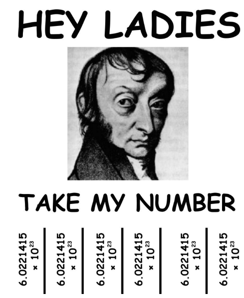
Chemistry 151: Basic Chemistry

Chapter 3 Part II: The Power of the Chemical Formula

The Power of the Chemical Formula

A **chemical formula** provides a lot of information to the chemist.

We will explore the value of **molar mass**, **Avogadro's number** and **percent composition** in order to find the **empirical formula** and **molecular formula**.



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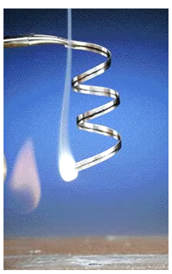
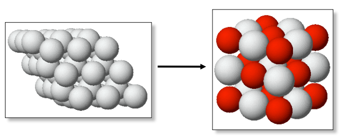
Counting Atoms



Mg burns in air (O_2) to produce white magnesium oxide, MgO.

How can we figure out how much oxide is produced from a given mass of Mg?



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Counting Atoms

Chemistry is a quantitative science - we need a "counting unit."

The MOLE!

A mole is similar to a *dozen* - you can have a dozen roses, a dozen donuts - you can also have a mole of roses, or a mole of donuts

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Particles in a Mole

Avogadro's Number (N_A), *named for* **Amedeo Avogadro,** *1776-1856*

$6.02214076 \times 10^{23}$

A mole is the amount of *any* substance containing 6.022×10^{23} particles

$$\frac{6.022 \times 10^{23} \text{ Cu atoms}}{1 \text{ mole Cu}} \qquad \frac{1 \text{ mole } CO_2}{6.022 \times 10^{23} \text{ molecules } CO_2}$$

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How Big is a Mole?

If you distribute equally 6×10^{23} dollars to every human being on the planet and spend a million dollars an hour it would would take more than 10,000 years to spend your share!

Traveling at the speed of light it would take more than a 100 billion years to travel 6×10^{23} miles!

A stack of 6×10^{23} pennies would be so tall that it would take 100,000 years traveling at the speed of light to go from one end of the stack to the other!

It would take more than a 100 trillion years to print 6×10^{23} dollars at a rate of 100 dollars per second!

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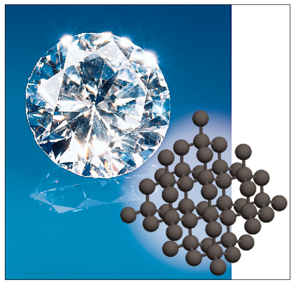
Molar Mass

1 mol of ^{12}C
= 12.00 g of C
= 6.022×10^{23} atoms of C

12.00 g of ^{12}C is its MOLAR MASS

Taking into account all of the isotopes of C, the molar mass of C is 12.011 g/mol



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Molar Mass

1 mol of Al = 26.9815 g of Al
1 mol of Al = 6.022×10^{23} atoms of Al
26.9815 g of Al is its MOLAR MASS
We will write this as: **26.9815 g Al / 1 mol Al**

Find molar mass from periodic table

13	← atomic number
Al	← symbol
26.9815	← atomic weight

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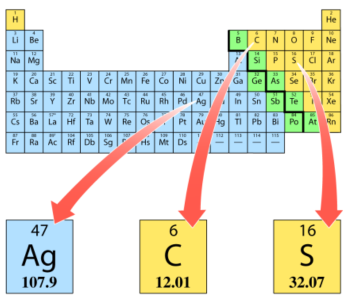
Molar Mass From the Periodic Table

Molar mass is the atomic weight expressed in grams per mol (g/mol), and these values come directly from the periodic table



1 mole Ag = 107.9 g
1 mole C = 12.01 g
1 mole S = 32.07 g

Molar mass of Ag = 107.9 g/mol

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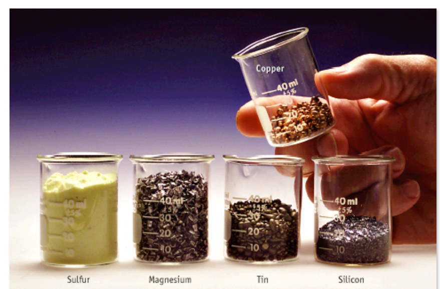
One mole Amounts



63.5 g Cu

32.1 g S   24.3 g Mg   118.7 g Sn   28.1 g Si

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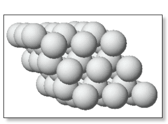

PROBLEM: What amount of Mg is represented by 0.200 g? How many atoms?

Mg has a molar mass of 24.3050 g/mol.

$$0.200 \text{ g} \bullet \frac{1 \text{ mol}}{24.31 \text{ g}} = 8.23 \times 10^{-3} \text{ mol}$$

How many atoms in this piece of Mg?

$$8.23 \times 10^{-3} \text{ mol} \bullet \frac{6.022 \times 10^{23} \text{ atoms}}{1 \text{ mol}}$$

= 4.96×10^{21} atoms Mg

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Atomic Weight

***Atomic Weight*:** The weighted average mass of an element's atoms in a large sample that includes all naturally occurring isotopes of that atom.

Atomic number and atomic weight displayed in periodic table

Atomic weight (amu) and **molar mass** (g/mol): *same number, different units!*

* *Atomic weight for **one** atom*
* *Molar mass for grams in a mole (**6.022×10^{23} atoms**)*

13	← atomic number
Al	← symbol
26.9815	← atomic weight

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Molecular Weight

Molecular weight: The sum of atomic weights for all atoms in a molecule

Example (use a periodic table):

- **Carbon**: **12.01 amu** *(the **atomic weight**)*
- **Oxygen**: **16.00 amu** *(the **atomic weight**)*
- **Carbon monoxide (CO)**: **28.01 amu** = 12.01 + 16.00 *(28.01 is the **molecular weight** for CO)*
- 28.01 *is also the* molar mass *of CO (in* g/mol*) - the mass in grams of 6.022x10*[23] *molecules of CO)*

Molecular weight and molar mass: same number, different units (and uses)

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Molar Mass

Example: Find the molar mass of H_2O.

Water has 2 H and 1 O

2*H = 2*1.008 = 2.016 *grams*

1*O = 1*15.999 = 15.999 *grams*

so: Molar mass =

15.999 + 2.016 = ***18.015 grams per mole***

This means that in 18.015 grams of water we have one mole of molecules of water

One mole of water molecules equals 6.022×10^{23} molecules of water

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We can convert mol of water to g and g of water to mol using "18.0 g / mol" and dimensional analysis:

Molar mass used as conversion factor

$$0.25\ \cancel{\text{mol H}_2\text{O}} \times \frac{18.0\ \text{g H}_2\text{O}}{1\ \cancel{\text{mol H}_2\text{O}}} = 4.5\ \text{g H}_2\text{O}$$

Molar mass used as conversion factor

$$27\ \cancel{\text{g H}_2\text{O}} \times \frac{1\ \text{mol H}_2\text{O}}{18.0\ \cancel{\text{g H}_2\text{O}}} = 1.5\ \text{mol H}_2\text{O}$$

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Molar Mass

What is the molar mass of Urea, $(NH_2)_2CO$?

Solution:

2 x N = 2 x 14.0067 =	**28.0134**
1 x C = 1 x 12.0111 =	**12.0111**
4 x H = 4 x 1.00794 =	**4.03176**
1 x O = 1 x 15.9994 =	**15.9994**
TOTAL =	**60.0556 g/mol**

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Test Yourself Part 1

What is the molar mass of potassium dichromate, $K_2Cr_2O_7$?

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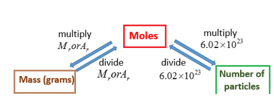
Test Yourself Part 2

How many moles in 35.013 g of $K_2Cr_2O_7$?



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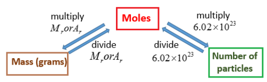
Test Yourself Part 3



How many molecules of $K_2Cr_2O_7$ in 35.013 g?

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Percent Composition

Chemists wish to determine the elements present in a compound and their **percent by mass**.

- Percent by mass also known as "percent by weight"

Example: A 100g sample of a new compound contains 55 g of element X and 45 g of element Y

Percent by mass can be calculated using:

$$\frac{\textit{Mass of element}}{\textit{Mass of compound}} \times 100 = \textbf{percent by mass}$$

55% X and 45% Y

Percents of all elements in compound must equal 100%

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Percent Composition from the Chemical Formula

If you know the chemical formula for a compound, you can calculate its percent composition:

1. Calculate the molar mass of each element in the compound formula unit
   a. Assume sample size is one mole
   b. Multiply the molar mass of the element by its subscript in the chemical formula
2. Divide the mass of the element by the molar mass of the compound unit and multiply by 100

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Percent Composition from the Chemical Formula

Example: Find the percent composition of **water, H_2O**

- Hydrogen – 1.01 x 2 = 2.02 g H in water
  Oxygen – 16.00 x 1 = 16.00 g O in water
  Molar mass = 2.02 + 16.00 = 18.02 g/mol of H_2O

- % of H: $\frac{2.02 \text{ g H}}{18.02 \text{ g } H_2O}$ x 100% = **11.2 %H in Water**
  % of O: $\frac{16.00 \text{ g O}}{18.02 \text{ g } H_2O}$ x 100% = **88.79 %O in Water**

Water is 11.2% H and 88.79% O
Check: 11.2 + 88.8 = 99.99% :)

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Percent Composition from the Chemical Formula

Determine the percent composition of Sodium Hydrogen Carbonate ($NaHCO_3$)

First find molar mass (g/mol)

Na = 1* 22.99 g = 22.99 g Na
H = 1* 1.01 g = 1.01 g H
C = 1* 12.01 g = 12.01 g C
O = 3* 16.00 g = <u>48.00 g O</u>
84.01 g/mol $NaHCO_3$

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Percent Composition from the Chemical Formula

Sodium: $\frac{22.99 \text{ g Na}}{84.01 \text{ g } NaHCO_3}$ x 100% = **27.37 % Na**

Hydrogen: $\frac{1.01 \text{ g H}}{84.01 \text{ g } NaHCO_3}$ x 100% = **1.20 % H**

Carbon: $\frac{12.01 \text{ g C}}{84.01 \text{ g } NaHCO_3}$ x 100% = **14.30 % C**

Oxygen: $\frac{48.00 \text{ g O}}{84.01 \text{ g } NaHCO_3}$ x 100% = **57.14 % O**

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check: 27.37% + 1.20% + 14.30% + 57.14% = 100.01%

Empirical Formula (EF) and Molecular Formula (MF)

Finding the molecular formula (MF) is a "holy grail" for chemists. If they can determine the MF, they know what the compound is, etc.

To find the MF, chemists first have to find the empirical formula (EF), then compare the EF to the molar mass.

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Empirical Formula (EF) and Molecular Formula (MF)

Molecular formula: the true number of atoms of each element in the formula of a compound.

Empirical formula: the lowest whole number ratio of atoms in a compound.

molecular formula = (empirical formula)$_n$

molecular formula = C_6H_6 = $(CH)_6$

empirical formula = CH

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Empirical Formula (EF) and Molecular Formula (MF)

Formulas for ionic compounds are **ALWAYS** empirical (lowest whole number ratio).

Examples:

$NaCl$ $Al_2(SO_4)_3$

$MgCl_2$ K_2CO_3

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Empirical Formula (EF) and Molecular Formula (MF)

Formulas for molecular compounds *MIGHT* be empirical (lowest whole number ratio).

Molecular:	H_2O	$C_6H_{12}O_6$	$C_{12}H_{22}O_{11}$
	↓	↓	↓
Empirical:	H_2O	CH_2O	$C_{12}H_{22}O_{11}$

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Empirical Formula (EF) and Molecular Formula (MF)

Molecular Formula	Empirical Formula
N_2O	N_2O
$C_2H_4O_2$	CH_2O
$C_2H_6O_2$	CH_3O
N_2O_4	NO_2

Notice:

1. The molecular formula and the empirical formula *can* be identical
2. You scale up from the empirical formula to the molecular formula by a whole number factor

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Empirical Formula via Mass Percentages

To find the Empirical Formula from mass percentages:

1. Assume 100 grams of the substance and convert % into grams.
2. Convert grams to moles by dividing the amount in grams by the molar mass of that element.
3. Select the SMALLEST mole value and divide ALL mole values by this smallest one.
4. The results of Step 3 will either be VERY close to whole numbers or will be recognizable mixed number fractions If any result from Step 3 is a decimal mixed number, you must multiply ALL values by some number to make it a whole number. Ex: 1.33 x 3, 2.25 x 4, 2.50 x 2, etc.

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Let's see some examples

Empirical Formula via Mass Percentages

Example: The percent composition of a sulfur oxide is 40.05 % S and 59.95 % O. Find the empirical formula.

Step 1: Convert % to grams (assume 100 g), then find moles of each element

$$\frac{40.05 \text{ g S}}{32.07 \text{ g/mol S}} = 1.249 \text{ mol S}$$

$$\frac{59.95 \text{ g O}}{16.00 \text{ g/mol O}} = 3.747 \text{ mol O}$$

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Empirical Formula via Mass Percentages

Example: The percent composition of a sulfur oxide is 40.05 % S and 59.95 % O. Find the empirical formula.

Step 2: Divide the mole values by the value of the element with the *smallest* number of moles (sulfur).

$$\frac{1.249 \text{ mol S}}{1.249} = 1 \text{ mol S}$$

$$\frac{3.747 \text{ mol O}}{1.249} = 3 \text{ mol O}$$

Empirical Formula = SO_3

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Empirical Formula via Mass Percentages

In this example, the simplest whole number mole ratio of S atoms to O atoms is 1:3. The empirical formula for the oxide of sulfur is **SO_3**

Note that the calculated mole values may not always be whole numbers.

In these cases all the mole values must be multiplied by the smallest factor that will make them whole numbers

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Practice Problem

Butene is hydrocarbon, a compound composed only of carbon and hydrogen. It is 85.63% carbon and 14.37% hydrogen. What is the empirical formula?

Assume 100 g total.

85.63 g C * (mol C / 12.01 g C) = 7.130 mol C

14.37 g H * (mol C / 1.008 g H) = 14.26 mol H

14.26 / 7.130 = 2.000 mol H

7.130 / 7.130 = 1.000 mol C

Empirical Formula = CH_2

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Molecular Formulas

Two or more substances with distinctly different properties can have the same percent composition and the same empirical formula

Example: NO_2 and N_2O_4: same EF, different compounds

Example: C_2H_4 and C_4H_8: same EF, different compounds

Empirical formulas do not always indicate the actual moles in the compound! Chemists need a molecular formula to fully describe a compound.

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Determining Molecular Formulas

A molecular formula specifies the actual number of atoms of each element in one molecule or formula unit of the substance

The **molar mass** must be determined through a separate experiment *(mass spectrometer)* and compared with the empirical formula to find the molecular formula.

Let's see an example!

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Determining Molecular Formulas

Example: The molar mass of a compound is 181.50 g/mol and the empirical formula is C_2HCl. What is the molecular formula?

First, find molar mass of empirical formula (C_2HCl):
2*C + 1*H + 1*Cl = 2*12.01 + 1*1.01 + 1*35.45
= 60.48 g/mol for C_2HCl

Now compare molar mass of compound (181.50) to molar mass of EF (60.48) - should always get a whole number!
181.50 / 60.48 = 3.001 which is essentially 3

Multiply this ratio by the EF to get the MF:
Molecular Formula = $(C_2HCl)_3$ = $\mathbf{C_6H_3Cl_3}$

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Test Yourself!

Analysis of a weak acid finds a chemical composition of 49.32 %C, 6.85 %H, and 43.84 %O. The molar mass is 146 g/mol. Determine the empirical and molecular formulas.

Steps:
- assume 100 g, so %s equal g of the element
- turn g of element into moles
- divide moles by smallest number to find EF
- turn EF into a molar mass
- compare molar mass of compound (146) to EF molar mass to find ratio, then MF

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Test Yourself!

Analysis of a weak acid finds a chemical composition of 49.32 %C, 6.85 %H, and 43.84 %O. The molar mass is 146 g/mol. Determine the empirical and molecular formulas.

49.32 %C = 49.32 g of C, etc. *Turn to moles:*
49.32 g C * (mol C / 12.01 g C) = 4.107 mol C
6.85 g H * (mol H / 1.01 g H) = 6.78 mol H
43.84 g O * (mol C / 16.00 g O) = 2.740 mol O

2.740 is smallest, so find EF:
C(4.107/2.740) H(6.78/2.740) O(2.740/2.740)
C(1.499) H(2.47) O(1.000) ≈ $C_{1.5}\ H_{2.5}\ O_1$

Multiply by 2 to eliminate fraction:
$(C_{1.5}\ H_{2.5}\ O_1)_2$ = $\mathbf{C_3H_5O_2}$ = *Empirical Formula*

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Test Yourself!

Analysis of a weak acid finds a chemical composition of 49.32 %C, 6.85 %H, and 43.84 %O. The molar mass is 146 g/mol. Determine the empirical and molecular formulas. (EF = $C_3H_5O_2$ via previous page)

To find MF, *find molar mass of EF ($C_3H_5O_2$) and compare to 146 g/mol:*

(3C*12.01 g/mol) + (5H*1.01 g/mol) + (2O*16.00 g/mol) = 73.07 g/mol *(molar mass of EF)*

146 / 73.07 = 2.00 *ratio should always be whole number*

$(C_3H_5O_2)_2$ = **$C_6H_{10}O_4$ = molecular formula (MF)**

This is adipic acid!

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Test Yourself!

A colorless liquid composed of 46.68% nitrogen and 53.32% oxygen has a molar mass of 60.01 g/mol. What is the molecular formula?

Answers: EF = NO, MF = N_2O_2

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End of Chapter 3 Part II