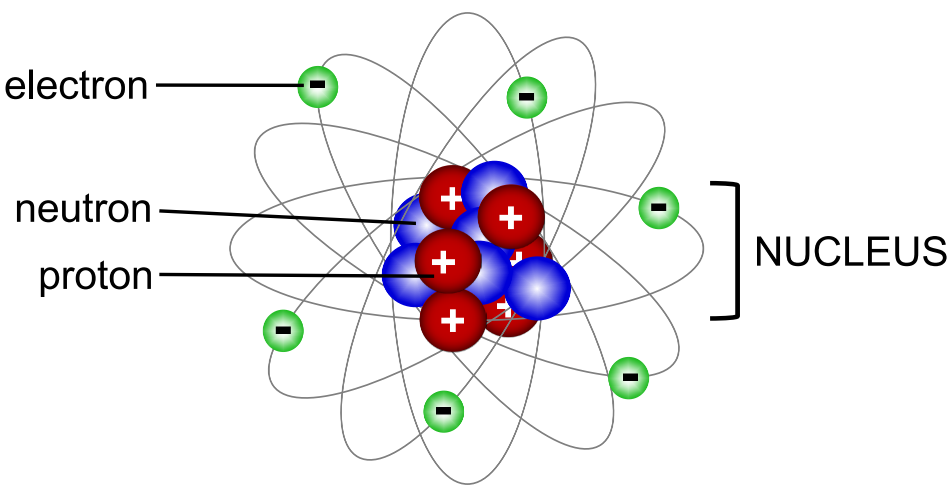
LAB 3 – Molecules, Water & pH

Objectives

1. Determine the molecular structure of small molecules.
2. Determine the densities of various liquids.
3. Assess the solubility of various substances in water.
4. Measure the pH of various liquid products.
5. Assess the buffering capacity of a liquid product.

Part 1: BUILDING MOLECULES

You most likely have already covered the nature of atoms and molecules to some degree in the lecture portion of this course. Nevertheless, let's remind ourselves of some key points with regard to atoms and how they form connections with each other to create molecules. All atoms are constructed of *positively charged* **protons**, *uncharged* **neutrons** and *negatively charged* **electrons**, and the nucleus of an atom is comprised of the protons and neutrons:



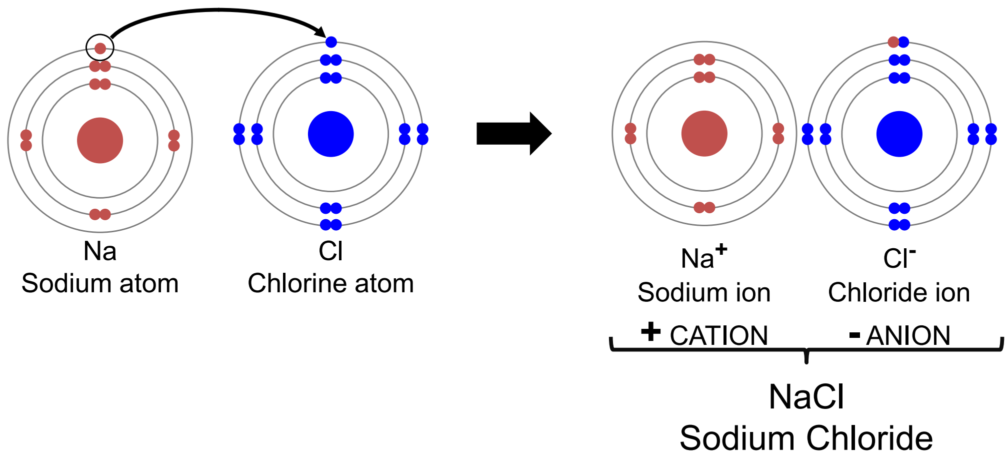
Electrons move around the nucleus at incredible speeds in regions referred to as **orbitals**, and electrons tend to occupy orbitals in pairs. Most atoms in their neutral state (same number of protons and electrons) have at least one ***unpaired* electron**, and atoms do whatever they can to avoid having *any* unpaired electrons. The 3 ways in which atoms avoid having unpaired electrons are to:

1) ***donate*** (give up) unpaired electrons to other atoms

2) ***accept*** unpaired electrons from other atoms

3) ***share*** unpaired electrons with other atoms

Atoms that **donate** (give up) or **accept** (gain) electrons end up with a number of electrons (*negative* charges) that does not equal the number of protons (*positive* charges). As a consequence the atom will have a net charge and is therefore referred to as an **ion**. Atoms that *gain* extra electrons become negatively charged ions (**anions**), whereas atoms that *give up* electrons become positively charged ions (**cations**).



Most elements, however, avoid having unpaired electrons by *sharing* them with other atoms that also have unpaired electrons. The sharing of unpaired electrons provides a partner for each and avoids the instability associated with unpaired electrons. The sharing of such a pair of electrons between 2 atoms constitutes a type of chemical bond referred to as a **covalent bond**. As a general rule, atoms form one covalent bond for every unpaired electron. Below is a summary of the number of unpaired electrons and covalent bonds formed in several elements of biological importance:

element	unpaired electrons	covalent bonds
hydrogen (H)	**1**	**1**
oxygen (O)	**2**	**2**
nitrogen (N)	**3**	**3**
carbon (C)	**4**	**4**

Covalent bonds are the connections that hold atoms together in **molecules**, and we can describe a molecule as simply ***2 or more atoms connected by covalent bonds***. Two atoms can be connected by 1 covalent bond (**single bond**), 2 covalent bonds (**double bond**) or even 3 covalent bonds (**triple bond**), depending on the elements and the number of unpaired electrons each contains. The electrons shared in covalent bonds are not always shared equally. If the sharing of electrons is *unequal*, the bond is said to be **polar** since the distribution of negatively charged electrons across the bond is uneven. If the sharing of electrons across the bond is *equal*, the bond is said to be **non-polar**. The polarity of covalent bonds in molecules is very important as we shall see when we look at the properties of water.

Now let's concern ourselves with how covalent bonds connect atoms together by looking at several small molecules…

Referring to the number of *unpaired* electrons for each element listed on the previous page (hence the number of covalent bonds each tends to form), you're going to build some small molecules containing these elements using your molecular model kit. A couple things you need to understand before doing so are the concepts of a **molecular formula** and a **structural formula**. *Molecular* formulas contain the chemical symbols for each element in the molecule, with subscripts to indicate the number of atoms of that element. A chemical symbol with no subscript indicates only 1 atom of that element. For example, the molecular formula for a molecule of water is:

$$H_2O$$

A water molecule therefore contains 2 hydrogen atoms and one oxygen atom. The 3 atoms in a water molecule are interconnected in some way by covalent bonds, however the *molecular* formula doesn't indicate how these bonds are arranged. *Structural* formulas indicate the arrangement of covalent bonds in a molecule using lines to represent each covalent bond. Since hydrogen atoms have 1 unpaired electron (and thus can participate in only 1 covalent bond), and oxygen atoms have 2 unpaired electrons (and thus can participate in 2 covalent bonds), we should come up with a structural formula for water such that each unpaired electron is involved in a covalent bond. In other words, *each **hydrogen** atom should be involved in **one** covalent bond, and each **oxygen** atom should be involved in **two** covalent bonds*:

$$H{-}O{-}H$$

The structural formula above satisfies this requirement and is, in fact, the correct structural formula for water. Each hydrogen atom is involved in 1 covalent bond, and the oxygen atom is involved in 2 covalent bonds. There are no longer any unpaired electrons in these atoms (each originally unpaired electron now has a partner), thus the molecule and the atoms it contains are relatively stable.

Let's look at the molecular and structural formulas of two more molecules, remembering that atoms can be joined by as many as 3 covalent bonds:

CO_2 (carbon dioxide)	**$O{=}C{=}O$**
N_2 (nitrogen gas)	**$N{\equiv}N$**

A *correct* structural formula for carbon dioxide requires that each oxygen atom be involved in 2 covalent bonds, and the carbon atom be involved in 4 covalent bonds. The only way to satisfy this requirement is with the structural formula shown above. To produce a correct structural formula for N_2, each nitrogen atom should be involved in 3 covalent bonds. Thus the structural formula shown above is the only option.

<u>Exercise 1</u> – Building small molecules

1. For practice, copy the structural formulas for water, nitrogen gas and carbon dioxide on your worksheet and construct these three molecules using your molecular model kit. Below is a key to the components of your kit:

   - **WHITE = *hydrogen atom***
   - **BLACK = *carbon atom***
   - **BLUE = *nitrogen atom***
   - **RED = *oxygen atom***
   - *short connectors* (use for single covalent bonds)
   - *long connectors* (use to create double & triple covalent bonds)

   Notice that each "atom" has a number of holes equal to the number of unpaired electrons in the atom. **If you've built your model correctly, all holes in each atom are plugged into connectors – i.e., each unpaired electron is involved in a covalent bond.**

   Once you've built each molecule, notice that the atoms and covalent bonds in the molecule have a specific 3-dimensional arrangement. This arrangement is difficult to convey on paper, however by building such models it's much easier to appreciate their *actual* structure.

2. To complete this exercise, determine the correct structural formulas for each molecule below on your worksheet, then build each molecule with your model kit and show them to your instructor:

H_2 **(hydrogen gas)**	NH_3 **(ammonia)**
O_2 **(oxygen gas)**	CH_4 **(methane)**
HCN (hydrogen cyanide)	C_2H_5OH **(ethanol)**

<u>Part 2: PROPERTIES OF WATER</u>

By weight, living organisms contain more water than any other substance. Other substances contained in living organisms include a wide variety of organic molecules, salts and minerals, but water is the medium in which all these substances exist and interact. Thus, essentially all processes of life occur in a watery environment, even for organisms such as human beings that live on land.

In light of the obvious importance of liquid water to all living things, let's look at some of the properties of this perfect "living medium"…

Density **of water**

The density of water, its weight per unit volume, is extremely relevant to life on our planet. We all know from experience that solid water (ice) floats in liquid water. This is because the arrangement of water molecules in ice crystals is less compact than the arrangement of water molecules in liquid water. In other words, ice floats because it is less dense than liquid water. If ice were denser than water, ice would sink and the depths of the oceans would be entirely frozen making earth a very different place.

You can also appreciate that all the sediment that washes into our oceans and waterways is denser than water, that's why it sinks and forms layers along the bottom. Imagine if this material was less dense than water and thus floated. The bodies of water on earth would have a permanent covering of floating particles, blocking all sunlight and affecting the formation of life as we know it. Density does indeed matter.

By convention, the density of a substance is the weight in grams of 1 ml of that substance. Conveniently enough, the density of pure liquid water is exactly 1 gram/ml! This is no coincidence since, by definition, a gram is the weight of 1 ml (or cubic centimeter, **cc**) of pure liquid water at standard conditions.

density = grams/ml

Density is dependent not only on the mass of the elements that make up the substance, but also how tightly the atoms or molecules are packed (think of ice vs liquid water). For example, a substance such as hydrogen gas (H_2) which is composed of loosely packed molecules containing a very light element has a very low density, whereas a substance composed of very heavy, tightly packed elements such as lead or gold has a very high density.

Exercise 2A – Determination of density

*To determine the density of a substance, all you need to know is the **volume in ml** of the sample, and its **weight in grams**. Once you have that information, simply **divide the weight (g) by the volume (ml)** to obtain a value for the **density (g/ml)**.*

In this exercise you will determine the densities of acetone, pure water and 20% salt water (20 g of NaCl dissolved per 100 ml of water) as follows:

1. Label and weigh *each* of the three 20 ml beakers you will use for each sample.*

2. Using a pipette, measure 10 ml of each sample into the corresponding beaker.*

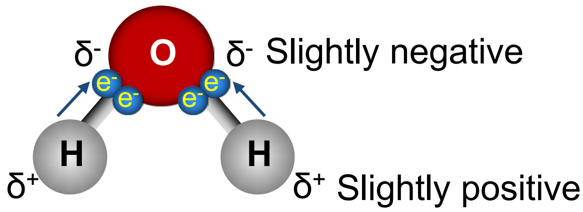
3. Weigh each beaker now containing the added sample.*

4. Calculate the weight of each sample and divide by its volume to get the density.

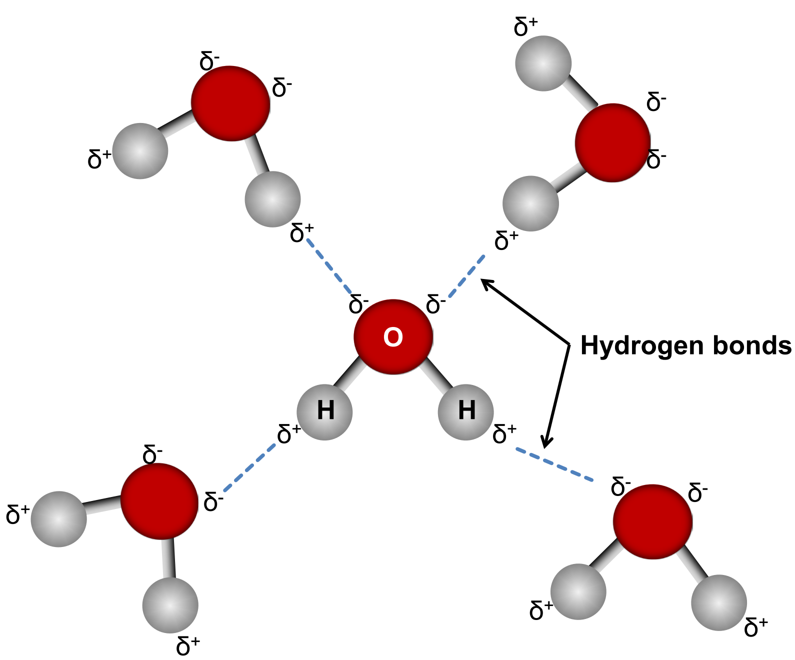
**** The more accurate your measurements, the more accurate your results will be!***

***Cohesion* of water**

Water is a **polar molecule** since the covalent bonds that hold the molecule together are polar. Specifically, the oxygen atom attracts the shared electron pair in each bond more strongly than the hydrogen atoms. As a result, the oxygen end of the molecule is slightly negative in charge, and the hydrogen ends of the molecule have a slight positive charge.



Because water is a polar molecule, the partial negative (δ^-) and partial positive (δ^+) charges on each side of the molecule are attracted to the opposing partial charges in other water molecules. These attractions between opposing partial charges are called **hydrogen bonds** (since they are due to polar covalent bonds involving hydrogen atoms).



Hydrogen bonding between water molecules is responsible for the **cohesion** of water, i.e., the “stickiness” between water molecules. The cohesion of water molecules via hydrogen bonding is responsible for many of the important properties of water, including its unusually high freezing temperature (becoming solid, i.e., ice), boiling temperature, and heat of vaporization (heat energy required to evaporate).

Ethanol (C_2H_6O), the substance we commonly refer to as “alcohol”, is a larger molecule than water with more than double the molecular weight, however its freezing temperature, boiling temperature, and heat of vaporization are all much lower than water. This is also true for **acetone**, the main ingredient in nail polish remover. This is largely because ethanol and acetone are less polar than water and thus exhibit less cohesion through hydrogen bonding. As a result, it takes much less energy for molecules of ethanol or acetone to evaporate than molecules of water, so they will evaporate much more readily. As a consequence, evaporating molecules of ethanol or acetone remove much less heat than do evaporating molecules of water. For this reason water is a much more effective coolant for the body than would be ethanol or acetone.

Exercise 2B – Evaporation rates of water vs acetone

Examine the relative heats of vaporization of water and acetone as follows:

1. Hypothesize which liquid will evaporate faster – acetone or water.
2. Simultaneously stick one cotton swab into a beaker of water and second swab in a container of acetone. (*press each swab against the inside of container while rolling to remove excess liquid*)
3. *Gently* draw thin lines of liquid (a few cm long) with each swab on your bench top and record on your worksheet how long it takes for each to evaporate.

Water as a *Solvent*

The polar nature of water molecules makes water a good **solvent** (liquid in which something is dissolved) for other substances that are polar (e.g. "table sugar" or sucrose) or charged/ionic (e.g. the ions in "table salt": Na^+Cl^-). This is because the partial + and – charges in polar water molecules can interact with and neutralize the opposing charges in polar and ionic **solutes** (substances dissolved in a liquid).

No such interactions are possible with substances that are **non-polar** (have non-polar covalent bonds and don't produce ions; e.g. "oils"), so non-polar solutes do not readily dissolve in water, they prefer to keep to themselves.

Exercise 2C – Solubility of various solutes in water

*To observe how water behaves as a solvent, you will attempt to dissolve a variety of substances in liquid water. Begin by hypothesizing which substances are soluble in water, then measure 30 ml of deionized water into each of four 125 ml flasks and attempt to dissolve each substance by **thoroughly** stirring or swirling. Record on your worksheet whether or not each substance dissolves, and if it is **polar, non-polar** or **ionic**:*

Flask #1 – one small packet of NaCl, also known as "table salt" (***ionic***)

Flask #2 – one small packet of sucrose, also known as "table sugar" (***polar***)

Flask #3 – 1 squeeze from a transfer pipet of vegetable oil (***non-polar***)

Flask #4 – 1 squeeze from a transfer pipet of ethanol (***polar***)

<u>Part 3: pH & BUFFERS</u>

The vast majority of liquid water consists of H_2O molecules, however a very small proportion of water molecules at any given moment are split into **H^+** and **OH^-** ions (see below):

$$\mathbf{H_2O \longleftrightarrow H^+ + OH^-}$$

The property of **pH** and the terms ***acidic*** and ***basic*** (*alkaline*) refer to the relative amounts of these two ions. In absolutely pure liquid water, there will always be equal amounts of H^+ & OH^- ions since every split water molecule yields one H^+ ion and one OH^- ion. Pure water, however, exists only in a vacuum since even gases such as N_2, O_2 and CO_2 in the air dissolve in water to some degree. So in reality, water always has other substances dissolved in it.

Many substances when dissolved in water will alter the balance of H^+ and OH^- ions by releasing additional H^+ or OH^- ions into solution, and/or by combining with H^+ and OH^- ions already present. Substances that cause an ***increase* in H^+** and a ***decrease* in OH^-** ions when added to water are referred to as **acids**. For example, hydrochloric acid (**HCl**) will split into H^+ and Cl^- ions when added to water, thus increasing the overall **concentration** (amount per unit volume) of H^+ ions, some of which then combine with OH^- ions to decrease the OH^- concentration. HCl is thus an acid:

$$\mathbf{HCl\ (an\ acid) \longrightarrow H^+ + Cl^-}$$

Substances that cause a ***decrease* in H^+** and an ***increase* in OH^-** ions when added to water are referred to as **bases**. For example, sodium hydroxide (**NaOH**) will split into Na^+ and OH^- ions when added to water, thus increasing the overall **concentration** of OH^- ions, some of which then combine with H^+ ions to decrease the H^+ concentration. NaOH is thus a base:

$$\mathbf{NaOH\ (a\ base) \longrightarrow Na^+ + OH^-}$$

An aqueous solution (water containing some sort of solute) that contains a higher concentration of H^+ than OH^- ions is referred to as **acidic**. An aqueous solution that contains a higher concentration of OH^- than H^+ ions is referred to as **basic**. An aqueous solution that contains equal concentrations of H^+ and OH^- ions is referred to as **neutral**:

solutions with $[H^+] > [OH^-]$ are *<u>acidic</u>*

solutions with $[H^+] < [OH^-]$ are *<u>basic</u>*

solutions with $[H^+] = [OH^-]$ are *<u>neutral</u>*

NOTE: $[H^+]$ refers to "concentration of H^+"; $[OH^-]$ refers to "concentration of OH^-"

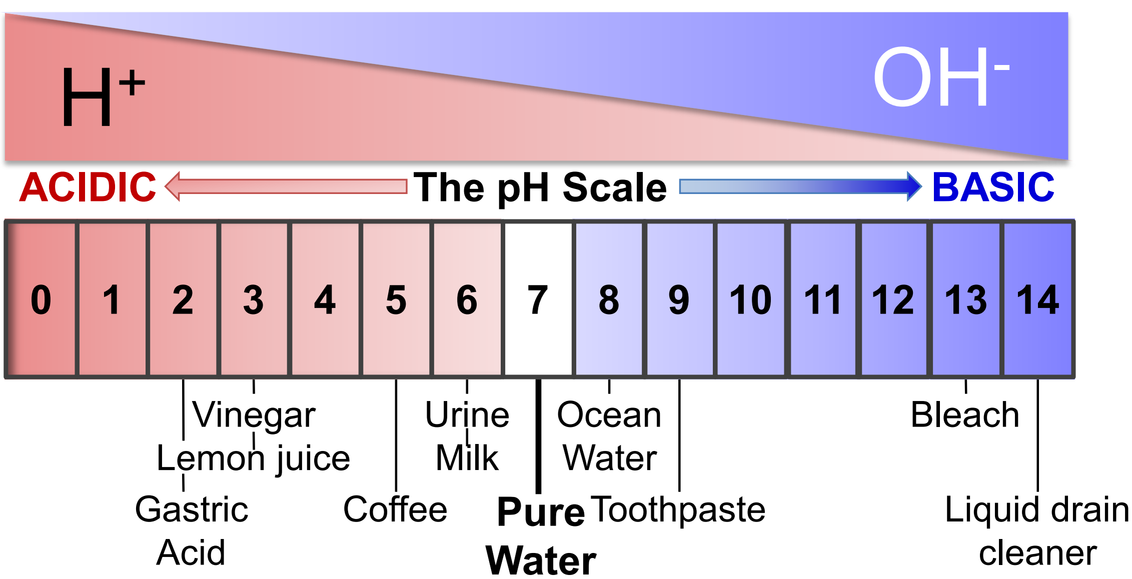
<u>The pH *Scale*</u>

Just as the terms "pair" and "dozen" refer to 2 and 12 of something, respectively, the term **mole** in chemistry refers to **6.02 x 10^{23}** (602,000,000,000,000,000,000,000!) of something. This is relevant since the *unit of concentration* used for H^+ and OH^- ions in a solution is **moles per liter** (also referred to as **molarity** and symbolized by **M**). For example, a solution containing 1 mole of H^+ ions per liter (1 M H^+) contains 6.02 x 10^{23} H^+ ions per liter. In an aqueous solution, the concentrations of H^+ and OH^- have an inverse relationship (as one increases, the other decreases) which when represented in moles/liter (M) is explained by the following equation:

$$[H^+] \times [OH^-] = 1 \times 10^{-14}$$

A neutral solution, in which the concentrations of H^+ and OH^- are equal, thus contains a concentration of 1 x 10^{-7} moles/liter (M) for each ion. The H^+ concentration in tomato juice (which is acidic) is 1 x 10^{-4} M, therefore the concentration of OH^- in tomato juice must be 1 x 10^{-10} M. The H^+ concentration in seawater is 1 x 10^{-8} M, therefore the concentration of OH^- must be 1 x 10^{-6} M. As you can see, the greater the H^+ concentration, the lower the OH^- concentration and vice versa.

The pH scale was devised to represent the H^+ concentration in a substance. The scale ranges from values of 0 to 14 and each number on the scale represents the **negative log of the H^+ concentration** in moles/liter (M). For example, the pH of gastric acid (stomach acid) is 2. This is because the H^+ concentration in gastric acid is 1 x 10^{-2} M, and the negative log of 1 x 10^{-2} is 2. Another way to think of this is to remember that **<u>the pH value of a solution means that the H^+ concentration is 1 x 10^{-pH} M</u>**, or in the case of gastric acid, 1 x 10^{-2} M. Examine the pH scale below and try to determine the H^+ and OH^- concentrations of some of the solutions indicated:



pH *Indicators*

The pH of an actual solution can be measured in several ways. These days, most labs use digital pH meters that give a numerical readout of pH values. Traditionally, pH has been determined using **pH indicators**, chemicals that change color depending on the pH (i.e., H^+ concentration). Although less accurate, this method is much less expensive and is sufficient for our purposes, so we will be measuring pH in this manner.

Exercise 3A – Determining unknown pH values

A simple way to determine an unknown pH value is with pH paper. pH paper is simply a strip of absorbent paper coated with a mixture of pH indicators. The color of the pH paper after wetting with liquid is compared to a chart indicating the colors associated with each pH value. In this way you can estimate the pH of a solution based on the color of the pH paper:

1. Tear off 6 pieces of pH paper (~2 to 3 cm or 1 inch each), one for each test liquid (soda, grape juice, bicarbonate, etc, located at the front of the lab).
2. For each test liquid, place 1 drop of the liquid onto a piece of pH paper.
3. Use the color chart that came with your pH paper to estimate the pH value and record on your worksheet.

pH *Buffers*

It is extremely important that the pH of fluids in living organisms (e.g., blood, lymph, cell cytoplasm) remain within a very narrow range. This is one aspect of maintaining **homeostasis** (a constant internal environment) within an organism. For example, the pH of human blood needs to be maintained at ~7.4. If blood pH drops below 7.0 or rises above 7.8, *death* may occur.

So how is a constant pH level maintained in biological fluids? The answer is pH **buffers**, substances in solution that resist changes in pH. Biological fluids such as blood contain a variety of pH buffers such as bicarbonate and the proteins albumin and hemoglobin. When blood pH decreases (i.e., the H^+ concentration *increases*), the buffers in blood combine with H^+ ions. When blood pH increases (i.e., the H^+ concentration *decreases*), the buffers in blood release H^+ ions. In this way the buffers in blood and other body fluids resist pH change and thus stabilize the pH. Because body fluids contain pH buffers, they are said to have **buffering capacity**.

Many other liquid solutions such as beverages and liquid medicines contain pH buffers. To test for buffering capacity, you simply add increasing amounts of acid or base to a solution, checking the pH after each addition, and look for any resistance to pH change as you will do below.

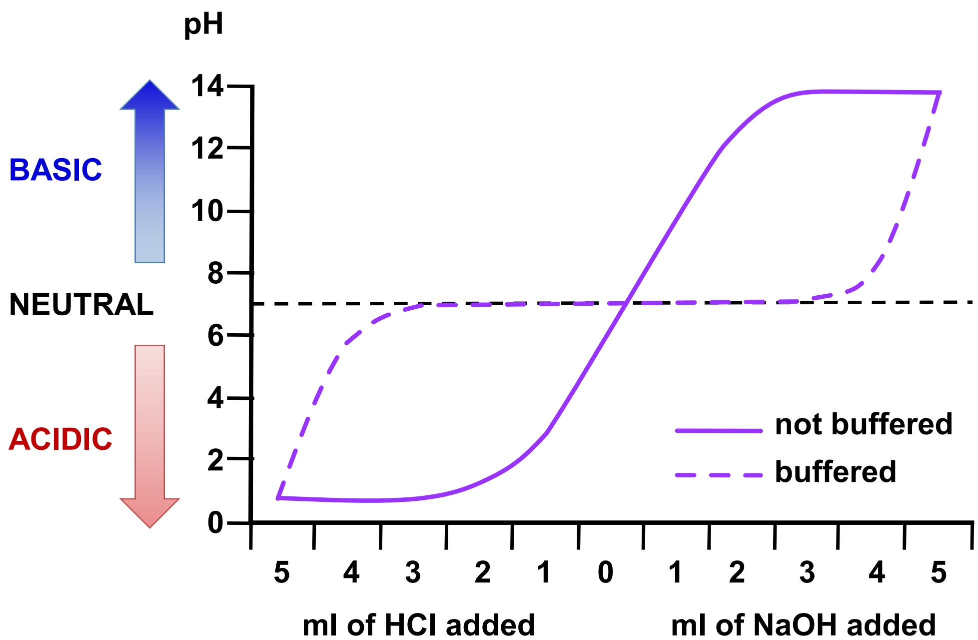
Exercise 3B – Assessment of buffering capacity

In this exercise, you will perform an experiment to determine if a test solution assigned by your instructor (e.g., milk, antacid, soda) contains pH buffers, i.e., if it has ***buffering capacity****. To do this you will add successive amounts of acid or base to your test solution, determine the pH at each step, graph the results, and look for evidence in the graph of buffering capacity.*

To do this experiment properly, you need to simultaneously test a solution that contains no pH buffers: plain water. This is a control experiment that is necessary for you to see how the pH changes in a solution with no buffering capacity. If your test solution shows a similar pattern of pH change, then you can conclude that it also lacks buffering capacity. However, if your test solution resists pH change relative to plain water, then you can conclude that it contains pH buffers and thus has buffering capacity:

1. Hypothesize whether or not your assigned test solution has buffering capacity.
2. Get 2 small beakers and label one for water, one for the test solution (see instructor).
3. Measure 20 ml of water or test solution into the corresponding beakers.
4. Determine the pH of each using pH paper and record the values on your worksheet.
5. Add 1 dropper full (1 ml) of 0.1 M HCl (an acid) to each solution, ***mix well***, determine the pH using pH paper, and record the value on your worksheet.
6. Repeat the previous step four more times (so a total of 5 ml of HCl is added).
7. Dispose of your solutions in the sink, rinse the beakers with water and dry.
8. Get fresh 20 ml samples of water and your test solution, and repeat steps 4 to 6 using 0.1 M NaOH (a base) *instead* of the HCl.

Once you have all your pH values, plot them on a graph set up as illustrated below, and ***determine whether or not your test solution has buffering capacity****.*



To interpret each curve on this graph, notice the pH value before any acid or base is added (i.e., the middle of each curve corresponding to "0 ml"), and then follow the curve in either direction as more acid or base is added and look for any changes in pH. You can see that the "not buffered" curve shows changes in pH with each ml of acid or base added until the pH of the acid or base itself is reached. In contrast, the "buffered" curve maintains a steady pH value until 3 or 4 ml of acid or base is added. The curve for this "buffered" solution clearly resists pH change until the amount of added acid or base exceeds its **buffering capacity** after which the pH clearly changes. The flattened appearance of this curve reveals a resistance to pH change in this solution and thus it has **buffering capacity**.

Before you leave, please make sure your table is clean, organized, and contains all supplies listed below so that the next lab will be ready to begin. Thank you!

Supply List

- Molecular model kit (please break down all molecular models before returning to bag)
- Marker pen or China marker
- Small containers of acetone, water, 20% salt, ethanol, vegetable Oil
- 3 - 20 ml beakers for acetone, water, 20% Salt
- 3 - 10 ml pipettes marked acetone, water, 20% Salt
- Scales
- 2 cotton swabs – blue for water and red for Acetone
- 4 – 125 ml flasks marked #1, #2, #3, #4
- 1 pkg NaCl, 1 pkg sucrose
- Transfer pipets for veg oil and ethanol (1 each)
- 50 ml graduated cylinder
- pH paper
- 2 small beakers labeled water and test solution
- 2 Stirring rods
- Two 25 ml Graduated cylinders

Also PLEASE be sure to do the following before you leave:

- *Used acetone should be poured into labeled container in the hood.*
- *Wash all glassware with soap and water using brush and then rinse with tap water.*

LABORATORY 3 WORKSHEET

Name ________________________

Section________________________

Exercise 1 – Building small molecules

Draw the structural formulas for the following molecules:

H_2O **CO_2** **N_2**

H_2 **O_2** **NH_3**

CH_4 **HCN** **C_2H_5OH**

Exercise 2A – Determination of density

sample	volume (ml)	empty beaker (g)	sample + beaker	sample (g)	density (g/ml)
pure water	**10**				
acetone	**10**				
20% salt water	**10**				

Exercise 2B – Evaporation of water vs acetone

- Hypothesis:

sample	time to evaporate
water	
acetone	

- Which substance has the higher heat of vaporization (i.e., took longer to evaporate)?
- Which is more polar, acetone or water?
- Which should have a higher heat of vaporization, a molecule that is less polar or more polar?

➢ Is this consistent with your result?

Exercise 2C – Water as a solvent

Fill in the chart below indicating which types of molecules should be soluble in water:

type of molecule	soluble in H_2O?
ion	
polar molecule	
nonpolar molecule	

➢ Hypothesis:

Indicate in the table below whether each substance is ionic, polar or non-polar, as well as whether or not each substance is soluble in water:

substance	polarity?	soluble?	substance	polarity?	soluble?
table salt			**vegetable oil**		
table sugar			**ethanol**		

➢ Were the insoluble substances ionic, polar or non-polar?

➢ Did the insoluble substances float on top or sink to the bottom?

➢ What does this tell you about the density of the insoluble substances (i.e., denser or less dense than water)?

Exercise 3A – Determining unknown pH values

Determine the pH values of all six test liquids and indicate H^+ and OH^- concentrations in mol/L (M):

test liquid	pH	$[H^+]$	$[OH^-]$	test liquid	pH	$[H^+]$	$[OH^-]$

<u>Exercise 3B</u> – Assessment of buffering capacity **test liquid (*see instructor*) ________**

- Define buffering capacity.

- State your hypothesis regarding whether or not your test liquid has buffering capacity:

Record the pH values for your buffering capacity experiment below:

WATER (control) ***test liquid ________________***

HCl added	pH	NaOH added	pH	HCl added	pH	NaOH added	pH
none		-----------	-------	***none***		-----------	-------
1 ml		1 ml		1 ml		1 ml	
2 ml		2 ml		2 ml		2 ml	
3 ml		3 ml		3 ml		3 ml	
4 ml		4 ml		4 ml		4 ml	
5 ml		5 ml		5 ml		5 ml	

On the next page graph your data (see example on page 47).

- Describe the characteristics of a graph in general that reveals buffering capacity.

- Based on *your* graph, is your hypothesis supported? Explain.