Empirical and Molecular Formulas

Things to Remember…

- Chemical formulas are very important; they:
  - state which elements are in the molecule
  - give the exact number of atoms of each element that are in the molecule
  - may give an indication as to how the elements are bonded together

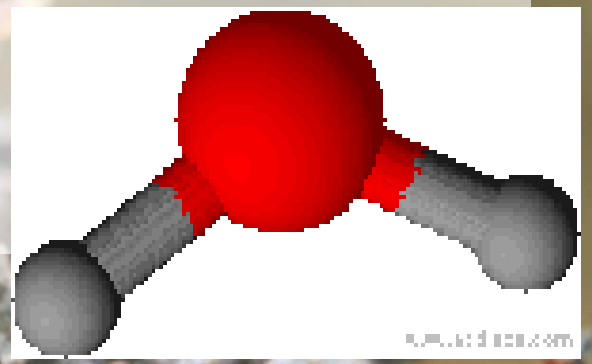
Law of Definite Proportions

- In 1779, Joseph Proust showed that the proportion of the mass of the elements in copper carbonate always stays the same.
- This is called the law of definite proportions; it is also sometimes called the law of constant composition.
- When elements combine to form compounds, they do so in a definite proportion.
- The percentage composition of an element can be expressed as:

$$\% \text{ mass} = \frac{\text{mass of the element}}{\text{mass of the compound}} \times 100\%$$

Law of Definite Proportions

- Water has the chemical formula H_2O.
- In terms of mass, its molecule is always made up of 11% hydrogen and thus the remaining mass (89%) must be oxygen.
- Notice how much more massive the oxygen atom is in this image of the water molecule.
- Similarly, CO_2 is always made up of 27.3% carbon.



Percentage composition of compounds

- The percentage composition is the percentage of an element in a compound, in relation to its total mass.

Calculate the percentage composition by mass of sodium sulphate, Na_2SO_4.

Na - $2 \times 22.9877 = 45.9754$ g/mol

S - $1 \times 32.06 = 32.06$ g/mol

O - $4 \times 15.9994 = 63.9976$ g/mol

molecule 142.03714 g/mol

Na% $= \frac{45.9754}{142.03714} \times 100\%$

$= 32.37\%$

S% $= \frac{32.06}{142.03714} \times 100\%$

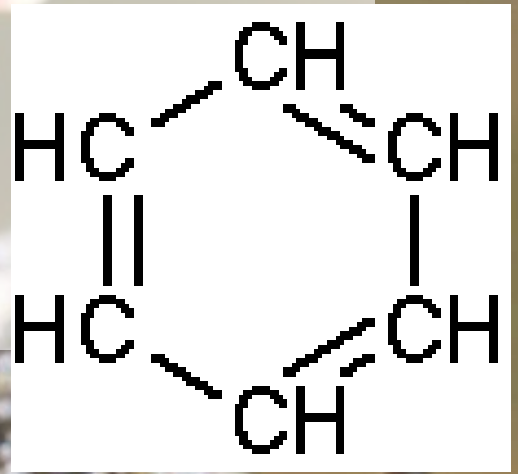
$= 22.57\%$

O% $= \frac{63.996}{142.0374} \times 100\%$

$= 45.06\%$

Empirical Formula

- A chemical's empirical formula indicates the simplest ratio in which the different atoms are combined. It is also called the simplest formula.
- For example the empirical formula for acetylene (C_2H_2) is CH, $HC{\equiv}CH$ since there is 1 C for every H.
- However, benzene also has the empirical formula CH; but its chemical formula is C_6H_6.
- Benzene and acetylene are not the same chemical; each compound is unique in terms of physical and chemical properties



Steps for Finding the Empirical Formula

- Consider the amounts you are given as being in units of grams.
- If percentages are given instead of grams, assume them to be grams (since percentages add up to 100, then your sample's mass will be 100 g).
- Convert the grams to moles for each element.
- Find the smallest whole number ratio of moles for each element.

A sample of calcium chloride contains 1.82 g of calcium and 3.23 g of chlorine. What is the empirical formula for the compound?

	Mass	Mol	Ratio
Ca	1.82 g	0.0454	1
Cl	3.23 g	0.09116	2
total			

$n = \frac{m}{MM}$

divide all moles by smallest value!

$n_{Ca} = \frac{1.82}{40.08}$

$= 0.0454$ mol

$n_{Cl} = \frac{3.23}{35.453}$

$= 0.09116$

∴ The empirical formula is $CaCl_2$

A sample of calcium chloride contains 1.82 g of calcium and 3.23 g of chlorine. What is the empirical formula for the compound?

The elemental analysis of an unknown organic compound returns the following data:

%C = 64.6%
%H = 10.8%
%O = 24.6%
What is the empirical formula for this compound?

	%	Assume 100g	mole	ratio	
C	64.6	64.6g	5.37	3.48 x2	7
H	10.8	10.8g	10.71	7 x2	14
O	24.6	24.6g	1.54	1 x2	2

$n = \frac{m}{mm}$

R.T. →

∴ Empirical $C_7H_{14}O_2$.

Please Try... Q 1–4 not 5-6

1. Suppose a compound is analyzed and reveals that is composed of 85.7% carbon and 14.3% hydrogen. Find the empirical formula for this compound.
2. Determine the empirical formula for a compound which is broken down into 6.16 g of sulphur and 8.84 g sodium.

H/C ratio = 14.19 mol H / 7.14 mol C = 2
There are 2 H for each C.
The empirical formula is CH_2

Na/S ratio = 0.3845 mol Na / 0.1921 mol S = 2
There are 2 Na for each S.
The empirical formula is Na_2S

	Empirical	Molecular	M.M
acetylene	$\boxed{CH}$	C_2H_2	~~24~~ 26.04
benzene	CH	C_6H_6	78.13

Molecular Formula

- The molecular formula indicates the number of atoms of each element in a molecule. It is determined using the empirical formula and the molar mass.

Steps for finding the molecular formula:

- Determine the compound's empirical formula.
- Divide the compound's molar mass by the mass of the empirical formula.
- Multiply each subscript in the empirical formula by this number.

Hydrogen peroxide is made of 5.03% hydrogen and 79.87% oxygen. Its molar mass is 34.01 g/mol. Find its molecular formula.

	%	Ass 100g	Moles	Ratio
H	5.03	5.03g	4.99	1
O	79.87	79.87g	4.99	1

$n = \frac{m}{Mm}$

Empirically

HO

1.0079 + 15.9994

= 17.... g/mol

34.01 ÷ 17

= 2

2(HO)

H_2O_2

If 4.04 g of nitrogen combine with 11.46 g of oxygen to produce a compound with a molar mass of 108.0 g/mol, what is the molecular formula of this compound?

	mass	mole	Ratio	
N	4.04g	0.288	1	2
O	11.46g	0.716	2.5	5

$n = \frac{m}{mm}$

N_2O_5

$N - 2 \times 14.0067$

$O - 5 \times 15.9994$

108

∴ The molecular formula is ~~HO_5~~ N_2O_5

Determine the molecular formula of a compound with an empirical formula of NH_2 and a molar mass of 32.06 g/mol.

Substance		Formaldehyde	Acetic acid	Glucose
Empirical formula		CH_2O	CH_2O	CH_2O
Molecular formula		CH_2O	$C_2H_4O_2$	$C_6H_{12}O_6$
Use		biological preservative	vinegar	sweetener
Physical properties	State	gas	liquid	solid
	Molar mass (g/mol)	30	60	180
	Melting point (°C)	-92	16	140
	Boiling point (°C)	-19.5	118	decomposes