Introduction Lecture

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- All cell phones must be silenced during the class period to minimize the disturbance for other students.
- If a cell phone goes off during my class the student must leave the class and he/she will receive and unexcused absence.

- <u>If you come late for more than five minutes please don’t try to enter the class</u>

- **Acid** is a substance that can **release hydrogen ions** (protons H+).
- **Base** is a substance that can **accept hydrogen ions.**
- **pH** is the concentration of hydrogen ions it determines the acidity of the solution
- The pH of a solution is the negative base 10 logarithm of its hydrogen ion concentration
- **pH** = -log10[H+]

pH	[H^+]	
0	(10^{0})	1.0
1	(10^{-1})	0.1
2	(10^{-2})	0.01
3	(10^{-3})	0.001
4	(10^{-4})	0.0001
5	(10^{-5})	0.00001
6	(10^{-6})	0.000001
7	$\mathbf{(10^{-7})}$	**0.0000001**
8	(10^{-8})	0.00000001
9	(10^{-9})	0.000000001
10	(10^{-10})	0.0000000001
11	(10^{-11})	0.00000000001
12	(10^{-12})	0.000000000001
13	(10^{-13})	0.0000000000001
14	(10^{-14})	0.00000000000001

pH	[H^+] (mol/l)	
1	10^{-1}	
2	10^{-2}	
3	10^{-3}	Increasing
4	10^{-4}	acidity
5	10^{-5}	
6	10^{-6}	
7	10^{-7}	Neutral
8	10^{-8}	
9	10^{-9}	
10	10^{-10}	Increasing
11	10^{-11}	alkalinity
12	10^{-12}	
13	10^{-13}	
14	10^{-14}	

- The following examples illustrate how to calculate the pH of acidic and basic solutions.
- ***Example 1:*** What is the pH of a solution whose hydrogen ion concentration is 3.2 X 10−4 mol/L?
- pH = -log [H+]

  = -log (3.2 X 10-4)
- = -log (3.2) - log(10-4)
- = -0.5 + 4
- pH = 3.5

Dissociation Constants (Ka)

When an acid loses a proton, its conjugate base is formed.

The tendency of any acid (HA) to lose a proton and form its conjugate base (A-) is called **dissociation constants (Ka).**

$$\underset{\text{Acid}}{HA} \rightleftharpoons \underset{\text{Conjugate Base}}{A^-} + H^+$$

$$Ka = \frac{[A^-]}{[HA]}$$

The stronger the acid, the greater its tendency to lose its proton.

<u>Strong acids</u>: are acids that dissociate completely in solution like HCl. **HCl** $\longrightarrow$ **Cl- + H+**

<u>Weak acids</u>: are acids that dissociate only to a limited extent like H2CO3. **H2CO3** $\longrightarrow$ **HCO3- + H+**

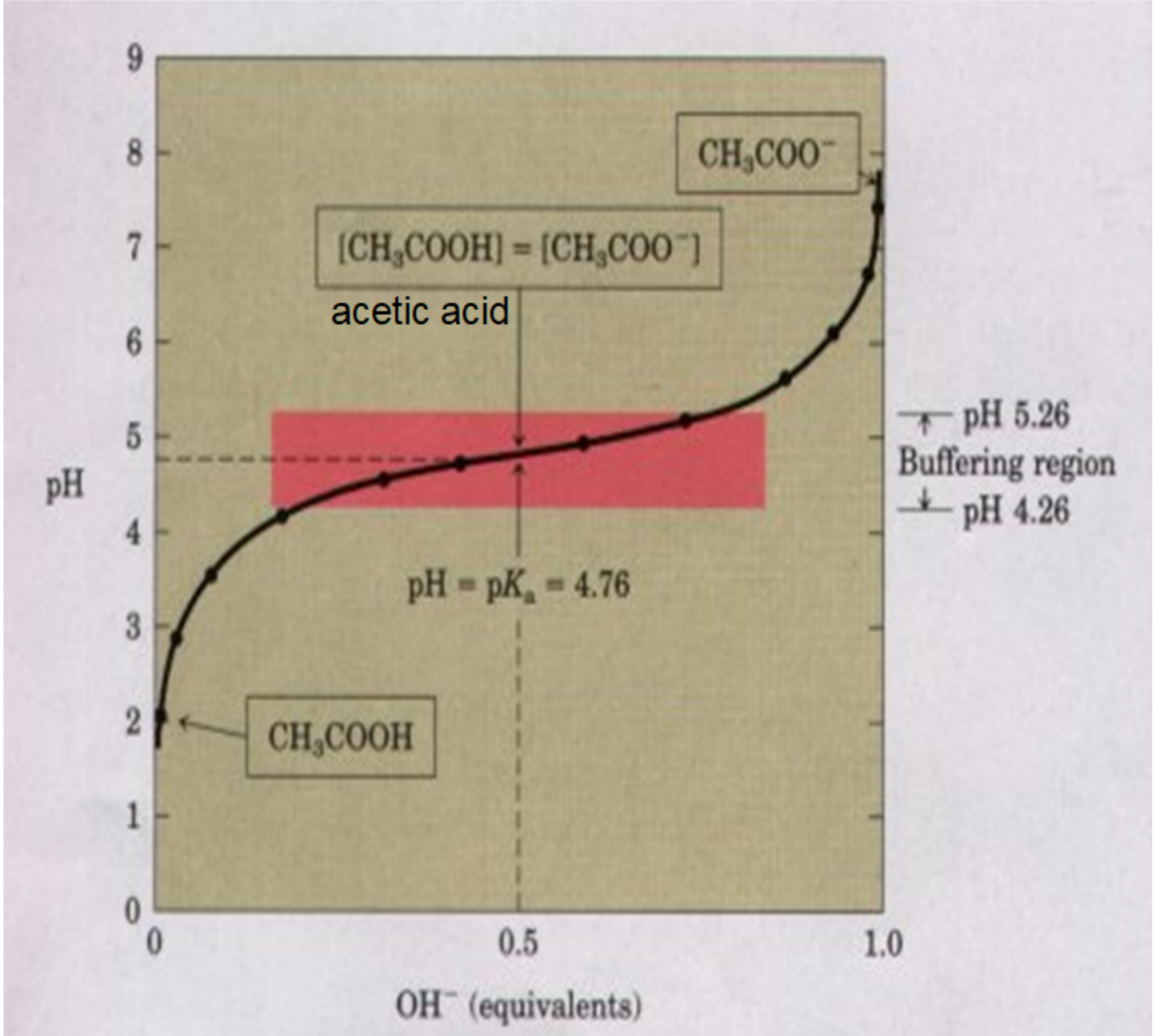
The weak **acid** (proton donor) dissociates into a hydrogen ion H+ and an anionic component (A-), called the **conjugate base** (or salt).

pKa

- **pKa = -log Ka**
- **pKa is the pH at which 50% dissociation occurs**
- pKa value is easier to work with and remember than Ka value.

- The stronger the tendency of an acid to dissociate the higher is the Ka and the lower is its p*K*a.

The maximum buffering capacity exists when the pH of the solution equals the pK' of the buffer, [conjugate base] = [acid], the buffer can then respond equally to both added acid and added base



<u>Buffers</u>

A buffer is a solution that resists pH changes when acids or bases are added to the solution.

Buffer solutions consist of a weak acid (undissociated acid) and its conjugate base (the form of the acid having lost its proton).

$$\underset{\text{Acid}}{HA} \rightleftharpoons \underset{\text{Conjugate Base}}{A^{-}} + H^{+}$$

A buffer works because added acids (H+) are neutralized by the conjugate base (A-) which is converted to the acid (HA).

Added bases are neutralized by the acid (HA), which is converted to the conjugate base (A-).

<u>Two factors determine the effectiveness of a buffer</u>:

1- its pKa relative to the pH of the solution

2- its concentration.

Henderson-Hasselbalch Equation

- Henderson-Hasselbalch adjusted equation shown below describe the relationship between the acid and its conjugate base with pH and pKa

$$pH = pKa + \log \frac{A^{-}}{HA}$$

$$pH = pKa + \log10 \frac{[\text{Conjugate Base}]}{[\text{Acid}]}$$

- The most effective buffers is when pH=pKa means it has equal concentrations of acid [HA] and its conjugate base [A-] (50% of both forms AH & A- present in solution).
- At pH = p*K*a ± 1 the buffer capacity falls to 33% of the maximum value. Therefore the buffer is effective one point up or down the pH pKa value.

Chemical bonds

- Refers to the attractive forces that hold atoms together in compounds.
- Chemically, bonding occurs when an atom give up electrons, accept electrons, or share electrons with another atom
- A stable compound occurs when the total energy of the combination has lower energy than the separated atoms.

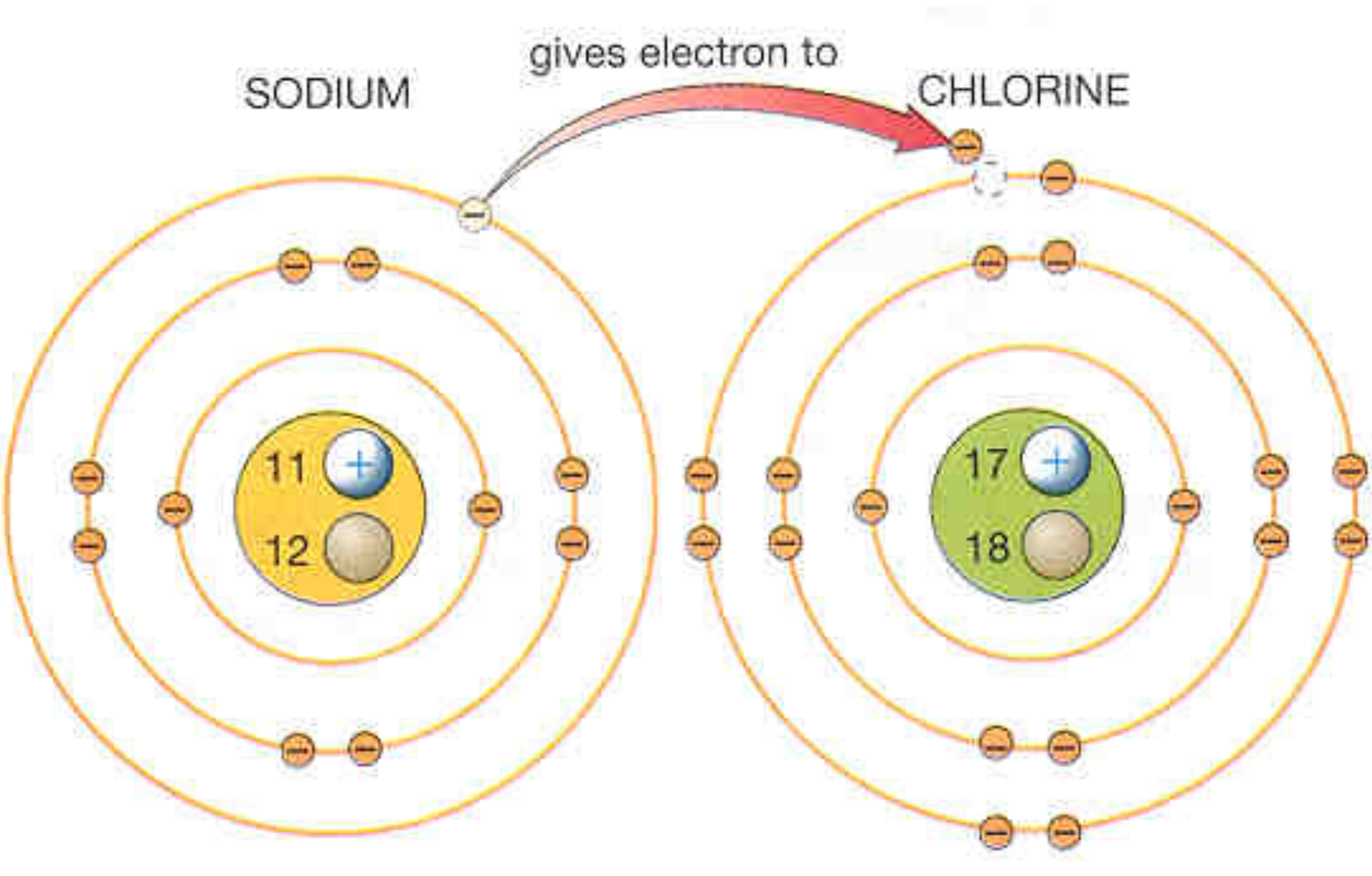
Major Bonds in Biological Molecules

1) **Ionic bonding**

In ionic bonding, electrons are completely transferred from one atom to another.

The oppositely charged ions are attracted to each other by electrostatic forces, which are the basis of the ionic bond.

Ionic Bond



Ionic compounds share many features in common including:

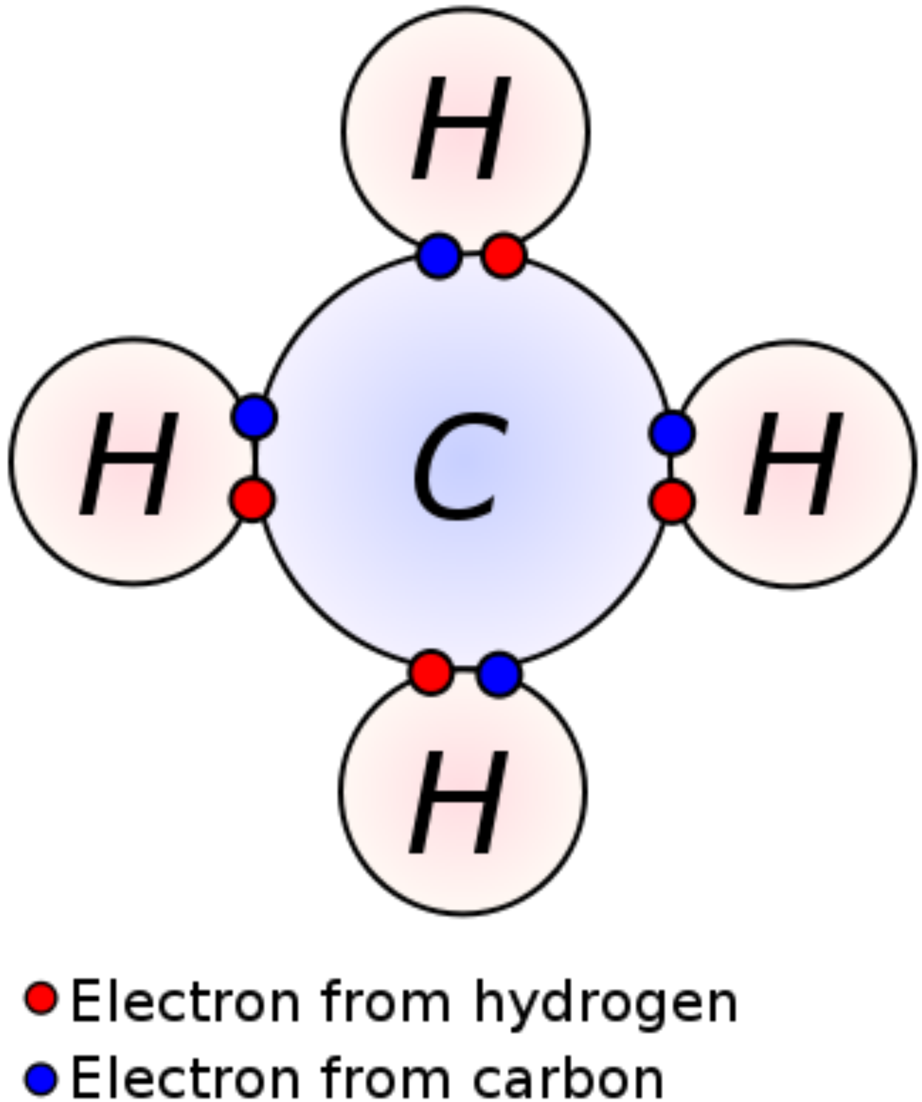
* Ionic bonds form between metals and non-metals.
* In naming simple ionic compounds, the metal is always first, the non-metal second (for example sodium chloride).
* Ionic compounds dissolve easily in water and other polar solvents.
* In solution, ionic compounds easily conduct electricity.
* Ionic compounds tend to form crystalline solids with high melting temperatures.

2- Covalent bonding

results from sharing one or more electron pairs between two atoms. Covalent bonding occurs because the atoms in the compound have a similar tendency for electrons (generally to gain electrons).

The elements involved will share electrons in an effort to fill their valence shells.

Covalent bonding in carbon

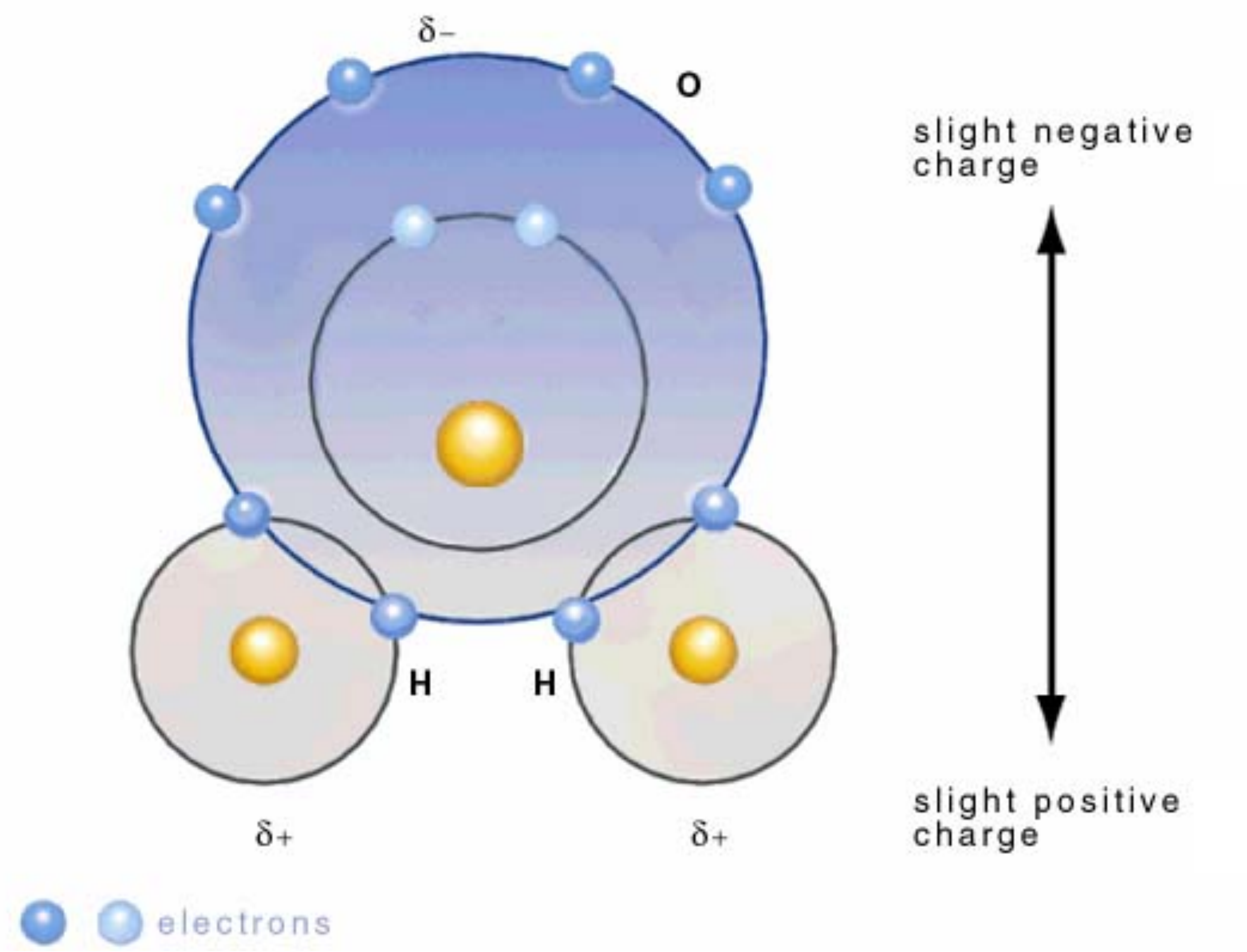


Polar Covalent Bonding

- A polar bond is formed when electrons are <u>unequally</u> shared between two atoms. Polar covalent bonding occurs because one atom has a <u>stronger affinity for electrons</u> than the other (yet not enough to pull the electrons away completely and form an ion).
- In a polar covalent bond, the bonding electrons will spend a greater amount of time around the atom that has the stronger affinity for electrons.

Polar bond in water molecule

The large oxygen atom has a stronger affinity for electrons than the small hydrogen atoms.



The Electronegativities of Selected Elements

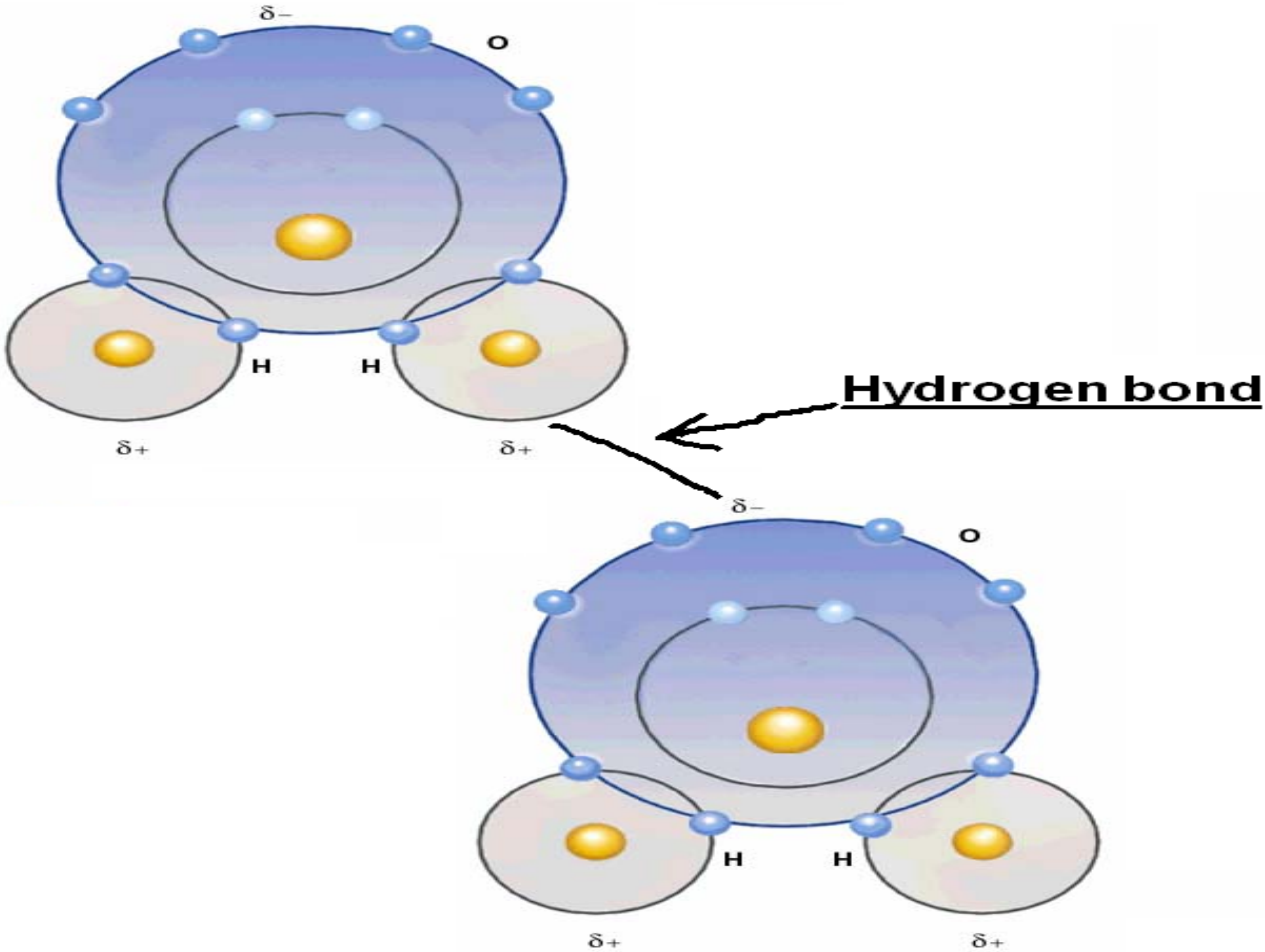
P 2.1	H 2.1	C 2.5	N 3.0	O 3.5	F 4.0
	K 0.8	Na 0.9	Ca 1.0	Mg 1.2	Cl 3.0

<u>Electronegativity</u> is the ability of an atom to attract electrons towards itself in a covalent bond

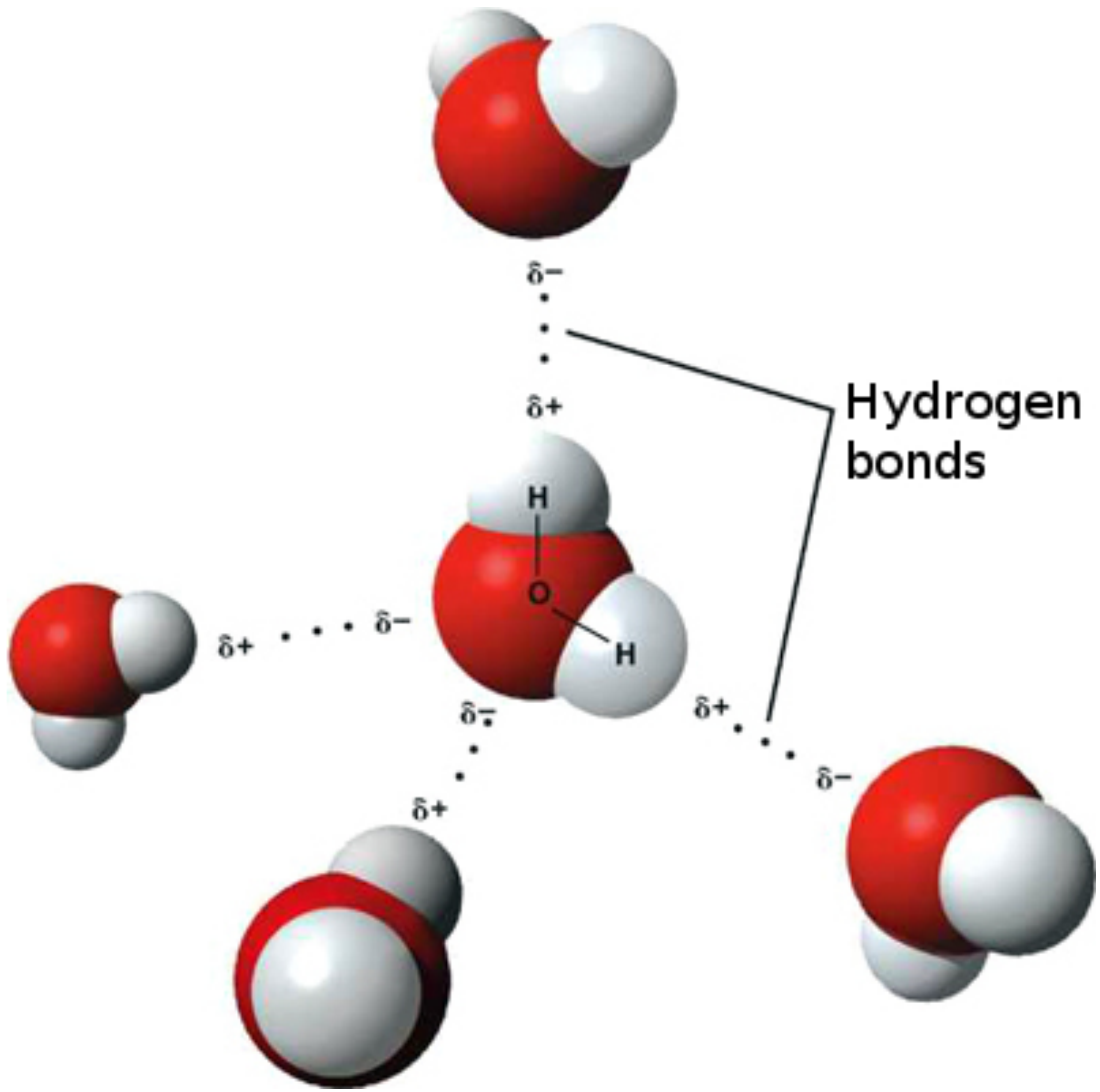
If the electronegativity difference between two atoms is less than about 0.5 it will be essentially non-polar and if the difference is more than 0.5 and less than 2 it is polar and if the difference is greater than 2.0 it is often considered to be ionic.

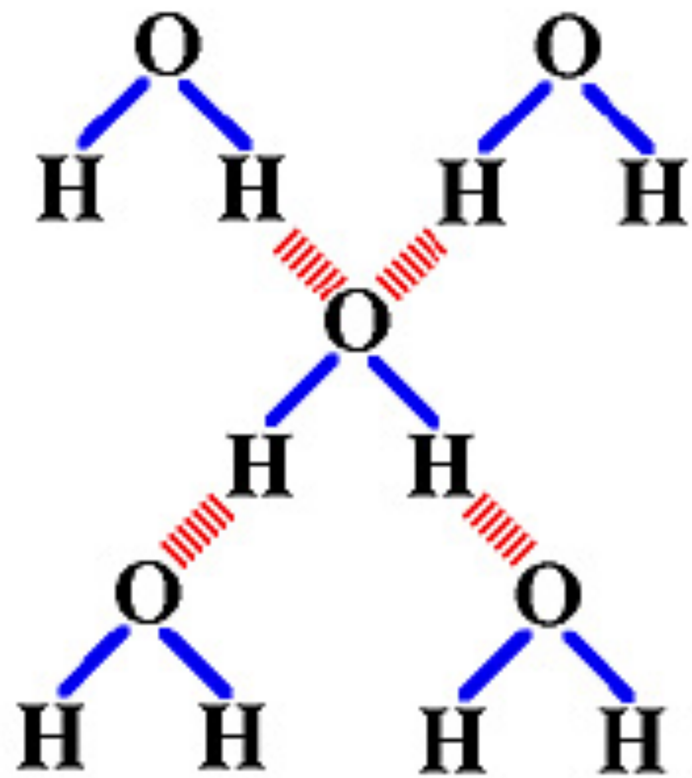
Hydrogen bond

Hydrogen bond is the attractive interaction of a hydrogen atom with an electronegative atom, like nitrogen, oxygen or fluorine. The partial positive region of hydrogen is attracted to the partial negative region of another molecule. The hydrogen must be covalently bonded to another electronegative atom to create the bond. The hydrogen bond is stronger than a van der Waals interaction, but weaker than covalent and ionic bonds.


δ−
O
H
H
δ+
δ+
Hydrogen bond
δ−
O
H
H
δ+
δ+

Hydrogen bond





- **4- Hydrophobic Interactions**

- Nonpolar groups do not form hydrogen bond to water so the are insoluble in water.

- Hydrophobic substances are “excluded” from aqueous solution this drive these molecules to cluster together.

- No affinity between nonpolar substances except van der Waals forces that promote the weak bonding of nonpolar substances.

- **<u>Van der Waals forces</u>**
- Van der Waals forces are weak attractive forces between electrically neutral atoms or molecules. They are much weaker than the ionic bond or the covalent bond. These forces may develop because the <u>rapid shifting of electrons within molecules</u> causes some parts of the molecule to become **<u>momentarily charged</u>**, either positively or negatively. For this reason, weak, transient forces of attraction can develop between particles that are actually neutral. The magnitude of the forces is dependent on the distance between neighbouring molecules.