

Chemistry 141
Samuel A. Abrash
Fall 2016

Lecture 1

Chemistry is the study of matter. In studying matter, we are particularly concerned with its composition, its properties, and the way that these can change. In order to study these characteristics of matter, we need to have ways to reproducibly describe matter. As such we look at a number of **measurable properties** of matter. **The collection of these properties, when they are unchanging over time, is called the state of the system.** In order to understand these properties better, we classify them in different ways.

The first important classification of properties that we make is the distinction between chemical and physical properties of matter. **Chemical properties** are those that involve a change in the substance's makeup. Some examples of chemical properties are toxicity (since poisoning is a chemical reaction), flammability, and the tendency of a substance to react with oxygen. **Physical properties** are those that can be changed without changing the chemical identity, i.e. the composition, of the substance. Examples of these are temperature, density, melting point, color, mass.

A lot of times we will measure one of these properties, and then record it. It is important in recording these numbers to recognize that some of these properties depend on how large the system is, and some do not. The reason that this is important is that if a property is dependent on the size of the system, we must record not just the property, but the system size, or our measurement is incomplete. An example of a property that depends on the size of the system is volume. For example, two gallons of milk take up twice as much space as one gallon of milk. Another example is mass – two gallons of

milk are twice as massive as one. Properties that depend on the size of the system are called **extensive properties**.

There are also properties that do not change with the size of the system. Examples of these are temperature, pressure and density. Each of these is unchanged when the size of the system changes. Properties that are independent of the size of the system are called **intensive properties**.

To distinguish between intensive and extensive properties I like to do the following thought experiment. Pretend we have a container that is filled with gas. The gas has a temperature, T ; a pressure p ; a volume, V ; and a mass, m . Now we take an infinitely thin sheet of glass and divide the container in two. What is the volume on each side? The mass? Since dividing the size of the container in two divided each of these parameters in two, volume and mass are extensive. Now, what is the temperature on each side? The pressure? Since changing the size had no effect on the temperature or pressure, these variables are intensive.

When we make measurements to describe the state of a system, the numbers that we measure are always associated with a unit to tell us what it was we measured. For example, you wouldn't measure your height and say I'm five. If you did that people would say "funny, you don't look a day younger than 18." So every measurement we make in chemistry will have a unit associated with it. Of all of the possible units that exist, the SI system chooses eight quantities and their units as basic.

TABLE 1.2 SI Base Units

Base Quantity	Name of Unit	Symbol
Length	meter	m
Mass	kilogram	kg
Time	second	s
Electrical current	ampere	A
Temperature	kelvin	K
Amount of substance	mole	mol
Luminous intensity	candela	cd

These units are called base units because all other units in the SI system can be written as a function of these units.

Sometimes we will want to measure quantities so large or so small that the base units are inconvenient. As a result, a series of prefixes has been generated to indicate common multiples of the base units. The most common of these are:

TABLE 1.3 Prefixes Used with SI Units

Prefix	Symbol	Meaning	Example
tera-	T	1,000,000,000,000, or 10^{12}	1 terameter (Tm) = 1×10^{12} m
giga-	G	1,000,000,000, or 10^9	1 gigameter (Gm) = 1×10^9 m
mega-	M	1,000,000, or 10^6	1 megameter (Mm) = 1×10^6 m
kilo-	k	1,000, or 10^3	1 kilometer (km) = 1×10^3 m
deci-	d	1/10, or 10^{-1}	1 decimeter (dm) = 0.1 m
centi-	c	1/100, or 10^{-2}	1 centimeter (cm) = 0.01 m
milli-	m	1/1,000, or 10^{-3}	1 millimeter (mm) = 0.001 m
micro-	μ	1/1,000,000, or 10^{-6}	1 micrometer (μ m) = 1×10^{-6} m
nano-	n	1/1,000,000,000, or 10^{-9}	1 nanometer (nm) = 1×10^{-9} m
pico-	p	1/1,000,000,000,000, or 10^{-12}	1 picometer (pm) = 1×10^{-12} m

As you can imagine, the number of properties that we can measure for a substance is not limited to the seven base SI quantities. Can anyone suggest a property other than these seven? The units for each property other than the seven base properties are derived as a function of the seven base units, and are therefore called derived units. For example, volume has the unit m^3 , and the unit of energy, the Joule, has the units $\text{kg m}^2/\text{s}^2$. For another example, density, symbolized the Greek letter ρ , is defined by

$$\rho \equiv \frac{m}{V}.$$

To determine the SI units for density, we simply take the unit for mass, kg, and divide it by the unit for volume, m^3 and get $\frac{\text{kg}}{\text{m}^3}$.

Often in chemistry, the amounts of matter that we measure are significantly less than the basic SI units, so we frequently use smaller units. For example, rather than use kg as the unit of mass, we commonly use grams. Similarly, rather than use m^3 as a volume unit we use liters, or dm^3 , or milliliters (ml) or cm^3 , as our units for volume. Thus the unit for density you'll commonly see in chemistry texts will be g/cm^3 . It is important that you develop the skill of converting between units.

Here's an example of a typical problem that we might solve:

Question: A block of platinum has a volume $V = 4.49 \text{ cm}^3$. What is the mass of the substance if $\rho = 21.5 \text{ g}/\text{cm}^3$?

We can solve this using the definition of the density:

Solution:

$\rho = \text{mass/volume}$. So, $mass = \rho \times volume = 21.5 \frac{g}{cm^3} \times 4.49 cm^3 = 96.5 g$. Notice that the units help us to confirm that we used the correct approach, since when the units are multiplied and cancelled, we are left with grams, the unit for mass, our desired quantity.

Lecture 2

Last time we talked about various **classifications of matter**. A deep understanding of the transformations of matter requires that we know the nature of matter, what it's made of and how it can be rearranged to make new substances.

The earliest model for the nature of matter in the Western world was that matter was composed of four elements, earth, fire, air and water. While the idea is old enough that it's impossible to trace its origin, such distinguished philosophers as Plato and Aristotle firmly believed this idea.

An alternative proposal came forth about the same time from the philosopher Democritus that matter could be subdivided into small pieces he called atoms, which had the characteristic nature of the bulk matter. In the Greek era, the alternative was not supported, in part because of the greater prestige of Plato and Aristotle. What was missing was a tradition of experimentation to test such theoretical predictions, and to determine the correctness of the proposals.

In the early 19th century, John Dalton rediscovered the atomic theory of Democritus, and expounded it in more detail. The **principle statements of Dalton's theory** are:

- 1) Matter is composed of tiny particles called atoms.
- 2) All atoms of a given element are identical. Atoms of the same element have the same mass. (Note that this is not quite correct, but we will refine this notion later in our lecture). Different elements have different mass.
- 3) Compounds are made of atoms of different elements. The ratio of the number of any two elements in a compound is an integer or simple fraction.

- 4) Atoms are indestructible and unchangeable. In chemical reactions, atoms combine but are not destroyed. This latter statement is also known as the law of the conservation of mass, and sometimes is simply stated as mass is neither created nor destroyed in a chemical reaction.

Dalton revived atomism in an age of experimentation, and framed his theory with statements that were testable. As a result, experimentation was able to demonstrate in relatively short order that the atomistic model was correct. Continued experimentation with increasingly sophisticated experimental equipment has only strengthened our confidence in the model.

In the course of studying the way in which chemicals could be transformed, 19th century chemists began to notice that certain chemicals tended to react the same way. For example, lithium, sodium and potassium tarnish very rapidly when exposed to air, and all of them react violently when they come in contact with water. Shortly after the Civil War, a Russian chemist named Dmitri Mendeleev decided to organize the chemical elements in a table starting with the lightest elements, and putting elements with similar chemical behaviors in the same column.

The Periodic Table

Mendeleev, D. (Russian, 1868):

Organized elements into a table emphasizing chemical properties

Accurately predicted, a number of elements : including, Sc, Ga, and Ge.

GROUP →

PERIOD ↓

	1 1A																			18 8A	
1	1 H	2 2A																			2 He
2	3 Li	4 Be																			
3	11 Na	12 Mg	3 3B	4 4B	5 5B	6 6B	7 7B	8 8B	9 8B	10 8B	11 1B	12 2B	13 Al	14 Si	15 P	16 S	17 Cl	18 Ar			
4	19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr			
5	37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe			
6	55 Cs	56 Ba	57 La	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn			
7	87 Fr	88 Ra	89 Ac	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112	(113)	114	(115)	116	(117)	(118)			

Metals	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu
Metalloids	80 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr
Nonmetals														

Mendeleev's original periodic table was incomplete. There were elements whose properties required him to leave blank spaces. One of the successes of his table, aside from his recognition that both mass and chemical properties could be organizing principles, was that he predicted that elements would be discovered that filled the empty spaces in the table, and in addition was able to predict their chemical properties. In this way he predicted the discovery of the elements scandium, gallium and germanium. However, in Mendeleev's time, chemists were unable to explain the reason for the periodic repetition of chemical properties that Mendeleev recognized. It was not until the early years of the 20th century that a combination of theory and experiment led to an understanding of the structure of atoms that explained the reason for this periodic behavior.

We will talk in great detail about atomic structure later in the course, but it is necessary that we introduce the basics before we proceed further. Atoms are indeed small, with radii ranging between 30 and 300 pm. The atom consists of a small positively charged nucleus surrounded by electrons in a large space around the nucleus.

The nucleus, which contains almost all of the mass of the atom, consists of two types of heavy particles: protons, which are positively charged, and neutrons, which are uncharged. Protons and neutrons have almost identical masses, although the neutrons are a tiny bit heavier. The electrons, which have negative charges, and surround the nucleus, are about 2000 times lighter than protons and neutrons.

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TABLE 2.1 Mass and Charge of Subatomic Particles

Particle	Mass (g)	Charge	
		Coulomb	Charge Unit
Electron*	9.10939×10^{-28}	-1.6022×10^{-19}	-1
Proton	1.67262×10^{-24}	$+1.6022 \times 10^{-19}$	+1
Neutron	1.67493×10^{-24}	0	0

*More refined measurements have given us a more accurate value of an electron's mass than Millikan's.

An element is characterized by the number of protons it has. In other words, the chemical identity of an element depends only on the number of protons. Because the number of protons in an atom is so crucial to its identity, the number of protons is given a special name, the atomic number, and a special symbol, Z . Z is routinely used to identify elements. To reiterate, atoms with the same number of protons are defined as the same element regardless of the number of electrons or the number of neutrons it has. Since protons are positively charged and electrons are negatively

charged, a neutral atom will have the same number of electrons and protons. Ions are species that have a net charge.

Not all atoms of a given element have the same number of neutrons. Atoms which have the same number of protons but differ in the number of neutrons are called isotopes. For example, chlorine has two stable isotopes, one of which has 18 neutrons, and one of which has 20. Since isotopes have the same number of protons, they have identical chemical properties. The biggest difference between isotopes is their mass. Their chemical properties are identical. Because the biggest difference between isotopes is their mass, isotopes are identified by a mass number, A . A is simply the sum of the number of protons and the number of neutrons in an isotope, i.e.

$$A = \# \text{ protons} + \# \text{ neutrons}$$

So for the case of chlorine we mentioned earlier, the two isotopes have mass numbers of $17+18 = 35$, and $17 + 20 = 37$. We identify an isotope with its chemical symbol, its atomic number and its mass number, arranged as follows:

$$\begin{array}{c} \text{mass number} \\ \text{atomic number} \end{array} E \Rightarrow \begin{array}{c} A \\ Z \end{array} E$$

According to this scheme, the symbols for the two isotopes of chlorine are ${}_{17}^{35}\text{Cl}$ and ${}_{17}^{37}\text{Cl}$. Alternatively, you can identify an isotope with the name of the element and the mass number, such as chlorine-35, or carbon-14.

There is one exception to the rule for identifying isotopes and that is for isotopes of hydrogen. Unlike other isotopes, the three isotopes of hydrogen have different names. The first, with one proton and no neutrons, is simply called hydrogen, H. The second, with one proton and one neutron, is called deuterium, D. The third, with

one proton and two neutrons, is called tritium, T. (Note that while chemical symbols are capitalized, the names of elements and compounds are not.)

If all matter were in the form of atoms, chemistry would be very boring. Fortunately, atoms combine in different ways to make a very wide variety of substances. The chemical abstract service of the American Chemical Society has registered more than three million different molecules, each constructed out of a little over 100 building blocks in the form of elements. We need to discuss the way we name and represent these combinations.

A **molecule** is **any combination of two or more atoms held together to form a stable entity**. We call the forces that hold the atoms together chemical bonds. A molecule can be an element if it is composed of only one element, as in the case of chlorine, which has two chlorine atoms joined by a bond, or buckminsterfullerene, which has 60 carbon atoms joined in the shape of a soccer ball. A substance made up of two or more elements is called a **compound**, such as table salt, which is made up of sodium and chlorine.

We typically represent a molecule with a molecular formula. The molecular formula shows the number of each type of atom in the smallest unit of the substance (i.e. the molecule). The molecule $A_aB_bC_c$ consists of a atoms of element A, b atoms of element B, and c atoms of element C. Some other simple examples of formulas are H_2O for water, with two hydrogen atoms and one oxygen atom, and $C_6H_{12}O_6$ for glucose, with 6 carbon atoms, 12 hydrogen atoms and 6 oxygen atoms. Other examples of chemical formulas are those for hydrogen gas (H_2), carbon dioxide (CO_2), ammonia (NH_3), propane (C_3H_8) and chlorophyll a ($C_{55}H_{72}O_5N_4Mg$).

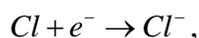
There are other common ways to represent a molecule, including structural formulas, ball and stick models, and space filling models. However, in this course we will use molecular formulas more than any other type.

Another important type of formula that we will use frequently is called an **empirical formula**. **The empirical formula is the smallest whole number ratio of atoms in a substance.** For example, the molecular formula of glucose is $C_6H_{12}O_6$. Since the numbers of each type of atom are multiples of 6, to obtain the empirical formula we divide by 6, yielding an empirical formula of CH_2O . Note that the empirical formula will either be the same as the molecular formula or simpler. Empirical formulas are important for two reasons. First, an experimental technique that we often use to determine the formulas of molecules is called elemental analysis, and this technique yields only empirical formulas. Second there are compounds, in particular ionic solids (also known as salts), for which the molecular formula is not well defined. This is because salt crystals come in many different sizes. They can be the size of a grain of sand, or as big as your father. For example, while all sodium chloride salt crystals will have an empirical formula of $NaCl$, individual crystals will have larger or smaller numbers of the individual ions. For this reason, empirical formulas are the only useful formulas with which to represent ionic compounds.

Lecture 3

Last time, in discussing the structure of atoms, we stated that all neutral atoms have the same number of protons and electrons. However, not all species are neutral.

A species, either atomic or molecular, that has a net charge is called an **ion**. If one or more electrons are removed from a neutral species, then the net charge is positive, and the species is called a **cation**. If one or more electrons are added to a neutral species the species now has a negative charge, and is called an **anion**. For example, if an electron is added to Cl,

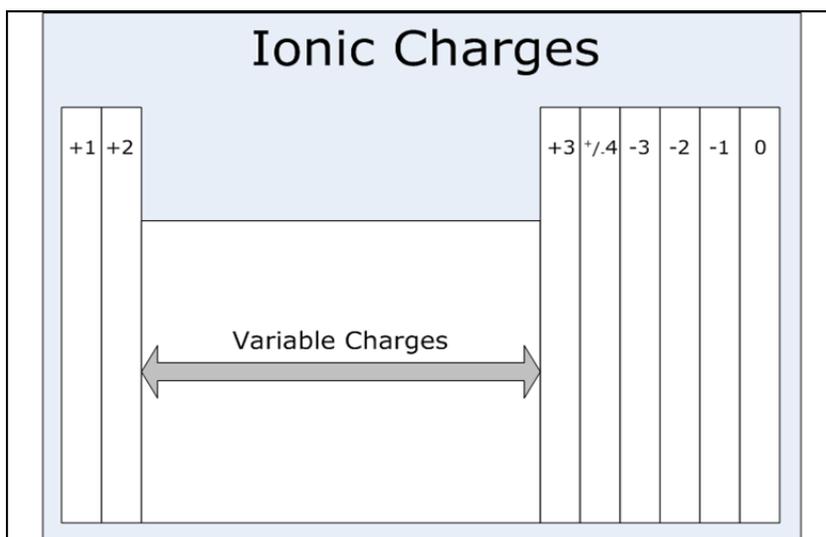


the result is an anion, called the chloride ion. As another example, if an electron is removed from a sodium atom,



the result is a cation, called the sodium ion.

The periodic table can give us a hint about which species are likely to form ions, and, if they do, what charge the ions will have. Notice that the columns of the periodic table are labeled both with numerals from 1-18 and numbers and letters from 1a-8a and 1b-8b. These labels are called the group numbers. The labels with a and b are most useful. The elements in columns ending in the letter “a” are called **main**



group elements. The group numbers are useful because they are related to the charges of the ions. For example, groups 1a and 2a tend to become cations, and tend to have charges of +1 (for group 1a) and +2 for group 2a. Elements in groups 6a and 7a tend to become anions, and will have charges of -2, and -1. The elements in columns ending with the letter “b” are called **transition metals**, and tend to be cations. Many transition metals can exist stably in more than one ionic form, i.e., two or more ions, each with a different charge, can form. For example, iron can exist stably with a charge of +2 or +3. The chart I’m giving you as a handout shows the most common trends for the main group elements. Examples are Li^+ , Mg^{+2} , Al^{+3} , $\text{C}^{\pm 4}$, N^{-3} , O^{-2} , F^{-1} , Ne. Note that there are some deviations from these trends, but that the deviations are more likely to occur the further down the periodic table an element is found. Also note that the elements in the center of the “a” group, in this case C and N, are usually not going to form ionic compounds.

Not all ions are atomic. Sometimes groups of atoms can form ions. These ions are called polyatomic ions. When compounds containing polyatomic ions dissolve in water, the polyatomic ions stay together. In other words, they are stable entities in solution. For example, when Na_2SO_4 , containing the SO_4^{-2} polyatomic ion, dissolves, it does not break into sulfur and oxygen atoms, rather it breaks into two Na^+ ions, and one SO_4^{-2} ion. Most polyatomic ions are anions, but there are some exceptions. Common examples include OH^- , CN^- , CO_3^{-2} , SO_4^{-2} , SO_3^{-2} , NO_3^{-1} , NO_2^{-1} and NH_4^+ . Unfortunately, the best way to learn the names and formulas of polyatomic ions is simply to memorize them. Please memorize the names and formulas of the ions in table 2.5 of your textbook, on page 63.

Most chemicals are in the form of compounds. Ionic compounds are formed by the combination of positive and negative ions. Ionic compounds tend to form strongly bound crystalline solids. These are often formed when elements from groups 1a, 2a or 3a combine with elements from groups 6a or 7a. For example, sodium metal (Na) from group 1a, combines with chlorine (Cl) from group 7a, to form table salt (NaCl). Other examples of ionic compounds are lithium fluoride, LiF; potassium permanganate, KMnO_4 ; magnesium fluoride, MgF_2 , and potassium chloride, KCl. When these ionic compounds form they form an ordered 3 dimensional assembly in which the cation and anion ion alternate, as in the diagram below for NaCl(s):



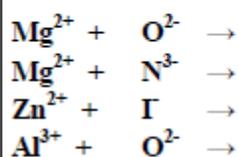
Note once again, that because ionic compounds form crystals of widely varying sizes (a salt crystal can be barely large enough to see or bigger than your head), they contain widely varying numbers of atoms. Therefore, they are best represented by empirical formulas (we represent table salt as NaCl, not $\text{Na}_{2,500,000}\text{Cl}_{2,500,000}$ for a small crystal and $\text{Na}_{\text{lots and lots}}\text{Cl}_{\text{also lots and lots}}$ for a really big one).

Stable ionic compounds are neutral, and therefore consist of a combination of cations and anions whose positive charges equal their negative charges. For example, to form a neutral compound from ammonium, NH_4^+ , which has a charge of plus one, and SO_4^{2-} , which has a charge of -2, we need a combination of two NH_4^+ s, and one SO_4^{2-} . Thus the formula of the resulting compound, ammonium sulfate, is

$(\text{NH}_4)_2\text{SO}_4$. Note that in general, the formula A_aB_b means that the compound is made from a A atoms and b B atoms. Note also that when, as in the example above, one of the ions is polyatomic, that the subscript after the parentheses indicates the number of polyatomic ions present.

Let's practice a few examples of figuring out formulas for some ionic compounds,

Practice Questions: Write down the formula for solids of the following combinations of cations and anions.



given the cations and anions they are formed from.

As you can tell from some of the examples above, all compounds have names in addition to formulas. Compounds are named using a series of rules. For binary ionic compounds, A_aB_b , ionic compounds made of two elements, the rule is simple:

- 1) Write down the name of element A first.
- 2) Then write down the name of the anion, B. The name of the anion of an element is formed by removing the last few letters of the element name, and replacing them with ide. For example, F^- is fluoride, O^{2-} is oxide, and N^{3-} is nitride.

Let's practice this a couple of times:



The rules are only slightly different for compounds that contain polyatomic ions. Many polyatomic ions have traditional names like sulfate (SO_4^{-2}). Examples of these are cyanide ion (CN^-), sulfate ion (SO_4^{-2}), hydroxide ion (OH^-) or carbonate ion (CO_3^{-2}). If polyatomic anions are combined with atomic cations, then the name is simply the name of the cation followed by the name of the anion. So for example, K_2SO_4 is called potassium sulfate, and $\text{Mg}(\text{CN})_2$ is called magnesium cyanide. If a polyatomic cation is combined with an atomic anion, then the name is the name of the polyatomic ion followed by the name of the atomic anion, i.e. NH_4Cl is simply ammonium chloride.

Finally, naming a compound made of two polyatomic ions is simple, name the cation first, and then the anion. For example, NH_4NO_3 is made of ammonium and nitrate, and is called (can you guess?) ammonium nitrate.

Check the handout if necessary, and name the following:

LiOH →

$\text{Mg}(\text{CO}_3)_2$ →

So far things have been relatively unambiguous. However, when we move to transition metals, we have the added complication that they can stably exist in more than one ionic form. For example, iron can exist stably as Fe^{+2} or Fe^{+3} , while copper can exist as Cu^{+1} and Cu^{+2} . We need names that distinguish between these different charges. There are two conventions that are used for naming these ions. The newer convention is the simpler one, and is the one we will be using. The ion is named by taking the name of the element, and adding the charge in roman numbers. Thus Fe^{+2} becomes Fe(II) or iron (II), and Fe^{+3} becomes Fe (III) or iron III. When a compound

is made with one of these ions, we just add the name of the anion to the name of the cation. So FeCl_2 becomes iron (II) chloride, and $\text{Fe}(\text{NO}_3)_3$ becomes iron (III) nitrate.

In the older convention the ion with the smaller charge is given the suffix *ous*, and the ion with the larger charge is given the suffix *ic*. So Fe^{+2} (with the smaller charge) is ferrous ion, and Fe^{+3} is ferric ion. For another example, Cu^+ (smaller charge) is cuprous ion, and Cu^{+2} is cupric ion. To name compounds with these ions, simply take the name of the cation and add the names of the anions. So FeCl_2 is ferrous chloride, and $\text{Fe}(\text{NO}_3)_3$ is ferric nitrate. Again we won't be using this nomenclature in lecture or on tests, but it is still found very frequently in the literature, so it's important for you to know.

Remember that ionic compounds are characterized by the formation of crystals containing large numbers of atoms. This is not the only way that compounds can form. The other large class of compounds are molecular compounds. Molecules are combinations of small numbers of atoms which are bound together by electrostatic forces, called chemical bonds, to form stable discrete entities. Molecules are usually combinations of non-metal atoms. Molecules can be elements, such as N_2 , O_2 , or C_{60} , or they can be compounds like CO_2 , or H_2O .

The biggest challenge in naming molecular compounds is that a pair of elements forming molecular compounds can combine in many different ways. For example, carbon and oxygen can combine to form either CO_2 or CO , and hydrogen and oxygen can combine to form H_2O and H_2O_2 . This means that when we name them, we need a way to distinguish between the ways in which they combine. Here is how we name molecular compounds made from two elements:

For a molecule A_aB_b

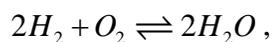
- 1) Name the first element, then the second
- 2) Add the suffix “ide” to the first part of element B.
- 3) Use a Greek prefix to indicate the number of each element in the molecule. Note that we don’t use a prefix for the first element when there is only one of that element.
 - a. The Greek prefixes are mono- for 1, di- for 2, tri- for 3, tetra- for four, penta- for 5, hexa- for 6, hepta- for 7, octa- for 8, nona- for 9, and deca- for 10.
 - b. For example, CO is carbon monoxide, while CO₂ is carbon dioxide. NO₃ is nitrogen trioxide, while N₂O₅ is dinitrogen pentoxide.

Note that under the right conditions molecules do form solids, but there are several differences between these solids and ionic solids. First when molecules form solids they keep their molecular identity. CO₂ is still a discrete unit within solid CO₂. Second, the forces holding the molecules together are much weaker than the forces that hold ionic solids together. Thus molecular solids evaporate or melt at much lower temperatures than ionic solids. As an extreme example, solid oxygen, a molecular solid, has a melting point of 54.7 K (-281.14 °C), while sodium chloride (NaCl), an ionic solid, melts at 1074 K, or 801 °C.

Lecture 4

One of the goals we stated at the beginning of the course was to understand the nature and transformation of chemicals. In order to do this, we need to be able to quantify the number of atoms and molecules making up a substance, and the number of atoms and molecules involved in chemical reactions.

The most fundamental units for counting in chemistry are the atom and the molecule. For example, when we talk of water, H_2O , we are saying that one molecule of water consists of two hydrogen atoms and one oxygen atom. When we talk of the reaction between hydrogen and oxygen to form water,



we are saying that two molecules of hydrogen and one of oxygen combine to form two molecules of water.

However, when we do experimental studies of reactions and the constitution of chemicals we have to use other means, typically mass measurements, to determine how much of each substance we have. Why? Because of the incredibly small size of atoms and molecules. Atoms and small molecules are on the scale of a few nanometers to a few tens of nanometers in size, a factor of more than 10,000 smaller than the smallest objects that can be seen with the naked eye. Unfortunately, single atoms and molecules, with masses on the order of 10^{-24} g to 10^{-21} g, are also too light to weigh conveniently.

For this reason, we usually resort to weighing convenient amounts of atoms and molecules. How do we determine this convenient amount? The answer lies in the periodic table. Below each element are the masses of each element. Originally these

were determined through a series of painstaking experiments that determined the relative masses of each element. Thus according to the periodic table, helium atoms have a mass approximately four times that of hydrogen atoms, and carbon has a mass just under 12 times that of hydrogen. The units of these masses were called atomic mass units, and as I said, originally only indicated the relative mass of the various elements.

We can also define an amount called the gram atomic mass, which is simply the number of grams of a substance equal to its atomic weight. So the gram atomic mass of hydrogen is 1.01g, of carbon is 12.011g, and of chlorine atoms is 35.453 grams. It turns out that the number of atoms in a gram atomic mass of a substance is always the same. This is known as Avogadro's principle. In other words, 1.01g of H, 12.011g of C, and 35.453g of Cl all contain the same number of atoms. We call this number of atoms a mole. Careful experimentation has allowed us to determine that the number of atoms in a mole is 6.023×10^{23} atoms. This number is also called Avogadro's number. So we now have two different definitions of a mole. I: A mole is 6.023×10^{23} of an object. 6.023×10^{23} uranium atoms is a mole of uranium atoms, 6.023×10^{23} basketballs is a mole of basketballs, and 6.023×10^{23} eggs is a mole of eggs. 6.023×10^{23} avocados, however, is called a guacamole. II. A mole is the number of atoms or molecules in a gram atomic or gram molecular mass.

The value of the mole concept is that because a mole of anything always contains the same number, the relative number of moles of atoms in a mole of molecules is the same as the relative number of atoms in a molecule. So when we say that water consists of two hydrogen atoms and one oxygen atom, we could equivalently say that

a mole of water contains two moles of hydrogen atoms and one mole of oxygen atoms.

Why is this valuable? It is valuable because the mass of a mole is easy to measure. Therefore, the mole concept allows us to study the composition of chemicals and their reactions by measuring the masses of the reactants and products in convenient amounts.

It is common for students to be confused by moles, in part because the number of objects in a mole is so large. However, a mole is just a number of objects, just as a dozen is. Five dozen eggs and 10 dozen apples are in a 1:2 ratio, just as 5 moles of oxygen and 10 moles of hydrogen are in a 1:2 ratio.

Knowing the number of atoms in a mole allows us to determine the absolute mass of atoms, and to assign a definite (not just relative) mass to the atomic mass unit. It turns out that an atomic mass unit is 1.6605×10^{-24} grams. This means that we can now calculate absolute masses for various atoms. All we need to do is to multiply the number of atomic mass units by 1.6605×10^{-24} grams. So for example, the mass of nitrogen is 14.067 amu. $m_N = 14.067 \text{ amu} \times 1.6605 \times 10^{-24} \text{ g/amu} = 2.3358 \times 10^{-23} \text{ g}$.

A logical question to ask at this point is why the masses in AMU of the various elements are not whole numbers? The answer is that the **masses on the periodic table are average masses**. Remember that elements can exist as a number of different isotopes. For example, carbon has two stable isotopes, carbon-12 and carbon-13 (carbon-14, which is used in dating old objects is radioactive, and is not a stable isotope). Because they have different mass numbers, they have different masses. Carbon-12 has a mass of exactly 12 AMU (by definition) with an abundance

of 98.90%, while carbon-13 has a mass of 13.003 amu and an abundance of 1.10%. The average mass on the periodic table takes into account that a typical sample has both isotopes in it, and that both contribute to the average mass. **To calculate the average mass of an element, we need to know both the mass of each isotope, and its abundance.** The average mass will be the sum of the products of the isotopic masses times their abundance. So for example, $m(\text{C}) = m(\text{C-12}) \times \text{abundance}(\text{C-12}) + m(\text{C-13}) \times \text{abundance}(\text{C-13}) = 12.00 \text{ AMU} \times .9890 + 13.003 \text{ AMU} \times .0110 = 12.0110 \text{ AMU}$. Note that you need to divide the percent abundance by 100 to get the proper abundance for this calculation.

Since we know the average masses of all the elements, we can also figure out average molecular masses or average formula weights. All we have to do is add up the atomic weights for all the atoms in our compound. For example, for NaCl, the formula weight is just the sum of the masses of the Na and the Cl, i.e.,

$$FW(\text{NaCl}(s)) = m_{\text{Na}} + m_{\text{Cl}} = 22.989 \text{ g/mol} + 35.453 \text{ g/mol} = 58.442 \text{ g/mol}$$

For the case of H_2SO_4 , we need to add the mass of two hydrogens, one sulfur and four oxygens, i.e.,

$$\begin{aligned} MW(\text{H}_2\text{SO}_4) &= 2 * m_{\text{H}} + m_{\text{S}} + 4 * m_{\text{O}} \\ &= 2 * 1.008 \text{ g/mol} + 32.065 \text{ g/mol} + 4 * 15.999 \text{ g/mol} = 98.077 \text{ g/mol} \end{aligned}$$

There are a number of other calculations involving masses and mols that we now have the knowledge to do. These include calculating the number of moles of a substance from the number of atoms or molecules and vice versa; and calculating the number of moles and the number of atoms from the mass of a substance. Let's practice some examples.

Example one: conversion of mass to number of atoms or molecules:

How many carbon atoms are there in 6.005 g of carbon?

Approach: first determine how many moles of carbon this is, and then convert to atoms: To determine the number of moles, we divide by the molar mass:

$$6.005\text{gC} \times \frac{1\text{molC}}{12.010\text{gC}} = 0.500\text{molC} .$$

Then we convert mols to number of atoms, by multiplying by Avogadro's number:

$$0.500\text{molC} \times \frac{6.023 \times 10^{23} \text{atomsC}}{\text{molC}} = 3.0115 \times 10^{23} \text{atomsC}$$

Notice that I was careful to include units for all steps of my calculation. The units are important not just to identify the quantities, but also can guide us in how to do the calculations. Note that in all of the calculations, the units cancelled to yield our desired units. If I had used them the wrong way, the units would not have cancelled. For example, suppose I had tried to convert from grams to mols by multiplying by the molar mass (WARNING: Do not try this at home. It is incorrect.)

$$6.005\text{gC} \times \frac{12.010\text{gC}}{\text{molC}} = \frac{72.120\text{g}^2\text{C}}{\text{molC}}$$

Notice that the units resulting from this calculation are not the correct units, so we know we used the conversion factor incorrectly.

Example two: How many molecules are there in 25.00 g of Cl₂? How many atoms are there?

Approach: First we convert grams to moles, then moles to molecules, then molecules to atoms.

In order to convert grams to moles, we need the molar mass of Cl₂. This is simply the mass of two chlorine atoms and is equal to 70.906 g/mol.

Note that we can combine the first two steps into one:

$$25.00 \text{ gCl}_2 \times \frac{1 \text{ molCl}_2}{70.906 \text{ gCl}_2} \times \frac{6.023 \times 10^{23} \text{ moleculesCl}_2}{1 \text{ molCl}_2} = 2.1235 \times 10^{23} \text{ moleculesCl}_2$$

Now that we know the number of molecules, we can figure out the number of atoms.

The key here is that the formula tells us the conversion factor that we need, that there are two Cl atoms for every Cl molecule, so

$$2.1235 \times 10^{23} \text{ moleculesCl}_2 \times \frac{2 \text{ atomsCl}}{1 \text{ moleculeCl}_2} = 4.2472 \times 10^{23} \text{ atomsCl}.$$

Example 3: Converting numbers of molecules to moles

If all the ozone in a column 1 cm^2 going from the surface of the planet to the top of the atmosphere were totaled, it would come to 8.25×10^{18} molecules of ozone. How many moles of ozone is this?

Approach: Since we are converting between molecules and moles, we need to use Avogadro's number, 6.023×10^{23} molecules/mol, as the conversion factor. The question is, do we multiply or divide by this number? Once again, the units guide us. The correct approach (dividing) is the one yielding the correct units for the answer.

$$8.25 \times 10^{18} \text{ molecules ozone} \times \frac{1 \text{ mol ozone}}{6.023 \times 10^{23} \text{ molecules ozone}} = 1.370 \times 10^{-5} \text{ mol ozone}$$

Example 4: Converting from molecules to mass.

In my experiments, I used to study the reactions of samples containing 1.807×10^{23} molecules of acetylene, C_2H_2 . What was the mass of one of these samples?

Approach: first convert to moles, using Avogadro's number, then to mass, using the molar mass. Before we do this we need the molar mass of acetylene. The formula tells us that acetylene consists of 2 C atoms and 2 hydrogen atoms, so

$$m_{C_2H_2} = 2m_C + 2m_H = 2 * 12.01g / mol + 2 * 1.01g / mol = 26.04g / mol.$$

As before we can do this in a single step:

$$1.807 \times 10^{23} \text{ molecules } C_2H_2 \times \frac{1 \text{ mol } C_2H_2}{6.023 \times 10^{23} \text{ molecules } C_2H_2} \times \frac{26.04 \text{ g } C_2H_2}{\text{mol } C_2H_2} = 7.68 \times 10^{-2} \text{ g } C_2H_2$$

A powerful application of these calculations we've just learned is that we can calculate empirical formulas of a molecule if we know its % composition. If in addition, we know the molar mass of the molecule, we can figure out its molecular formula. This is an important type of problem that is still used to determine the formulas of newly synthesized organic molecules.

Before we start, we need to define the mass percentage. The definition is simple enough – it's simply how many grams an element is out of 100 grams of a molecule. It's defined as

$$\text{Mass\%} = (\text{Mass of element} / \text{Mass of molecule}) \times 100\%.$$

For example, water is H₂O.

$$\text{Mass\%H} = 2.02\text{g}/18.02\text{g} \times 100\% = 11.21\% \text{ H}$$

$$\text{Mass\%O} = 16.00\text{g}/18.02\text{g} \times 100\% = 88.79\% \text{ O}$$

This means that a 100 g sample of water would contain 11.21g H and 88.79g O.

Example: An unknown molecule is composed only of nitrogen and oxygen and has the following composition by mass: N=30.4%, and O=69.6%. An independent experiment has shown that the molar mass is 92.02 g/mol. What is the empirical formula and what is the molecular formula?

Approach: To find the empirical formula: Convert mass % to mass by choosing a sample size (the results will be the same no matter what sample size you choose.)

Convert masses to moles. Determine the smallest whole number mole ratio. This will be the empirical formula.

To find the molecular formula: Calculate the formula weight from the empirical formula. Divide molar mass by formula weight. This should be a whole number.

Multiply the empirical formula by this number. The result is the molecular formula.

Let's try this for our example. For simplicity, I'm going to assume a sample size of 100g, but the choice of sample size is not important. You will get the same result no matter what sample size you choose.

The masses of N and O are obtained as follows:

$$m_{\text{element1}} = m_{\text{total}} * \frac{\text{mass}\%(\text{element1})}{100\%}$$

So

$$m_N = 100\text{ g} * \frac{30.4\%}{100\%} = 30.4\text{ g}$$

$$m_O = 100\text{ g} * \frac{69.6\%}{100\%} = 69.6\text{ g}$$

Now that we have the masses we convert to moles of each element by dividing by the average atomic mass.

$$n_N = 30.4\text{ g N} * \frac{1\text{ mol N}}{14.0067\text{ g N}} = 2.17\text{ mol N}$$

$$n_O = 69.6\text{ g O} * \frac{1\text{ mol O}}{15.9999\text{ g O}} = 4.35\text{ mol O}$$

Note that the symbol for moles is a lower case n.

Now we make our empirical formula, by using the moles of each substance as the subscripts, and dividing by the smallest number

$$EF = N_{\frac{2.17}{2.17}} O_{\frac{4.35}{2.17}} = NO_2$$

Sometimes this procedure may yield formulas in which the subscripts are not whole numbers, i.e., $SO_{1.5}$. In those cases, you multiply by a number that yields the smallest whole number ratio, in this case multiplying by two and yielding S_2O_3 .

Finally, we use our empirical formula and our molar mass to determine the molecular formula.

First we calculate our formula weight:

$$FW(NO_2) = M_N + 2 * M_O = 14.0067 \text{ g / mol} + 2 * 15.9999 \text{ g / mol} = 46.0065 \text{ g / mol}$$

Now we divide our molar mass by the formula weight. The result must be a whole number (or at least be easily roundable to one).

$$\frac{\text{Molar Mass}}{\text{Formula Weight}} = \frac{92.02 \text{ g / mol}}{46.0065 \text{ g / mol}} = 2.0001$$

In our last step, we multiply our empirical formula by this number to get the molecular formula:

$$\text{Molecular Formula} = 2 * EF = 2 * NO_2 = N_2O_4$$

Let's practice this together by figuring out the formula for hydrogen peroxide, which is composed only of hydrogen and oxygen. The mass% of H is 5.94%, the mass % of O is 94.06%, and the molar mass is 34.0 g/mol.