Empirical Formulas

Empirical Formulas vs Molecular Formulas

Molecular Formula: The exact number of atoms of each element that is combined (for example, glucose: $C_6H_{12}O_6$)

Empirical Formula: The simplest ratio of atoms of each element in a particular compound (for example, glucose: $C_1H_2O_1$)

The relationship between molecular formula and empirical formula:

The molecular formula is equal to the empirical formula times some integer, n, where n = 1, 2, 3 …

Why do we distinguish between molecular formulas and empirical ones?

Two separate experiments are often needed to evaluate the molecular formula

A brief review :

Calculating the Chemical Composition of Substances by Relative Mass

Consider the substance: NaCl

What % by mass of NaCl is sodium?

Na: 23 g/mol

Cl: 35.5 g/mol

NaCl: 58.5 g/mol

Na: 23g/58.5 =

0.393

Cl: 35.5/58.5 =

0.607

0.393+0.607 = 1.0

Empirical Formulas

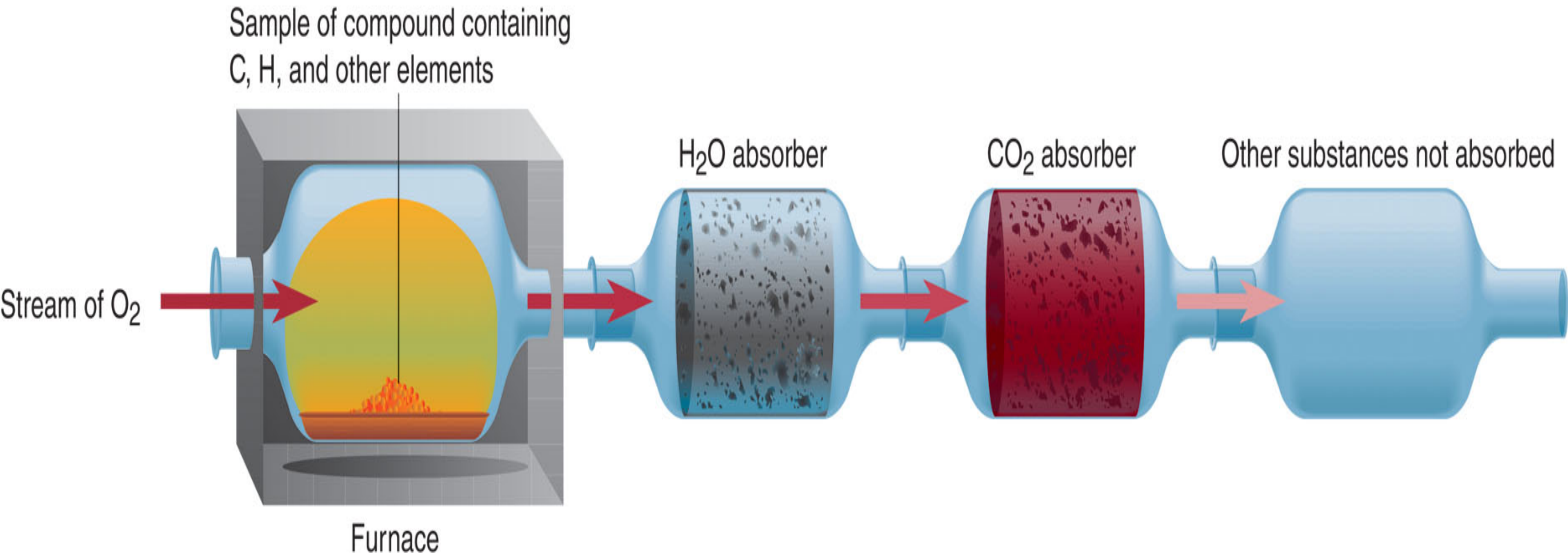
Consider glucose, $C_6H_{12}O_6$: How was the molecular formula of glucose determined?

Combustion of organic compounds:

Most organic compounds when burned in an excess of oxygen form CO_2 and H_2O quantitatively.

$$C_6H_{12}O_6 + O_2 = CO_2 + H_2O$$

$$C_6H_{12}O_6 + 6O_2 = 6CO_2 + 6H_2O$$


Sample of compound containing
C, H, and other elements
Stream of O_2
H_2O absorber
CO_2 absorber
Other substances not absorbed
Furnace

When 1.0 g glucose is burned it gives rise to 1.467 g of CO_2 and 0.6 g H_2O

Can we determine the empirical formula of glucose from this information?

Before beginning we need to know one more thing: the elements present in glucose – C, H, O.

If all of the carbon in CO_2 comes from the carbon in glucose, how much of the 1.467 g of CO_2 isolated is due to the mass of carbon?

Since we know the composition of CO_2, we can determine this exactly;

In one mol of CO_2, we have 12 g of C combined with 32 g of O_2

The fractional mass due to C in CO_2 is? 12g/(12 + 32) = 0.2727

1.467 g * 0.2727 = 0.400 g C in 1.0 g of glucose

In H_2O 2 gH/18 g/mol = 0.111

Similarly for hydrogen: 0.111 * 0.6g = 0.0666 g H

When 1.0 g glucose is burned it gives rise to 1.467 g of CO_2 and 0.6 g H_2O

$$C_6H_{12}O_6 + 6O_2 = 6CO_2 + 6H_2O$$

0.400 g C + 0.0666 g H = 0.4666 g accounted for,

Therefore, the remainder must be due to oxygen

1.0g – 0.466g = 0.534 g oxygen

0.40 g C

0.0666 g H

0.534 g O

0.40 g C/12 g/mol = 0.033 mol

0.066 g H/1 g/mol = 0.066 mol

0.534 g O/16 g/mol = 0.033 mol

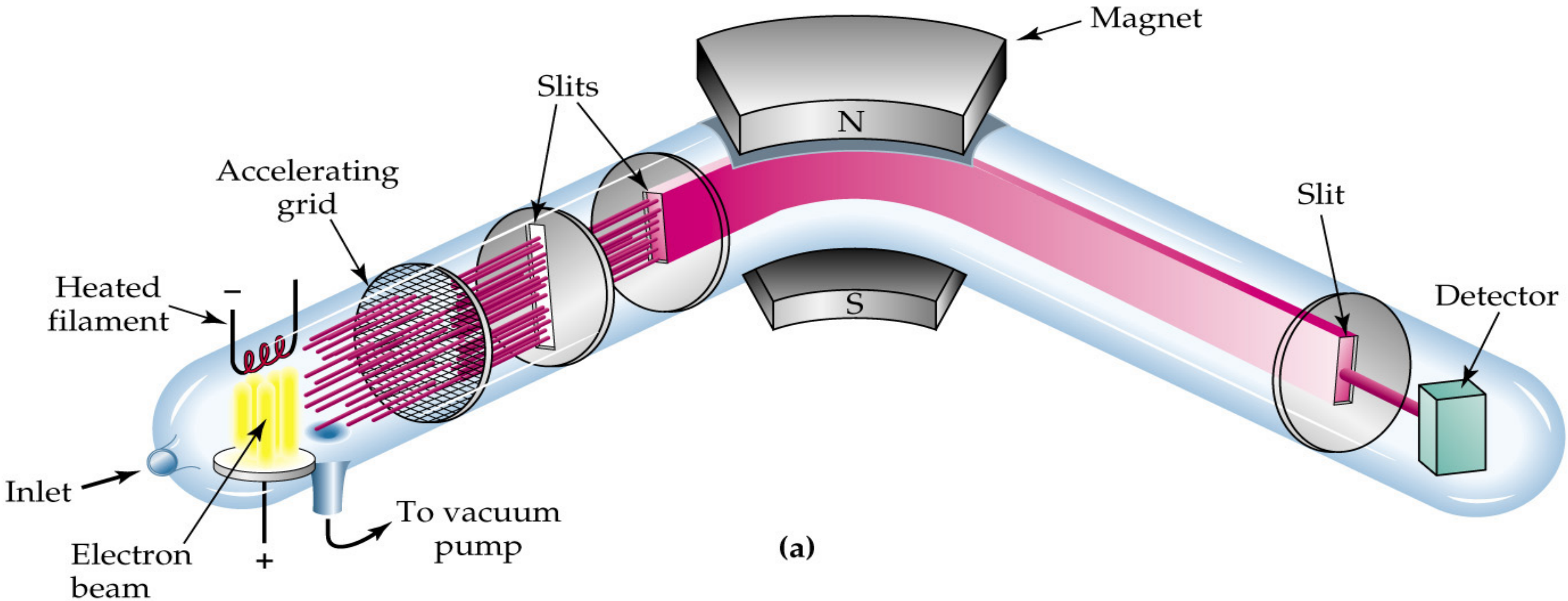
The ratio of C: H: O atoms in glucose is 1: 2: 1

The ratio of atoms in glucose (empirical formula) must be $C_1H_2O_1$

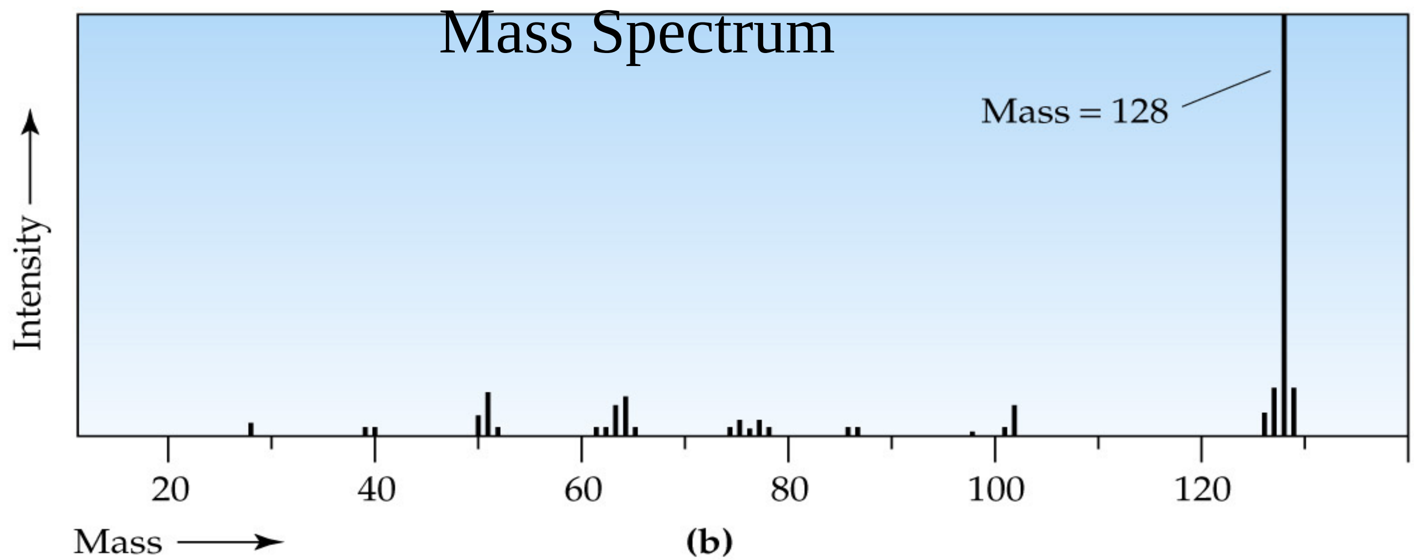
Unless we know the molecular weight of glucose we cannot proceed any further.

Numerous methods have been developed over the years to measure molecular weight.

Mass spectrometry, Melting point depression, …



Sample → Sample^{+} → mass/charge is analyzed



The ratio of atoms in glucose (empirical formula) must be $C_1H_2O_1$

If we assume a molecular weight of 180 g /mol obtained by mass spectrometry

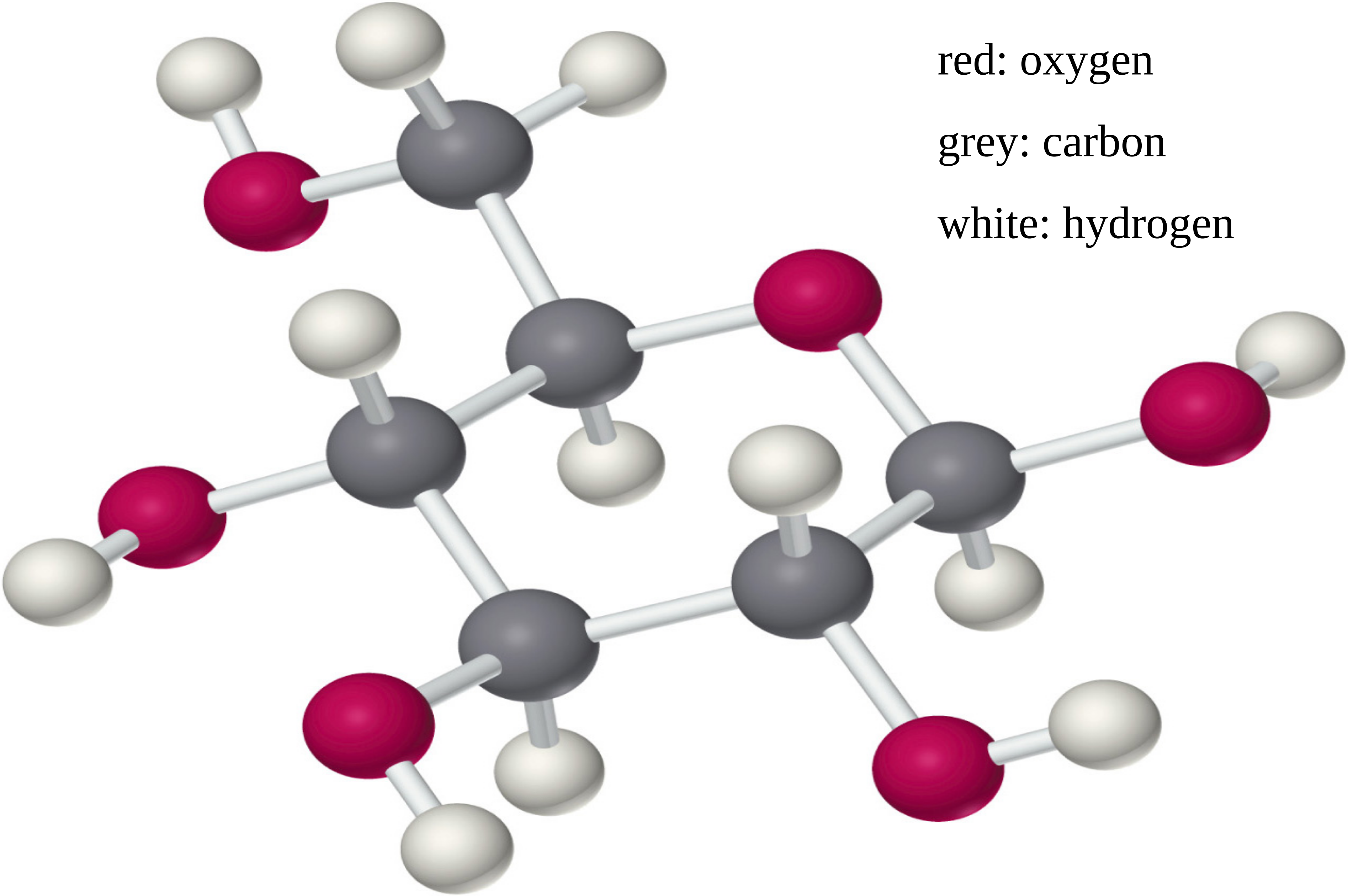
$C_1H_2O_1$ = (12 + 2 +16) = 30 g/mol

180/30 = 6

Molecular formula = $C_6H_{12}O_6$

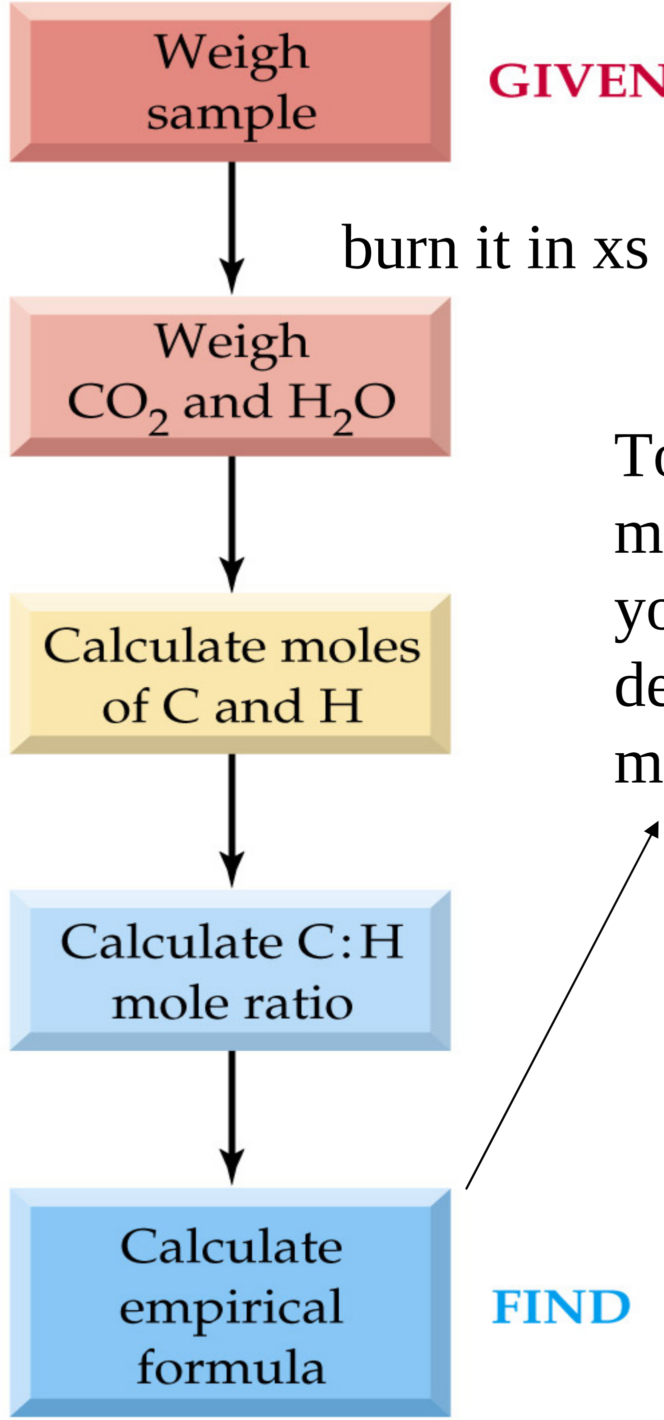
Other methods of determining molecular weights include:

Freezing point depression; Boiling point elevation, Osmotic pressure; Titration



Glucose

In Summary



burn it in xs O_2

To determine the molecular formula, you need to determine the molecular weight

Solutions

Solute: substance present is the smallest amount

Solvent: the most abundant substance present

Define molarity (<u>M</u>) as: mols of solute /liter of solution

What is the molarity of water?

How do we calculate it?

How many grams of H_2O in 1000 mL?

1000 g

How many mols in 1000g?

1000g/18 g/mol = 55.5 <u>M</u>

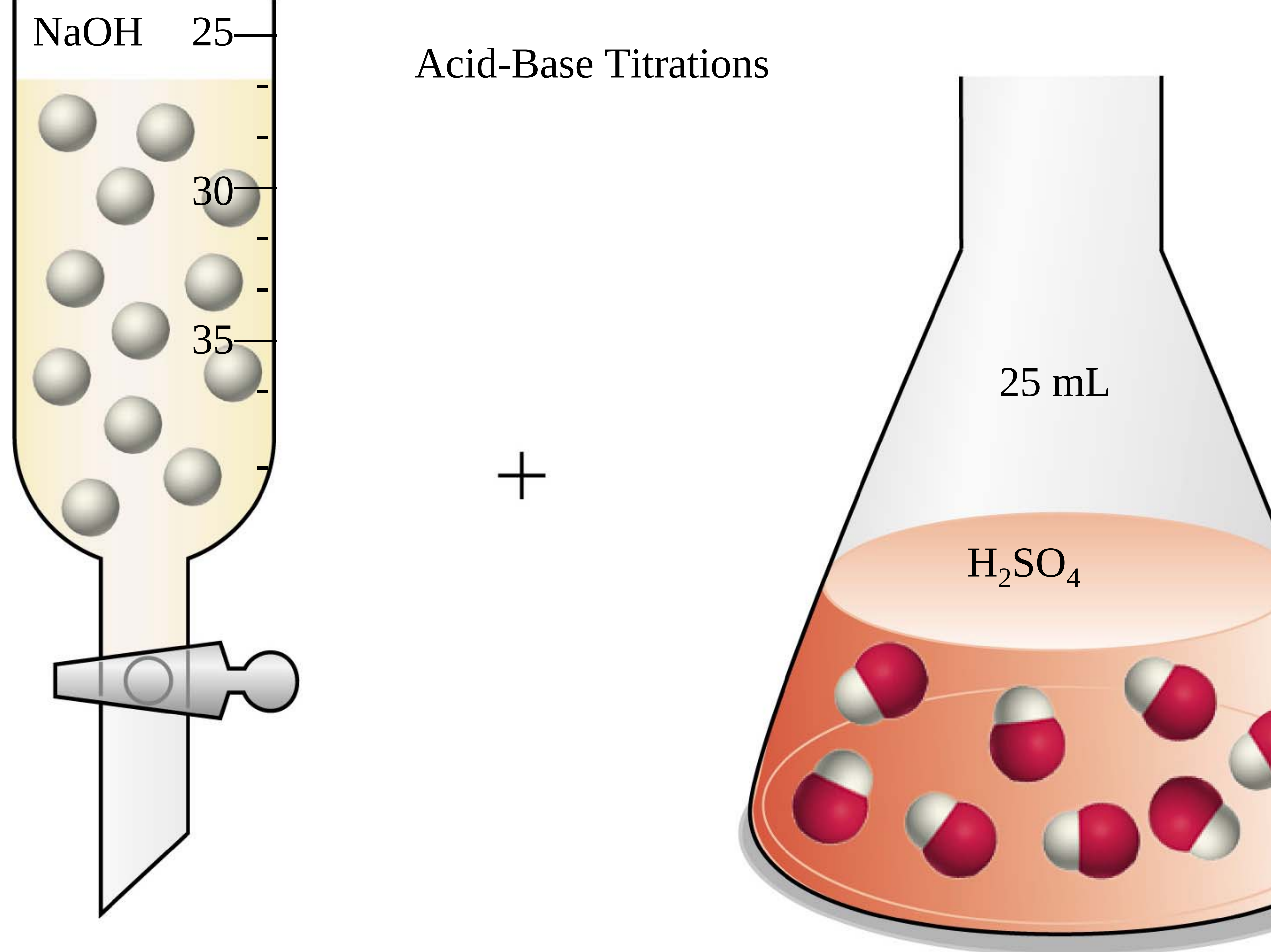
The molarity of concentrated pure sulfuric acid is 18 M. What is the density of sulfuric acid?

g MW of H_2SO_4 = 98 g/mol

One liter of sulfuric acid contains 18 mol.

How many grams?

18 M x 98 g /mol = 1764g/1000 mL = 1.764 g/mL


Acid-Base Titrations
NaOH
25
30
35
+
25 mL
H2SO4

Acid-Base Titrations

Suppose we had a solution of NaOH and we wanted to determine its concentration in mols/L (M)

A titration is often performed to achieve this goal. Suppose we had available to us a solution of H_2SO_4 with a known concentration. Lets say the concentration of sulfuric acid was 0.1 M. Now suppose we use a volumetric flask designed to deliver exactly 25 mL of solution. If we placed 25 mL of this sulfuric acid solution in a flask, how many mols of H_2SO_4 would we have in the flask?

$$0.1 \text{ mol/L} * 0.025 \text{ L} = 0.0025 \text{ mol } H_2SO_4$$

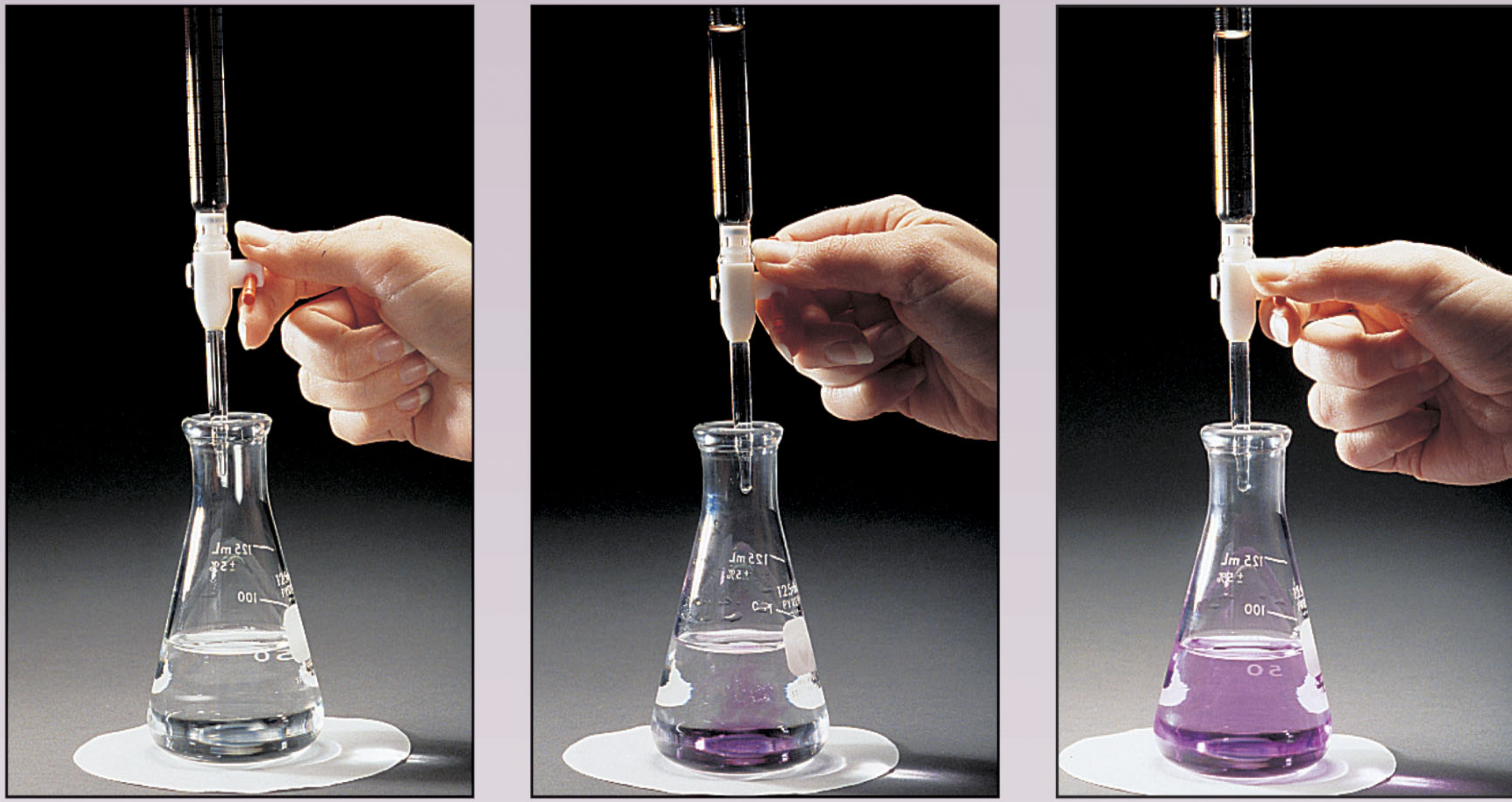
$$H_2SO_4 + NaOH \rightarrow Na_2SO_4 + H_2O$$

First let’s balance the equation

$$H_2SO_4 + 2NaOH \rightarrow Na_2SO_4 + 2H_2O$$

How can we determine when the reaction is complete?

Acid base indicators: usually weak organic acids that have a neutral and ionic form with very different but intense colors. Phenolphthalein is such a substance; in solutions that are acidic or neutral, is completely colorless. In mildly basic conditions it is converted to a red form whose intensity is very strong. By using a very little amount of this substance, it is possible to identify the point at which the solution switches from being slightly acidic to one becoming slightly basic.



A B C

Suppose in our titration we find that it takes 25.0 mL of our base to make the phenolphthalein change to a pink color. What is the concentration of our base?

$$H_2SO_4 + 2NaOH \rightarrow Na_2SO_4 + 2H_2O$$

1 mol of H_2SO_4 neutralizes 2 mol of NaOH

In the flask we added 0.025 L*0.1<u>M</u> H_2SO_4 = 0.0025 mol

0.0025 mol of H_2SO_4 must neutralize 0.005 mol of NaOH

That 0.005 mol of NaOH must have been present in 0.025 L of NaOH solution

0.005 mol/0.025L = 0.2 mol/L = 0.2 <u>M</u> NaOH

Suppose we want to prepare 250 mL of a 0.1 M solution of $AgNO_3$. How could we do this

a: using solid $AgNO_3$?

A drop of a dilute solution of $AgNO_3$ has been used on new born babies at birth to prevent contraction of gonorrhea from the mother.


A
B
C
D

Suppose we want to prepare 250 mL of a 0.1 <u>M</u> solution of $AgNO_3$. How could we do this

a: using solid $AgNO_3$?

Molecular weight of $AgNO_3$?

Ag = 107.9

N =14

O = 16

$AgNO_3$ =107.9+14+3*16 = 169.9 g/mol

250 mL = 0.25 L; 0.25 L x0.1 <u>M</u> = 0.025 mol $AgNO_3$

0.025 mol $AgNO_3$ x 169.9 g/mol = 4.25 g

dissolve 4.25 g in enough H_2O to form 250 mL of solution

b: using a solution of 1.0 M $AgNO_3$?

0.25 L x0.1 <u>M</u> = 0.025 mol $AgNO_3$ (V_1 x $\underline{M}_1$ = mol_1)

0.025 mol = 1.0 $\underline{M}_2$x V_2; V = 0.025 L or 25 mL diluted to 250 mL

$V_1\underline{M}_1 = V_2 \underline{M}_2$

Practice Problems

NaN_3 has been used in automobile air bags. When heated to 300 °C it basically explodes according to the following reaction:

$$NaN_3 \rightarrow Na + N_2$$

If 1 mole of N_2 gas at 1 atm pressure and room temperature occupies 27 L, how many liters of gas can be formed by heating 38.5 g of NaN_3

What's the first thing we need to do?

$$2NaN_3 \rightarrow 2Na + 3N_2 \; ; \qquad NaN_3 \rightarrow Na + 1.5\, N_2$$

gMW of NaN_3: 23+ 3*14 = 65 g/mol

38.5 g/65 g/mol = 0.59 mol NaN_3

How many mol of N_2 will be formed?

1.5 mol of N_2/mol of NaN_3; 3/2x0.59 mol = 0.89 mol N_2

* 27 L/mol x 0.89 mol = 24.0 L

Cisplatin, a compound used in the treatment of certain cancers, is prepared by reacting ammonia with potassium tetrachloroplatinate:

$$2\ NH_3 \quad + \quad K_2PtCl_4 \quad = \quad 2\ KCl \ + \ Pt(NH_3)_2Cl_2$$

How many grams of Cisplatin are formed from 55.8 g of K_2PtCl_4 and

35.6 g NH_3 if the reaction takes place in 95% yield based on the limiting reagent.

K_2PtCl_4 mw = 2x 39.1 +195.1 +4x 35.5; gmw = 415.3 g / mol

NH_3 = 14 + 3; gmw = 17 g / mol

$Pt(NH_3)_2Cl_2$ gmw = 195.1 + 2x 17 + 2x 35.5 = 300.1 g / mol

mol of K_2PtCl_4: 55.8 g /415.3 g /mol = 0.134 mol;

mol of NH_3: 35.6 g / 17 g/mol = 2.09 mol;

K_2PtCl_4 is the limiting reagent

0.95x 300.1 g/mol x 0.134 mol = 38.2 g $Pt(NH_3)_2Cl_2$

Copper reacts with concentrated nitric acid in the following manner:

$$Cu + 4\ HNO_3 = Cu(NO_3)_2 + 2NO_2 + 2H_2O$$

If an old copper penny (3.045 g) is completely dissolved in nitric acid and the solution diluted to 50 mL with water, what is the molarity of the $Cu(NO_3)_2$?

Cu: gmw = 63.5 g/mol

Cu: 3.045 g/63.5 = 0.048 mol

mol Cu consumed = mol of $Cu(NO_3)_2$ formed

$Cu(NO_3)_2$ = 0.048 mol/ 0.050 L

The solution is = 0.96 M $Cu(NO_3)_2$

cunacid

Balance the following:

Reaction of ammonia with iodine:

$$NH_3 \quad + \quad I_2 \quad \rightarrow \quad NI_3 \quad + \quad HI$$

$$NH_3 \; + \; 3I_2 \quad \rightarrow \quad NI_3 + 3HI$$

When nitrogen triiodide is agitated, the following occurs:

$$NI_3 \quad \rightarrow \quad N_2 \; + \; I_2$$

$$2\,NI_3 \; \rightarrow \; N_2 \; +3\,I_2$$

NI3.mov

Let's balance the following reactions:

1. $NaHCO_3 + H_2SO_4 = Na_2SO_4 + H_2O + CO_2$

$2\ NaHCO_3 + H_2SO_4 = Na_2SO_4 + 2\ H_2O + 2\ CO_2 \uparrow$

2. $Pb(NO_3)_2 + H_2SO_4 = PbSO_4 + HNO_3$

$Pb(NO_3)_2 + H_2SO_4 = PbSO_4 \downarrow + 2\ HNO_3$

3. $C_2H_5OH + H_2SO_4 = C_4H_{10}O + H_2O + H_2SO_4$

$2\ C_2H_5OH + H_2SO_4 = C_4H_{10}O + H_2O + H_2SO_4$

$2\ C_2H_5OH + H_2SO_{4\ (conc)} = C_4H_{10}O + H_2O + H_2SO_{4\ (dilute)}$

4. $C_{12}H_{22}O_{11} + H_2SO_4$ (conc) = cca3 formC1

$KMnO_4$ reacts with oxalic acid in dilute sulfuric acid as follows:

$2KMnO_4 + 5H_2C_2O_4 + 3H_2SO_4 = 2\ MnSO_4 + 10\ CO_2 + 8\ H_2O + K_2SO_4$

How many mL of a 0.25 M $KMnO_4$ solution are needed to react completely with 3.225 g of oxalic acid?

What's the limiting reagent?

$H_2C_2O_4$ (OA)

$0.4KMnO_4 + H_2C_2O_4 + 0.6H_2SO_4 = 0.4\ MnSO_4 + 2CO_2 + 1.6\ H_2O + 0.2K_2SO_4$

$H_2C_2O_4$: mw = 2 +24+64 ; gmw = 90 g/mol

mol $H_2C_2O_4$ = 3.225 g/90 g/mol; mol = 0.036

the amount of $KMnO_4$ needed is 0.036 mol x 0.4 = 0.014 mol

V x M = mol; V = 0.014mol $KMnO_4$ /0.25 mol/L;

V = 0.057 L or 57 mL

The empirical formula of benzoic acid is $C_7H_6O_2$

A sample of benzoic acid, 0.122 g, required 10.0 mL of a 0.1**M** solution of NaOH to reach a phenolphthalein endpoint. What is the likely molecular weight of benzoic acid

0.1M NaOH * 0.01L = 0.001 mol of NaOH

0.122g/MW(benzoic acid) = 0.001

Assuming that benzoic acid is a monoprotic acid (has only one acidic H)

MW = 0.122/0.001 = 122

MW ($C_7H_6O_2$) = 7*12 +6*1+32 = 122

Empirical formula = molecular formula

What are the formulas of the following compounds?

1. sodium phosphate
2. magnesium sulfate
3. aluminum chloride
4. zinc II chloride
5. iron III bromide
6. calcium carbonate

Name the following

1. Li_2S
2. BCl_3
3. $NaHCO_3$
4. $KCLO_4$
5. $NaNO_3$
6. Li_3N

Elements A and B form two compounds. The ratio (mass A)/(mass B) for compound **1** is 2 and ratio (mass A)/(mass B) for compound **2** is 0.666. If compound **1** has the chemical formula AB, what is the chemical formula for compound **2**?

A/B = 200/100

Since the ratio of A to B is smaller for compound 2, the ratio must be A/B_n where $n > 1$

$AB_2 = 200/200 = 1$

$AB_3 = 200/300 = 0.666$