Chemical Formulae

Chemical formulae are used as shorthand to indicate how many atoms of one element combine with another element to form a compound.

C_2H_6, 2 atoms of carbon combine with 6 atoms of hydrogen to form ethane.
$Mn(Cr_2O_7)_2$, one Mn combines with 4 Cr and 14 O to form manganese(II) dichromate.

If we know the formula of a compound, determining the molar mass is simple. Since we know the atomic masses of the elements, we can sum the atomic masses to obtain the molecular masses.

1 atom of C_2H_6 contains 2 atoms of C	12.01 amu =	24.02
1 atom of C_2H_6 contains 6 atoms of H	1.0079 amu =	6.0474
		30.0674 = 30.07 amu

We also know that 1 mole of C atoms weighs 12.01 g and 1 mol of H atoms weighs 1.0079 g. So, we know the molar mass of ethane also.

1 mole C_2H_6, 2 moles of C	12.01 g x 2	24.02 g
1 mole C_2H_6, 6 moles of H	1.0079 g x 6	6.0474 g
		30.0674 = 30.07 g/mole

Or, 30.07 g in 1 mole C_2H_6. So, we say the molar mass of ethane is 30.07 g/mol (that's grams per mole).

1 mole $Na_2Cr_2O_7$, 2 mole of Na	22.989 g x 2	47.978 g
1 mole $Na_2Cr_2O_7$, 2 mole of Cr	51.996 g x 2	103.992 g
1 mole $Na_2Cr_2O_7$, 7 moles of O	15.9994 g x 7	111.9958 g
		263.9658 = 263.97 g/mole

MW (which means molar mass) of $(C_5(CH_3)_5)Re(NO)(CO)_2BF_4$.

$$12 \text{ mol C} \times \frac{12.01 \text{ g C}}{1 \text{ mol C}} = 144.12 \text{ g C}$$

$$15 \text{ mol H} \times \frac{1.0079 \text{ g H}}{1 \text{ mol H}} = 15.1185 \text{ g H}$$

$$1 \text{ mol B} \times \frac{10.81 \text{ g B}}{1 \text{ mol B}} = 10.81 \text{ g B}$$

$$4 \text{ mol F} \times \frac{18.998 \text{ g F}}{1 \text{ mol F}} = 75.992 \text{ g F}$$

$$1 \text{ mol N} \times \frac{14.01 \text{ g N}}{1 \text{ mol N}} = 14.01 \text{ g N}$$

$$3 \text{ mol O} \times \frac{15.9994 \text{ g O}}{1 \text{ mol O}} = 47.9982 \text{ g O}$$

$$1 \text{ mol Re} \times \frac{186.207 \text{ g Re}}{1 \text{ mol Re}} = 186.207 \text{ g Re}$$

$$\text{MW} = 494.26 \text{ g/mol}$$

Percent Composition

Why do we care about percent composition?

When an elemental analysis is performed we do not get the molecular formula. The result of an elemental analysis is always reported as a percent mass of each of the elements for which the analysis was performed.

An elemental analysis of a white crystalline compound believed to be $C_6H_{12}O_6$, analyzed for C, H and O gave the following results.

C = 40.00 % , H = 6.71 %, O = 53.28 % by wt.

Is the compound actually $C_6H_{12}O_6$?

Start the problem with the assumption that you have 100.0 g of sample. The percent composition tells you how much of each element is present:

$$100.0 \text{ g sample} \times \frac{40.00 \text{ g C}}{100.0 \text{ g sample}} = 40.00 \text{ g C}$$

$$100.0 \text{ g sample} \times \frac{6.71 \text{ g H}}{100.0 \text{ g sample}} = 6.71 \text{ g H}$$

$$100.0 \text{ g sample} \times \frac{53.28 \text{ g O}}{100.0 \text{ g sample}} = 53.28 \text{ g O}$$

Now we have to determine the number of atoms/moles of each element present.

$$100.0 \text{ g sample} \times \frac{40.00 \text{ g C}}{100.0 \text{ g sample}} = 40.00 \text{ g C} \times \frac{1 \text{ mol C}}{12.01 \text{ g C}} = 3.330 \text{ mol}$$

$$100.0 \text{ g sample} \times \frac{6.71 \text{ g H}}{100.0 \text{ g sample}} = 6.71 \text{ g H} \times \frac{1 \text{ mol H}}{1.0079 \text{ g H}} = 6.66 \text{ mol}$$

$$100.0 \text{ g sample} \times \frac{53.28 \text{ g O}}{100.0 \text{ g sample}} = 53.28 \text{ g O} \times \frac{1 \text{ mol O}}{15.9994 \text{ g O}} = 3.33 \text{ mol}$$

Finally we reduce the number of moles to the smallest whole number ratio.

1 C for 2 H for 1 O.

According to our calculations we have CH_2O or formaldehyde (which is a gas)!

Are we wrong...NO! We have determined the *ratios* in which the elements are combined to form the compound, but not the actual amount of the elements present. To determine the actual amount of each element present we need to know the Molar Mass (often referred to as the molecular weight or MW).

The molar mass must be determined using another experiment (A mass spectrometer could determine the molar mass. There are other less expensive ways to determine molar mass, and we will discuss some of them next semester.)

The molar mass was determined to be 180.16 g/mol.

To determine the molecular formula we will use the empirical formula which

$$CH_2O$$

we just found. The molecule must be made up of some number of empirical formula units; that way the ratio of the elements remains the same:

molecular formula = (a number) x (empirical formula)

If we knew any two of these numbers then we could find the third, but we only know one.

We are not dead in the water though, because we also know molar mass = (a number) x (empirical mass)

Since, empirical mass CH_2O = 30.25 g/mole

180.16 g/mol = (a number) x 30.25 g/mol

(a number) = 5.956 or 6

molecular formula = (6) x (CH_2O) So, we did have $C_6H_{12}O_6$
Essentially we found how many empirical formula units are in the whole.

A bottle of improperly labeled "iron oxide" is found in a laboratory. Elemental analysis reveals that the sample is iron and oxygen, and the sample is 69.94 % iron by mass. What is the formula of the material, and what should the bottle be labeled; that is, name the compound?

To find the formula we need to know the % mass of each of the elements.
Since, there are only 2 different elements in iron oxide we know...

%Fe + %O = 100 %

100 % - %Fe = %O

100 % - 69.94 % = %O

%O = 30.06 %

now that we have % mass of both elements let's find the formula

assume 100 g sample

$$30.06 \text{ g O} \times \frac{1 \text{ mol O}}{15.9994 \text{ g O}} = 1.8788 \text{ mol O}$$

$$69.94 \text{ g Fe} \times \frac{1 \text{ mol Fe}}{55.85 \text{ g Fe}} = 1.2523 \text{ mol Fe}$$

reduce to lowest ratio by dividing each number by the smallest number...

$$\frac{1.8788 \text{ mol O}}{1.2523} = 1.500 \text{ mol O}$$

$$\frac{1.2523 \text{ mol Fe}}{1.2523} = 1 \text{ mol Fe}$$

do not want fractions in a formula so we must find the lowest common whole number multiple

Multiplying 1.5 by 2 gives a whole number; i.e., 3

So, multiply each number by 2

1.5 x 2 = 3 mol O and 1 Fe x 2 = 2 mol Fe

So, the formula is

Fe_2O_3

The name is iron(III) oxide

To find a formula we do not need to have % composition.

If we are told the mass of each element present in a compound we can find the formula. The mass of the elements can be converted to moles of the elements. The mole ratio tells us the empirical formula

For example,

A compound containing only Mn and Cl contains 1.9228 g Mn and 2.4817 g Cl. Determine the empirical formula.

We simply need to convert the masses of the elements to moles. The empirical formula is determined by the mole ratio of Mn to Cl.

$$1.9228 \text{ g Mn} \times \frac{1 \text{ mol Mn}}{54.938 \text{ g Mn}} = 0.034999 \text{ mol Mn}$$

$$2.4817 \text{g Cl} \times \frac{1 \text{ mol Cl}}{35.453 \text{ g Cl}} = 0.070000 \text{ mol Cl}$$

reducing to 1 by dividing by 0.034999

$$1.9228 \text{ g Mn} \times \frac{1 \text{ mol Mn}}{54.938 \text{ g Mn}} = 0.034999 \text{ mol Mn} \quad = 1$$

$$2.4817 \text{g Cl} \times \frac{1 \text{ mol Cl}}{35.453 \text{ g Cl}} = 0.070000 \text{ mol Cl} \quad = 2$$

The formula is

$MnCl_2$

Combustion analysis is used to determine the formula of hydrocarbons (a compound containing on hydrogen and carbon).

Combustion of a hydrocarbon with a molar mass of 78.11 g/mol produced 2.6406 g CO_2 and 0.5400 g H_2O. Determine the molecular formula.

$$C_{(?)}H_{(?)} + (?)\ O_2 \longrightarrow (?)\ CO_2 + (?)\ H_2O$$

Since we do not know the formula we cannot balance the equation.

> The important thing to note is that all the carbon in the CO_2 must come from the hydrocarbon. All the hydrogen in the water must also come from the hydrocarbon!

If we determine the number of moles of C in the CO_2 we will have the number of moles of carbon in the hydrocarbon. If we determine the number of moles of H in the H_2O we have the number of moles of H in the hydrocarbon.

$$2.6406\ \text{g}\ CO_2 \times \frac{1\ \text{mol}\ CO_2}{44.01\ \text{g}\ CO_2} \times \frac{1\ \text{mol C}}{1\ \text{mol}\ CO_2} = 0.06000\ \text{mol C}$$

$$0.5400\ \text{g}\ H_2O \times \frac{1\ \text{mol}\ H_2O}{18.00\ \text{g}\ H_2O} \times \frac{2\ \text{mol H}}{1\ \text{mol}\ H_2O} = 0.06000\ \text{mol H}$$

the empirical formula is

CH

So, the molecular formula is made up of some number of empirical formula units. Use the molar mass and the empirical formula mass to determine that number.

$$78.11 \text{ g/mol} = (\text{A \#}) \times \;\; 13.018 \text{ g/mol}$$

$$(\text{A \#}) = 6.000$$

The molecule contains 6 empirical formula units. The molecular formula is

$$C_6H_6$$