EMPIRICAL AND MOLECULAR FORMULA

Percent Composition: law of constant composition states that any sample of a pure compound always consists of the same elements combined in the same proportions by mass

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

EXAMPLE:

Here is CH_3COOH.

First, figure out the molar mass from the formula. It is 60.05 g/mol.

Second, figure out the grams each atom contributes by multiplying the atomic weight by the subscript.

Carbon = 2 x 12.011 g = 24.022 g

Hydrogen = 4 x 1.008 = 4.032 g

Oxygen = 2 x 16.00 = 32.00 g

Third, divide the answer for each atom by the molar mass and multiply by 100 to get a percentage.

Carbon's percentage: (24.022 g / 60.05 g) x 100 = 40.00 %

Hydrogen's percentage: (4.032 g / 60.05 g) x 100 = 6.71 %

Oxygen's percentage: (32.00 g / 60.05 g) = 53.29 %

Empirical and Molecular Formulas: assume 100 g sample if given %'s

Empirical formula: subscripts represent the smallest ratio of atoms in a formula unit:

1) convert all grams (=%) to moles
2) divide by smallest # of moles
3) create whole number ratio of subscripts (multiply through by integer if needed)

EXAMPLE:

In an unknown molecule, there is 4.15 g carbon and 1.38 g hydrogen. Determine the empirical formula for the substance.

Step 1. Divide mass of each substance by atomic mass to determine number of moles of each substance

4.15 g C/12.0 g C = .346 mol C

1.38 g H/1 g H = 1.38 mol H

Step 2. Divide number of moles of each substance by smallest number of moles to determine what the ratio of carbon is to hydrogen

.346 mol C/.346 mol C = 1

1.38 mol H/.346 mol C = 4

This indicates that for every 1 carbon atom there are 4 hydrogen atoms.

The empirical formula would be CH_4.

EXAMPLE:

Phenol, a general disinfectant, is 76.57% C, 6.43% H, and 17.00% O. Determine its empirical formula.

Step 1. A 100.00g sample of phenol contains 76.57g C, 6.43g H, 17.00g O.

Step 2. Convert the masses of C, H, and O to numbers of moles.

$$76.57\text{g C} \times \frac{1 \text{ mol C}}{12.011 \text{ g C}} = 6.375 \text{ mol C}$$

$$6.43\text{g H} \times \frac{1 \text{ mol H}}{1.008 \text{ g H}} = 6.38 \text{ mol H}$$

$$17.00\text{g O} \times \frac{1 \text{ mol O}}{15.999 \text{ g O}} = 1.063 \text{ mol O}$$

Step 3. Divide each of the quantities above by the smallest, and use the result as subscripts in a tentative formula.

C = 6.375/1.063 = 5.997
H = 6.38/1.063 = 6.00
O = 1.063/1.063 = 1.000
C_6H_6O

Since all the subscripts are integers, there is no need to multiply each subscript by a common factor to convert them all to integers.

The empirical formula of phenol is C_6H_6O.

Molecular formula represents the actual # of atoms in a molecule:

1) Need to be given molar mass of actual compound.
2) Calculate molar mass of your empirical formula
3) Molar mass of compound ÷ molar mass of empirical formula= multiple of number of atoms in molecular formula
4) Apply multiple to empirical ratio

The empirical formula of hydroquinone, a chemical used in photography, is C_3H_3O, and its molecular weight is 110 g/mol.

What is its molecular formula?

The formula weight based on the empirical formula is 55g/mol. If all the subscripts are multiplied by two
(110/55.0 = 2), the molar mass of the empirical formula becomes equal to the molecular weight or molar mass of the compound
2(55.0g/mol) = 110g/mol.
The molecular formula is $2(C_3H_3O)$ or $C_6H_6O_2$

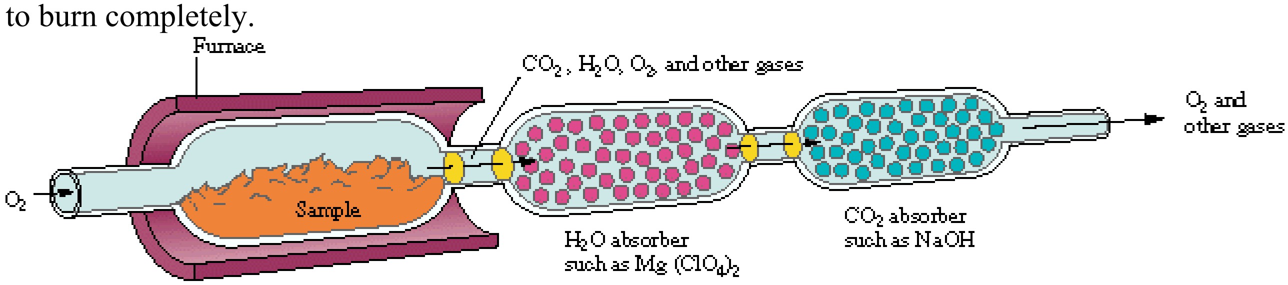
ANALYSIS BY COMBUSTION

$C_?H_?$ + O_2 → CO_2 + H_2O

- All carbons go to carbon dioxide
- All hydrogens go to water

  - ✓ To find formulas we need grams of carbon and grams of hydrogen in original hydrocarbon.
  - ✓ Grams of Carbon → the molar mass of CO_2 provides a conversion factor between g C and g CO_2 (12.01 g C = 44.01 g CO_2)
  - ✓ Grams of Hydrogen → the molar mass of H_2O provides a conversion factor between g of H and g of H_2O (2.02 g H = 18.02 g H_2O)
  - ✓ If compound also contains oxygen,
    g of oxygen = sample mass - [g of C + g of H]
  - ✓ Grams are converted to moles

In practice, a combustible sample is placed in an oven under an oxygen stream and heated to burn completely.



The H_2O formed gas stream is trapped in a desiccant such as $Mg(ClO_4)_2$, the CO_2 is absorbed in a base (like NaOH), and the excess O_2 just vents off. Weighing the traps before and after the combustion gives one the weight of the evolved CO_2 and H_2O.

EXAMPLE:
Imagine that a 5.0000 g sample of some unknown containing the elements C, H and O (actually acetic acid) is subjected to such a combustion analysis. The traps yield 7.3285 g CO_2 and 3.000 g H_2O.
$C_?H_?O_?$ + O_2 → CO_2 + H_2O

Find grams of C and H to find oxygen subtract grams of H and C from mass of sample:
But CO_2 isn't C, and H_2O isn't H.

We need the molar mass of CO_2 and water

Molar masses CO_2 = (AW C) + 2×(AW O)
= 12.011 g/mol + 2(15.999 g/mol) = 44.009 g CO_2 / mol CO_2

$$\mathbf{7.3285\ g\ CO_2 \times \frac{12\ g\ C}{44.009\ g\ CO_2} = 1.998\ g\ C\ or\ 2.00\ g\ C}$$

MW H_2O = (AW O) + 2×(AW H)
= 15.999 g/mol + 2(1.008 g/mol) = 18.015 g H_2O / 1 mol H_2O

$$\mathbf{3.00\ g\ H_2O \times \frac{2\ g\ H}{18.015\ g\ H_2O} = 0.3357\ g\ H}$$

Grams O = So a total of 2.000 g C+0.3357 g H=2.336 g of the unknown is C and H. The rest, 5.0000 g sample - 2.336 g C and H =**2.664 g O**

Convert g to MOLES

$$C = \frac{2.00\ g}{12\ g/mol} = 0.1666666\ \text{mole of C}$$

$$H = \frac{0.3357\ g}{1\ g/mol} = 0.3357\ \text{mole H}$$

$$O = \frac{2.6664\ g}{16\ g/mol} = 0.16665\ \text{mole O}$$

Determine molar ratio:

C = 0.166666 mole/.16665 mole = 1
H = 0.3357/0.16666 mole = 2
O= 0.16665 mole/ 0.16665 mole = 1

CH_2O

Exercises

1. The molecular formula of the antifreeze ethylene glycol is $C_2H_6O_2$. What is the empirical formula?

2. A well-known reagent in analytical chemistry, dimethylglyoxime, has the empirical formula C_2H_4NO. If its molar mass is 116.1 g/mol, what is the molecular formula of the compound?

3. Nitrogen and oxygen form an extensive series of oxides with the general formula NxOy. One of them is a blue solid that comes apart, reversibly, in the gas phase. It contains 36.84% N. What is the empirical formula of this oxide?

4. A sample of indium chloride weighing 0.5000 g is found to contain 0.2404 g of chlorine What is the empirical formula of the indium compound?

5. A combustion device was used to determine the empirical formula of a compound containing only carbon, hydrogen, and oxygen. If the data determined from a .6349 g sample of the unknown is that 1.603 g of CO_2 and .2810 g of H_2O were produced, determine the empirical formula of the compound.

6. The analysis of a rocket fuel showed that it contained 87.4% nitrogen and 12.6% hydrogen by weight. Mass spectral analysis showed the fuel to have a molar mass of 32.05g. What are the empirical and molecular formulas of the fuel?

<u>Answers</u>:
1. CH_3O
2. Molar mass of empirical formula is 58.06 g/mol. Thus molecular formula is $C_4H_8N_2O_2$.
3. The empirical formula is thus N_2O_3. (The name is dinitrogen trioxide.)
4. $InCl_3$.
5. $C_7H_6O_2$
6. empirical formula: NH_2
molecular formula: N_2H_4
(the compound is called hydrazine)