CH301 REVIEW: CHEMICAL FORMULAS , COMPOSITION STOICHIOMETRY

Summary. Much of high school chemistry was devoted to introducing the concept of Dalton's ATOMIC THEORY which provides a foundation for a more quantitative description of matter. By combining the idea of the atom with the LAW OF MULTIPLE PROPORTIONS, the concept of the MOLECULE was developed. Chemical formulas and the associated names for small molecules and IONS were introduced. From the idea that the individual atom representing each element has its own unique mass, the concept of ATOMIC WEIGHT was developed. Then, in order to operate with experimentally-manageable amounts of matter, the MOLE was introduced, and the fun with calculations began.

The simple numerical relationship between atoms in molecules allows a collection of calculations called COMPOSITIONAL STOICHIOMETRY problems to be performed. Most of this chapter is devoted to reviewing every kind of problem in which mass, numbers of atoms, moles, atomic and molecular formula, elemental formula and percent composition are related to one another.

The good news is that there is a common approach to solving all stoichiometry problems: the use of a UNIT FACTOR. Thus, in the same way that you have learned to convert inches into miles, by making the units in UNIT FACTORS cancel, you can perform all the conversions in compositional stoichiometry by making units in unit factors cancel. You will start with some known quantity like:

atoms of A and be asked to convert it into **grams of molecule AB**

Now as you work problems like this you will find that there are patterns that you will use over and over in putting together unit factors. The last half of the chapter is spent looking at almost every permutation of unit factors. We will look at a collection of examples, and then try to come up with a general procedure for working the problems.

One word of caution. You must learn to do COMPOSITIONAL STOICHIOMETRY problems in this chapter effortlessly because the next review material considers REACTION STOICHIOMETRY which assumes you can do COMPOSITIONAL STOICHIOMETRY blindfolded.

Atomic Theory

Early scientists had figured out that a very complex world could be reduced to a collection of ELEMENTAL materials. John Dalton came along in the early 1800s and proposed that these elemental materials were made up of very small, indivisible particles he called ATOMS. Dalton was to provide the framework for a theory, which although not perfect, launched the modern age of chemistry and physics.

Here are some ideas of DALTON'S ATOMIC THEORY:

1. An element is composed of small indivisible particles called ATOMS.

2. All atoms of a given element have identical properties which are unique from other elements.

3. Atoms cannot be created, destroyed or converted into other elements.

4. MOLECULES are formed when atoms of different elements combine in simple whole number ratios.

5. The relative number and type of atoms is constant for a given MOLECULE.

Flaws in Dalton's Theory

Note some of the flaws in this theory. Obviously in the nuclear age, atoms can be created and destroyed. In addition, the theory does not recognize the existence of different ISOTOPES of an atom. Nonetheless, the theory works extremely well as a platform for describing almost every chemical and physical process we will examine in this course.

TIME OUT. We all know that atoms are made up of ELECTRONS and PROTONS and NEUTRONS, but Dalton didn't in the early 1800s. And we don't need to know this either to appreciate descriptive chemistry and stoichiometry calculations that are covered in this review material. So kick back and enjoy the simplicity of believing that atoms are small indivisible particles: tiny billiard balls of different sizes.

Chemical Formulas: ATOMS

Before we can start working all our stoichiometry problems, we have to be able to develop a NOMENCLATURE, a short-hand language, for describing atoms and molecules. We will use as a starting place, the shorthand notation for elements found in every periodic table. Try memorizing a few dozen elements and their abbreviations from early in the periodic table to speed up your test taking. Here are a dozen to get you started.

Atomic number	Name	Symbol	Period	Group	Chemical series	Mass (g/mol)
1	Hydrogen	H	1	1	Nonmetal	1.00794
2	Helium	He	1	18	Noble gas	4.002602
3	Lithium	Li	2	1	Alkali metal	6.941
4	Beryllium	Be	2	2	Alkaline earth	9.012182
5	Boron	B	2	13	Metalloid	10.811
6	Carbon	C	2	14	Nonmetal	12.0107
7	Nitrogen	N	2	15	Nonmetal	14.0067
8	Oxygen	O	2	16	Nonmetal	15.9994
9	Fluorine	F	2	17	Halogen	18.9984032
10	Neon	Ne	2	18	Noble gas	20.1797
11	Sodium	Na	3	1	Alkali metal	22.98976928
12	Magnesium	Mg	3	2	Alkaline earth	24.3050

By the way, do you HAVE to memorize the elements? Of course not. There is always a periodic table handy. But if you find yourself having to look up oxygen's atomic mass of 16 for the 300th time, you are probably not finishing the exams on time.

Chemical Formulas: MOLECULES

Recall that Dalton's theory suggests that MOLECULES can be made from simple combinations of atoms. We can write a shorthand notation for this by using a subscript beside the atom abbreviation. In its simplest form with a single type of element we can have

Monatomic molecules	He	helium
	Ne	neon
Diatomic molecules	O_2	dioxygen
	H_2	dihydrogen
Polyatomic molecules	P_4	tetraphosphorous
	S_8	octasulfur

We can also mix elements together in various combinations to form the vast array of MOLECULES that make up our universe:

one hydrogen and one chloride	HCl	hydrochloric acid
two hydrogens and one oxygen	H_2O	water
one nitrogen and three hydrogens	NH_3	ammonia
three carbons and eight hydrogens	C_3H_8	propane

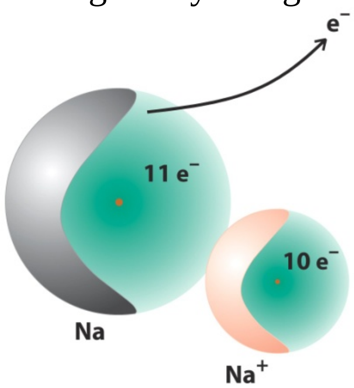
The entire first half of the course is in fact spent discussing bonding theories so that you can draw three dimensional structures of the compounds above, and thousands more, in your sleep.

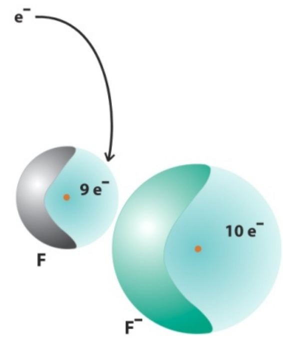
Ions: Compounds with charge

Life is never simple and chemistry being part of life, chemistry is never simple either. For reasons we will learn about later, it is possible to find compounds which are not neutral but instead possess a charge.

CATION: a positively charged compound Na^{+} NH_4^{+}

ANION: a negatively charged compound F^{-} SO_4^{-2}





IONIC compounds: What you get when you put together anions and cations to obtain a neutral species (no charge)

NaCl $(NH_4)_2SO_4$

IONS are not MOLECULES

Now Davis makes a big deal about IONS not being able to form MOLECULES. Thus, NaCl is not a molecule, it is just a simple way of describing the appropriate ratio of ions which come together to form regularly packed crystals. For example, shown in Figure 2 are ball and stick and space-filled models of table salt. So what kind of word do we use if we can't use the word MOLECULE to describe NaCl?

FORMULA UNIT: the simplest whole number ratio of ions in a compound.

Thus,

NaCl is the FORMULA UNIT for sodium chloride.

But

NaCl is NOT a MOLECULAR UNIT for sodium chloride

Naming Compounds: Ions

As a start on the very important but very difficult process of naming chemical compounds, we will look at some rules of naming IONIC compounds.

- The formula of an ionic compound is adjusted to make the FORMULA UNIT neutral.
- The positive cation species are written first and followed by the negative anion species.
- The common ionic nomenclature for individual ions is used to assemble an ion's FORMULA UNIT.

Examples:

NaCl	$Na^+ Cl^-$	sodium chloride
$(NH_4)_2S$	$2NH_4^+ \; S^=$	ammonium sulfide
$MgBr_2$	$Mg^{+2} \; 2Br^-$	magnesium bromide

Atomic Weight

You'll recall that early scientists were able to reduce mixtures to their elemental forms. In the process they weighed these materials and not only came up with the law of multiple proportions, but also a relative ratio of weights of the different elements. For example, they found that by assigning hydrogen, the lightest element, an ATOMIC MASS UNIT of one, the following approximate relative ratios of other elements were:

hydrogen	1	magnesium	24
carbon	12	and so on...	

With more precise measurements, it was found that these whole number values were not exact (we'll learn about isotopes and mass defects later). But this concept did give way to the idea of ATOMIC WEIGHT which can be found for each element in the periodic table. This value represents an average weight for *naturally occurring* amounts of each element. Hence, the atomic weights which are not even close to whole numbers.

For example

Cl has an atomic weight of 35.45 amu.

The rest of the atomic weights are listed in the periodic table.

The Mole

Recall that Dalton suggested atoms were very small. In contrast, we are very big. So if we want to work with reasonable quantities of materials (like amounts we can hold in our hand and see), we have to deal with incredibly large numbers of atoms. It is out of this need to hold an amount we can see, but not want to have to deal with such big numbers, that the idea of a mole was born--in exactly the same way that chicken farmers dealt with DOZENS of eggs to reduce the magnitude of the number describing eggs, and Lincoln used SCORE as a way to reduce the size of the number describing years ('four score and seven years ago' let him use the numbers four and seven rather than the number 87). In the same way, we use the MOLE to reduce the size of the numbers we use to describe atoms and molecules.

dozen	=	12
score	=	20
mole	=	6.02×10^{23}

Where did 6.02×10^{23} (Avagadro's number) come from?

Arbitrarily it was decided to allow a mole to be equal to the atomic weight of an element in atomic mass units. This mass is called the molar mass and has units of grams/mole.

So a mole of hydrogen atoms weighs about 1 gram.

A mole of oxygen atoms weighs about 16 grams.

And exactly how many molecules are in a mole of a sample? Like we said, Avagadro's number:

$6.02213167 \times 10^{23}$ particles.

This is an extraordinarily large number--a larger number than you will ever deal with in just about any other area of science. The kind of magnitude that makes talking about billions (10^9) and trillions (10^{12}) of things like people or dollars, comparatively minuscule.

Summarizing, why do we bother to use moles?

Because it allows us to scale up using the law of multiple proportions in putting together simple ratios of atoms to make a molecule. This way, when we get a can of diet coke, we can say:

> "Hey, that 360 milliliters = 360 grams = 20 moles of Diet Coke = 40 moles of hydrogens combined with 20 moles of oxygens, sure tasted good!!"

Instead of saying

> "Hey, that 360 milliliters = 360 grams = 120×10^{23} molecules = 240×10^{23} atoms of hydrogen combined with 120×10^{23} atoms of oxygen, sure tasted good!!"

That is all there is to it. We use moles so we don't have to run around saying "times ten to the twenty-third" all the time.

It is as simple as that.

LET'S DO SOME PROBLEMS.

Stoichiometry problem solving is all about setting up and canceling unit factors, until the unit you want results from the unit with which you begin.

The best news of all is that there are only three unit factors you will use .commonly.

Unit factor:

Density	volume to mass
Avagadro's number	moles to number of particles
Atomic weight	moles to mass

The second best news is that the problems are ALWAYS set up exactly the same way:

what you don't know **=** *what you do know* **(unit factors)(unit factors)(unit factors)**

You find the answer to what you don't know by taking the value you are given in the problem and then using unit factors that turn the units of what you do know into the units of what you don't know.

It is that simple. Proof: let's look at a dozen examples.**Example 1**: Calculate the mass of a magnesium, Mg, atom in grams.

$$?\ \text{mass of Mg atom} = \left(24.3\frac{\text{g}}{\text{mole Mg}}\right)\left(\frac{1\ \text{mole Mg}}{6.02\ \text{X}\ 10^{23}\ \text{atoms}}\right)$$
$$= 4.04\ \text{X}\ 10^{-23}\ \text{g / atom}$$

Example 2: Calculate the number of atoms in one-millionth of a gram of magnesium, Mg.

$$?\ \text{atoms} = \left(1\ \text{X}\ 10^{-6}\ \text{g Mg}\right)\left(\frac{1\,\text{mole Mg}}{24.3\ \text{g}}\right)\left(\frac{6.0\,2\ \text{X}\ 10^{23}\ \text{atoms}}{1\,\text{mole Mg}}\right)$$
$$= 2.47\ \text{X}\ 10^{16}\ \text{atoms}$$

Example 3: How many atoms are in 1.67 moles of magnesium?

$$? \text{ atoms} = (1.67 \text{ moles Mg})\left(\frac{6.02 \text{ X } 10^{23} \text{ atoms}}{1 \text{ mole Mg}}\right)$$
$$= 1.00 \text{ X } 10^{24} \text{ atoms}$$

Example 4: How many moles of magnesium are in 73.4 grams of magnesium?

$$? \text{ moles of Mg atoms} = (73.4 \text{ g Mg})\left(\frac{1 \text{ mole Mg}}{24.3 \text{ g}}\right)$$
$$= 3.0 \text{ moles}$$

FORMULA WEIGHT (MOLECULAR WEIGHT)

To this point, we've dealt with moles of atoms. Now we deal with MOLES of MOLECULES by introducing the concept of formula or molecular weight (these are the same if dealing with molecules. If dealing with ionic materials, it is more appropriate to describe a formula weight.)

FORMULA WEIGHT: The FORMULA WEIGHT of a substance is found by summing the atomic weights of each atom in the molecular formula (or formula unit).

Example 5. Calculate the formula weight of propane, C_3H_8.

atomic weight C = 12.01 g/mole
atomic weight H = 1.0079 g/mole
formula weight = 3 x 12.01 + 8 x 1.0079 = 44.09 g/mole

Now we can start to play games involving moles and molecules. One mole of a substance is 6 x 10^{23} particles of the substance and is equal to the formula weight in grams of the substance.

Example 6. Lets play fill in the blank:

The mole of the molecule, chlorine, Cl_2, weighs <u>2 x 35.45 = 70.9</u>

grams. It contains ____2____ moles of chlorine atoms,

<u>6.02×10^{23}</u> Cl_2 molecules and <u>$2 \times 6.02 \times 10^{23}$</u> Cl atoms.

Some more examples:

Example 7. Calculate the number of propane, C_3H_8 molecules, in 74.6 grams of propane.

$$\begin{aligned} ?\text{ propane molecules} &= 74.6\text{ g}\left(\frac{1\text{ mole}}{44.09\text{ g}}\right)\left(\frac{6.02\text{ X }10^{23}\text{ molecules}}{1\text{ mole}}\right) \\ &= 1.01\text{ X }10^{24}\text{ molecules} \end{aligned}$$

Example 8. What is the mass of 10.0 billion molecules of propane?

$$\begin{aligned} ?\text{ g molecules} &= \left(10.0\text{ X }10^{9}\text{ molecules}\right)\left(\frac{1\text{ mole}}{6.02\text{ X }10^{23}\text{ molecules}}\right)\left(\frac{44.09\text{ g}}{1\text{ mole}}\right) \\ &= 7.33\text{ X }10^{-13}\text{ g} \end{aligned}$$

Example 9. How many moles, molecules, and oxygen atoms are contained in a 60 gram sample of ozone, O_3?

$$?\text{ moles} = \left(60\text{ g O}_3\right)\left(\frac{1\text{ mole}}{3\text{ X }15.9994\text{ g}}\right) = 1.25\text{ moles}$$

$$?\text{ molecules} = \left(1.25\text{ moles}\right)\left(\frac{6.02\text{ X }10^{23}}{1\text{ mole}}\right) = 7.53\text{ X }10^{23}\text{ molecules}$$

$$?\text{ atoms} = \left(7.53\text{ X }10^{23}\text{ molecules}\right)\left(\frac{3\text{ O atoms}}{1\text{ O}_3\text{ molecules}}\right) = 2.26\text{ X }10^{24}\text{ atoms}$$

Now let's get a little fancier with our stoichiometry and some famous kinds of chemistry problems:

Percent Composition

The usual method for counting amounts of chemical compounds uses the mole as currency: a mole of propane, C_3H_8 contains 3 moles of carbon and eight moles of hydrogen.

Unfortunately, many of the devices we use for measuring chemicals actually measure the MASS of individual samples. Thus we need to be able to readily convert between MOLES of individual atoms in a molecule to percent by weight of each atom in the molecule.

Example 10. What is the percent composition of each element in propane?

$$\begin{aligned}
1 \text{ mole } C_3H_8 &= (3 \text{ moles C})\left(\frac{12.01 \text{ g}}{1 \text{ mole}}\right) = 36.03 \text{ g C} \\
&= (8 \text{ moles H})\left(\frac{1.0079 \text{ g}}{1 \text{ mole}}\right) = 8.06 \text{ g H} \\
\text{total weight} &= 36.03 \text{ g C} + 8.06 \text{ g H} = 44.09 \text{ g} \\
\%\text{ C} &= \left(\frac{36.03 \text{ g C}}{44.09 \text{ g sample}}\right) \text{X } 100 = 81.7\% \\
\%\text{ H} &= (100 - 81.7)\% = 18.3\%
\end{aligned}$$

Empirical Formula

We have learned by experimental means that it is possible to determine the % composition of an unknown compound. This percent composition can easily be turned into a molar ratio of elements which the law of simple proportions tells us will be a simple whole number ratio. This simple whole number ratio is the smallest possible ratio of atoms in the sample, the EMPIRICAL FORMULA or SIMPLEST FORMULA. But the MOLECULAR FORMULA may be some multiple of the EMPIRICAL FORMULA.

Example 11. A compound that is 24.74% K, 34.76% Mn and 40.40% O by mass has what empirical formula?

1. Convert grams to moles, assume 100 g sample

$$24.74\text{ g K}\left(\frac{1\text{ mole}}{39.09\text{ g}}\right) = 0.633\text{ mole}$$

$$34.76\text{ g Mn}\left(\frac{1\text{ mole}}{54.93\text{ g}}\right) = 0.633\text{ mole}$$

$$40.50\text{ g O}\left(\frac{1\text{ mole}}{15.9994\text{ g}}\right) = 2.53\text{ mole}$$

2. Divide by smallest number of moles

$$\frac{0.633}{0.633} = 1$$

$$\frac{2.53}{0.633} = 4$$

$\therefore$ the empirical formula is $KMnO_4$

Determination of Molecular Formula

We can take the elemental composition problem one step further by adding knowledge about a compound's actual molecular weight. (There are a variety of analytical techniques for determining the molecular weight of a compound, MASS SPECTROMETRY being the most famous of the bunch.)

Thus if we know:

1. The empirical (simplest) formula
2. The molecular weight

We can obtain the molecular formula of the compound.

For example, if the empirical formula of a hydrocarbon is C_2H_5 (empirical weight = 12+12+5 = 29) and the molecular weight is 116, then the molecular formula is simply (116/29) = a four-fold multiple of C_2H_5 = C_8H_{20}.

Example 12. A compound is found to contain 85.63% C and 14.37% H by mass. In another experiment its molecular weight is found to be 56.1 grams/mole. What is the molecular formula of the compound?

First, find the empirical formula. Convert g $\rightarrow$ mole

$$85.63 \text{ g C} \left(\frac{1 \text{ mole}}{12 \text{ g}}\right) = 7.12 \text{ moles}$$

$$14.37 \text{ g H} \left(\frac{1 \text{ mole}}{1.0079 \text{ g}}\right) = 14.25 \text{ moles}$$

$$\text{so we have } \frac{14.25 \text{ moles H}}{7.12 \text{ moles C}} \Rightarrow CH_2 \quad \text{as the empirical formula}$$

Second, the empirical weight of $CH_2 \approx 14$

$$\text{so the } \frac{\text{molecular weight}}{\text{empirical weight}} \approx \frac{56}{14} = 4$$

$$\therefore \text{ the molecular formula is } C_4H_8$$

Example 13. What mass of phosphorous is contained in 45.3 grams of $(NH_4)_3PO_4$?

$$(NH_4)_3PO_4 = \text{M.W. of } 149.08 \text{ g / mole}$$

$$? \text{ g P} = 45.3 \text{ g } (NH_4)_3PO_4 \left(\frac{1 \text{ mole}}{149.08 \text{ g}}\right) = 0.304 \text{ moles}$$

$$= 0.304 \text{ moles } (NH_4)_3PO_4 \left(\frac{1 \text{ mole P atom}}{1 \text{ mole } (NH_4)_3PO_4}\right)\left(\frac{30.97 \text{ g P}}{1 \text{ mole P}}\right)$$

$$= 9.41 \text{ g P}$$

Example 14. What mass of ammonium phosphate would contain 15.0 g of nitrogen?

$$? \text{ g } (NH_4)_3PO_4 = 15 \text{ g N} \left(\frac{1 \text{ mole N}}{14.00 \text{ g}}\right)\left(\frac{1 \text{ mole } (NH_4)_3PO_4}{3 \text{ mole N atoms}}\right)\left(\frac{149.08 \text{ g}}{1 \text{ mole } (NH_4)_3PO_4}\right)$$

$$= 53.2 \text{ g } (NH_4)_3PO_4$$

Example 15. What mass of propane, C_3H_8, contains the same mass of carbon as is contained in 1.35 grams of barium carbonate, $BaCO_3$?

$$? \text{ mole C in } BaCO_3 = (1.35 \text{ g } BaCO_3)\left(\frac{1 \text{ mole}}{197.3 \text{ g}}\right)\left(\frac{1 \text{ mole C}}{1 \text{ mole } BaCO_3}\right)$$

$$= 6.8 \text{ X } 10^{-3} \text{ moles of C}$$

want the same number of mole of C in C_3H_8 as $BaCO_3$

$$\text{g } C_3H_8 = (6.8 \text{ X } 10^{-3} \text{ mole C})\left(\frac{1 \text{ mole } C_3H_8}{3 \text{ moles C atoms}}\right)\left(\frac{44 \text{ g } C_3H_8}{1 \text{ mole}}\right)$$

$$= 0.1 \text{ g of } C_3H_8$$

Purity of Samples:

The percent purity of a compound can be used in a collection of unit factors which make problems more difficult. In these problems, it is necessary to have an appropriate scaling factor or multiplier added to the problem to get the right answer. For example, it you have a bottle of ethanol which contains 0.5% benzene impurity, then the ethanol is 99.5 % pure. We can set up a collection of unit factors:

$$\frac{0.5 \text{ g benzene}}{100 \text{ g sample}} \qquad \frac{99.5 \text{ ethanol}}{100 \text{ g sample}} \qquad \frac{0.5 \text{ g benzene}}{99.5 \text{ g ethanol}}$$

Example 16: A bottle of sodium phosphate, Na_3PO_4, is 98.3% pure Na_3PO_4. What are the masses of sodium phosphate and impurities in 250 grams of sample?

$$250 \text{ g sample}\left(\frac{98.3 \text{ g } Na_3PO_4}{100 \text{ g sample}}\right) = 245.8 \text{ g } Na_3PO_4$$

$$250 \text{ g sample}\left(\frac{1.7 \text{ g impurity}}{100 \text{ g sample}}\right) = 4.25 \text{ g impurity}$$

And now on to reaction stoichiometry in which we apply these ideas of STOICHIOMETRY to chemical reactions.