Molecular Mass

Molecular Mass

synonymous with molar mass and molecular weight

is the sum of the atomic masses of all the atoms in a molecule

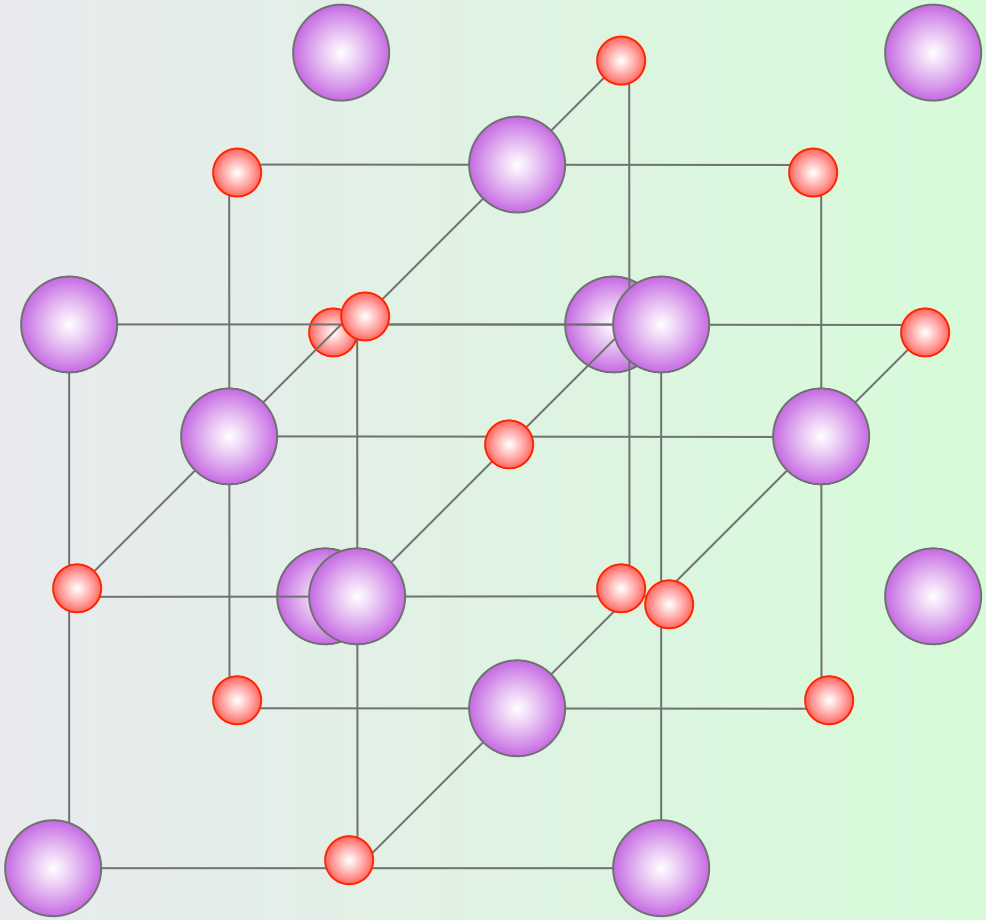
the mass in grams of one mole of a compound

Formula Mass

not all compounds are molecular

calculated exactly the same way as molecular mass

Solid structure of NaCl



Example

Calculate the number of moles of chloroform ($CHCl_3$) in 198 g of chloroform.

Molecular mass of chloroform:

1 mol C = 12.01 g

1 mol H = 1.008 g

3 mol Cl = 3(35.46 g) = 106.38 g

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1 mol $CHCl_3$ = 119.4 g

$$198\ \cancel{g}\ CHCl_3 \times \frac{1\ mol\ CHCl_3}{119.4\ \cancel{g}\ CHCl_3} = 1.66\ mol\ CHCl_3$$

Percent Composition of Compounds

Percent composition is the percent by mass of each element the compound contains.

Obtained by dividing the mass of each element in one mole of the compound by the molar mass of the compound and multiplying by 100%

$$\% \text{ Element} = \frac{(\text{number of atoms})(\text{atomic weight})}{(\text{FW of the compound})} \times 100$$

Example

A sample of a compound containing carbon and oxygen had a mass of 88g. Of this sample 24g was carbon, 64g was oxygen. What is the percent composition of this compound.

$$\% \text{carbon} = \frac{24\text{g}}{88\text{g}} \times 100\% = 27\%$$

$$\% \text{oxygen} = \frac{64\text{g}}{88\text{g}} \times 100\% = 73\%$$

Example

Calculate the percent composition by mass of H,P and O for one mole of phosphoric acid (H_3PO_4)

Molar mass = 3(1.008g) + 30.97g + 4(16.00) = 97.99

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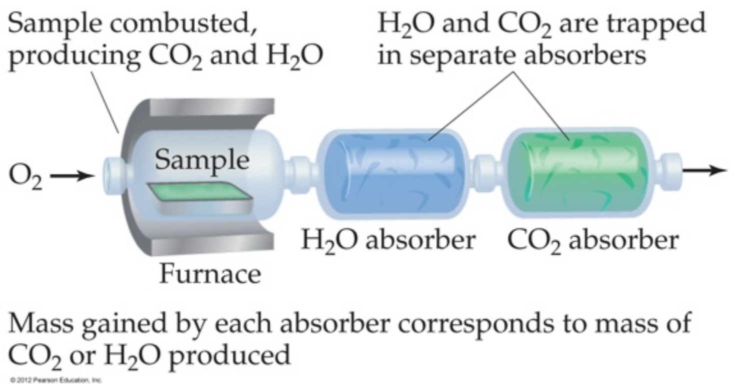
$$\%H = \frac{3(1.008g)}{97.99g} \times 100\% = 3.086\%$$

$$\%P = \frac{30.97g}{97.99g} \times 100\% = 31.61\%$$

$$\%O = \frac{4(16.00)}{97.99g} \times 100\% = 65.31\%$$

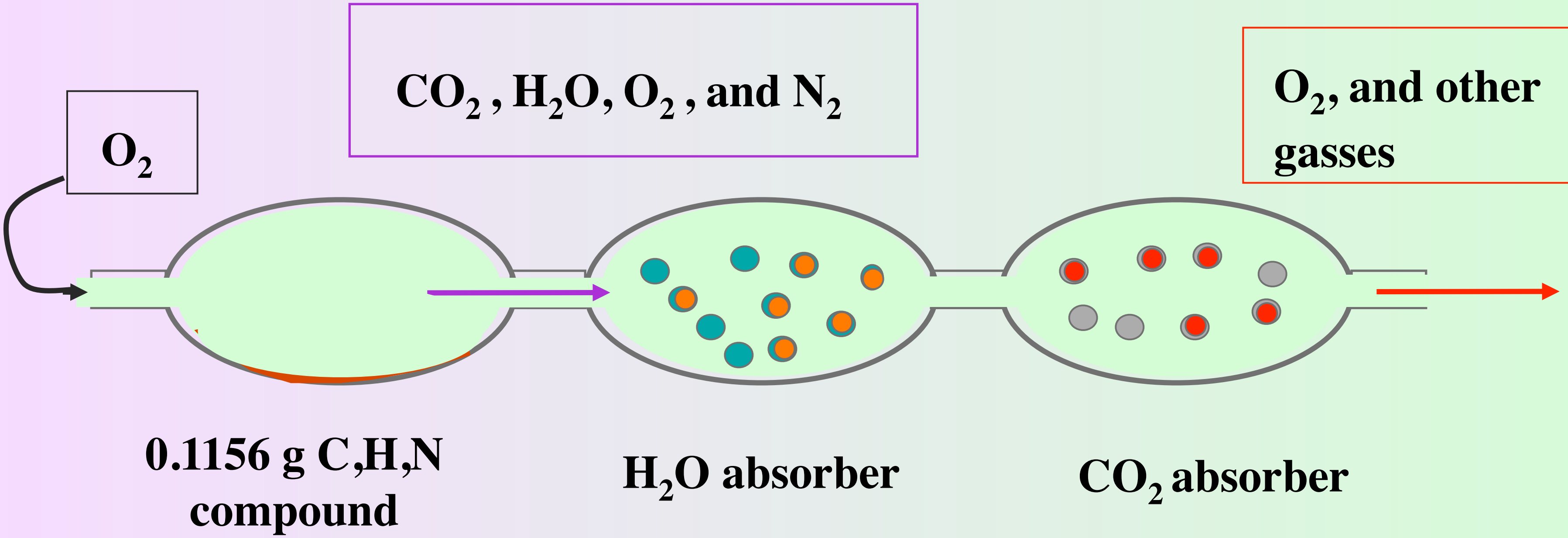
Determining Formula

Combustion Analysis



- Compounds containing C, H, and O are routinely analyzed through combustion in a chamber like the one shown in Figure 3.14.
  - C is determined from the mass of CO_2 produced.
  - H is determined from the mass of H_2O produced.
  - O is determined by difference after the C and H have been determined.

Determining the Formula



Burning the sample completely

compound + O_2 $\longrightarrow$ H_2O + CO_2 + other gasses

Determining the Formula

Reacting the C,H,N sample with O_2 , we assume all of the hydrogen and carbon present in the 0.1156g sample is converted to H_2O and CO_2 respectfully

grams collected

$$0.1638\text{g } CO_2 \times \frac{12.01\text{g C}}{44.009\text{ g } CO_2} = 0.04470\text{ g C}$$

$$0.1676\text{g } H_2O \times \frac{2.016\text{g H}}{18.015\text{ g } H_2O} = 0.01876\text{ g H}$$

Determining the Formula

Remembering the original mass of the sample the percentages of the components can be determined

$$\frac{0.04470 \text{ g C}}{0.1156 \text{ g sample}} \times 100\% = 38.67\% \text{ C}$$

$$\frac{0.01876 \text{ g H}}{0.1156 \text{ g sample}} \times 100\% = 16.23\% \text{ H}$$

$$38.67\% \text{ C} + 16.23\% \text{ H} + \% \text{ N} = 100\%$$

$$\% \text{ N} = 45.10\%$$

Levels of Structure

Elemental Composition

Empirical Formula

Molecular Formula

Constitution

Configuration

Conformation

Elemental Composition

Examples:

Formaldehyde	**Glucose**
C: 40.00%	**C: 40.00%**
H: 6.73%	**H: 6.73%**
O: 53.27%	**O: 53.27%**

Levels of Structure

Elemental Composition √

Empirical Formula

Molecular Formula

Constitution

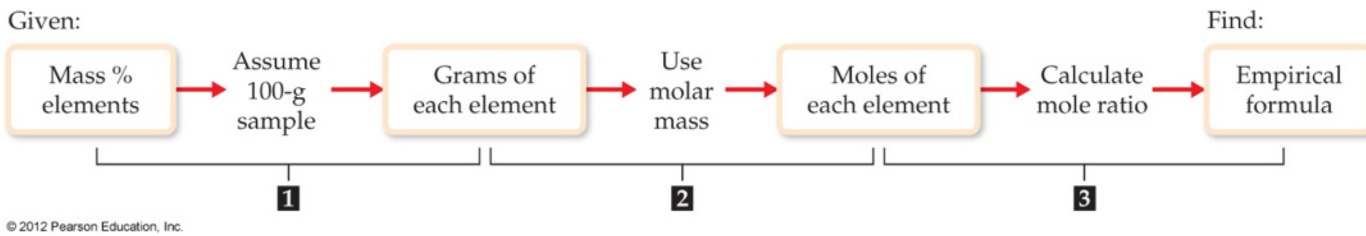
Configuration

Conformation

Empirical Formula

The empirical formula tells us which elements are present and the simplest whole-number ratio of their atoms.

Calculating Empirical Formulas



One can calculate the empirical formula from the percent composition.

Empirical Formula

Examples: Formaldehyde and Glucose

Elemental Composition

C: 40.00% 40.00 g

H: 6.73% 6.73 g

O: 53.27% 53.27 g

assume a 100g sample

calculate atom ratios by dividing by atomic weight

Calculating Empirical Formula

$$\textbf{C:} \quad 40.00\ \cancel{g} \times \frac{1\ \text{mol}}{12.01\ \cancel{g}} = 3.33\ \text{mol}$$

$$\textbf{H:} \quad 6.73\ \cancel{g} \times \frac{1\ \text{mol}}{1.00\ \cancel{g}} = 6.73\ \text{mol}$$

$$\textbf{O:} \quad \underline{53.27\ \cancel{g}} \times \frac{1\ \text{mol}}{16.0\ \cancel{g}} = 3.33\ \text{mol}$$

100 g

Empirical Formula

Examples: Formaldehyde and Glucose

Elemental Composition

C:	40.00%	40.00 g	3.33 mol
H:	6.73%	6.73 g	6.73 mol
O:	53.27%	53.27 g	3.33 mol

assume a 100g sample

calculate atom ratios by dividing by atomic weight

determine the smallest whole number ratio by dividing by the smallest molar value

Calculating Empirical Formula

$$\text{C:}\quad \frac{40.00\ \cancel{g}}{100\ g} \times \frac{1\ \text{mol}}{12.01\ \cancel{g}} = \frac{3.33\ \text{mol}}{3.33\ \text{mol}} = 1.00$$

$$\text{H:}\quad 6.73\ \cancel{g} \times \frac{1\ \text{mol}}{1.00\ \cancel{g}} = \frac{6.73\ \text{mol}}{3.33\ \text{mol}} = 2.02$$

$$\text{O:}\quad \frac{53.27\ \cancel{g}}{100\ g} \times \frac{1\ \text{mol}}{16.0\ \cancel{g}} = \frac{3.33\ \text{mol}}{3.33\ \text{mol}} = 1.00$$

Empirical Formula

Examples: Formaldehyde and Glucose

Elemental Composition

C:	40.00%	40.00 g	3.33 mol	1
H:	6.73%	6.73 g	6.73 mol	2
O:	53.27%	53.27 g	3.33 mol	1

Empirical Formula: CH_2O

Example

A 1.723 g sample of aluminum oxide (which consists of aluminum and oxygen only) contains 0.912g of Al. Determine the empirical formula of the compound.

1.723 g sample - 0.912 g Al = 0.811 g O

Al_2O_3

$$0.912 \text{ g Al} \times \frac{1 \text{ mol Al}}{26.98 \text{ g Al}} = \frac{0.0338 \text{ mol}}{0.0338 \text{ mol}} = 1.0 \times 2 = \boxed{2}$$

$$0.811 \text{ g O} \times \frac{1 \text{ mol O}}{16.0 \text{ g O}} = \frac{0.0507 \text{ mol}}{0.0338 \text{ mol}} = 1.5 \times 2 = \boxed{3}$$

Calculating Empirical Formulas

The compound *para*-aminobenzoic acid (you may have seen it listed as PABA on your bottle of sunscreen) is composed of carbon (61.31%), hydrogen (5.14%), nitrogen (10.21%), and oxygen (23.33%). Find the empirical formula of PABA.

Calculating Empirical Formulas

Assuming 100.00 g of *para*-aminobenzoic acid,

C: $61.31\text{ g} \times \dfrac{1\text{ mol}}{12.01\text{ g}} = 5.105\text{ mol C}$

H: $5.14\text{ g} \times \dfrac{1\text{ mol}}{1.01\text{ g}} = 5.09\text{ mol H}$

N: $10.21\text{ g} \times \dfrac{1\text{ mol}}{14.01\text{ g}} = 0.7288\text{ mol N}$

O: $23.33\text{ g} \times \dfrac{1\text{ mol}}{16.00\text{ g}} = 1.456\text{ mol O}$

Calculating Empirical Formulas

Calculate the mole ratio by dividing by the smallest number of moles:

$$\text{C:} \quad \frac{5.105 \text{ mol}}{0.7288 \text{ mol}} = 7.005 \approx 7$$

$$\text{H:} \quad \frac{5.09 \text{ mol}}{0.7288 \text{ mol}} = 6.984 \approx 7$$

$$\text{N:} \quad \frac{0.7288 \text{ mol}}{0.7288 \text{ mol}} = 1.000$$

$$\text{O:} \quad \frac{1.458 \text{ mol}}{0.7288 \text{ mol}} = 2.001 \approx 2$$

Calculating Empirical Formulas

These are the subscripts for the empirical formula:

$C_7H_7NO_2$

Example

Write the empirical formulas for the following molecules: (a) acetylene (C_2H_2), (b) dinitrogen tetroxide (N_2O_4), (c) glucose ($C_6H_{12}O_6$), diiodine pentoxide (I_2O_5).

This problem is not realistic. Molecular formulas are derived from empirical formulas, not vice versa. Empirical formulas come from experiment.

Levels of Structure

Elemental Composition √

Empirical Formula √

Molecular Formula

Constitution

Configuration

Conformation

Molecular Formula

determined from empirical formula and experimentally determined molecular mass

Compound	Empirical Formula	Molar mass
formaldehyde	CH_2O	30
glucose	CH_2O	180

Calculation of empirical mass

1 mol C = 12.01 g

2 mol H = 2 x 1.016 g

1 mol O = 16.00g

30.026g

<u>*Molecular mass*</u>

glucose $\frac{180g}{30g}$ **= 6**

<u>*Empirical mass*</u>

formaldehyde $\frac{30g}{30g}$ **= 1**

Molecular Formula

determined from empirical formula and experimentally determined molecular mass

Compound	Empirical Formula	Molar mass	Molecular formula
formaldehyde	CH_2O	30	CH_2O
glucose	CH_2O	180	$C_6H_{12}O_6$

Elemental Composition

Example:

Lysine

C: 49.20%

H: 9.66%

N: 19.20%

O: 21.94%

Levels of Structure

Elemental Composition √

Empirical Formula

Molecular Formula

Constitution

Configuration

Conformation

Elemental Formula

Example:

Lysine

C:	**49.20%**	**49.20 g**	**4.10 mol**
H:	**9.66%**	**9.66 g**	**9.58 mol**
N:	**19.20%**	**19.20 g**	**1.37 mol**
O:	**21.94%**	**21.94 g**	**1.37 mol**

assume a 100-g sample

calculate atom ratios by dividing by atomic weight

determine smallest whole-number ratio
by dividing by smallest number

Elemental Formula (cont'd)

Example:

Lysine

C:	**4.10 mol C atoms**	**3**
H:	**9.58 mol H atoms**	**7**
N:	**1.37 mol N atoms**	**1**
O:	**1.37 mol O atoms**	**1**

determine smallest whole-number ratio by dividing by smallest number (1.37 mol)

$\boxed{C_3H_7ON}$

Levels of Structure

Elemental Composition √

Empirical Formula √

Molecular Formula

Constitution

Configuration

Conformation

Molecular Formula

determined from empirical formula and molar mass

Compound	Empirical Formula	Molar mass	Molecular formula
lysine	C_3H_7ON	~150	$C_6H_{14}O_2N_2$

Alternative Method for determining Molecular Formula

the molar mass and the percentages by mass of each element present can be used to compute the moles of each element present in one mole of compound.

Example

Caffeine contains 49.48% carbon, 5.15% hydrogen, 28.87% nitrogen, and 16.49% oxygen by mass and has a molar mass of 194.2g. Determine the molecular formula formula of caffeine

Example

First determine the mass of each element in one mole of caffeine

$$\frac{49.48\text{g C}}{100\text{g caffeine}} \times \frac{194.2\text{g caffeine}}{1\text{ mol}} = \frac{96.09\text{g C}}{1\text{ mol caffeine}}$$

$$\frac{5.15\text{g H}}{100\text{g caffeine}} \times \frac{194.2\text{g caffeine}}{1\text{ mol}} = \frac{10.0\text{g H}}{1\text{ mol caffeine}}$$

$$\frac{28.87\text{g N}}{100\text{g caffeine}} \times \frac{194.2\text{g caffeine}}{1\text{ mol}} = \frac{56.07\text{g N}}{1\text{ mol caffeine}}$$

$$\frac{16.49\text{g O}}{100\text{g caffeine}} \times \frac{194.2\text{g caffeine}}{1\text{ mol}} = \frac{32.02\text{g O}}{1\text{ mol caffeine}}$$

Example

$C_8H_{10}N_4O_2$

then convert to moles

$$\frac{96.09\text{g C}}{1\text{ mol caffeine}} \times \frac{1\text{ mol C}}{12.011\text{g C}} = \frac{8.00\text{ mol C}}{1\text{ mol caffeine}}$$

$$\frac{10.0\text{g H}}{1\text{ mol caffeine}} \times \frac{1\text{ mol H}}{1.008\text{g H}} = \frac{9.92\text{ mol H}}{1\text{ mol caffeine}}$$

$$\frac{56.07\text{g N}}{1\text{ mol caffeine}} \times \frac{1\text{ mol N}}{14.01\text{g N}} = \frac{4.00\text{ mol N}}{1\text{ mol caffeine}}$$

$$\frac{32.02\text{g O}}{1\text{ mol caffeine}} \times \frac{1\text{ mol O}}{16.00\text{g O}} = \frac{2.00\text{ mol O}}{1\text{ mol caffeine}}$$