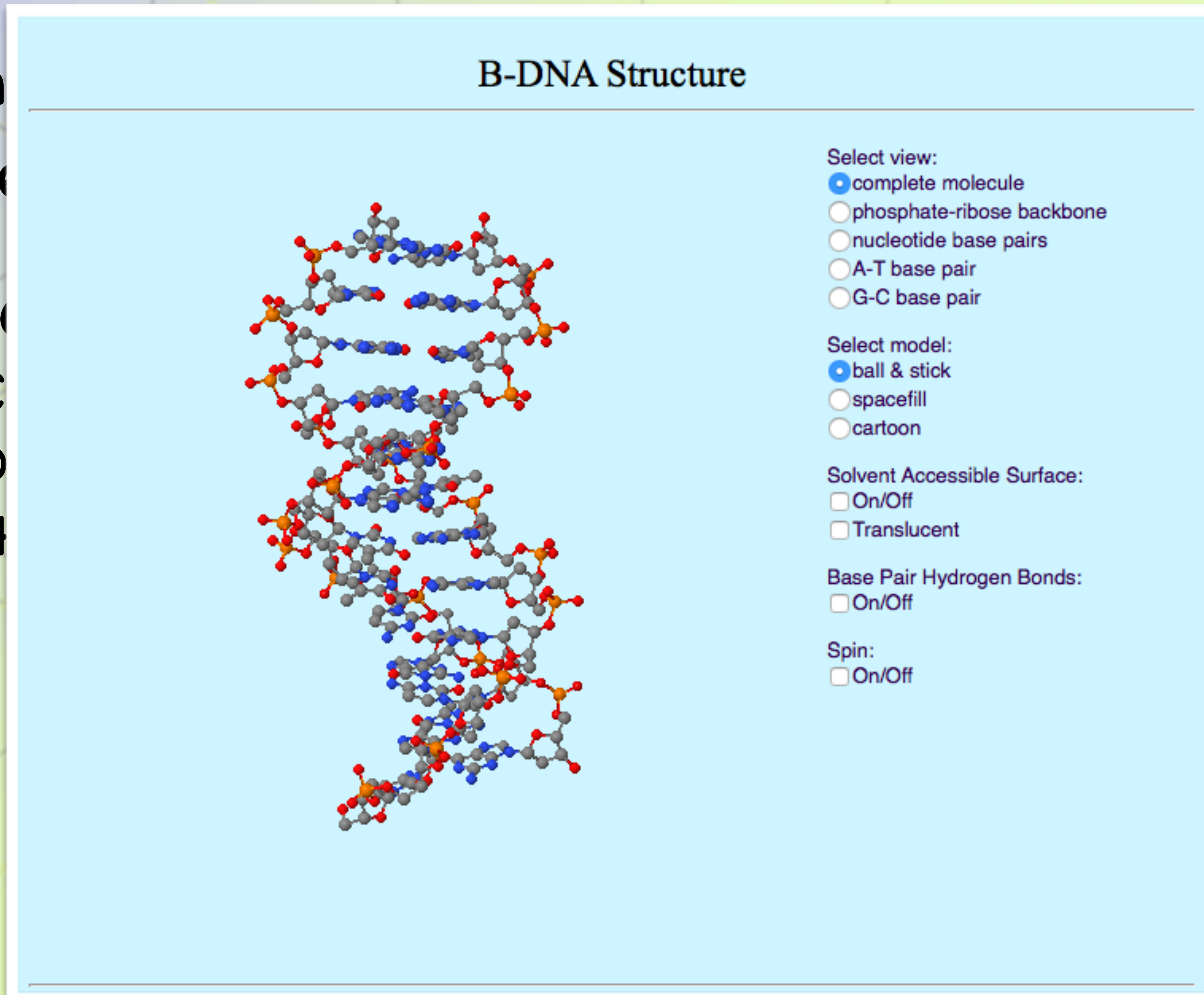

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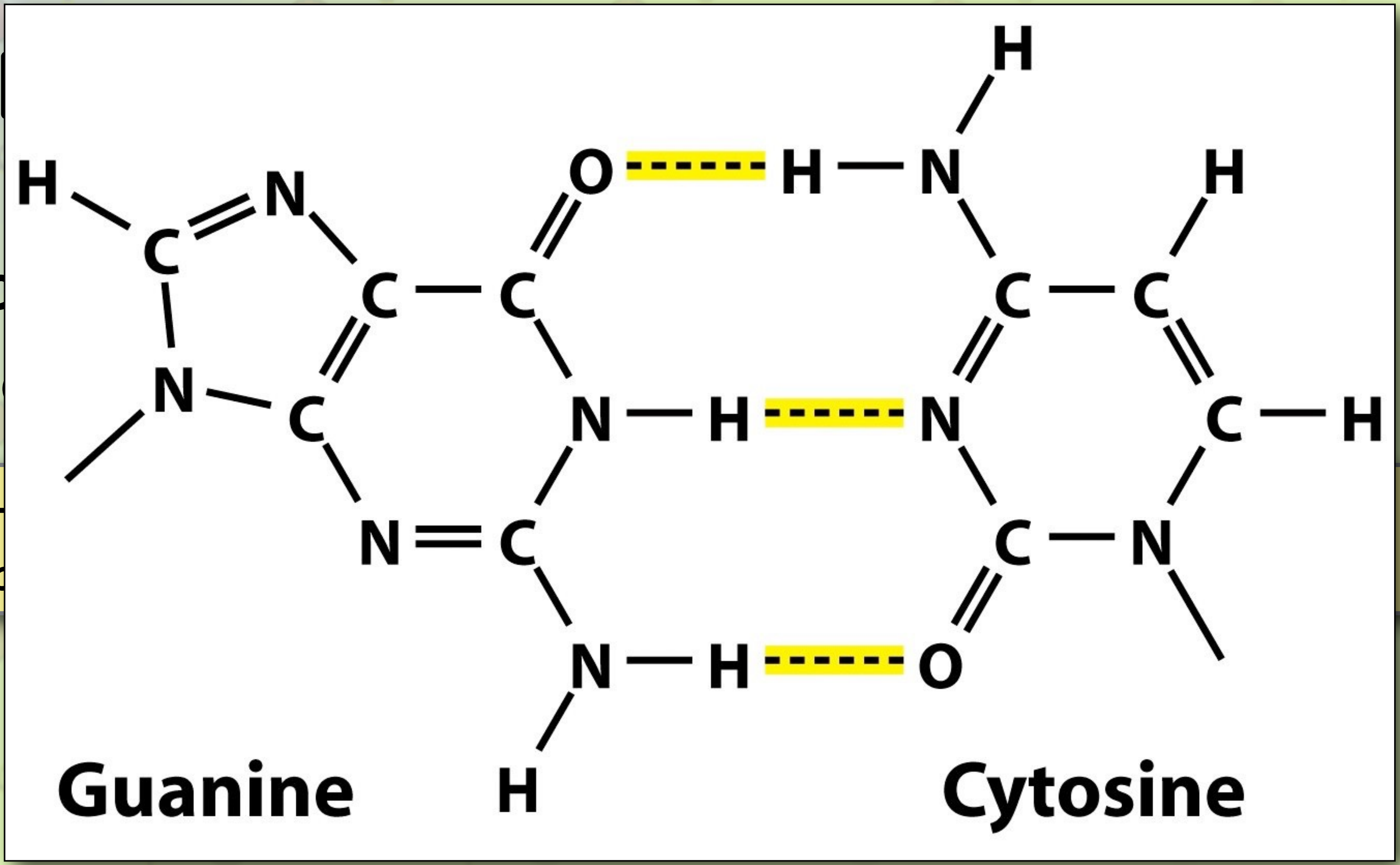

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- vander Waals interactions include
  - dipole/induced dipole
  - induced/induced dipole (London Dispersion)
  - electron repulsion

Noncovalent Interactions

The stabilizing noncovalent interactions

Ion–induced dipole		Ion charge–polarizable e$^-$ cloud	3–15	$Fe^{2+} \cdots O_2$
Dipole–induced dipole		Dipole charge–polarizable e$^-$ cloud	2–10	$H—Cl \cdots Cl—Cl$
Dispersion (London)		Polarizable e$^-$ clouds	0.05–40	$F—F \cdots F—F$

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Noncovalent Interactions

The vander Waals radius

- Defined by a balance between
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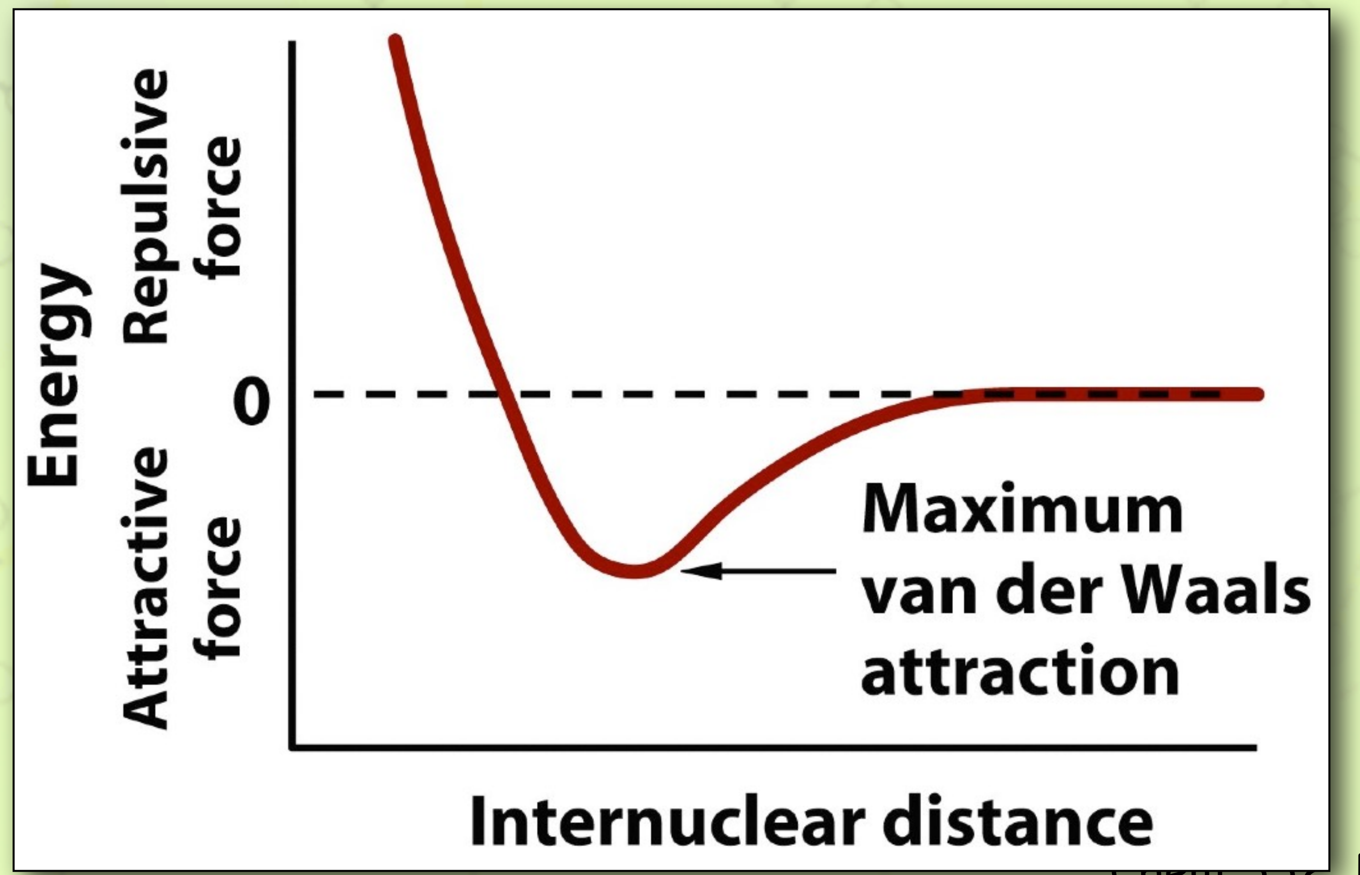

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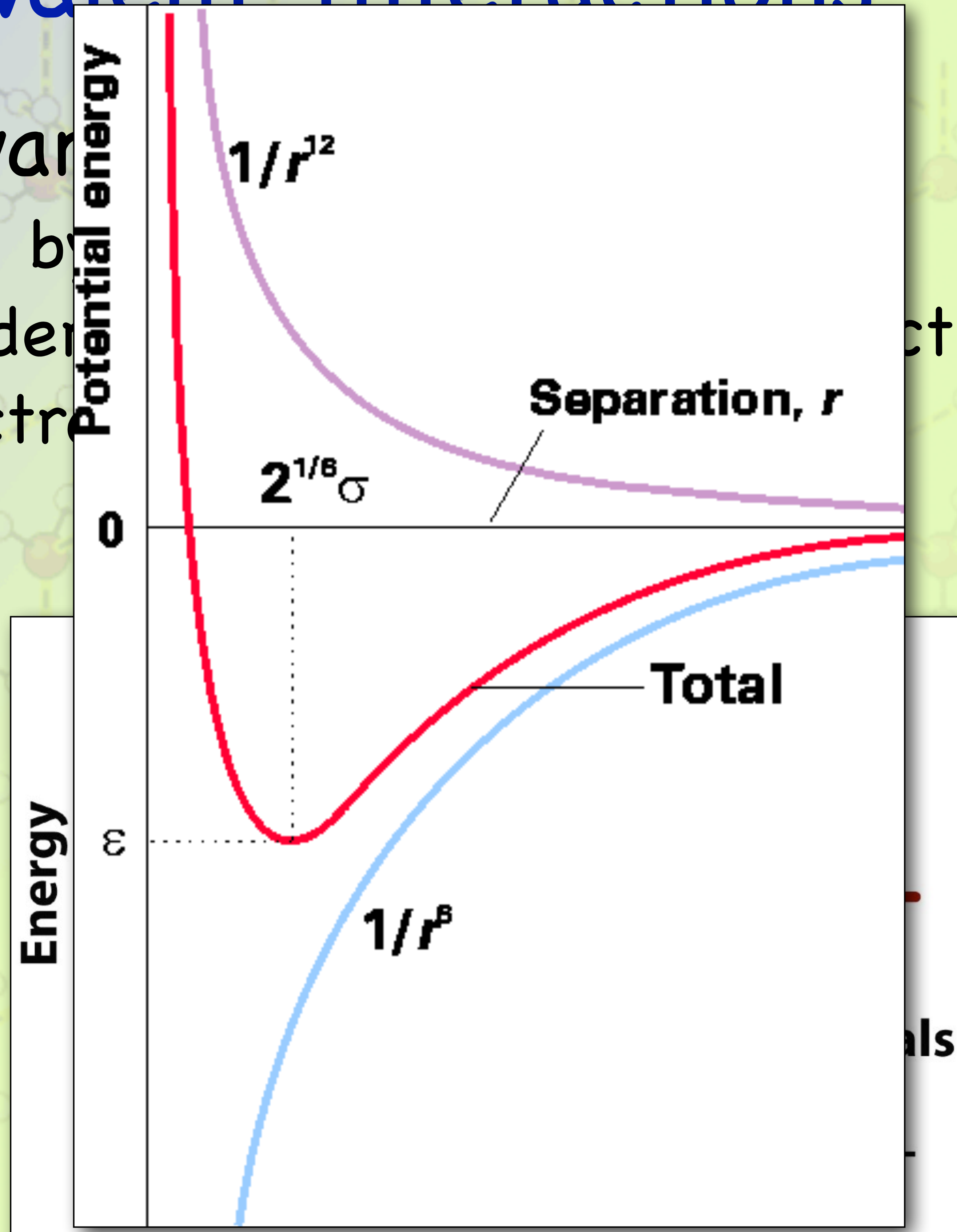

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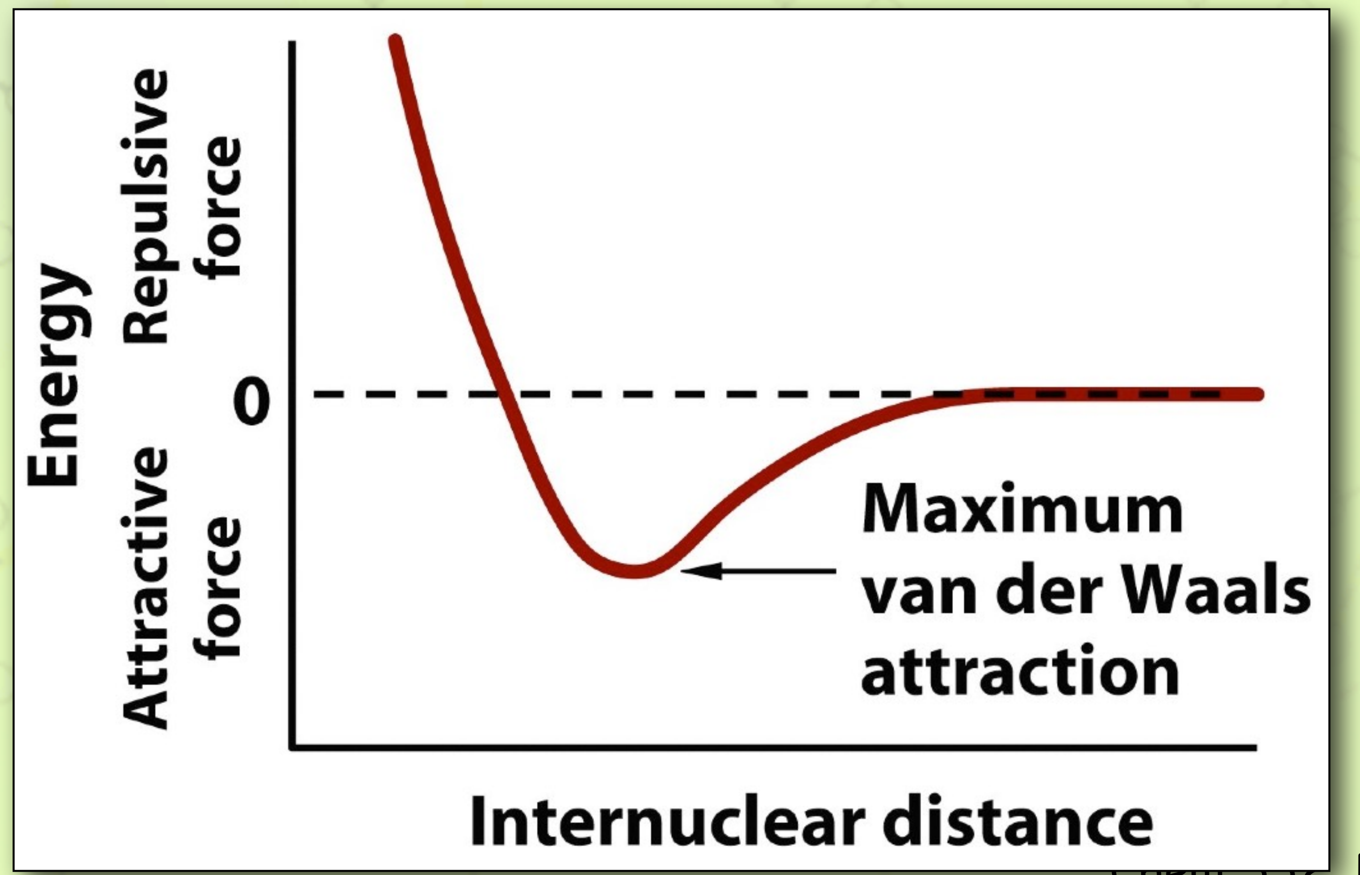

Noncovale... ons

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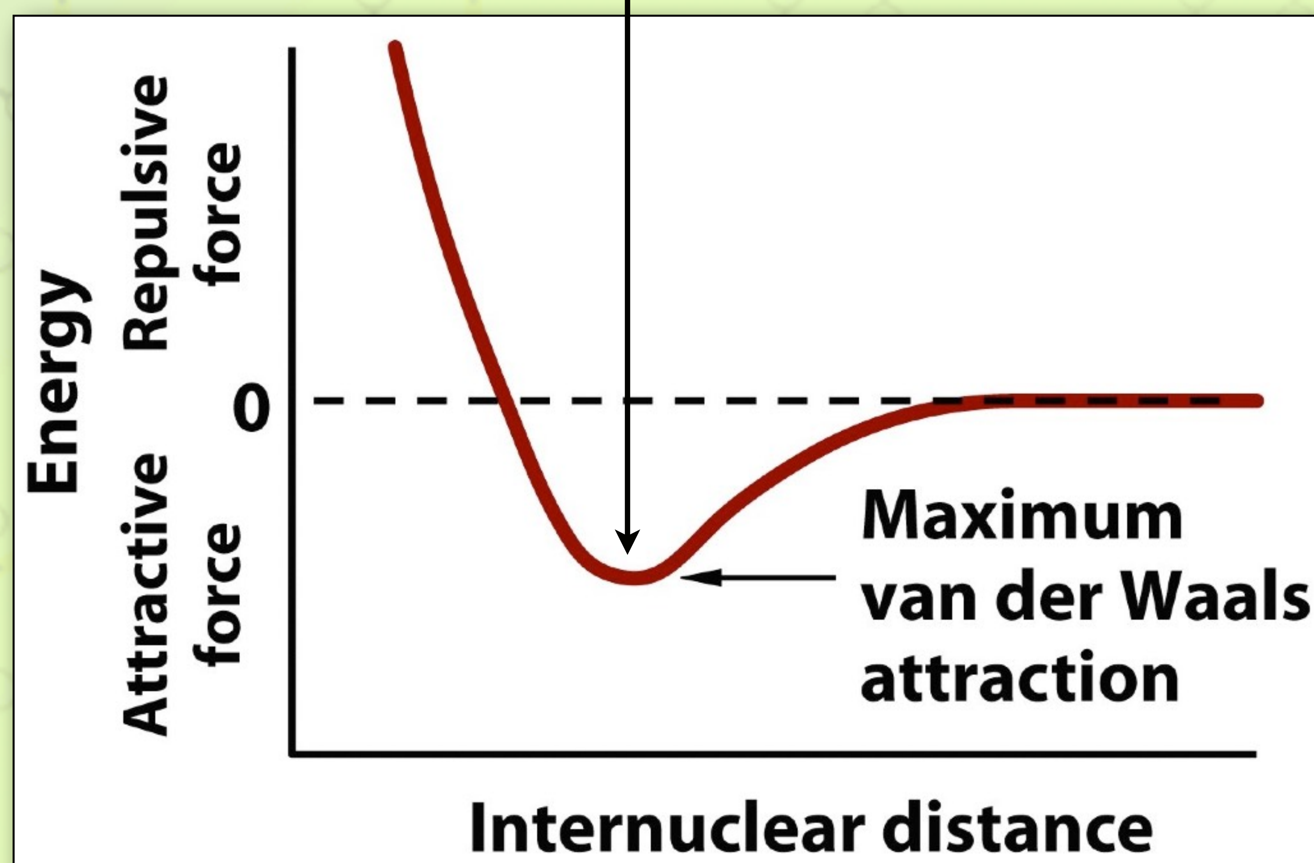

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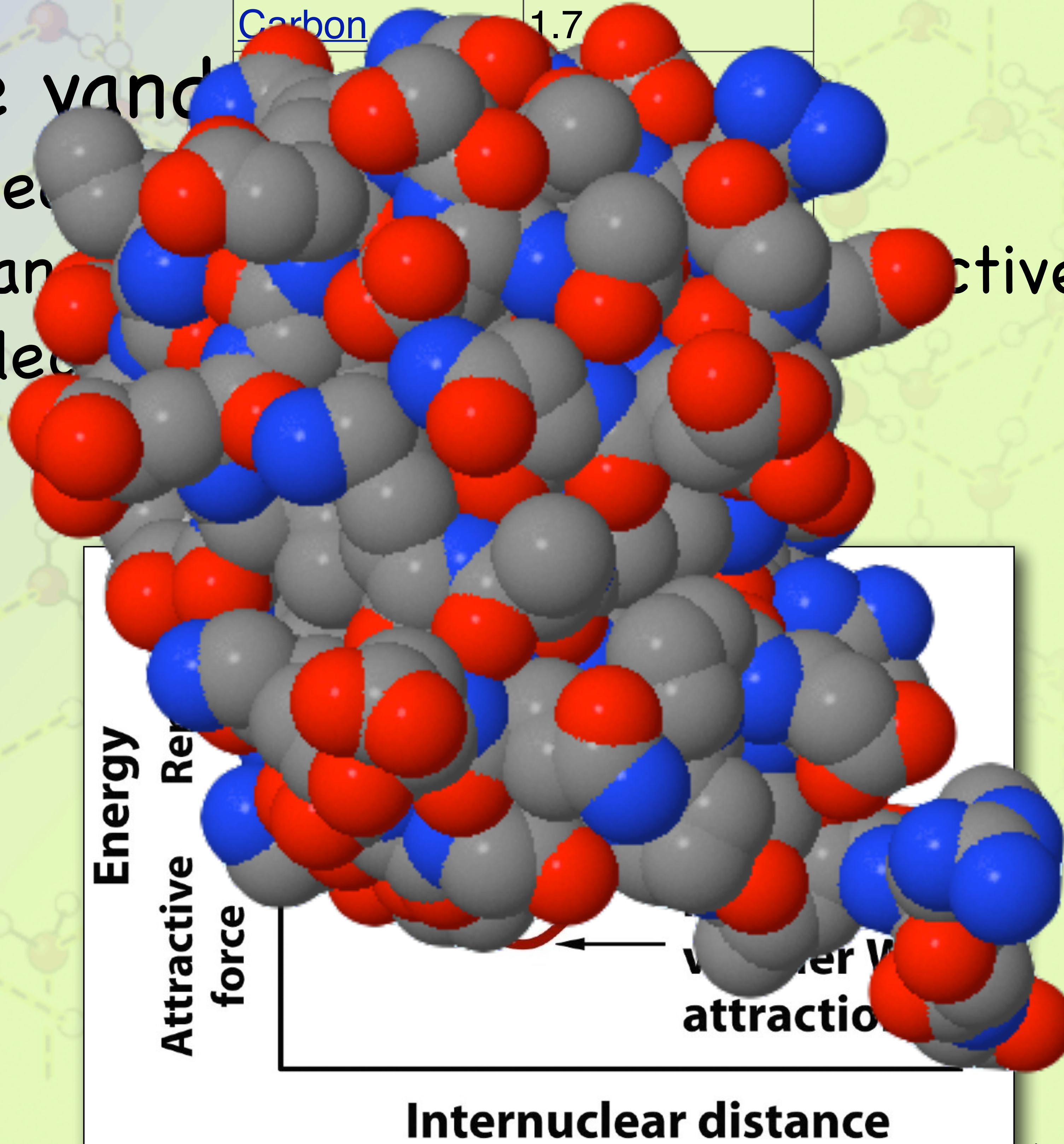

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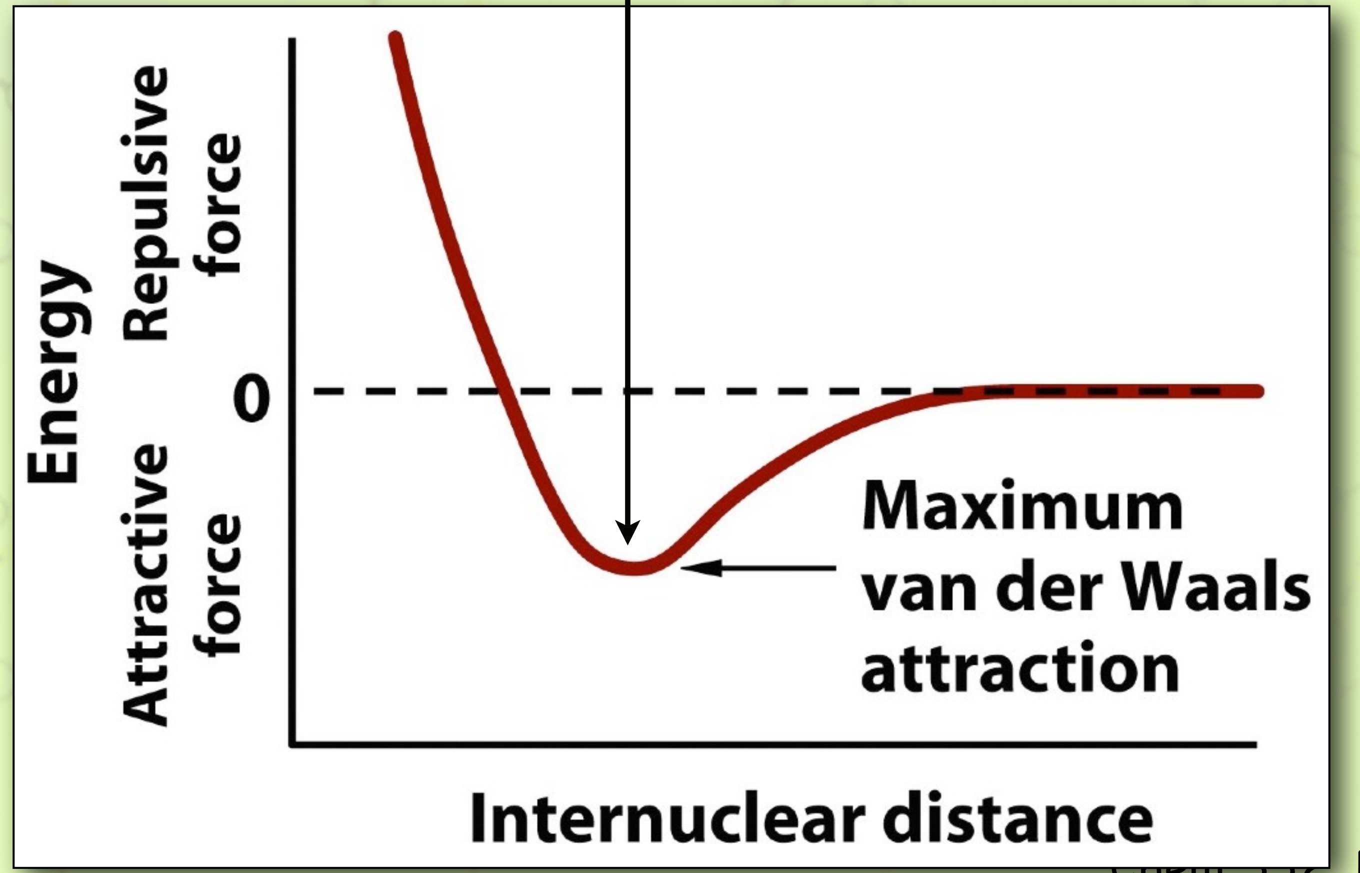
Sulfur	1.8
Chlorine	1.75
Copper	1.4



Noncovalent Interactions

Interaction	Distance dependence	Typical Energy {kJ/mol}	Comment
Ion/ion	$1/r$	± 250	In a vacuum
Ion/ion	$1/r$	± 3.1	In water
Ion/dipole	$1/r^2$	± 15	
Dipole/Dipole	$1/r^3$	± 2	Between stationary polar molecules
Dipole/Dipole	$1/r^6$	– 0.3	Between rotating polar molecules
London (Dispersion)	$1/r^6$	-2	Between all types of molecules
Compare to C–C bond		-348	Covalent bond

Noncovalent Interactions

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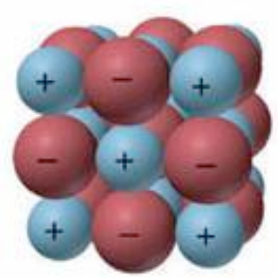
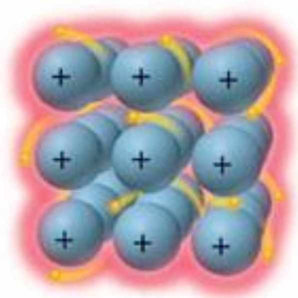
$RT = (8.314 \times 10^{-3}\ kJ/mol \bullet K)(310\ K) = 2.5\ kJ/mol$

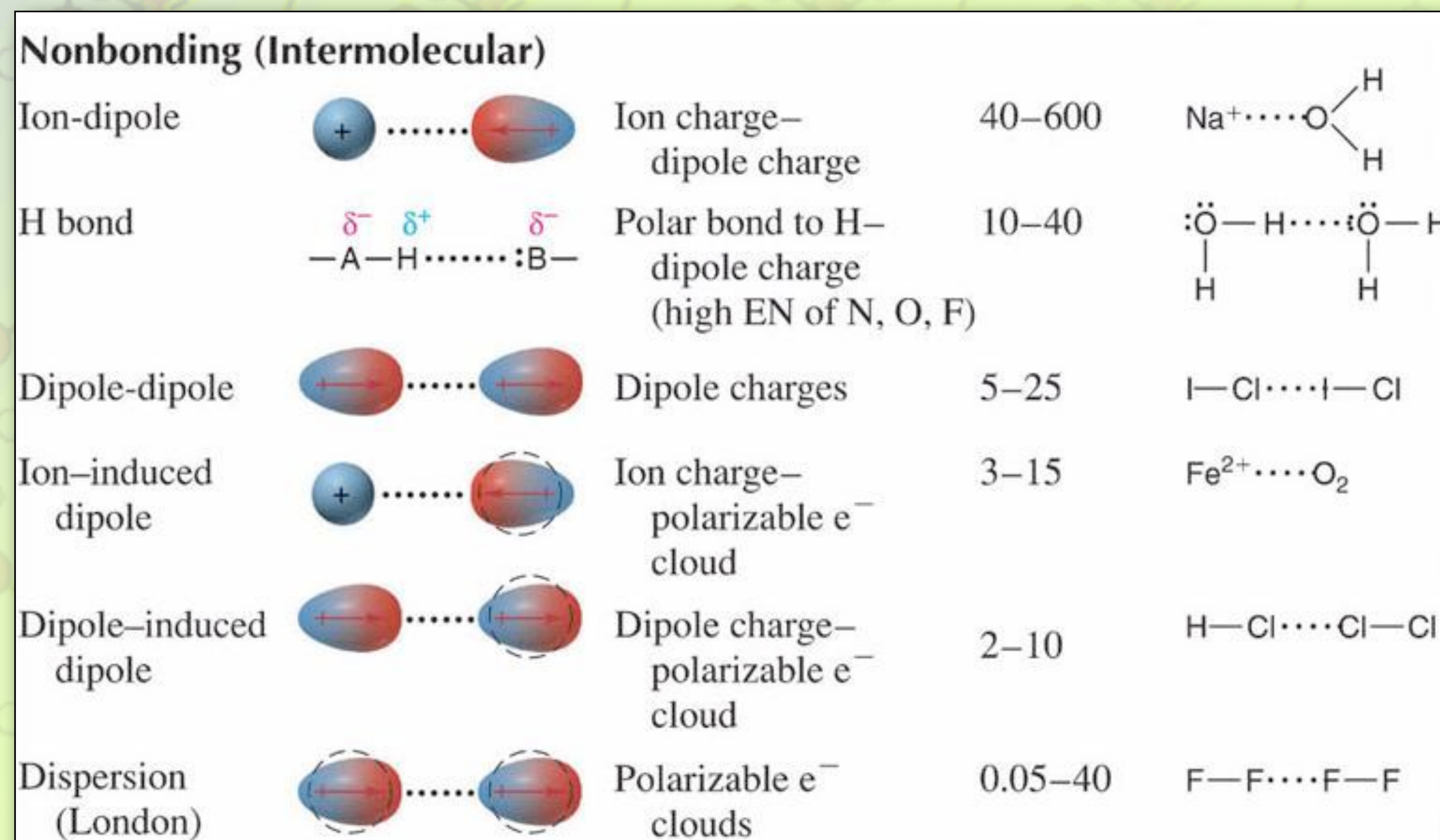
Noncovalent Interactions

- Summary of intermolecular interactions:
  - Bonding Interactions

Force	Model	Basis of Attraction	Energy (kJ/mol)	Example
Bonding				
Ionic		Cation–anion	400–4000	NaCl
Covalent		Nuclei–shared e^- pair	150–1100	H—H
Metallic		Cations–delocalized electrons	75–1000	Fe

Noncovalent Interactions

- Summary of intermolecular interactions:
  - ✦ Noncovalent (Nonbonding) Interactions



Nonbonding (Intermolecular)				
Ion-dipole		Ion charge– dipole charge	40–600	$Na^+ \cdots OH_2$
H bond	δ^- δ^+ δ^- —A—H·······:B—	Polar bond to H– dipole charge (high EN of N, O, F)	10–40	:Ö(H)—H····:Ö(H)—H
Dipole-dipole		Dipole charges	5–25	I—Cl····I—Cl
Ion–induced dipole		Ion charge– polarizable e⁻ cloud	3–15	$Fe^{2+} \cdots O_2$
Dipole–induced dipole		Dipole charge– polarizable e⁻ cloud	2–10	H—Cl····Cl—Cl
Dispersion (London)		Polarizable e⁻ clouds	0.05–40	F—F····F—F

↕ vander Waals

Review

Question:

What is the vander Waals radius of an atom and how is it defined?

Review

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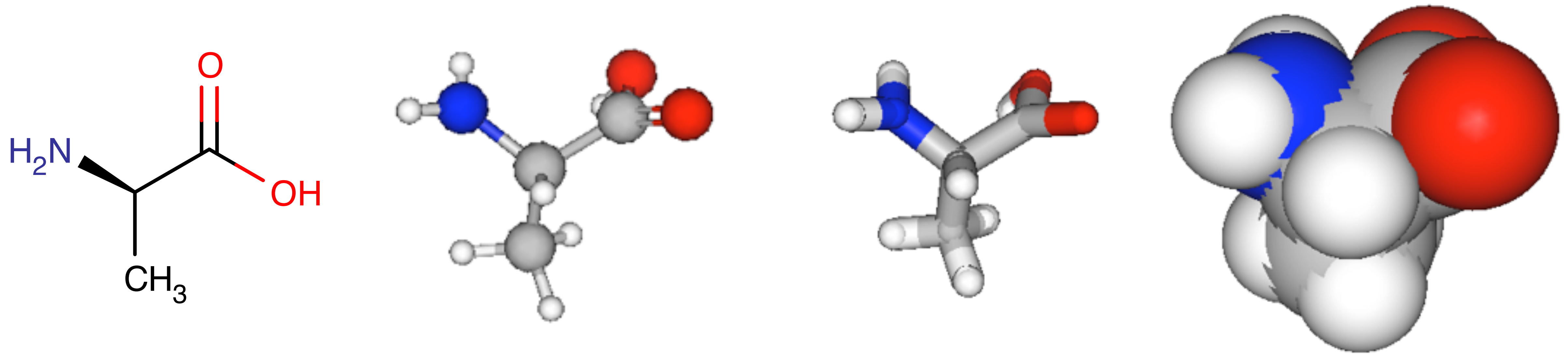
What is the vander Waals radius of an atom and how is it defined?

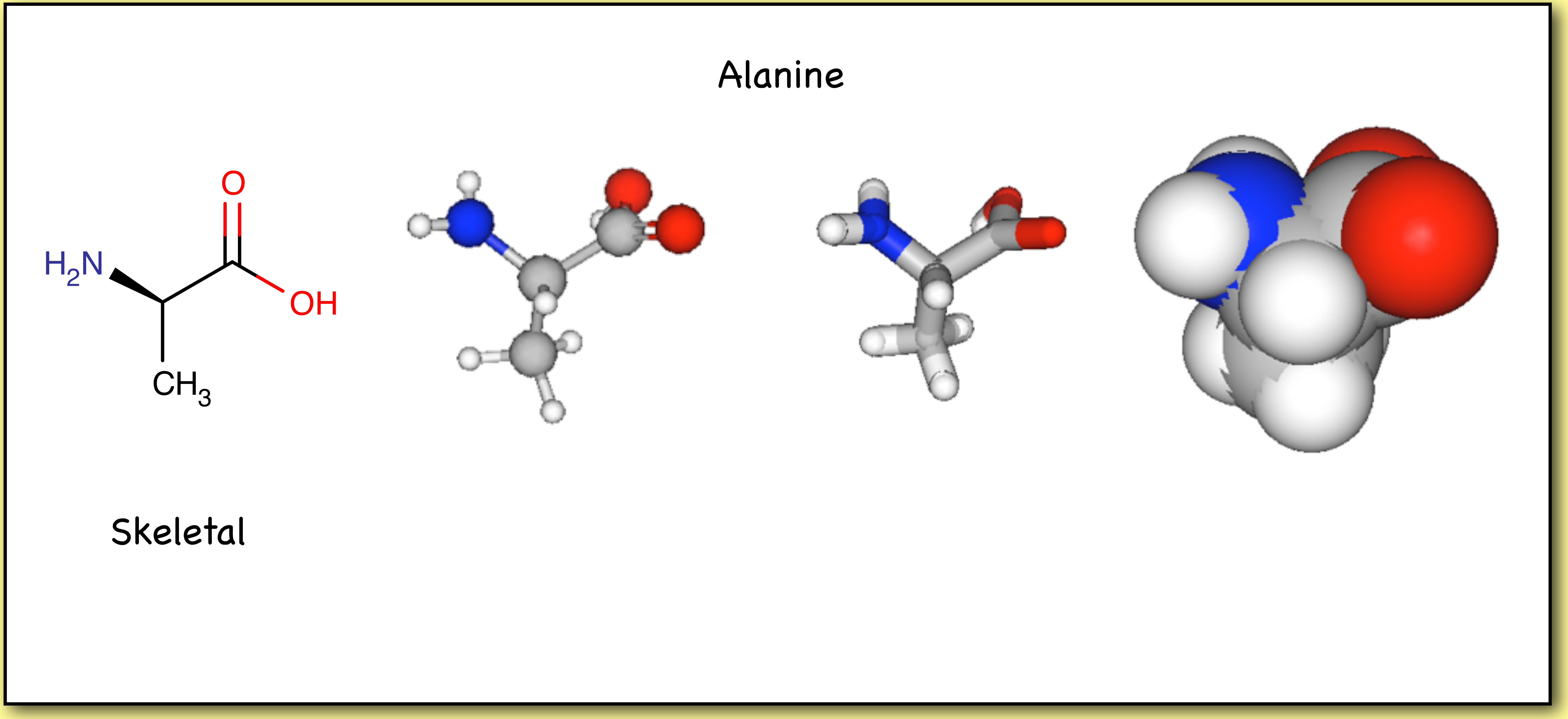
Alanine



Review

Question:

What is the vander Waals radius of an atom and how is it defined?



Review

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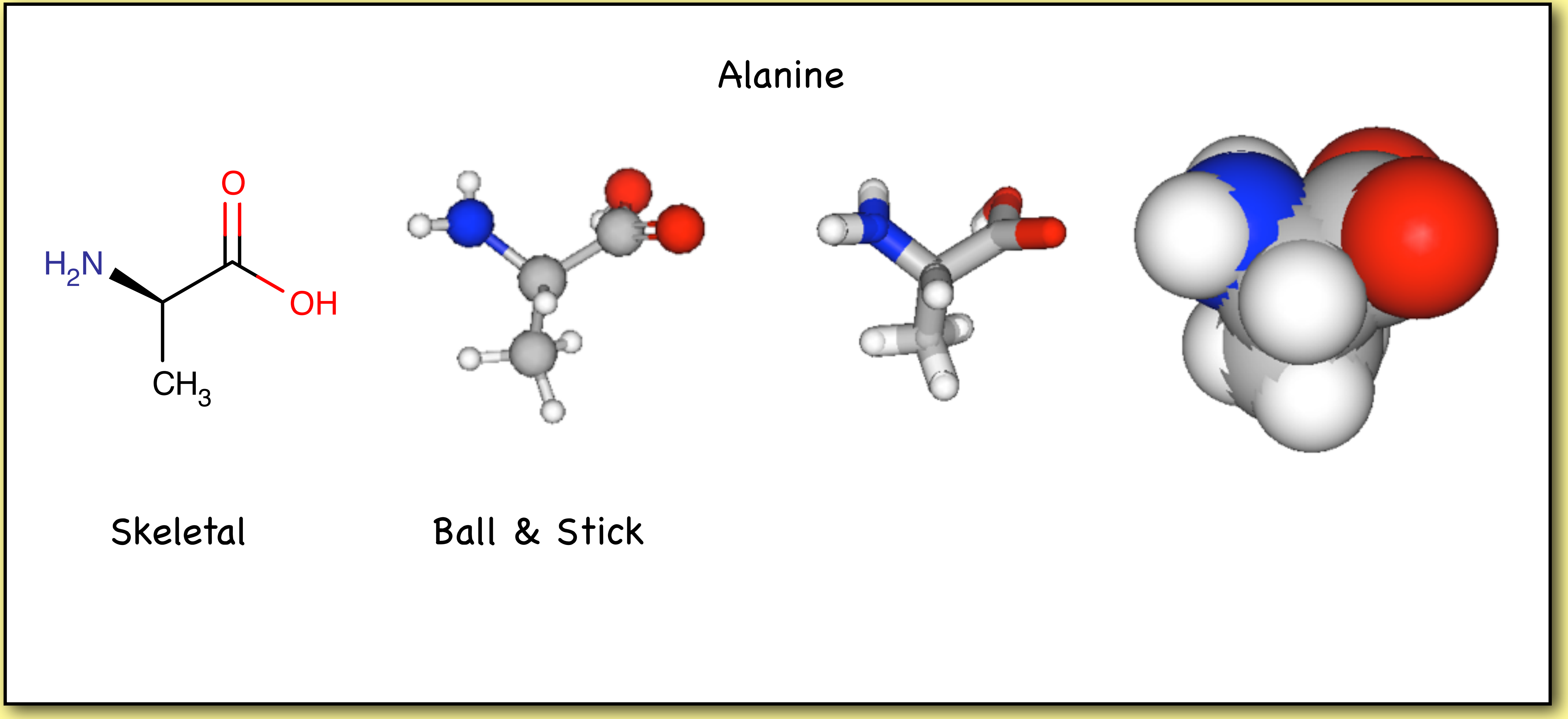

Review

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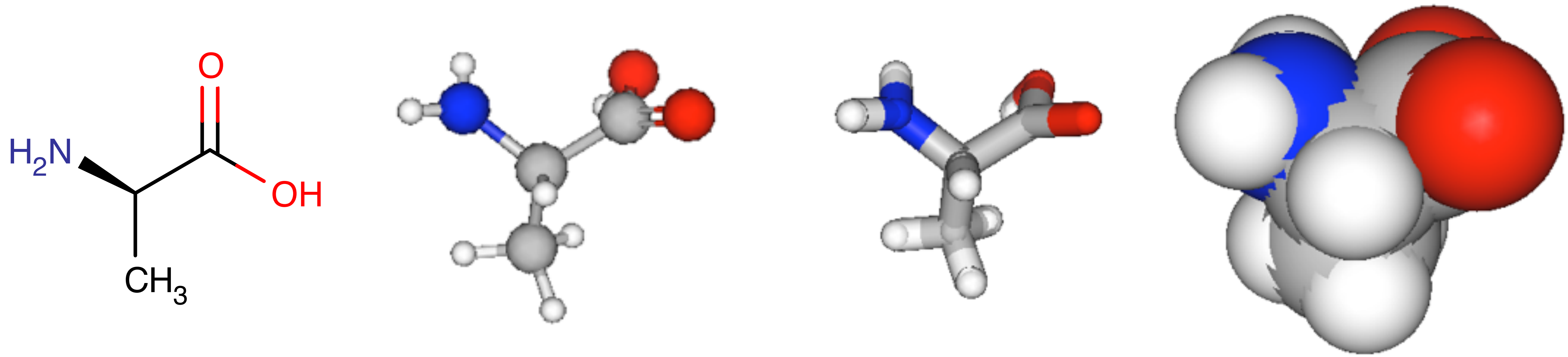

Skeletal | Ball & Stick | Stick

Review

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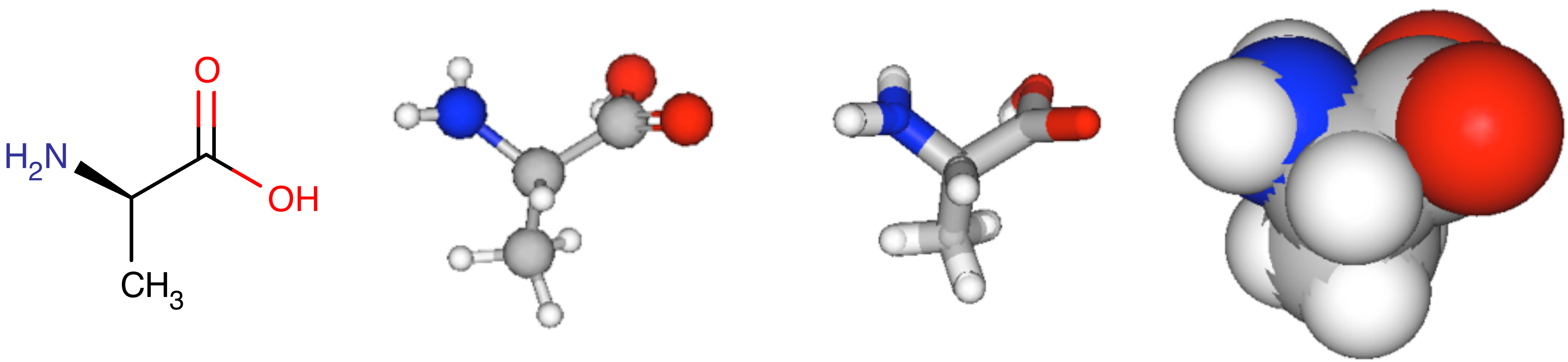
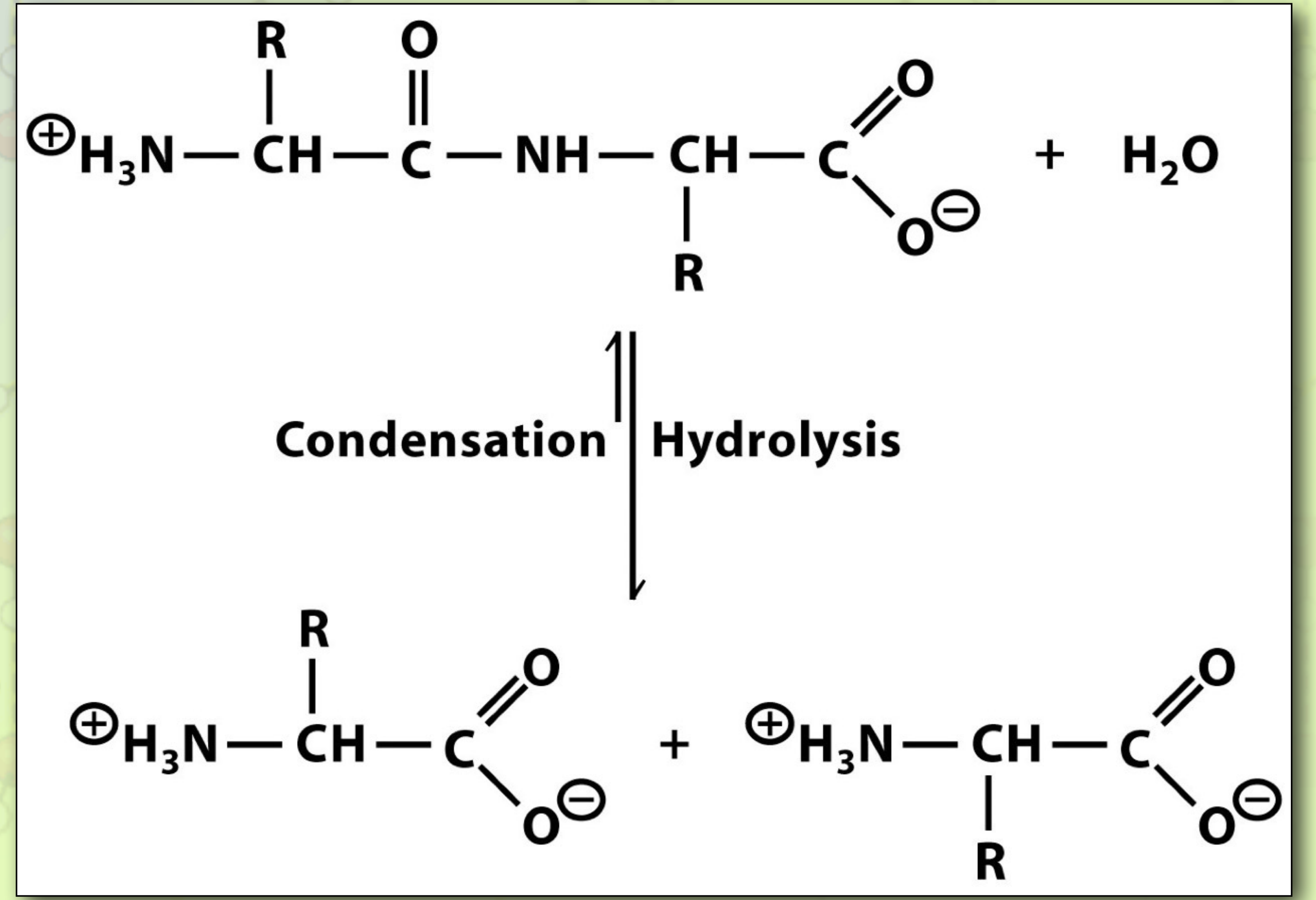


Skeletal | Ball & Stick | Stick | Spacefill

Chemical Properties of Water

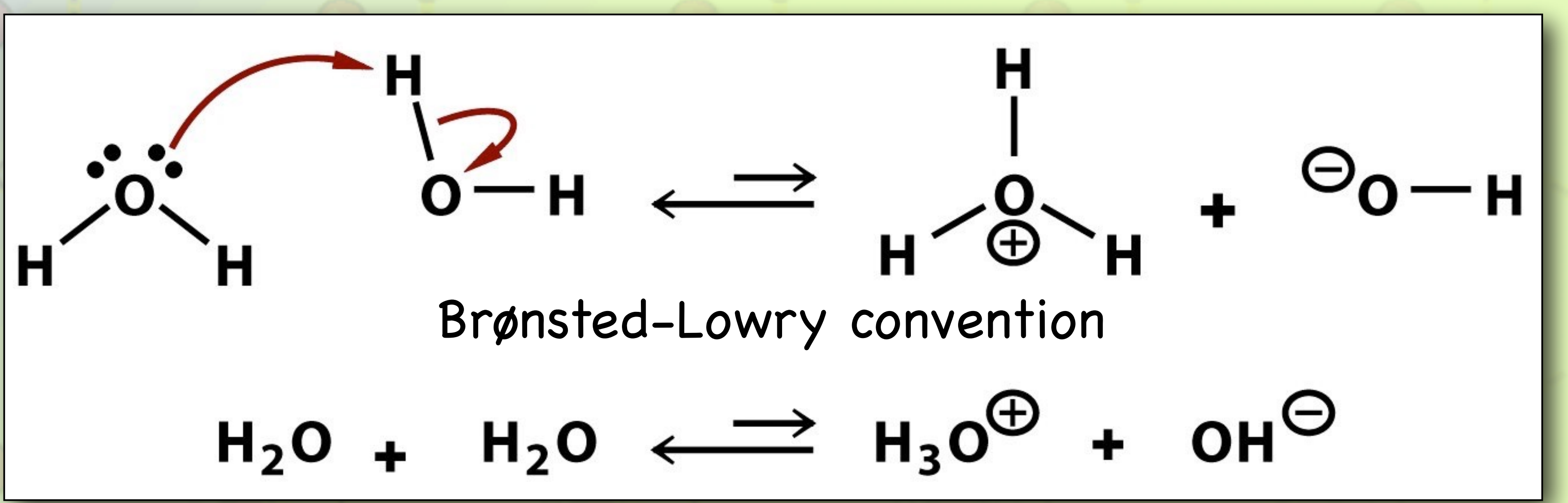
Chemical Properties of Water

- Water is a nucleophile
  - hydrolysis reactions



Chemical Properties of Water

- Water can self-ionize
  - K_w, the ion product for water



$$K_w = \left[\mathrm{H_3O^+}\right]\left[\mathrm{OH^-}\right]$$

$$K_w = 1.0 \text{ x } 10^{-14} \text{ M}^2$$

Chemical Properties of Water

- Water can self-ionize
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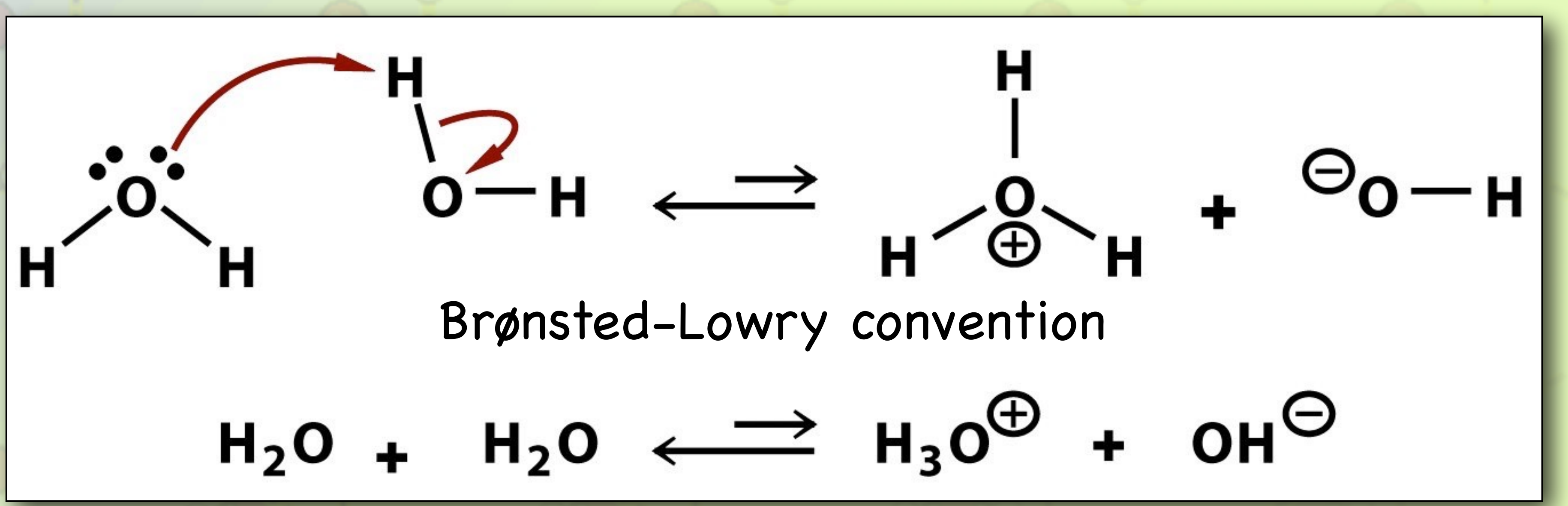

This can be thought of as an extension of the hydrogen bonding interaction

$$K_w = \left[H_3O^+\right]\left[OH^-\right]$$

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Chemical Properties of Water

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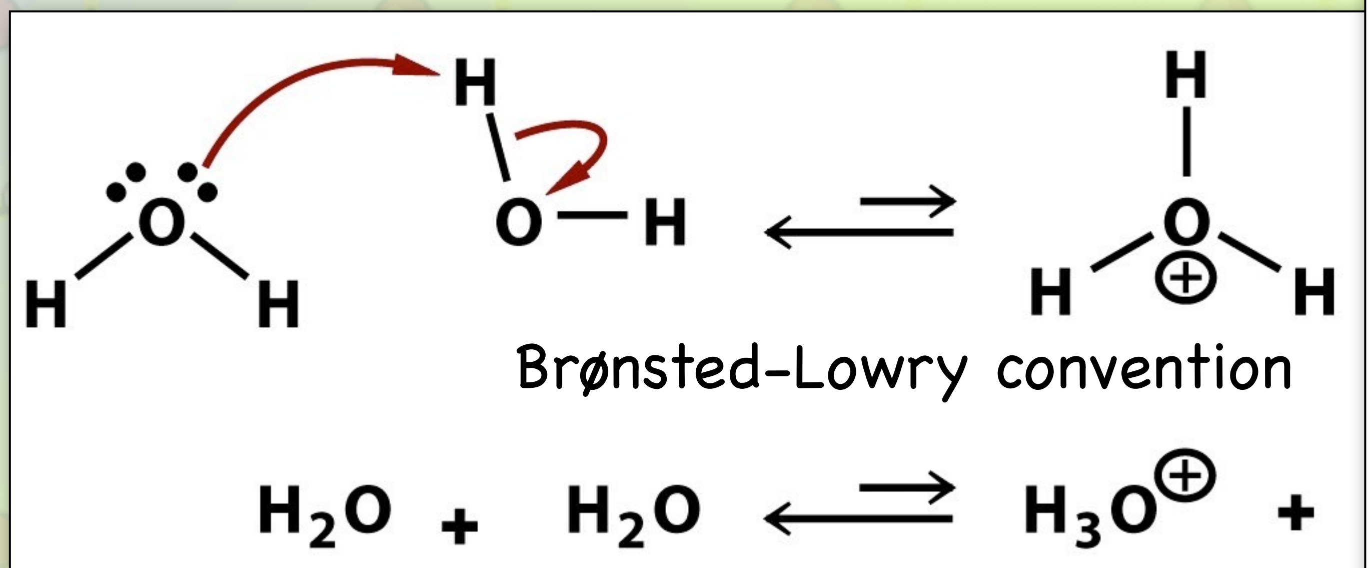


This can be thought of as an extension of the hydrogen bonding interaction

$$K_w = \left[H_3O^+\right]\left[OH^-\right]$$

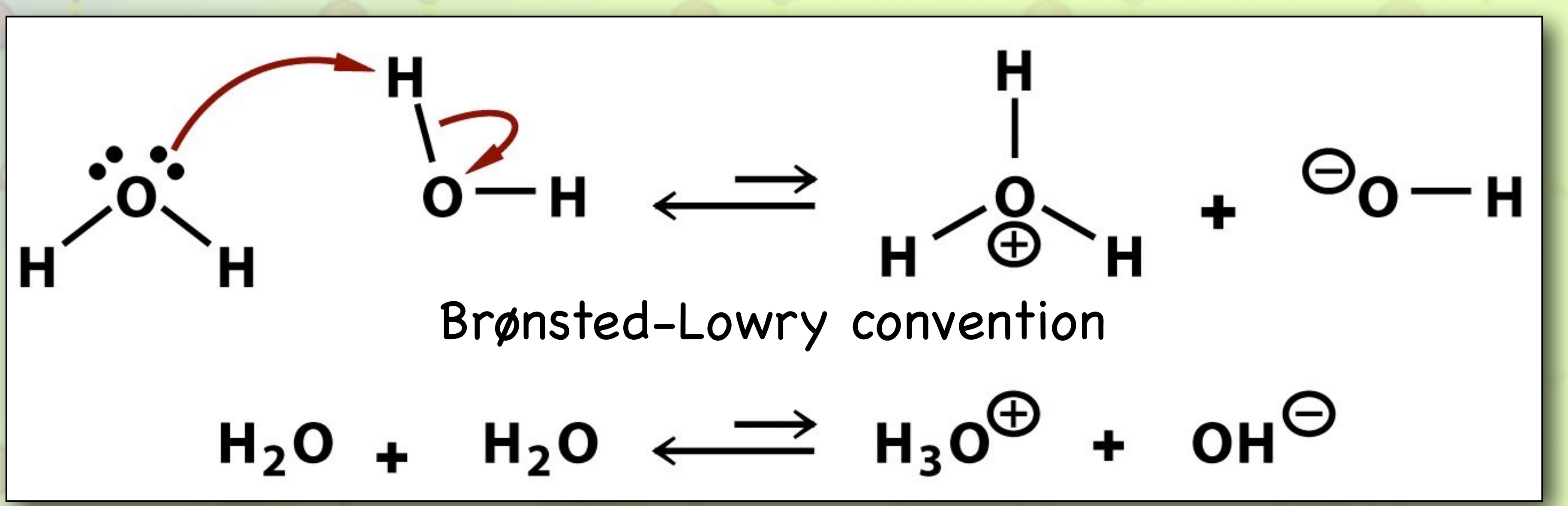
$$K_w = 1.0 \text{ x } 10^{-14} \text{ M}^2$$

TABLE 2.3 Relation of $[H^{\oplus}]$ and $[OH^{\ominus}]$ to pH

pH	$[H^{\oplus}]$ (M)	$[OH^{\ominus}]$ (M)
0	1	10^{-14}
1	10^{-1}	10^{-13}
2	10^{-2}	10^{-12}
3	10^{-3}	10^{-11}
4	10^{-4}	10^{-10}
5	10^{-5}	10^{-9}
6	10^{-6}	10^{-8}
7	10^{-7}	10^{-7}
8	10^{-8}	10^{-6}
9	10^{-9}	10^{-5}
10	10^{-10}	10^{-4}
11	10^{-11}	10^{-3}
12	10^{-12}	10^{-2}
13	10^{-13}	10^{-1}

Chemical Properties of Water

- Water can self-ionize
  - K_w, the ion product for water



This can be thought of as an extension of the hydrogen bonding interaction

$$K_w = [H_3O^+][OH^-]$$

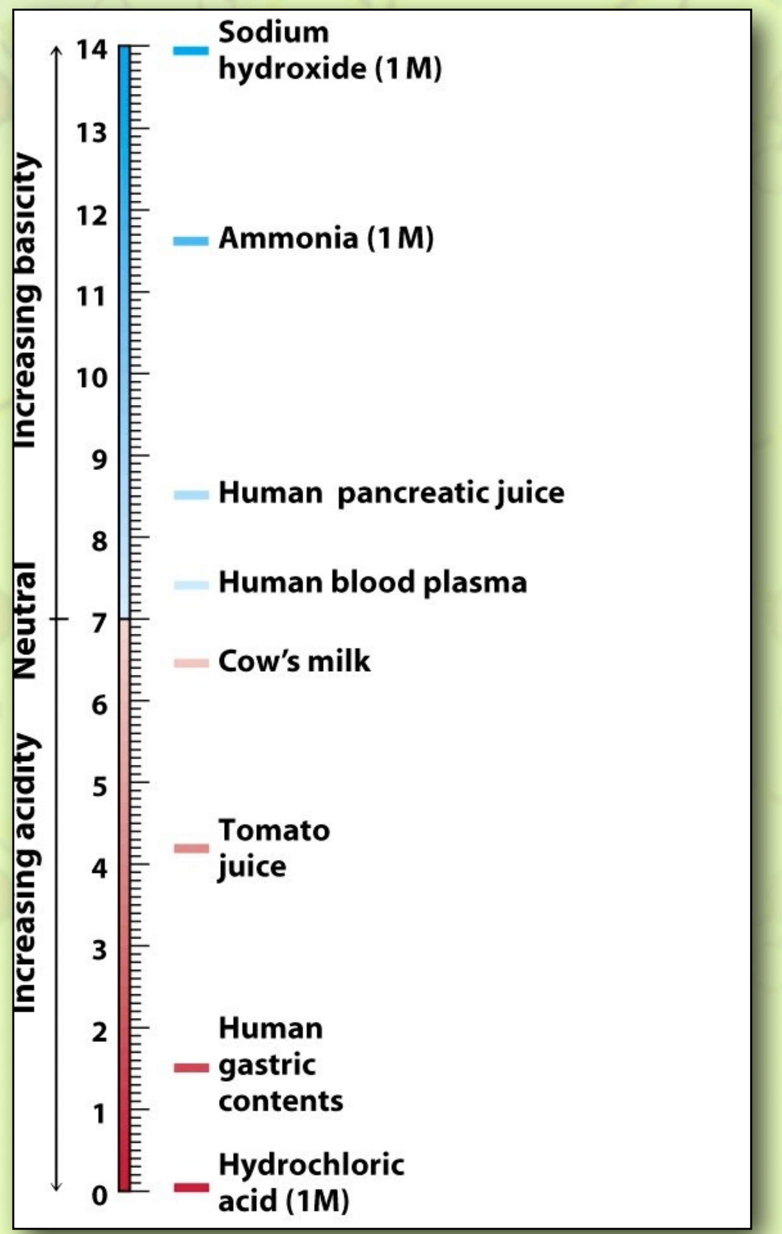
$$K_w = 1.0 \text{ x } 10^{-14} \text{ M}^2$$

Chemical Properties of Water

- The pH Scale

$$pH = -\log\left(\left[H^+\right]\right) \quad \text{(Arrhenius definition)}$$

$$pH = -\log\left([H_3O^+]\right) \quad \text{(Brønsted-Lowry definition)}$$



Chemical Properties of Water

Elaborations:

- Acids and bases
  - Operational Definition
  - Arrhenius Definition
  - Brønsted-Lowry Definition
- Strength of acids and bases
  - Strong acids
  - Weak acids
- Neutralization of acids and bases
  - Titration curves

(Virtual Laboratory)

Chemical Properties of Water

Definitions of Acids and Bases

- **Operational Definition**

Chemical Properties of Water

Definitions of Acids and Bases

- **Operational Definition**
  - Acids, when dissolved in water cause the pH to go down from pH7

Chemical Properties of Water

Definitions of Acids and Bases

- **Operational Definition**
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  - Bases, when dissolved in water cause the pH to go up from pH7

Chemical Properties of Water

Definitions of Acids and Bases

- **Operational Definition**
  - Acids, when dissolved in water cause the pH to go down from pH7
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$$pH = -\log([H^+])$$

Chemical Properties of Water

Definitions of Acids and Bases

- **Operational Definition**
  - Acids, when dissolved in water cause the pH to go down from pH7
  - Bases, when dissolved in water cause the pH to go up from pH7

$$pH = -\log([H^+])$$

$$[H^+] = 10^{-pH}$$

Chemical Properties of Water

Definitions of Acids and Bases

- **Arrhenius Definition**

Chemical Properties of Water

Definitions of Acids and Bases

- **Arrhenius Definition**
  - Acids, when dissolved in water release H^+ ions.

Chemical Properties of Water

Definitions of Acids and Bases

- **Arrhenius Definition**
  - Acids, when dissolved in water release H^+ ions.
  - Bases, when dissolved in water release $[OH^-]$ ions.

Chemical Properties of Water

Definitions of Acids and Bases

- **Arrhenius Definition**
  - Acids, when dissolved in water release H^+ ions.
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$$K_w = [H^+][OH^-] = 1.0 \times 10^{-14}\ M^2$$

Chemical Properties of Water

Definitions of Acids and Bases

- **Arrhenius Definition**
  - Acids, when dissolved in water release H^+ ions.
  - Bases, when dissolved in water release $[OH^-]$ ions.

$K_w = [H^+][OH^-] = 1.0 \times 10^{-14}\ M^2$

For pure water, $[H^+] = [OH^-] = 1.0 \times 10^{-7}\ M$

Chemical Properties of Water

Definitions of Acids and Bases

- **Arrhenius Definition**
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  - Bases, when dissolved in water release $[OH^-]$ ions.

$K_w = [H^+][OH^-] = 1.0\times10^{-14}\ M^2$

For pure water, $[H^+] = [OH^-] = 1.0\times10^{-7}\ M$

$$\left[H^+\right] = \frac{1.0\times10^{-14}M^2}{\left[OH^-\right]}; \quad \left[OH^-\right] = \frac{1.0\times10^{-14}M^2}{\left[H^+\right]}$$

Chemical Properties of Water

Definitions of Acids and Bases

- **Brønsted-Lowrey Definition**

Chemical Properties of Water

Definitions of Acids and Bases

- **Brønsted-Lowrey Definition**
    - Acids, donate a proton (H^+ ion) from a base.

Chemical Properties of Water

Definitions of Acids and Bases

- **Brønsted-Lowrey Definition**
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  - Bases, accept a proton (H^+ ion) from an acid.

Chemical Properties of Water

Definitions of Acids and Bases

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  - Acids, donate a proton (H^+ ion) from a base.
  - Bases, accept a proton (H^+ ion) from an acid.

$$K_w = \left[H_3O^+\right]\left[OH^-\right]$$

$$K_w = 1.0 \times 10^{-14}\ M^2$$

Chemical Properties of Water

- pH of a strong acid or a strong base

Chemical Properties of Water

- pH of a strong acid or a strong base
  - When a strong acid is dissolved in water it completely dissociates its H^+ ions.

Chemical Properties of Water

- pH of a strong acid or a strong base
  - When a strong acid is dissolved in water it completely dissociates its H^+ ions.
  - When a strong base is dissoved in water, it completely dissociates it OH^- ions.

Chemical Properties of Water

- pH of a strong acid and a strong base
- Neutralization of an acid by a base

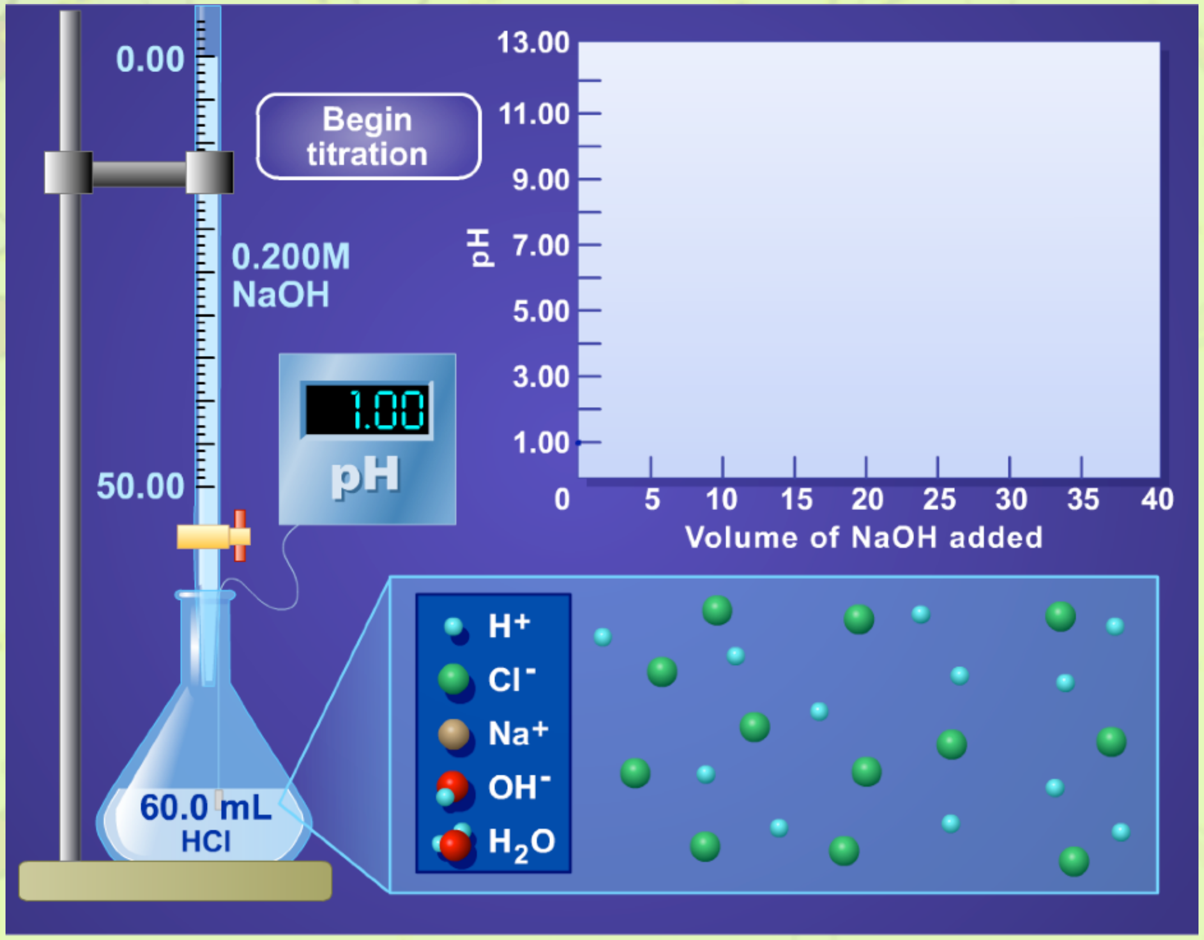
Chemical Properties of Water

- pH of a strong acid and a strong base
- Neutralization of an acid by a base
- Titration curve for a strong acid.

Chemical Properties of Water

Neutralization of an acid with a base (pH titration)

- Titrations can be used to determine the unknown concentration of an acid

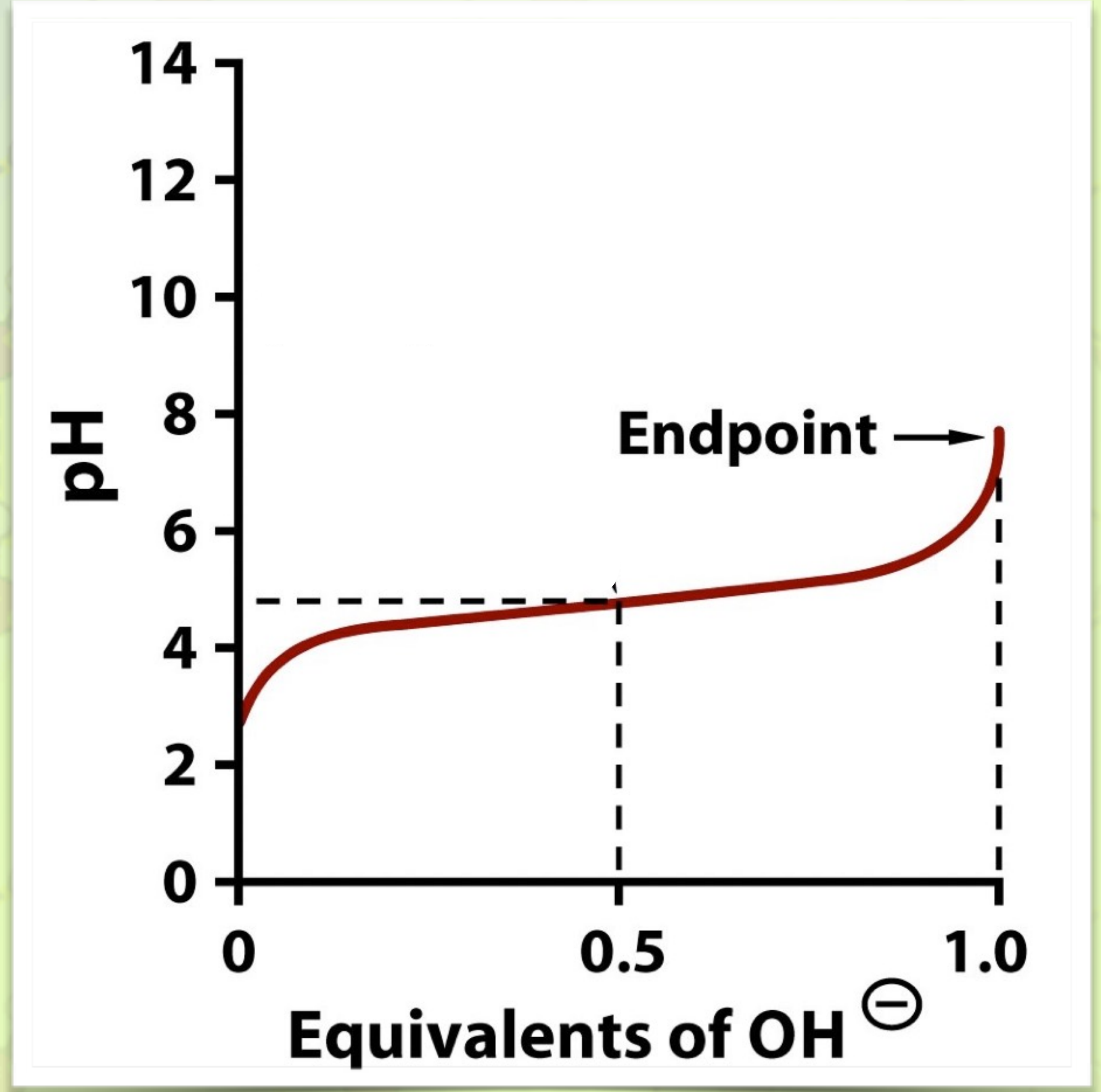


Chemical Properties of Water

- pH of a strong acid and a strong base
- Neutralization of an acid by a base
- Titration curve for a strong acid.
- Titration curve for a weak acid.

Chemical Properties of Water

- Titration curve for a weak acid

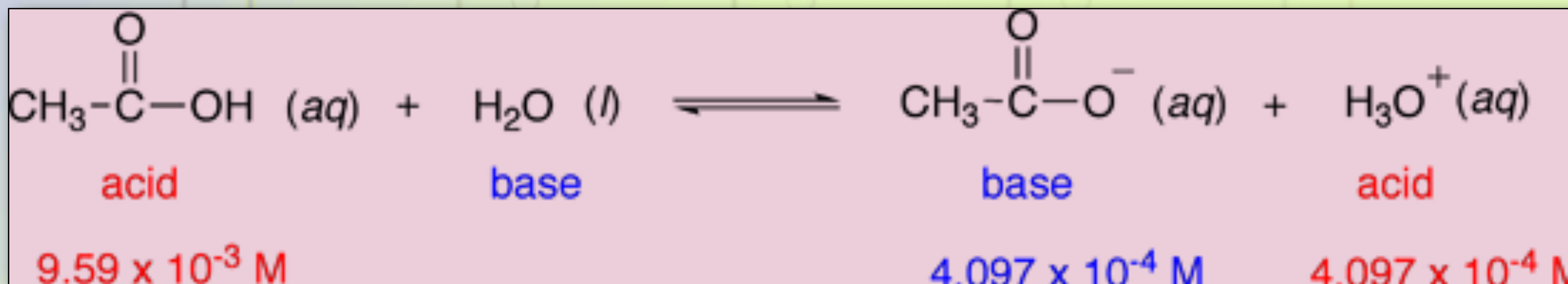


Chemical Properties of Water

- pH of a strong acid and a strong base
- Neutralization of an acid by a base
- Titration curve for a strong acid.
- Titration curve for a weak acid.
- Calculating the pH of a weak acid solution.

Chemical Properties of Water

- pH of a weak acid solution
  - 0.01 M acetic acid



Chemical Properties of Water

- pH of a weak acid solution
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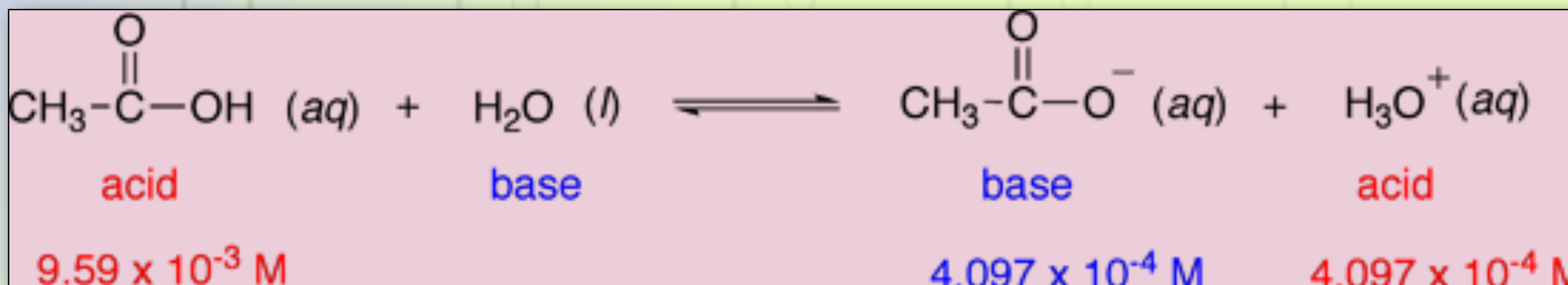
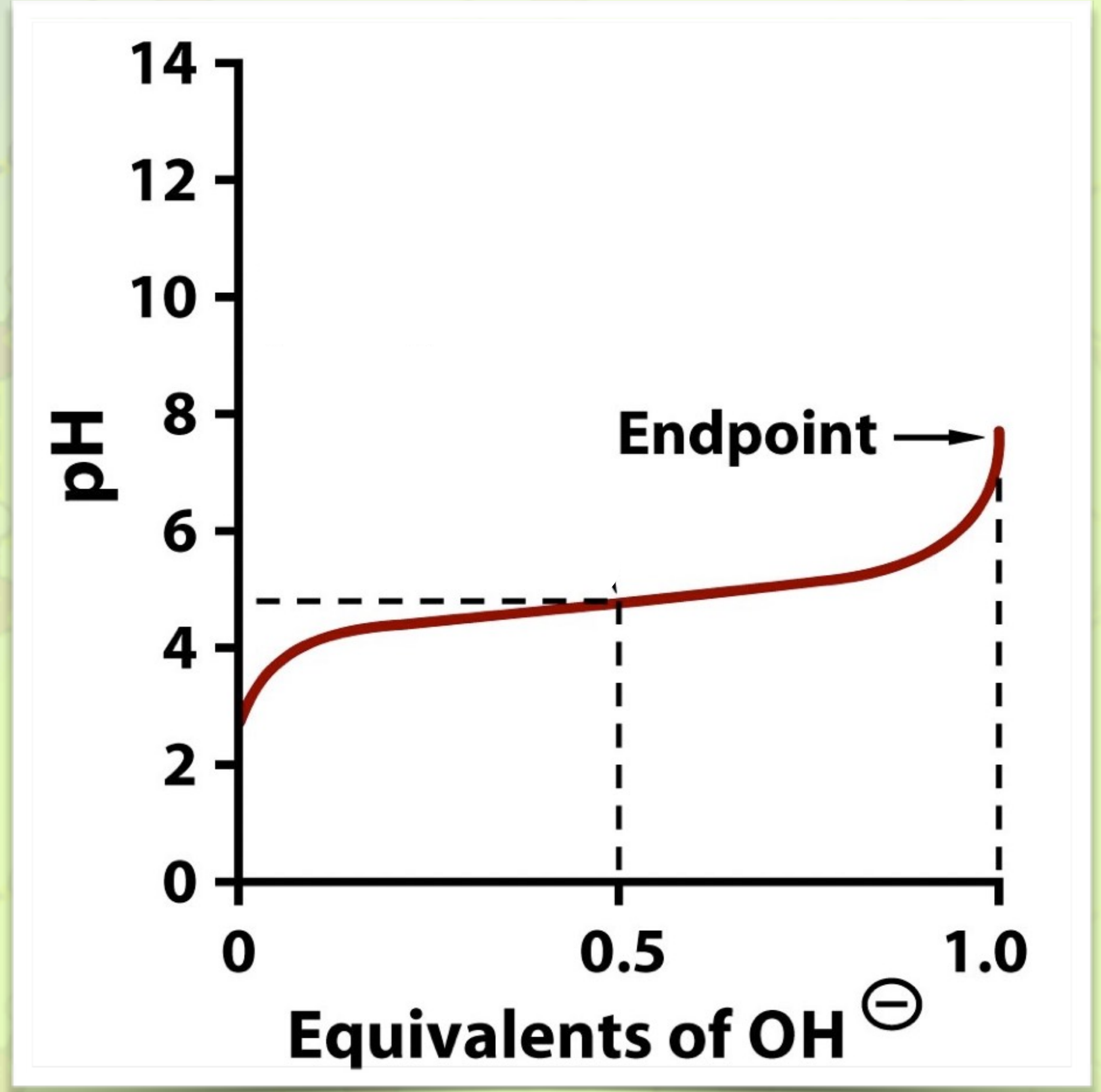


$$\left[\mathrm{H}^{+}\right] \approx \sqrt{K_a C}$$

$$pH \approx \frac{1}{2}\left(pK_a - \log(\mathrm{C})\right)$$

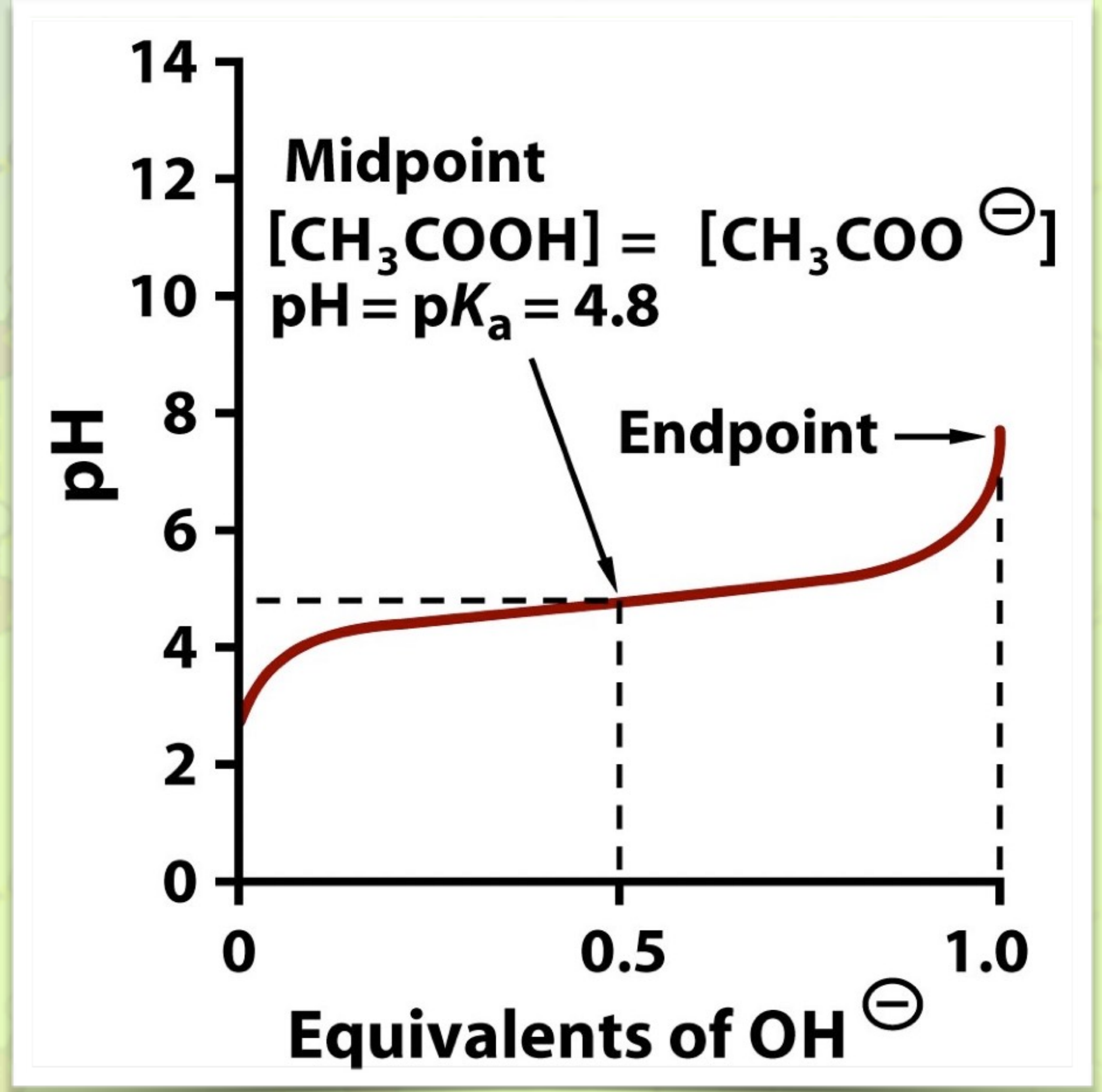
Chemical Properties of Water

- Titration curve for a weak acid



Chemical Properties of Water

- Titration curve for a weak acid



Chemical Properties of Water

TABLE 2.4 Dissociation constants and pK_a values of weak acids in aqueous solutions at 25°C

Acid	K_a(M)	pK_a
HCOOH (Formic acid)	1.77×10^{-4}	3.8
CH_3COOH (Acetic acid)	1.76×10^{-5}	4.8
$CH_3CHOHCOOH$ (Lactic acid)	1.37×10^{-4}	3.9
H_3PO_4 (Phosphoric acid)	7.52×10^{-3}	2.2
$H_2PO_4^{\ominus}$ (Dihydrogen phosphate ion)	6.23×10^{-8}	7.2
HPO_4^{2-} (Monohydrogen phosphate ion)	2.20×10^{-13}	12.7
H_2CO_3 (Carbonic acid)	4.30×10^{-7}	6.4
$HCO_3^{\ominus}$ (Bicarbonate ion)	5.61×10^{-11}	10.2
$NH_4^{\oplus}$ (Ammonium ion)	5.62×10^{-10}	9.2
$CH_3NH_3^{\oplus}$ (Methylammonium ion)	2.70×10^{-11}	10.7

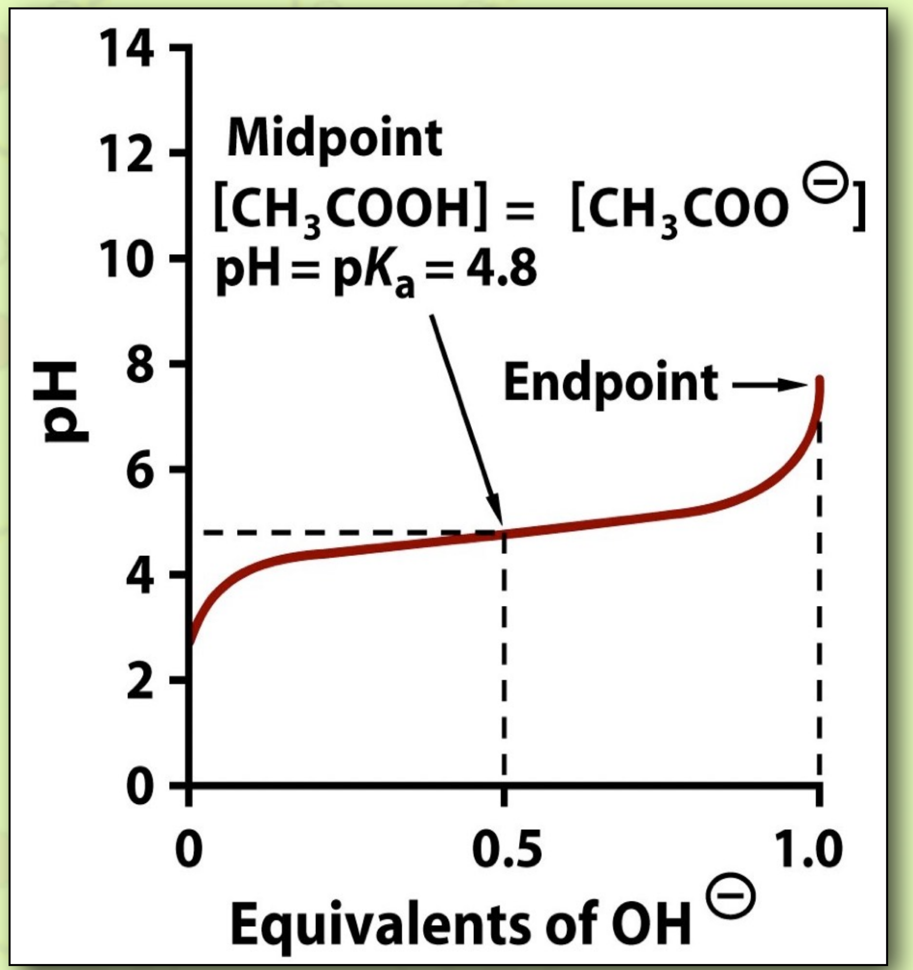
Chemical Properties of Water

- pH of a strong acid and a strong base
- Neutralization of an acid by a base
- Titration curve for a strong acid.
- Titration curve for a weak acid.
- Calculating the pH of a weak acid solution.
- The Henderson-Hasselbalch Equation and Buffers

pH Buffers

- The titration curve for a weak acid demonstrates that the pH of a solution changes very slowly when a weak acid and its conjugate base are present in a solution at nearly equal concentrations.

- This is the essence of a pH buffer



pH Buffers

- A **pH buffer** is defined as a mixture of a weak acid and its conjugate base
  - The weak acid component resists changes to the pH by neutralizing any strong bases that are added to the solution.

$$HA + OH^- \longrightarrow A^- + HOH$$

HA	OH⁻	A⁻	HOH
weak acid	strong base	weak base	weak acid

  - And the conjugate base component resists changes to the pH by neutralizing any strong acids that are added to the solution.

$$A^- + H^+ \longrightarrow HA + HOH$$

A⁻	H⁺	HA	HOH
weak acid	strong acid	weak base	weak acid

pH Buffers

- A **pH buffer** buffers best when the concentrations of the weak acid, [HA], and its conjugate base [A^-] are equal.
- The Henderson–Hasselbach equation be used to show that this occurs when the pH of the solution equals the pK_a of the weak acid component.

Chemical Properties of Water

- Henderson-Hasselbalch Equation

$$\mathrm{HA} + \mathrm{H_2O} \rightarrow \mathrm{A^-} + \mathrm{H_3O^+}$$

$$K_a = \frac{[\mathrm{H_3O^+}][\mathrm{A^-}]}{[\mathrm{HA}]}; \quad \left(= \frac{[\mathrm{H^+}][\mathrm{A^-}]}{[\mathrm{HA}]} \right)$$

$$pH = pK_a + \log\left(\frac{[\mathrm{A^-}]}{[\mathrm{HA}]} \right)$$

Chemical Properties of Water

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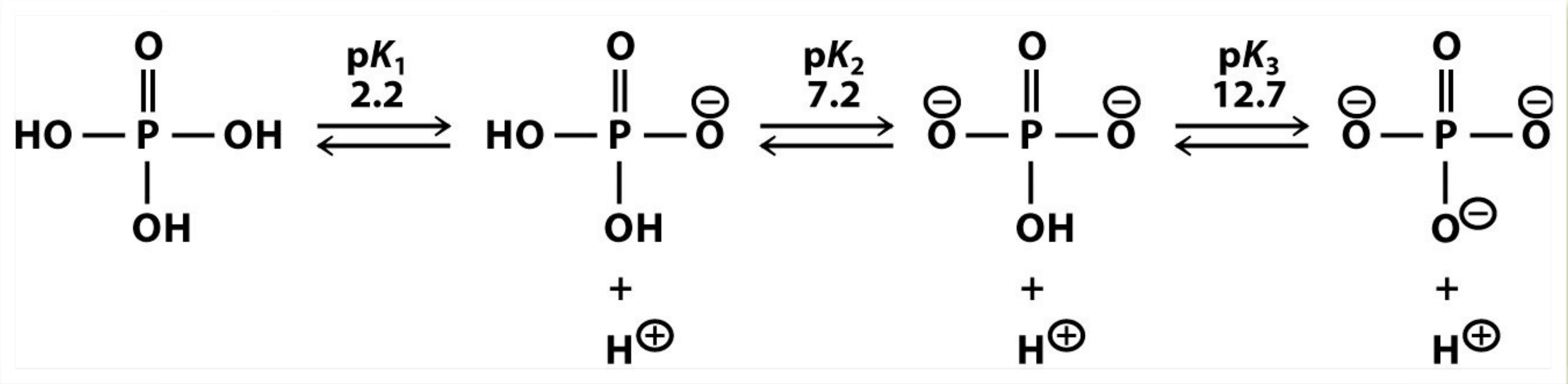
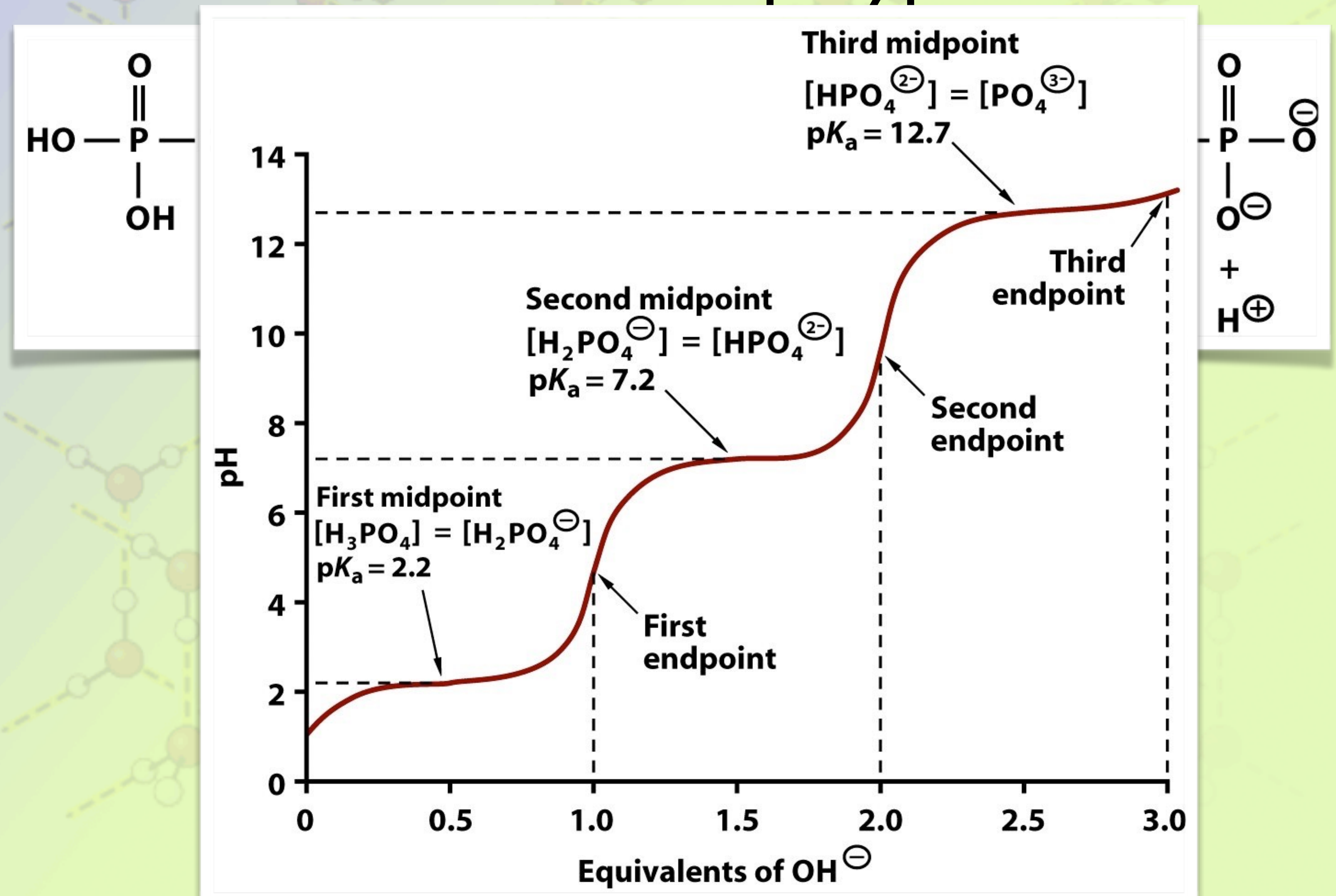
Chemical Properties of Water

Titration curve for a polyprotic acid



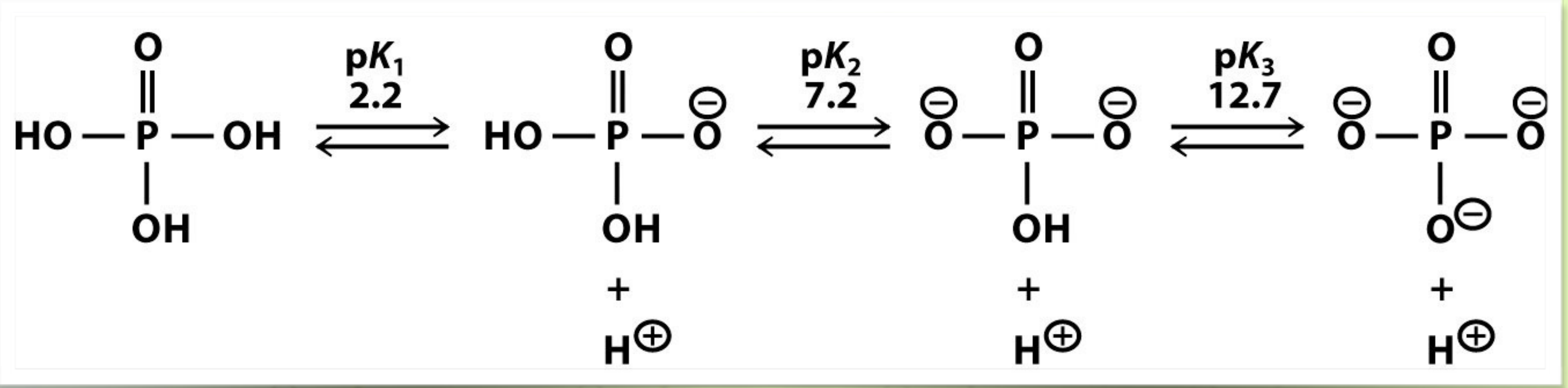
Chemical Properties of Water

Titration curve for a polyprotic acid



Chemical Properties of Water

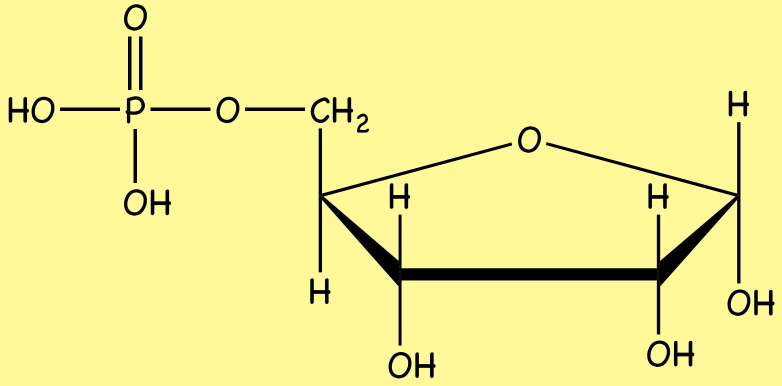
Titration curve for a polyprotic acid



Chemical Properties of Water

Problem: (Check your work with Marvin)

Many phosphorylated sugars (phosphate esters of sugars) are metabolic intermediates. the two ionizable -OH groups of the phosphate group of the monophosphate ester of ribose (ribose 5-phosphate) have pKa values 1.2 and 6.6. The fully protonated form of α-D-ribose 5-phosphate has the structure shown below.



A. Draw, in order, the ionic species formed upon titration of this phosphorylated sugar from pH 0.0 to pH 10.0.

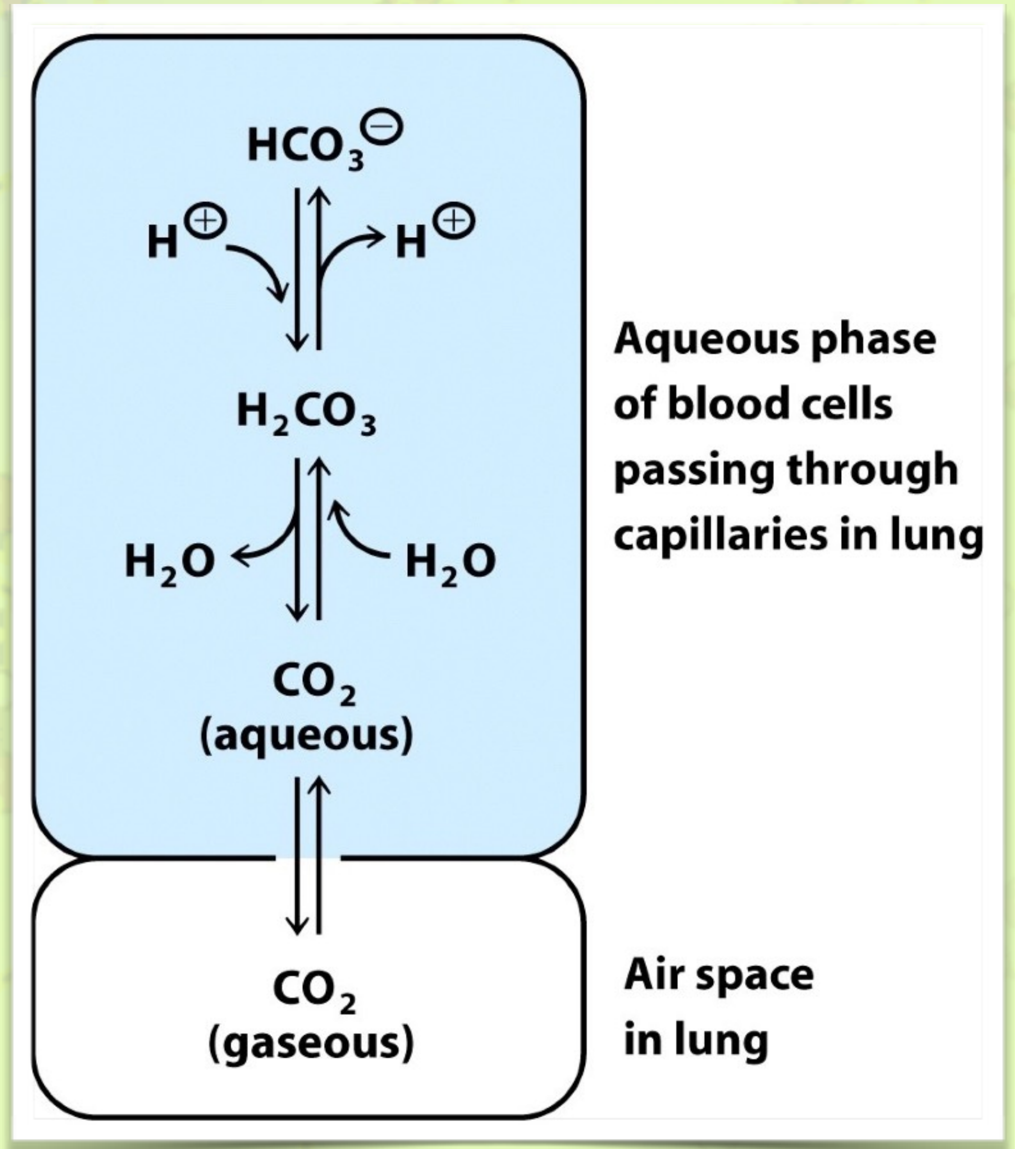
B. Sketch the titration curve for ribose 5-phosphate.

Molecular Resources

- Marvin
  - A tool for drawing and analyzing small molecules
- The Protein Data Bank (PDB)
  - A database where you can find and observe the structures of biological macromolecules and aggregates of these molecules.
  - Not limited to proteins

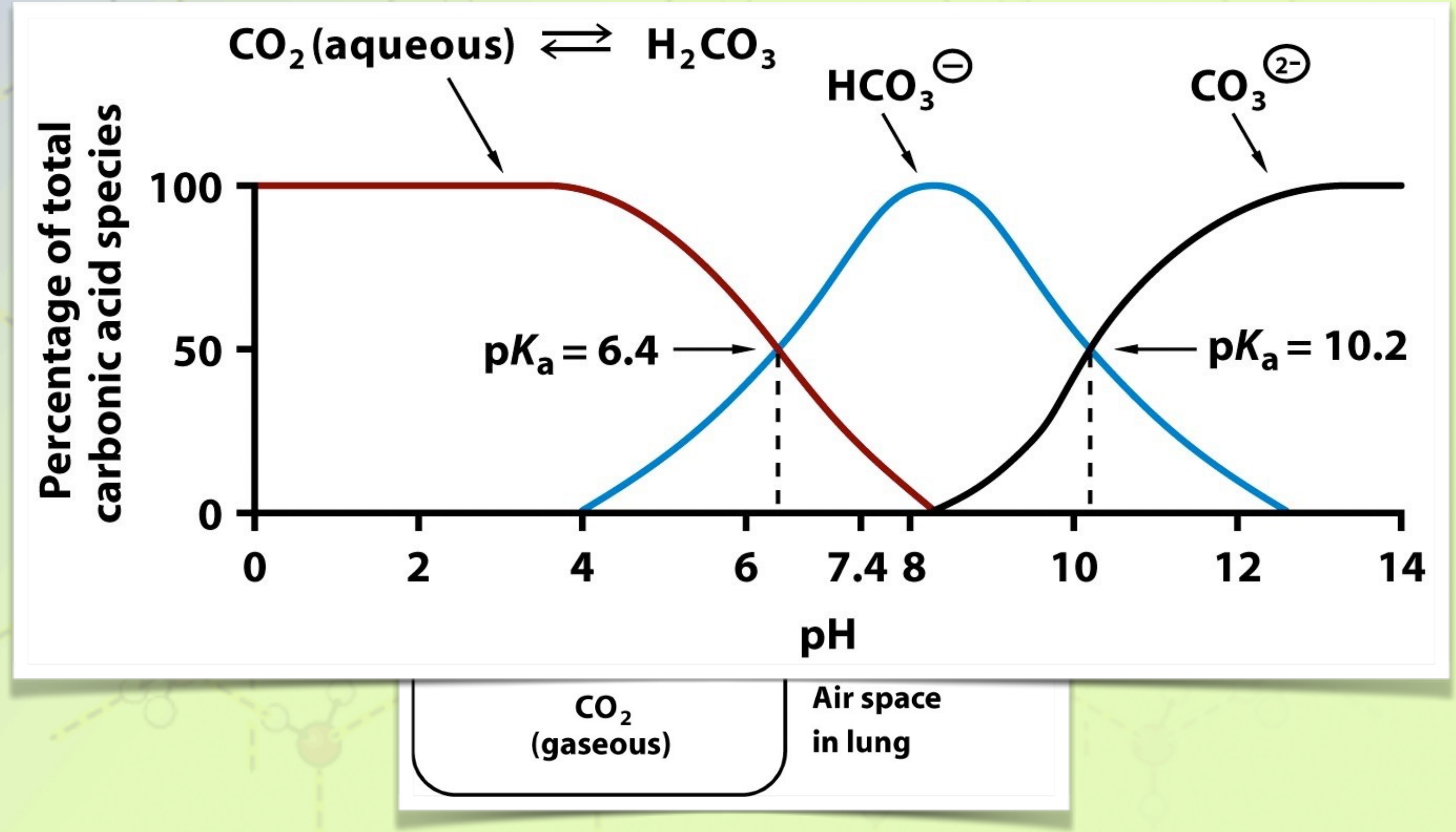
Chemical Properties of Water

The bicarbonate buffer and regulation of blood pH



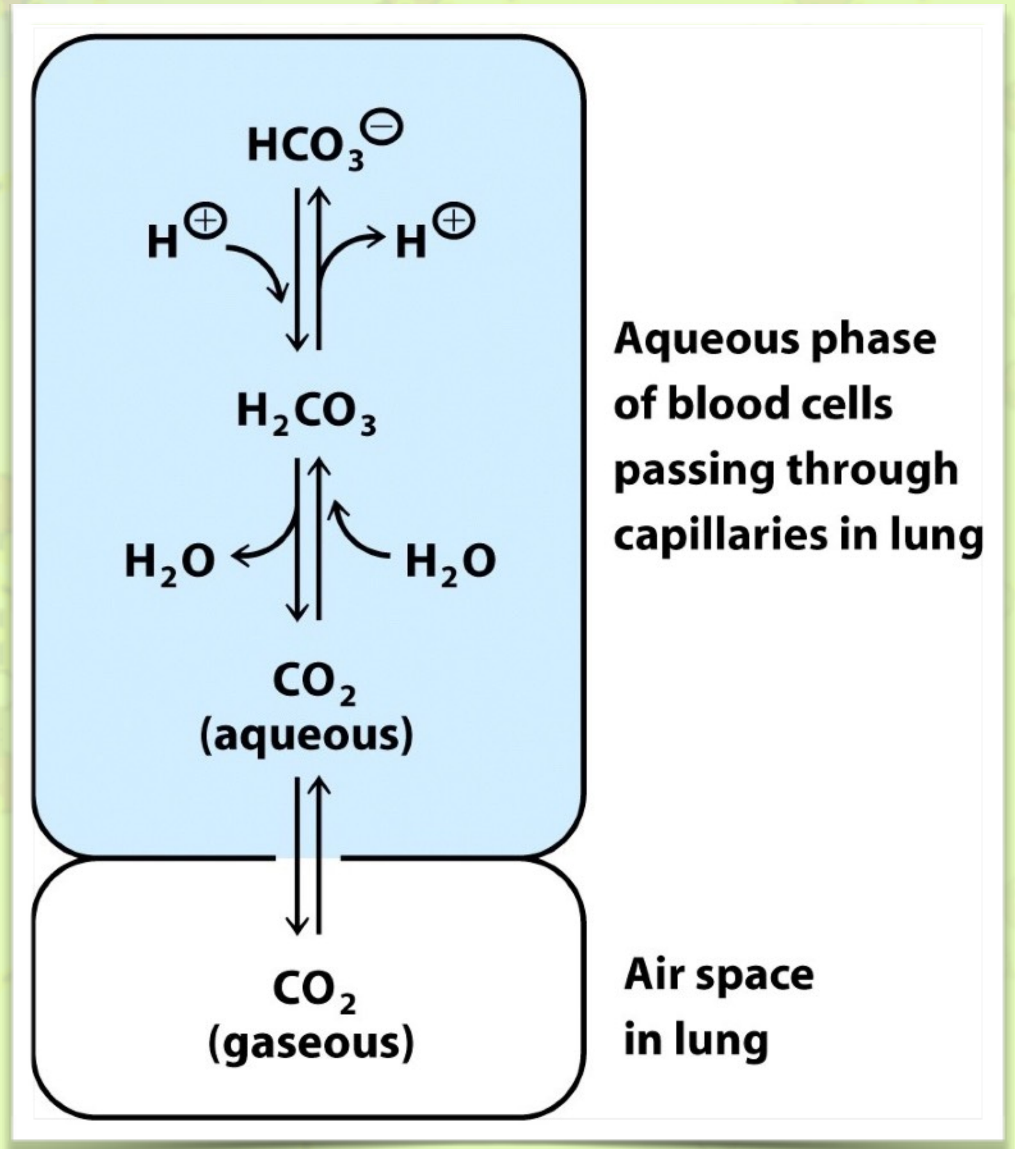
Chemical Properties of Water

The bicarbonate buffer and regulation of blood pH



Chemical Properties of Water

The bicarbonate buffer and regulation of blood pH



Next up

Lecture 3 - Amino Acids and Protein Primary Structure

- Read Chapter 3 of Moran et al.