بسم الله الرحمن الرحيم

BioChemistry | Lecture 2

Introduction to BioChem pt.2

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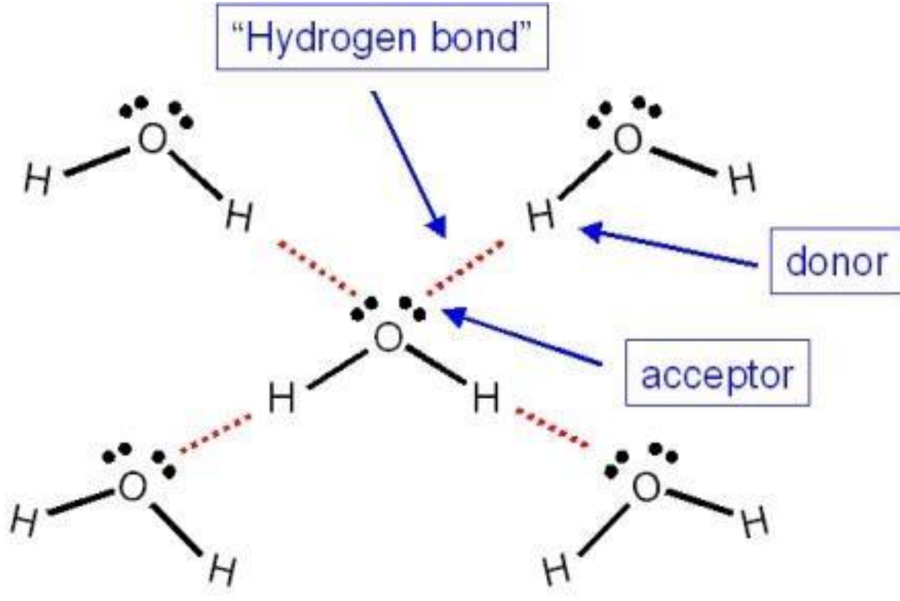
Water

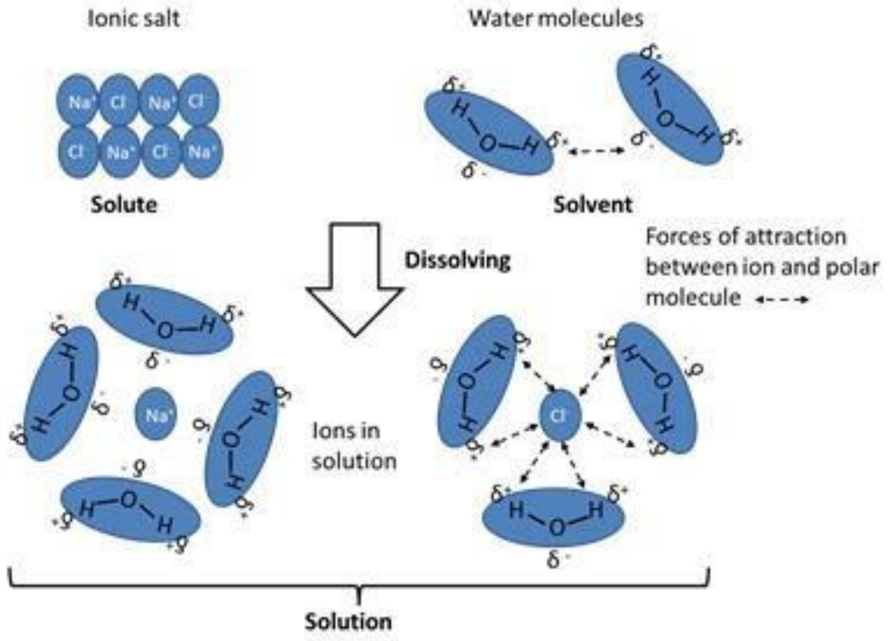
Properties of water (1)



H_2O

polar compound

- Polar
- Angular
- Dipole-dipole interactions and dipole-charge interactions
- Highly cohesive → Due to Hydrogen bonding, each water molecule can form up to 4 Hydrogen bonds, thus forming a lattice by the interactions it makes.
- produces a network
- Water is an excellent solvent



Small

Weakens electrostatic forces and hydrogen between polar molecules

- Water is a dipole molecule (it has a positive and negative end). So, between water molecules, there are dipole-dipole interactions. And if there are some charged atoms in the water, dipole-charge interactions occur (water surrounds and interacts with the charged particles). So, I have the capacity to form these two interactions.
- Solvent: a substance that can make hydrogen bonds with its solute molecules. Solvent surrounds solutes and detaches them from one another and forms multiple hydrogen bonds all around it.
- Why water is an excellent solvent?!
  Because it's a small molecule, meaning?

  If we compare one liter of water with one liter of another solvent, the number of moles will differ. Water is very small (composed of two hydrogen atoms and one oxygen atom only) so its number of moles is much higher than that of most other solvents in the same volume.
- When a molecule is big it has a big molecular weight so it will have less particles in the same volume.
- What's a Mole?

A mole of a substance indicates a **specific** quantity it tells us how much do we have of a substance (how many particles).

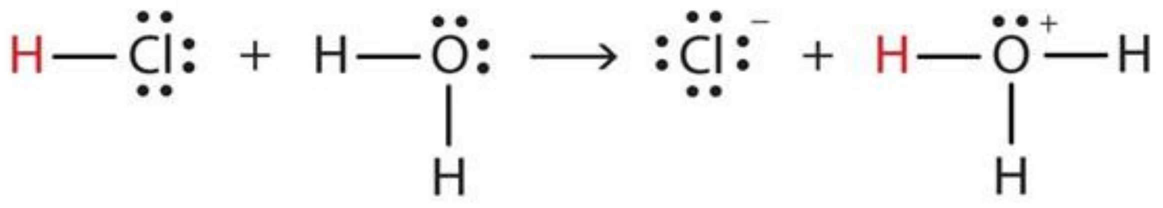
- So, the more that we have of certain solvents (the more number of molecules) the best this solvent can dissolve the solute.
- So, in case of H2O, we have more number of molecules, and each molecule can form up to 4 Hydrogen bonds.
- When the size of the solvent molecule is big it can't penetrate well (meaning it can't easily get between or surround solute particles) but when the solvent molecule is small, it can more easily diffuse between solute particles and interact with them.

- H_2O also has a high heat capacity because of the lattice of hydrogen bonds between its molecules. Any change in energy must be distributed throughout this hydrogen bond network, which slows down the response. That's why a large amount of energy – either added or removed – is required to significantly increase or decrease the temperature of water.

Recall that heat capacity refers to how much a substance resists changes in its temperature.

Properties of water (2)

- It is reactive because it is a nucleophile:
- – A nucleophile is an electron-rich molecule that is attracted to positively-charged or electron-deficient species (electrophiles).
- It can be ionized



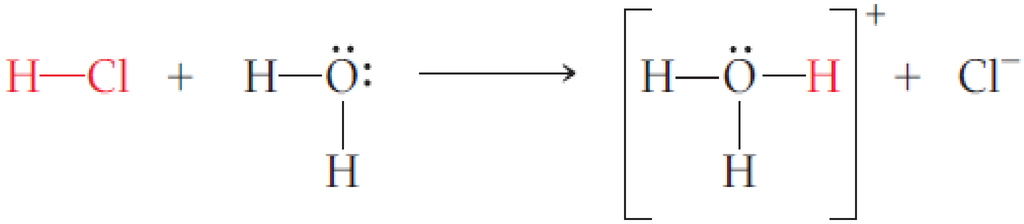
$$H_2O + H_2O \rightleftharpoons H_3O^{\oplus} + OH^{\ominus}$$

Acids and bases

Definitions and terms

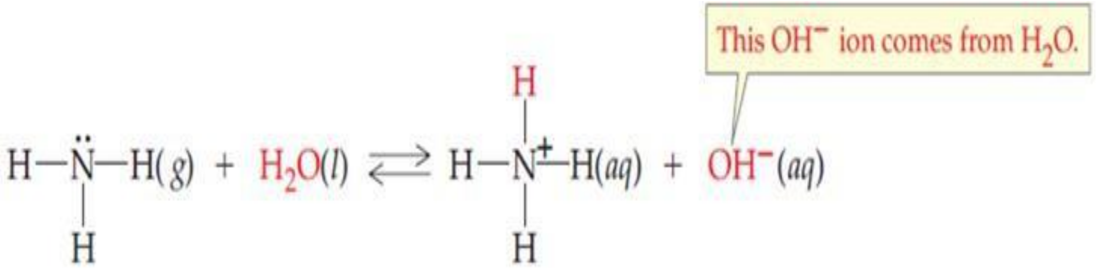
Proton (H+) is one of the ionization states of hydrogen
Hydrogen has 2 ionization states
1.(H+): proton
2.(H-): hydride

- Acid: A material that can donate a proton, when put inside a solution
  - A substance that produces H^+ (H_3O^+) when dissolved in water or reacts with other substances
  - Monoprotic acid: HCl, HNO_3, CH_3COOH Donates 1 proton
  - Diprotic acid: H_2SO_4 Donates 2 protons
  - Triprotic acid: H_3PO_3 Donates 3 protons



- Base:
  - A substance that produces OH^- when dissolved in water or accepts H^+ when reacts with other molecules
  - NH_3

A material that accepts the donated proton is a base.



- After an acid donates a proton to the solution, it can accept it again(in case of weak acids).(The conjugate base of an acid is the form that accepts the proton from the solution.)

- The same substance can act as either an acid or a base depending on the status of the proton – whether it's bound or free.

- The concept of acids and bases is based on their interaction with each other.

- What determines the strength of an acid – its ability to donate a proton?

A. The polarity of the bond holding the proton

B. The stability (stregnth) of the conjugate base after the proton is donated

C. The overall chemical structure of the molecule

- The chemical structure plays a major role in determining how easily an acid can release its proton into the solution.

- So, what distinguishes one acid from another?

- It's their strength – their ability to donate a proton.

- If an acid has a specific structure, it has a specific proton-donating ability; when the structure changes, its ability to donate protons also changes
- For diprotic and triprotic acids, which can donate multiple protons, the acid donates the first proton with a certain strength; after that, it becomes deficient of one proton, so the chemical structure has changed, meaning the strength differs as well.

Water = amphoteric

- Ampho = ‘both’ or ‘dual’
- Substances that can act as an acid in one reaction and as a base in another
- With ammonia (NH_3), water acts as an acid because it donates a proton (hydrogen ion) to ammonia
- $NH_3 + H_2O \leftrightarrow NH_4^+ + OH^-$
- With hydrochloric acid, water acts as a base
- $HCl + H_2O \rightarrow H_3O^+ + Cl^-$

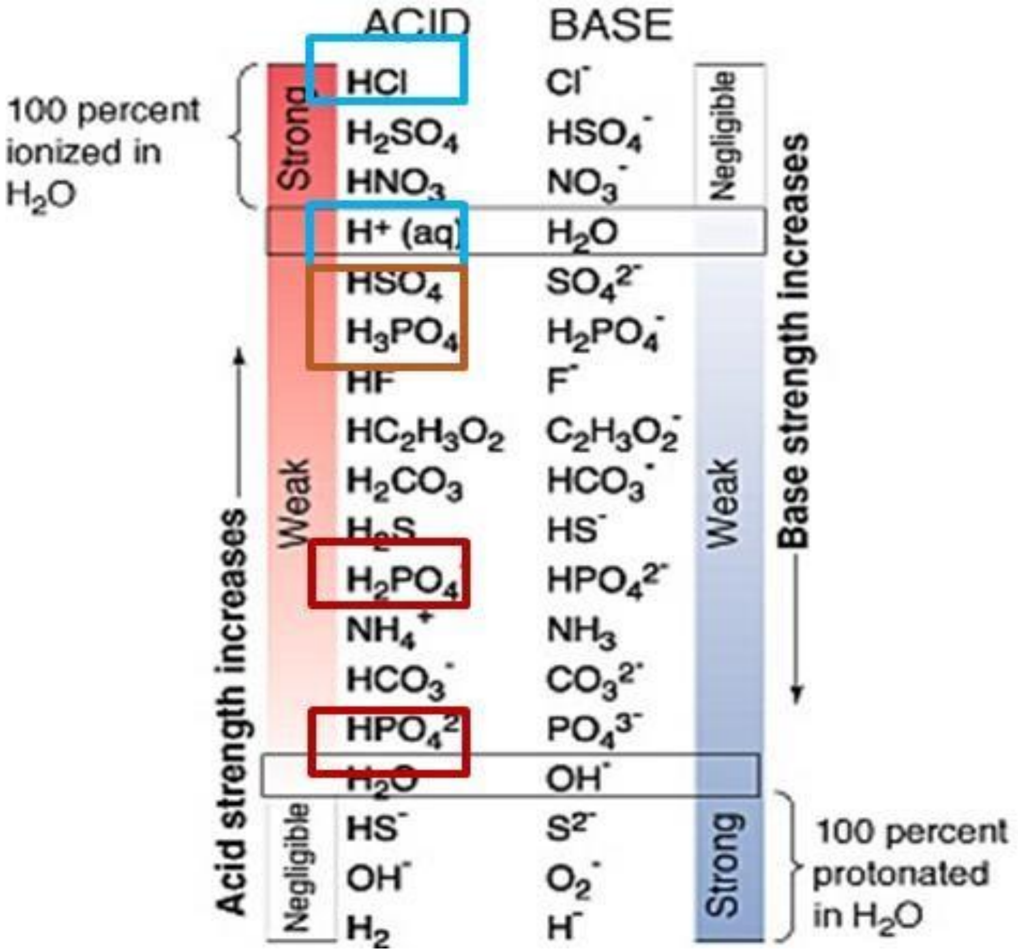
Depending on what the amphoteric substance reacts with. If amphoteric substance reacts with a base, then it acts as an acid and vice versa.

Carboxyl group is "the strongest functional group". So that if the molecule contains it, it will be a carboxylic acid even if it had other functional groups.
Carboxylic acids are weak acids.

Acid/base strength

- Acids differ in their ability to release protons
  - Strong acids dissociate 100%. For example,(almost) all the HCl molecules will dissociate into H+ (H3O+) and Cl- .
  - Full dissociation means that the reaction occurs in one direction and isn't reversible.
  - Biologically inside the body what's important is **weak** acids rather than strong because the full dissociation of strong acids produces large amounts of H+ in the solution therefore greatly affecting the PH making them harder to control
- Bases differ in their ability to accept protons
  - Strong bases have a strong affinity for protons.
- For multi-protic acids (H2SO4, H3PO4), each proton is donated at different strengths

Memorize strong acids



Rule

- The stronger the acid, the weaker the conjugate base
- Strong acids and bases are one-way reactions
- $HCl \rightarrow H^+ + Cl^-$ $NaOH \rightarrow Na^+ + OH^-$

- Weak acids and bases do not ionize completely
- $HC_2H_3O_2 \leftrightarrow H^+ + C_2H_3O_2^-$ $NH_3 + H_2O \leftrightarrow NH_4^+ + OH$

Equilibrium constant and Acid dissociation constant

- Acid/base solutions are at constant equilibrium
  - Equilibrium constant (Keq) for such reactions

Calculated or defined only at equilibrium. It is **ratio of concentrations of products to reactants at equilibrium** for a reversible chemical reaction at a given temperature.
For a strong acid there will be a large number in the nominator with a very low number in the denominator.

- **HA ↔ H^{+}+ A^{-}**

$$K_a = \frac{[H_3O^+] \cdot [A^-]}{[HA]}$$

[H3O+]=[A−]

- Value of the Ka indicates the direction of the reaction

Since weak acids and bases dissociation rxns are reversable, they reach equilibrium.

- Why?

To be stable. (everything is leaning toward having lower energy (more stability) when equilibrium is reached the difference in energy between the reactants and the products is zero).

- How ?

Equilibrium happens when the rates of the forward and backward reactions are equal and the concentrations of the reactants and products stay constant over time (not necessarily [Reactants]=[Products]) which makes sense because the rates of the reactions are equal.

- Equilibrium doesn’t mean death and it keeps biological systems functioning properly. The reactions are still occurring but at equal rates because there isnt a driving force (there isnt a rxn that has more energy than the other.

Ka vs. pKa

As Ka increases, acidity increases. Because high value of ka means that [H+] is high relative to [acid] and acidity is defined by how much H+ you have in the solution.
K can't be zero.

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
$HPO_4^{2\ominus}$ (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

TABLE | 9.4 K_A AND pK_A VALUES FOR SELECTED ACIDS

Name	Formula	K_a	pK_a
Hydrochloric acid	HCl	1.0×10^{7}	−7.00
Phosphoric acid	H_3PO_4	7.5×10^{-3}	2.12
Hydrofluoric acid	HF	6.6×10^{-4}	3.18
Lactic acid	$CH_3CH(OH)CO_2H$	1.4×10^{-4}	3.85
Acetic acid	CH_3CO_2H	1.8×10^{-5}	4.74
Carbonic acid	H_2CO_3	4.4×10^{-7}	6.36
Dihydrogenphosphate ion	$H_2PO_4^-$	6.2×10^{-8}	7.21
Ammonium ion	NH_4^+	5.6×10^{-10}	9.25
Hydrocyanic acid	HCN	4.9×10^{-10}	9.31

pKa is the **negative** logarithm **of the acid dissociation** constant **Ka.**

$$pK_a = -\log K_a$$

To make ka values easier to understand.

Measurements of acids and bases

Molarity: Measurement of concentration

- Moles = grams / MW moles are quantity
- M = moles / volume (L)
- Grams = M x volume (L)x MW

  – How many grams do you need to make 5M NaCl solution in 100 ml (MW =58.4)?
  – grams = 58.4 x 5 M x 0.1 liter = 29.29 g

How much charge do I need to neutralize the charge that I have.

Number of equivalents of an acid equals its moles when: it's a monoprotic acid.

Equivalents

- An equivalent is the number of moles of hydrogen ions that an acid can donate or a base can accept.
- For ions, one equivalent (Eq) is equal to the number of ions that carry 1 mol of charge.
- For acids:
  - 1 mole HCl = 1 mole [H+] = 1 equivalent which means I should have 1 negative charges to neutralize it.
  - 1 mole H_2SO_4 = 2 moles [H+] = 2 equivalents which means I need 2 negative charges to neutralize it.(I need 2 molecules of a base each with 1 negative charge to neutralize one molecule of this acid)
  - 1 eq of H_2SO_4 = ½ mol (because 1 mole gives two moles of H+ ions)
- For ions:
  - 1 eq of Na^+ = 23.1 g, 1 eq of Cl^- = 35.5 g, 1 eq of Mg^{2+} = (24.3)/2 = 12.15 g

Problems to solve

- How many equivalents are in the following:

- 5.0 g HNO_3 MW=63

5/(63/1)=

- 12.5 g $Ca(OH)_2$

12.5/(74/2)=

- 4.5 g H_3PO_4

4.5/(98/3)=

A way to calculate equivalence:

- You divide the mass that you have of the material by the equivalent mass.(it is atomic mass of that substance divided by how many charges it can give)

- The typical concentration of Mg^{2+} in blood is 3 mEq/L. How many milligrams of Mg^{2+} are in 250 mL of blood?

Exercise

- Calculate milligrams of Ca^{+2} in blood if total concentration of Ca^{+2} is 5 mEq/L.
- Note: atomic weight of Ca^{+2} is 40.1 grams/mole

- – 1 Eq of Ca^{+2} = 40.1 g/2 =20.1 g
  - Grams of Ca^{+2} in blood =
  - (5 mEq/L) x (1 Eq/1000 mEq) x (20.1 g/ 1 Eq)
- – = 0.1 g/L
- – =100 mg/L

Electrolytes

- Electrically-charged minerals when dissolved in water
- Sodium, potassium, chloride, calcium, magnesium, phosphate, and bicarbonate
- Vital for various bodily functions such as nerve and muscle function, fluid balance, acid-base balance, and blood pressure
- Heavy and continuous diarrhea can result in dehydration and very low sodium levels in the body (hyponatremia) hyponatremia can lead to hallucination and confusion.
- Heavy sweating leads to dehydration and loss of electrolytes

Electrolytes are very important to our bodies.
They can be lost along with water during diarrhea, vomiting and sweating.
Excessive loss of electrolytes can lead to severe complications therefore should be restored for example by IV electrolyte replacement in hospitals.
Also athletes drink electrolyte rich drinks to restore what is lost by excessive sweating during strenuous exercise.

Molarity and equivalents

- Equivalents = n x M x volume (L)
- One equivalent of any acid neutralizes one equivalent of base
- Basis of titration (neutralization)

“how much acid do I need to neutralize a base (ph=7) and vice versa”.

10.92 Titration of a 12.0 mL solution of HCl requires 22.4 mL of 0.12 M NaOH. What is the molarity of the HCl solution?

Eq of base = Eq of acid

$n \times M_1 \times Vol_1 = n \times M_2 \times Vol_2$

$1 \times 0.12 \times 22.4 = 1 \times M_1 \times 12$

$M_1 = (0.12 \times 22.4) / 12$

$M_1 = 0.224$ M

Problem to solve

10.93 What volume of 0.085 M HNO_3 is required to titrate 15.0 mL of 0.12 M $Ba(OH)_2$ solution?

- Note that 1 mole of HNO3 produces 1 mole of H+, but 1 mole of Ba(OH)2 produces 2 moles of OH-. In other words, the n is different.

- Eq of acid = Eq of base
- n x M1 x Vol1 = n x M2 x Vol2 1 x 0.085 x Vol = 2 x 0.12 x 15
- Vol = (2 x 0.12 x 15) / 1 x 0.085 Vol = 42.35 mL

Antacids

$$CaCO_3 + 2\ HCl \rightarrow CaCl_2 + H_2O + CO_2$$
$$NaHCO_3 + HCl \rightarrow NaCl + H_2O + CO_2$$
$$Al(OH)_3 + 3\ HCl \rightarrow AlCl_3 + 3\ H_2O$$
$$Mg(OH)_2 + 2\ HCl \rightarrow MgCl_2 + 2\ H_2O$$

- Alkaline (basic) compounds (neutralize HCl) of the stomach.
- Reduce stomach acidity and providing relief from heartburn and indigestion (dyspepsia)
- Reduce digestion of proteins by pepsin (pH 1-2 vs. 3.5-5)(activity of pepsin declines as PH reaches 3.5 and above)
  Antacids neutralize (HCl).This raises the pH of the stomach. At a higher pH (less acidic), pepsin becomes less active or inactive. This can slow or reduce protein digestion in the stomach.
- Examples: Magnesium Hydroxide, Aluminum Hydroxide, Calcium Carbonate, Sodium Bicarbonate

Water is a weak acid.

Ionization of water

- For simplicity, we refer to the hydronium ion as a hydrogen ion (H+) and write the reaction equilibrium as:

Water undergoes Self Ionisation

$$H_2O_{(l)} \rightleftarrows H^+_{(aq)} + OH^-_{(aq)}$$

or

$$H_2O_{(l)} + H_2O_{(l)} \rightleftarrows H_3O^+_{(aq)} + OH^-_{(aq)}$$

Equilibrium constant

The concentration of H+ and OH- are very low compared to concentration of H2O which means that a very small fraction of water molecules ionizes. They can be negligible; therefore we can say that the concentration of water inside a liter for example, isnt changing.

- The equilibrium constant Keq of the dissociation of water is:

$$K_{eq} = \frac{[H^{\oplus}]\,[OH^{\ominus}]}{H_2O}$$

- The equilibrium constant for water ionization under standard conditions is 1.8 x 10^-16 M. (memorize)

The ion product of water (Kw)

- Since there are 55.6 moles of water in 1 liter, the product of the hydrogen and hydroxide ion concentrations results in a value of 1 x 10-14 for: (If we multiply [H2O] (55.5M) in one L by Keq we get Kw:)

$$K_{eq}(55.5\ M) = [H^{\oplus}][OH^{\ominus}]$$

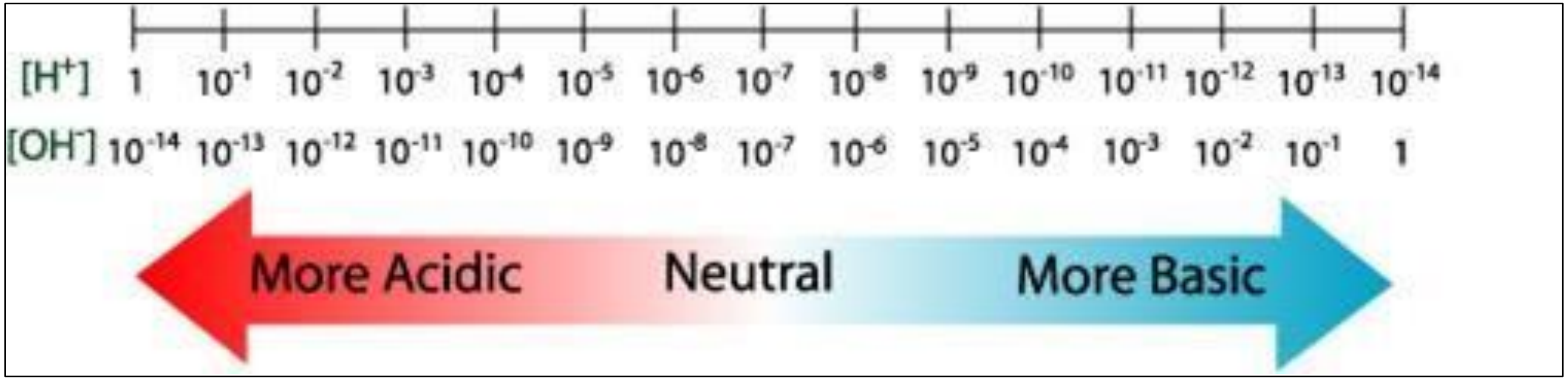
- This constant, Kw, is called the ion product for water

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

[H+]=[OH-]= 1.0 x 10^-7 If [H+] increases, [OH-] decreases and vice versa

$[H^+]$ and $[OH^-]$

- For pure water, there are equal concentrations of [H+] and [OH-], each with a value of 1 x 10-7 M.
- Since Kw is a fixed value, the concentrations of [H+] and [OH-] are inversely changing.
- If the concentration of H+ is high, then the concentration of OH- must be low, and vice versa. For example, if [H+] = 10-2 M, then [OH-] = 10-12 M



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اللهمّ نصرًا قريبًا وفرجًا جميلًا

For any feedback, scan the code or click on it.

Corrections from previous versions:

Versions	Slide # and Place of Error	Before Correction	After Correction
V0 → V1	19	The number of equivalents of an acid equals its concentration when it's a monoprotic	The number of equivalents of an acid equals its moles when it's a monoprotic
V1 → V2			