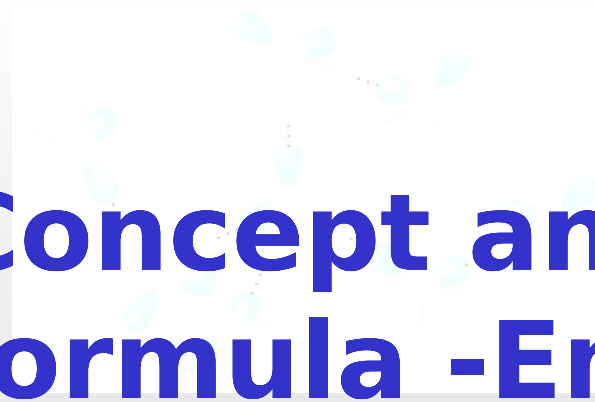


The Mole Concept and Chemical formula -Empirical and Molecular Formula OR Counting Atoms

REF: CHAPTER 6 OF TEXTBOOK

TOPICS COVERED:

- ✓THE LAW OF DEFINITE PROPORTIONS
- ✓CALCULATIONS OF FORMULA UNIT AND MOLECULAR MASSES
- ✓PERCENT COMPOSITION OF A COMPOUND
- ✓THE MOLE: THE CHEMIST'S COUNTING UNITS
- ✓RELATIONSHIP BETWEEN MOLE AND AVOGADRO NUMBER

- ✓RELATIONSHIP BETWEEN ATOMIC MASS UNITS (amu) AND MOLAR MASS OR GRAM UNITS (g/mol)
- ✓THE MOLE AND CHEMICAL CALCULATIONS
- ✓EMPIRICAL AND MOLECULAR FORMULAS
- ✓DETERMINATION OF EMPIRICAL FORMULAS
- ✓DETERMINATION OF MOLECULAR FORMULAS

THE LAW OF DEFINITE PROPORTIONS OR

The Law of Constant Composition

Compounds are fixed species. They are described by formulas. They are considered pure substances since:

- THEY ARE *CHEMICAL* COMBINATIONS OF TWO OR MORE ELEMENTS.
- THEY *CAN* BE BROKEN DOWN INTO ELEMENTS BY *CHEMICAL* MEANS BUT *NOT* BY *PHYSICAL* MEANS.
- THEY HAVE A *DEFINITE* AND *CONSTANT* ELEMENTAL COMPOSITION.

THE LAW OF DEFINITE PROPORTIONS OR THE LAW OF CONSTANT COMPOSITION.

THE LAW OF DEFINITE PROPORTIONS STATES:

- IN A PURE COMPOUND THE ELEMENTS ARE ALWAYS PRESENT IN THE SAME DEFINITE PROPORTION BY MASS.
- COMPOUNDS HAVE CHEMICAL AND PHYSICAL PROPERTIES BASED ON THIS LAW OF DEFINITE PROPORTIONS.
- NO MATER HOW MUCH WATER IS IN A CONTAINER, IT WILL ALWAYS BOIL AT 100°C. IT’S COMPOSITION DOESN’T CHANGE WITH MASS.

<u>Composition of Water</u>

- Water always contains the same two elements: hydrogen and oxygen.
- WATER IS ALWAYS 11.2% HYDROGEN <u>BY MASS</u>.
- WATER IS ALWAYS 88.8% OXYGEN <u>BY MASS</u>.
- WATER ALWAYS HAS THESE PERCENTAGES. IF THE PERCENTAGES WERE DIFFERENT THE COMPOUND WOULD NOT BE WATER.

Composition of Ammonia

- NH_3 always contains the same two elements: nitrogen and hydrogen.
- AMMONIA IS ALWAYS 82.24% NITROGEN BY MASS.
- AMMONIA IS ALWAYS 17.76% HYDROGEN BY MASS.
- AMMONIA ALWAYS HAS THESE PERCENTAGES. IF THE PERCENTAGES WERE DIFFERENT THE COMPOUND WOULD NOT BE AMMONIA.

PERCENT COMPOSITION OF COMPOUNDS

FROM THE FORMULA OR FROM EXPERIMENT

Percent Composition From the Formula

- IF THE FORMULA OF A COMPOUND IS KNOWN, A TWO-STEP PROCESS IS NEEDED TO CALCULATE THE PERCENT COMPOSITION.

Step 1 Calculate the formula mass or molecular mass.

Step 2 Divide the mass of each element in the formula by the total mass and multiply by 100.

FORMULA MASS AND MOLECULAR MASS

- **FORMULA MASS**: THE SUM OF THE ATOMIC MASSES OF THE ATOMS IN ONE FORMULA UNIT, EXPRESSED IN ATOMIC MASS UNITS (AMU).
- **MOLECULAR MASS**: THE SUM OF THE ATOMIC MASSES OF THE ATOMS IN ONE MOLECULE.

  MAY ALSO BE CALLED **FORMULA WEIGHT** OR **MOLECULAR WEIGHT**.

Formula Mass for NaCl	Formula Mass for $MgCl_2$	Molecular Mass for H_2O
22.99 amu (Na)	24.30 amu (Mg)	[2 x 1.01 amu (H)]
+ 35.45 amu (Cl)	+ [2 x 35.45 amu (Cl)]	+ 16.00 amu (O)
58.44 amu NaCl	95.20 amu $MgCl_2$	18.02 amu H_2O

Reference : Section 5.6 of Textbook, page 145 mass of the element X 100 = Percentage of the Element

total mass of compound

Calculate the percent composition of hydrosulfuric acid: H_2S.

Step 1 Calculate the molecular mass of H_2S.

$$2\ H = 2 \times 1.01\text{amu} = 2.02\ \text{amu}$$

$$\underline{1\ S = 1 \times 32.07\ \text{amu} = 32.07\ \text{amu}}$$

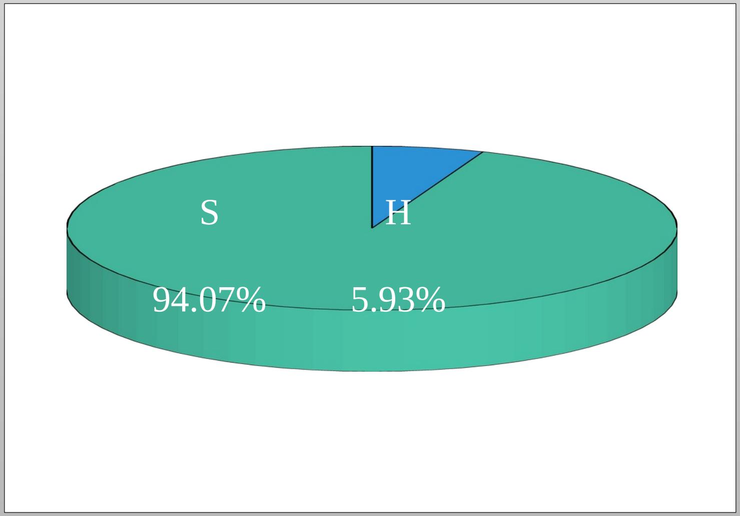
$$34.09\ \text{amu}$$

Calculate the percent composition of hydrosulfuric acid: H_2S.

Step 2 Divide the mass of each element by the molecular mass and multiply by 100.

%H = 2.02 amu / 34.09 amu x 100 = 5.93%

%S = 32.07 amu / 34.09 amu x 100 = 94.07%



Percent Composition From Experimental Information

- PERCENT COMPOSITION CAN BE CALCULATED FROM EXPERIMENTAL DATA WITHOUT KNOWING THE COMPOSITION OF THE COMPOUND.

Step 1 Calculate the mass of the compound formed.

Step 2 Divide the mass of each element by the total mass of the compound and multiply by 100.

A compound containing nitrogen and oxygen is found to contain 1.52 g of nitrogen and 3.47 g of oxygen. Determine its percent composition.

Step 1 Calculate the total mass of the compound

1.52 g N

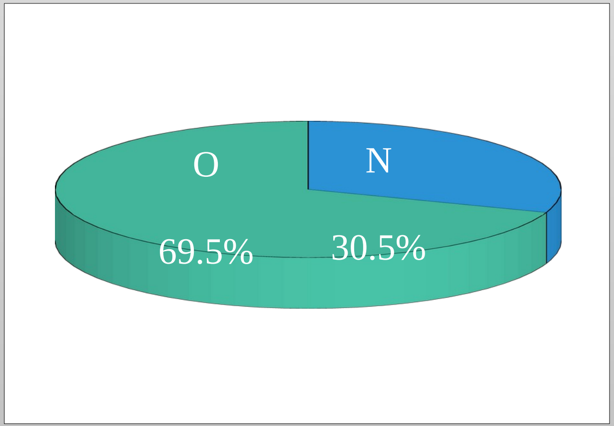
<u>3.47 g O</u>

4.99 g = total mass of product

A compound containing nitrogen and oxygen is found to contain 1.52 g of nitrogen and 3.47 g of oxygen. Determine its percent composition.

Step 2 Divide the mass of each element by the total mass of the compound formed.

$$\left(\frac{1.52\ \text{g N}}{4.99\ \text{g}}\right)(100) = 30.5\%$$



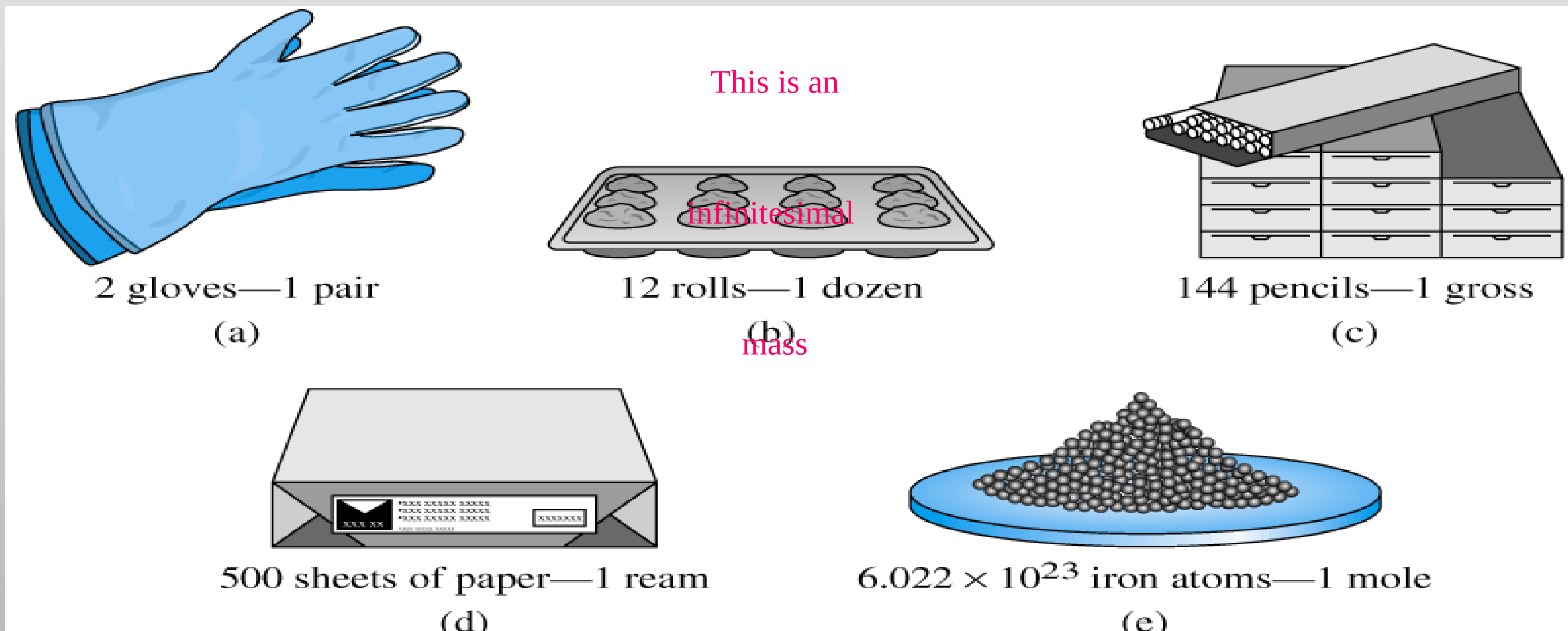
$$\left(\frac{3.47\ \text{g O}}{4.99\ \text{g}}\right)(100) = 69.5\%$$

COUNTING ATOMS AND MOLECULES

ATOMS AND MOLECULES ARE SO TINY, THAT YOU GENERALLY NEED BILLIONS OF THEM TO HAVE A MEASURABLE AMOUNT.

CHEMISTS REQUIRED A UNIT FOR COUNTING WHICH COULD EXPRESS LARGE NUMBERS OF ATOMS USING SIMPLE NUMBERS. THUS, THE UNIT WOULD BE LIKE OTHER COUNTING UNITS WE EMPLOY…

mass of hydrogen atom = 1.673×10^{-24} g



COUNTING ATOMS AND MOLECULES

- ATOMS ARE TOO SMALL TO COUNT INDIVIDUALLY. WE COUNT ATOMS IN GROUPS.
- THE ACTUAL NUMBER OF ATOMS IN 12.01g OF C-12 DETERMINED EXPERIMENTALLY.
- ITS NUMERICAL VALUE IS 6.0221415×10^{23} ATOMS.
- THEREFORE, A 12.01 g SAMPLE OF CARBON CONTAINS 6.0221415×10^{23} CARBON ATOMS.
- OUR OPERATIONAL RULE WILL USE VALUE 6.022×10^{23} FOR AVOGADRO'S NUMBER.

- **Well, chemists have chosen a unit for counting atoms.**
- **That unit is the…**

MOLE

1 mole = 6.022×10^{23} objects

1 mole of atoms = 6.022×10^{23} atoms

1 mole of molecules = 6.022×10^{23} molecules

1 mole of ions = 6.022×10^{23} ions

6.022×10^{23}

is a very

LARGE

number

$$6.022 \times 10^{23}$$

This number is called:

Avogadro's Number

Named after Lorenzo Romano Amedeo Carlo Avogadro, an Italian physicist.

SPECIES

H

QUANTITY

1 mole of H atoms

NUMBER OF H

6.022×10^{23}

SPECIES	H_2
QUANTITY	1 mole of molecules
	6.022×10^{23}
NUMBER OF H	

SPECIES

Na

QUANTITY

1 mole of atoms

6.022×10^{23}

NUMBER OF NA

SPECIES

Fe

QUANTITY

1 mole of atoms

NUMBER OF FE

6.022×10^{23}

SPECIES C_6H_6

QUANTITY 1 mole of molecules

NUMBER OF C_6H_6 MOLECULES 6.022×10^{23}

- **CURIOUSLY ENOUGH, CHEMISTS DECIDED ON THE FOLLOWING ABBREVIATION FOR THE MOLE UNIT:**
- **mol**

THE MASS OF A MOLE

- THE MASS OF THE MOLE, ***MOLAR MASS***, IS NOT THE SET NUMBER, IT VARIES FOR EACH CHEMICAL.
- THE ***MOLAR MASS*** OF AN ELEMENT, IS A MASS IN GRAMS NUMERICALLY EQUAL TO THE ATOMIC MASS OF THE ELEMENT, WHEN THE ELEMENT IS PRESENT IN ATOMIC FORM.
- IF WE KNOW THE ATOMIC MASS OF AN ELEMENT, WE KNOW THE MASS OF 1 MOLE OF ATOMS OF THE ELEMENT.

THE MASS OF A MOLE

- THE MOLECULAR FORM OF AN ELEMENT WILL HAVE DIFFERENT MOLAR MASS THAN IT'S ATOMIC FORM.
  - MOLAR MASS OF OXYGEN ATOM 'O'= 16.00 g
  - MOLAR MASS OF AN OXYGEN GAS 'O_2'= 32.00 g
  - MOLAR MASS OF OZONE GAS 'O_3' = 48.00 g
- THE **MOLAR MASS** IS THE MASS, IN GRAMS, OF ONE MOLE OF ATOMS, MOLECULES OR FORMULA UNITS OF A SUBSTANCE.

THE **MOLAR MASS** OF A COMPOUND IS A MASS IN GRAMS THAT IS **NUMERICALLY EQUAL** TO THE **FORMULA MASS** OR **MOLECULAR MASS** OF THE COMPOUND.

MOLECULAR MASS OF H_2O = 18.02 amu

MASS OF 1 MOLE H_2O MOLECULES = 18.02 g

So the units of molar mass are given as g/mol.

Moles of Substance	⟷ Molar mass	Grams of Substance

Avogadro's Number of Particles

6.022 x 10^{23} Particles

1 MOLE

Molar Mass

Avogadro's Number of Ca atoms

6.022 x 10^{23} Ca atoms

1 MOLE Ca

40.08 g Ca

Avogadro's Number of H_2O molecules

6.022×10^{23} H_2O molecules

1 MOLE H_2O

18.02 g H_2O

Avogadro's Number of H_2SO_4 molecules

6.022×10^{23} H_2SO_4 molecules

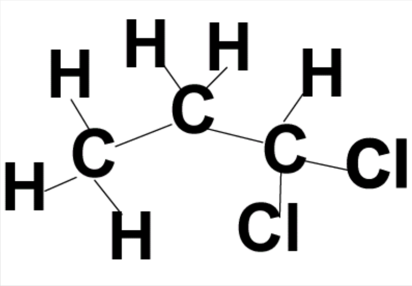
1 MOLE H_2SO_4

98.08g H_2SO_4

- **THE SUBSCRIPTS OF CHEMICAL FORMULAS DENOTE THE RATIO OF ATOMS TO EACH OTHER.**

One molecule of $C_3H_6Cl_2$ contains:

3 atoms C
6 atoms H
2 atoms Cl



One dozen molecules of $C_3H_6Cl_2$ contains:

3 dozen atoms C
6 dozen atoms H
2 dozen atoms Cl

One mole of $C_3H_6Cl_2$ contains:

3 mol C
6 mol H
2 mol Cl

HOW MANY MOLES OF IRON REPRESENTS IN 25.0 g OF IRON?

- MOLAR MASS IRON = 55.85 g/mol

Conversion sequence: grams Fe → moles Fe

Set up the calculation using a conversion factor between moles and grams.

$$(\text{grams Fe})\left(\frac{1\ \text{mol Fe}}{55.85\ \text{g Fe}}\right)$$

$$(25.0\ \cancel{\text{g Fe}})\left(\frac{1\ \text{mol Fe}}{55.85\ \cancel{\text{g Fe}}}\right) = 0.448\ \text{mol Fe}$$

MORE EXAMPLES

What is the mass, in grams, of 4.6 mol $MgCl_2$?

$$4.6\ \cancel{\text{mol } MgCl_2} \left(\frac{95.20 \text{ g } MgCl_2}{1\ \cancel{\text{mol } MgCl_2}} \right) = 4.4 \times 10^2 \text{ g } MgCl_2$$

How many $MgCl_2$ formula units are in 4.6 mol $MgCl_2$?

$$4.6\ \cancel{\text{mol } MgCl_2} \left(\frac{6.022 \times 10^{23} \text{ formula units } MgCl_2}{1\ \cancel{\text{mol } MgCl_2}} \right)$$

$$= 2.8 \times 10^{24} \text{ formula units } MgCl_2$$

How many oxygen ***molecules*** are present in 2.00 mol of oxygen molecules?

Conversion factor needed:

$$\left(\frac{6.022 \text{ x } 10^{23} \text{ molecules } O_2}{1 \text{ mol } O_2}\right)$$

Conversion sequence:

moles O_2 → molecules O_2

$$(2.00 \cancel{\text{mol } O_2})\left(\frac{6.022 \text{ x } 10^{23} \cancel{\text{molecules } O_2}}{1 \cancel{\text{mol } O_2}}\right)$$

$$= 1.20 \text{ x } 10^{24} \text{ molecules } O_2$$

How many moles of benzene, C_6H_6, are present in 390.0 grams of benzene?

The molar mass of C_6H_6 is 78.12 g/mol.

Conversion sequence: grams C_6H_6 → moles C_6H_6

Use the conversion factor: $\dfrac{78.12 \text{ grams } C_6H_6}{1 \text{ mole } C_6H_6}$

$$(390.0 \cancel{\text{g } C_6H_6})\left(\frac{1 \text{ mole } C_6H_6}{78.12 \cancel{\text{g } C_6H_6}}\right) = 5.000 \text{ moles } C_6H_6$$

How many grams of $(NH_4)_3PO_4$ are contained in 2.52 moles of $(NH_4)_3PO_4$?

The molar mass of $(NH_4)_3PO_4$ is 149.12 g/mol.

Conversion sequence: moles $(NH_4)_3PO_4$ → grams $(NH_4)_3PO_4$

Use the conversion factor: $\dfrac{149.12 \text{ grams } (NH_4)_3PO_4}{1 \text{ mole } (NH_4)_3PO_4}$

$$(2.52 \cancel{\text{ mol } (NH_4)_3PO_4}))\left(\frac{149.12 \text{ g } (NH_4)_3PO_4}{1 \cancel{\text{ mol } (NH_4)_3PO_4}}\right)$$

$$= 376\text{g } (NH_4)_3PO_4$$

56.04 g of N_2 contains how many N_2 molecules?

The molar mass of N_2 is 28.02 g/mol.

Conversion sequence: g N_2 → moles N_2 → molecules N_2

Use the conversion factors

$$\frac{1 \text{ mol } N_2}{28.02 \text{ g } N_2} \qquad \frac{6.022 \times 10^{23} \text{ molecules } N_2}{1 \text{ mol } N_2}$$

$$(56.04 \cancel{\text{ g } N_2})\left(\frac{1 \cancel{\text{ mol } N_2}}{28.02 \cancel{\text{ g } N_2}}\right)\left(\frac{6.022 \times 10^{23} \text{ molecules } N_2}{1 \cancel{\text{ mol } N_2}}\right)$$

$$= 1.204 \times 10^{24} \text{ molecules } N_2$$

Knowing moles or atoms or grams or molecules you can calculate the other units

Moles of substance	Avagadro's ⟷ Number	Particles of substance
Moles of substance	Molar ⟷ Mass	Grams of substance
Moles of Compound	Formula ⟷ Subscripts	Moles of Element within compound

EMPIRICAL FORMULA VERSUS MOLECULAR FORMULA

- THE **EMPIRICAL FORMULA** OR *SIMPLEST FORMULA* GIVES THE SMALLEST WHOLE-NUMBER **RATIO** OF THE ATOMS PRESENT IN A FORMULA UNIT OR COMPOUND.

- The **empirical formula** gives the relative number of atoms of each element present in the molecule of a covalent compound.

- The **molecular formula** represents the total number of atoms of each element present in one molecule of a compound.

- THE **MOLECULAR FORMULA** IS THE TRUE FORMULA OF A MOLECULAR COMPOUND AND CAN BE FOUND FROM THE EMPIRICAL FORMULA *AND* MOLAR MASS.

EXAMPLES OF FORMULA UNITS AND EMPIRICAL FORMULAS

Formula Unit $CaCl_2$

–

Empirical Formula $CaCl_2$

Smallest Whole Number Ratio Ca:Cl 1:2

EXAMPLES OF MOLECULAR FORMULAS AND EMPIRICAL FORMULAS

Molecular Formula C_2H_4

–

Empirical Formula CH_2

Smallest Whole Number Ratio C:H 1:2

Molecular Formula	C_6H_6
–	
Empirical Formula	CH
Smallest Whole Number Ratio	C:H 1:1

Molecular Formula H_2O_2

–

Empirical Formula HO

Smallest Whole Number Ratio $H:O$ 1:1

Some Empirical and Molecular Formulas

Compound	Empirical formula	Molecular formula	Compound	Empirical formula	Molecular formula
Acetylene	CH	C_2H_2	Diborane	BH_3	B_2H_6
Benzene	CH	C_6H_6	Hydrazine	NH_2	N_2H_4
Ethylene	CH_2	C_2H_4	Hydrogen	H	H_2
Formaldehyde	CH_2O	CH_2O	Chlorine	Cl	Cl_2
Acetic acid	CH_2O	$C_2H_4O_2$	Bromine	Br	Br_2
Glucose	CH_2O	$C_6H_{12}O_6$	Oxygen	O	O_2
Hydrogen chloride	HCl	HCl	Nitrogen	N	N_2
Carbon dioxide	CO_2	CO_2			

CALCULATING EMPIRICAL FORMULAS

STEP 1 ASSUME A DEFINITE STARTING QUANTITY (USUALLY 100.0 g) OF THE COMPOUND, IF NOT GIVEN, AND EXPRESS THE MASS OF EACH ELEMENT IN GRAMS.

Step 2 CONVERT THE GRAMS OF EACH ELEMENT INTO MOLES OF EACH ELEMENT USING EACH ELEMENT’S MOLAR MASS.

STEP 3 DIVIDE THE MOLES OF ATOMS OF EACH ELEMENT BY THE MOLES OF ATOMS OF THE ELEMENT THAT HAD THE SMALLEST VALUE

- If the numbers obtained are whole numbers, use them as subscripts and write the empirical formula.
- If the numbers obtained are not whole numbers, go on to step 4.

STEP 4 MULTIPLY THE VALUES OBTAINED IN STEP 3 BY THE SMALLEST NUMBERS THAT WILL CONVERT THEM TO WHOLE NUMBERS

Use these whole numbers as the subscripts in the empirical formula.

EXAMPLE:

$FeO_{1.5}$

$Fe_{1 \times 2}O_{1.5 \times 2} \longrightarrow Fe_2O_3$

- THE RESULTS OF CALCULATIONS MAY DIFFER FROM A WHOLE NUMBER.
  - If they differ ±0.1 round off to the next nearest whole number.

    2.9 3

  - Deviations greater than 0.1 unit from a whole number usually mean that the calculated ratios have to be multiplied by a whole number.

PROBLEMS

The analysis of a salt shows that it contains $\boxed{56.58\%}$ potassium (K); $\boxed{8.68\%}$ carbon (C); and $\boxed{34.73\%}$ oxygen (O). Calculate the empirical formula for this substance.

Step 1 Express each element in grams. Assume 100 grams of compound.

$$K = \boxed{56.58\text{ g}}$$

$$C = \boxed{8.68\text{ g}}$$

$$O = \boxed{34.73\text{ g}}$$

The analysis of a salt shows that it contains 56.58% potassium (K); 8.68% carbon (C); and 34.73% oxygen (O). Calculate the empirical formula for this substance.

Step 2 Convert the grams of each element to moles.

$$\text{K:}\ (56.58\ \cancel{\text{g K}})\left(\frac{1\ \text{mol K atoms}}{39.10\ \cancel{\text{g K}}}\right) = 1.447\ \text{mol K atoms}$$

$$\text{C:}\ (8.68\ \cancel{\text{g C}})\left(\frac{1\ \text{mol C atoms}}{12.01\ \cancel{\text{g C}}}\right) = 0.723\ \text{mol C atoms}$$

0.723 mol C atoms

C has the smallest number of moles

$$\text{O:}\ (34.73\ \cancel{\text{g O}})\left(\frac{1\ \text{mol O atoms}}{16.00\ \cancel{\text{g O}}}\right) = 2.171\ \text{mol O atoms}$$

The analysis of a salt shows that it contains 56.58% potassium (K); 8.68% carbon (C); and 34.73% oxygen (O). Calculate the empirical formula for this substance.

Step 3 Divide each number of moles by the smallest value.

$$K = \frac{1.447 \text{ mol}}{0.723 \text{ mol}} = \boxed{2.00} \qquad C: \frac{0.723 \text{ mol}}{0.723 \text{ mol}} = 1.00$$

$$O = \frac{2.171 \text{ mol}}{0.723 \text{ mol}} = \boxed{3.00}$$

0.723 mol C atoms

C has the smallest number of moles

The simplest ratio of K:C:O is 2:1:3

Empirical formula $K_{\boxed{2}}CO_{\boxed{3}}$

The percent composition of a compound is $\boxed{25.94\%}$ nitrogen (N), and $\boxed{74.06\%}$ oxygen (O). Calculate the empirical formula for this substance.

Step 1 Express each element in grams. Assume 100 grams of compound.

$$N = \boxed{25.94\ g}$$

$$O = \boxed{74.06\ g}$$

The percent composition of a compound is 25.94% nitrogen (N), and 74.06% oxygen (O). Calculate the empirical formula for this substance.

Step 2 Convert the grams of each element to moles.

$$\text{N:}\ \left(25.94\ \cancel{\text{g N}}\right)\left(\frac{1\ \text{mol N atoms}}{14.01\ \cancel{\text{g N}}}\right) = 1.852\ \text{mol N atoms}$$

$$\text{O:}\ \left(74.06\ \cancel{\text{g O}}\right)\left(\frac{1\ \text{mol O atoms}}{16.00\ \cancel{\text{g O}}}\right) = 4.629\ \text{mol O atoms}$$

The percent composition of a compound is 25.94% nitrogen (N), and 74.06% oxygen (O). Calculate the empirical formula for this substance.

Step 3 Divide each number of moles by the smallest value.

$$N = \frac{1.852 \text{ mol}}{1.852 \text{ mol}} = \boxed{1.000} \qquad O: \frac{4.629 \text{ mol}}{1.852 \text{ mol}} = \boxed{2.500}$$

This is not a ratio of whole numbers.

The percent composition of a compound is 25.94% nitrogen (N), and 74.06% oxygen (O). Calculate the empirical formula for this substance.

Step 4 Multiply each of the values by $\boxed{2}$.

N: $(1.000)\boxed{2} = \boxed{2.000}$

O: $(2.500)\boxed{2} = \boxed{5.000}$

Empirical formula $N_{\boxed{2}}O_{\boxed{5}}$

CALCULATING THE MOLECULAR FORMULA FROM THE EMPIRICAL FORMULA

- THE MOLECULAR FORMULA CAN BE CALCULATED FROM THE EMPIRICAL FORMULA IF THE MOLAR MASS IS KNOWN.
- The molecular formula will be equal to the empirical formula or some multiple *n* of it.
- To determine the molecular formula evaluate *n*.
- *n* is the number of units of the empirical formula contained in the molecular formula.

$$n = \frac{\text{molar mass}}{\text{mass of empirical formula}} = \text{number of empirical formula units}$$

What is the molecular formula of a compound which has an empirical formula of CH_2 and a molar mass of $\boxed{126.2\text{ g}}$?

Let n = the number of formula units of CH_2.

Calculate the mass of each CH_2 unit

$$1\text{ C} = 1(12.01\text{ g}) = 12.01\text{g}$$

$$2\text{ H} = 2(1.01\text{ g}) = \underline{2.02\text{g}}$$

$$14.03\text{g}$$

$$n = \frac{\boxed{126.2\text{ g}}}{14.03\text{ g}} = 9 \text{ (empirical formula units)}$$

The molecular formula is $(CH_2)_9 = C_9H_{18}$