CHEM 6.1 BALANCING CHEMICAL EQUATIONS 1

Chemical reactions – balancing chemical equations/stoichiometry

Reactants $\longrightarrow$ **Products** (must have atom & charge conservation for balance)

Examples: $2.C + O_2 \longrightarrow 2\,CO$

$Al^{3+}P^{3-}{}_{(s)} + 3.H_2O_{(l)} \longrightarrow Al(OH)_{3(s)} + PH_{3(g)}$

$Cu^{2+} + Zn \longrightarrow Cu + Zn^{2+}$

$Cl_2 + 2.I^- \longrightarrow 2.Cl^- + I_2$

Combustion [burning in air (20 %v/v oxygen) or in pure oxygen]

Eg. $2.\,C_2H_6 + 7.\,O_2 \longrightarrow 4.CO_2 + 6.H_2O$

Acid/Base Water forms hydrogen ions (**H^+**), which are the abbreviated form of the hydronium ion (H_3O^+), and hydroxide ions (**OH^-**) when it self-ionizes :
(δ = lower case delta (a small amount of charge) to indicate polarity eg., $H^{\delta+}$)

H δ+   H δ+
\   \
δ- : O :   : O : δ-   ⇆ H_3O^+ + HO^-
| | Acid   Base (or alkali)
δ+ H   H δ+

What is meant by the term, "**CHEMICAL EQUILIBRIUM**" as represented by ⇆ ?

Physical equilibrium is when we have a balanced static system. In contrast, a **chemical equilibrium** is **dynamic**, with reactants continually changing into products, and vice-versa, until no overall change in the concentrations of either reactants or products occurs, although they never stop interchanging.

Since at equilibrium there is no change in the overall concentrations of reactants or products, the ratio, [products]/[reactants] is constant, at constant temperature, so we can write the **equilibrium constant, K,** for the following reaction as:

$$H_2O + H_2O \overset{K}{\leftrightarrows} H_3O^+ + OH^- \qquad \mathbf{K} = [H_3O^+].[OH^-] / [H_2O]^2$$

Because this is in water, and the $[H_2O]$ is essentially constant, the product, $K.[H_2O]^2$ is constant, and given the special symbol, $K_{water} = K_w$ which has the value 10^{-14} @ 25^oC.

$$H_2O + H_2O \overset{K_w}{\leftrightarrows} H_3O^+ + OH^- \qquad \mathbf{K_w = [H_3O^+].[OH^-] = 10^{-14} \ @\ 25^oC}$$

WHAT IS AN ACID?

Brønsted concept: **an ACID is an entity which produces H_3O^+ ions** (aquated protons) in aqueous solution.

Why is the proton released? Because H is bound to a very electronegative element, eg O, Cl.
(Electronegativity is the ability of an atom/ion to attract electrons).

$$\overset{\delta-\ \ \delta+}{\text{ELEMENT – H}} \quad + \quad H_2O \quad \rightleftharpoons \quad \text{ELEMENT}^- \quad + \quad H_3O^+$$

δ = lower case delta (a small amount of charge) eg., $H^{\delta+}$
Δ = capital delta (a larger amount of charge) eg., $H^{\Delta+}$
$\pm$ = integral value of charge eg., H^+

so magnitude of charge follows the sequence $H^+ > H^{\Delta+} > H^{\delta+}$

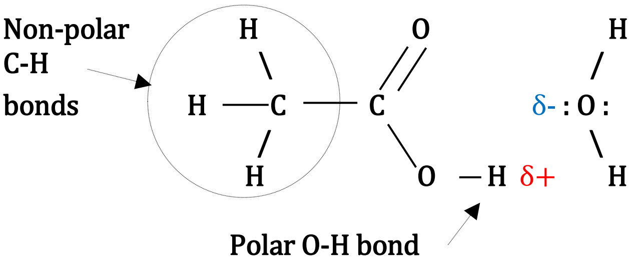
ELECTRONEGATIVITY VALUES OF SOME COMMON ELEMENTS

H 2.20		**B** 2.04	**C** 2.55	**N** 3.04	**O** 3.44	**F** 3.98
Li 0.98	**Be** 1.57	**Al** 1.61	**Si** 1.90	**P** 2.19	**S** 2.58	**Cl** 3.16
Na 0.93	**Mg** 1.31	**Ga** 1.81	**Ge** 2.01	**As** 2.18	**Se** 2.55	**Br** 2.96
K 0.82	**Ca** 1.00	**In** 1.78	**Sn** 1.96	**Sb** 2.05	**Te** 2.1	**I** 2.66

HCℓ (strong acid) H-Cℓ(g) ---water → H_3O^+ + $C\ell^-$ (aq) (virtually complete dissociation)

a large amount per mol, so a strong acid

ACETIC ACID (weak acid)



$\overset{K_a}{\leftrightarrows}$ CH_3COO^- + H_3O^+

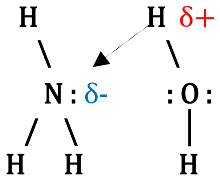
only a small amount per mol, so only a weak acid

CH_3COOH + H_2O ← (only about 1 % dissociation) K_a → CH_3COO^- + H_3O^+

Na^+OH^- (strong base) Na^+OH^-(s) ---water → Na^+(aq) + HO^-(aq) (virtually complete dissociation)

a large amount per mol, so a strong base

AMMONIA (weak base)

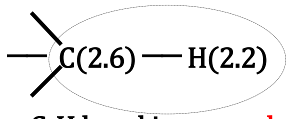


$\overset{K_b}{\leftrightarrows}$ NH_4^+ + HO^-

only a small amount per mol so only a weak base

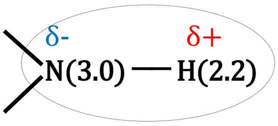
NH_3 + H_2O ← (only about 1 % dissociation) K_b → NH_4^++ OH^-

As an example, compare Δ(EN) (polarity) of hydrogen (H) bound to C, N, O, F:



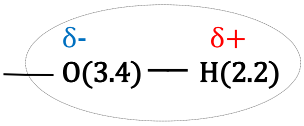
Δ(EN) = 0.4 ie., <u>C **has similar EN** to H</u>,

so **C-H bond is non-polar**, so H (in hydrocarbon) is **not acidic** when bound only to C.



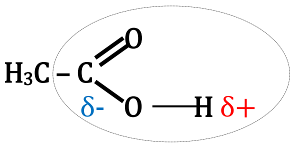
Δ(EN) = 0.8 ie., <u>N is **slightly more EN** than H</u>,

so **N-H bond is slightly polar**, but H (in amine) is **not acidic in water** when bound only to N.



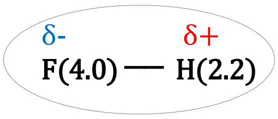
Δ(EN) = 1.2 ie., <u>O is **more EN** than H</u>,

so **O-H bond is polar**, but H (in alcohol) is **not acidic** in water when bound only to O.



Δ(EN) > 1.2 (due to proximity of another O in C=O),

so **O-H bond in carboxyl group is even more polar than –O-H in alcohol or water due to presence of >C=O**, and so H (in carboxylic acid) is **slightly acidic.**

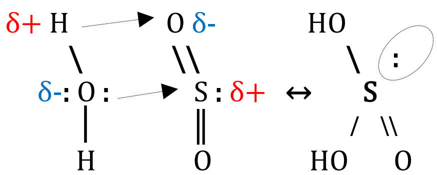


Δ(EN) = 1.8 ie., <u>F is **much more EN** than H</u>,

so **F-H bond is polar**, so H (in HF) is **quite acidic**.

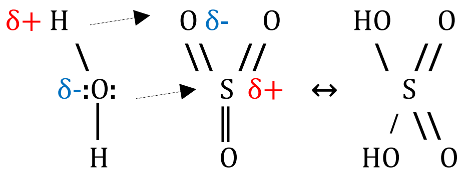
<u>Other examples:</u>

Sulphurous acid, dissolved SO_2 gas



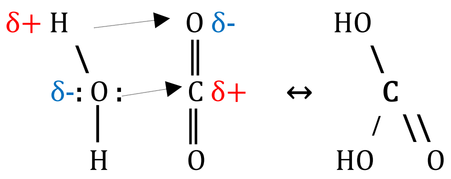
$H_2SO_3 \leftrightarrows H^+ + HSO_3^- \leftrightarrows H^+ + SO_3^{2-}$ an acid

Sulphuric acid, dissolved SO_3 gas



$H_2SO_4 \leftrightarrows H^+ + HSO_4^- \leftrightarrows H^+ + SO_4^{2-}$ an acid

Carbonic acid, dissolved CO_2 gas



$H_2CO_3 \rightleftarrows H^+ + HCO_3^- \rightleftarrows H^+ + CO_3^{2-}$ an acid

(Note that H^+ and $H^+(aq)$ are abbreviations for the hydronium ion, H_3O^+, in fact all ions in aqueous solution are always hydrated/solvated)

A scale for reporting acidity/basicity (alkalinity) – the pH scale

p NOTATION is a convenient means of expressing concentrations.
p means '$-\log_{10}$', and we use 'log' to signify '$\log_{10}$' (ie log to the base 10)

So, $\quad pX = -\log_{10}(X) = -\log(X)$ and $pK_a = -\log_{10}(K_a) = -\log(K_a)$

Hence, $\quad X = 10^{-pX}$ and $Ka = 10^{-pKa}$

What do we use this "p" notation for?

To express very low concentrations, especially for acid (H^+)/base (OH^-) solutions:

Eg $\boxed{pH = -\log_{10}[H^+] \quad [H^+] = 10^{-pH}\ M}$ & $\boxed{pOH = -\log_{10}[OH^-] \quad [OH^-] = 10^{-pOH}\ M}$

If $[H^+] = 0.000\,000\,01$ **M** $= 10^{-8}$ **M** $= 10^{-pH}$ then $pH = 8$;
If the pH = 3, then $[H^+] = 10^{-3}$ **M** (because $[H^+] = 10^{-pH}$ **M**) so $[H^+] = 0.001$ **M**

Since:

$$H_2O + H_2O \overset{K_w}{\rightleftarrows} H_3O^+ + OH^- \quad \text{and} \quad K_w = [H_3O^+].[OH^-] = 10^{-14} \text{ @ } 25^oC$$

then, in **pure water**, $[H_3O^+] = [OH^-] = 10^{-7}$ M @ 25^oC.

Now, the pH Scale is defined by : $pH = -\log_{10}[H^+]$ so, $[H^+] = 10^{-pH}$
so in pure water where $[H^+] = 10^{-7}$ M $= 10^{-pH}$ M, the pH = 7 (neutral)
and $\boxed{pH + pOH = 14}$

So the pH scale is a measure from 1 to 14 of the acidity (pH = 1-6), or alkalinity (pH =8-14), of an aqueous solution.

	pH = 2	pH = 7	pH = 12	
$[H^+] = 10^{-pH}$	$[H^+] = 10^{-2}$	$[H^+] = 10^{-7}$	$[H^+] = 10^{-12}$	mol/L

pH = 0—1—2—3—4—5—6—7—8—9—10—11—12—13—14

very acidic **neutral** **very basic(alkaline)**

$[OH^-] = 10^{-pOH}$	$[OH^-] = 10^{-12}$	$[OH^-] = 10^{-7}$	$[OH^-] = 10^{-2}$	mol/L
	pOH = 12	pOH = 7	pOH = 2	

stomach pH = 1– 3 intestines pH =7.6-8.2 dishwasher detergent pH =12

STRONG ACIDS completely dissociate (ionize) in water. e.g., HCl, HNO_3, H_2SO_4.

HNO_3 + H_2O ------- 100 % dissociation → $H_3O^+(aq)$ + $NO_3^-(aq)$

i.e., a strong acid dissociates / ionizes completely in solution (about 95 – 100 %). In the stomach HCl forms the strong acid H^+ Cl^- which kills bacteria and activates digestive enzymes .

For a Strong ACID dissolved in water : eg. $HC\ell + H_2O \rightarrow H_3O^+ + C\ell^-$
If $[HC\ell] = 0.1$ M $= 10^{-1}$ M, then $[H_3O^+] = [H^+] = 10^{-1}$ M, so, since $[H^+] = 10^{-pH}$, pH = 1

WEAK ACIDS only partly dissociate (partially ionize, about 1-10 %) in water. e.g. carboxylic acids (RCOOH), H_3PO_4, carbonic acid (H_2CO_3), H_2S, HF, boric acid (H_3BO_3).

Acetic acid – found in vinegar :

CH_3COOH + H_2O ← (1 % dissociation) → $CH_3COO^-(aq)$ + $H_3O^+(aq)$ (over the arrow: K_a)

BASES or ALKALIS

An alkali (or base) is an entity which produces hydroxide (OH^-) ions in solution. e.g.

NaOH (Na^+OH^-) + H_2O → $Na^+(aq)$ + $OH^-(aq)$

STRONG BASES completely dissociate in water(about 95 – 100 %) i.e. tend to completely ionize in solution to produce OH^- ions, eg NaOH, KOH, $Ba(OH)_2$

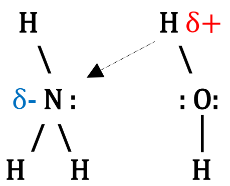
KOH(K^+OH^-) + water ------ 100 % dissociation → $K^+(aq)$ + $OH^-(aq)$

For a Strong BASE dissolved in water : eg. KOH(K^+OH^-) + H_2O → $K^+(aq)$ + $OH^-(aq)$
If [KOH] = 0.1 M $= 10^{-1}$ M, then $[OH^-] = 10^{-1}$ M, so since $[OH^-] = 10^{-pOH}$, pOH = 1,

Since, pH + pOH = 14, so pH + 1 = 14, so pH =13.

WEAK BASES only partially ionize in water (about 1-10 %); indeed, they tend to remain as molecules e.g., ammonia and amines (RNH_2, R'R"NH etc.) react with water to produce OH^- ions.

eg NH_3 + H_2O ← (1 % dissociation) → $NH_4^+(aq)$ + $OH^-(aq)$ (over the arrow: K_b)



↔ $NH_4^+(aq)$ + $OH^-(aq)$

NEUTRALISATION is usually the formation of water from an *acid* (H^+) and a *base* (eg. OH^- or $:NH_3$), and this is always accompanied by the formation of an ionic salt :

$HBr(aq) + KOH(aq) \rightarrow Br^- + H^+ + OH^- + K^+ \rightarrow K^+ + Br^-$ (soluble salt) $+ H_2O$

("spectator ions")

$H_2SO_4 = SO_4^{2-} + 2.H^+ + 2.OH^- + 2.Na^+ \longrightarrow 2.H_2O + 2.Na^+ + SO_4^{2-}$

Acetic acid (in vinegar) $CH_3COOH + OH^- + K^+ \longrightarrow H_2O + CH_3COO^- + K^+$

Neutralisation can also occur when an acid and a base react to give just a salt:

Eg., $HC\ell(aq) + :NH_3(aq) \rightarrow C\ell^- + H^+ + :NH_3(aq) \rightarrow NH_4^+ + C\ell^-$ soluble salt

(ammonia molecule) (ammonium ion)

With $Na_2CO_3 = 2.Na^+ + CO_3^{2-} + H^+ + C\ell^- \rightarrow Na^+ + HCO_3^- + Na^+ + C\ell^-$

Then $Na^+ + HCO_3^- + H^+ + C\ell^- \rightarrow Na^+ + C\ell^- + H_2CO_3 \rightarrow H_2O + CO_2$

overall

$$\mathbf{2.Na^+ + CO_3^{2-} + 2.H^+ + 2.C\ell^- \rightarrow 2.Na^+ + 2.C\ell^- + H_2O + CO_2}$$

Notice that during the acid/base reaction the Na^+ and $C\ell^-$ "spectator" ions do not take part in the reaction.

BUFFER SOLUTIONS

A BUFFER is an aqueous solution which resists changes in pH when acids or bases are added to it.

To do this, they must contain both an acidic component (to react with added base) and a basic (alkaline) component (to react with added acid).

Eg., base $HPO_4^{2-} + H^+ \leftrightarrows H_2PO_4^-$ acid

comprises the major buffer inside cells where pH = 7.4

and, base $HCO_3^- + H^+ \leftrightarrows H_2CO_3$ (dissolved CO_2) acid

comprises the major buffer in blood where pH = 7.4

A mixture of acetic acid (CH_3COOH) and sodium acetate ($Na^+ CH_3COO^-$) provides a buffer having a pH of 5, whilst a mixture of ammonium chloride ($NH_4^+ Cl^-$) and ammonia (NH_3) provides a buffer of pH 9.