Chapter 3
Mass Percent and Empirical Formula

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Molecular and Formula Mass

- Molecular mass is for molecules (covalent compounds)
- Formula mass is for ionic compounds.
- Masses are calculated by adding the mass of all the elements in the formula.
- It is really important to be good in nomenclature by now. The most common error is not knowing the formula of the compound.

Solved Examples

Calculate the formula weight of the following compounds from their formulas. Report your answers to three significant figures.

Calcium hydroxide, $Ca(OH)_2$

1 Ca	1(40.08) =	40.08 amu
2 O	2(16.00) =	32.00 amu
2 H	2(1.008) =	2.016 amu
Total		74.096 amu; correct SF = 74.10 amu

Methylamine, CH_3NH_2

1 C	1(12.01) =	12.01 amu
1 N	1(14.01) =	14.01 amu
5 H	5(1.008) =	5.040 amu
Total		31.060 amu; correct SF = 31.06 amu

Nitric acid, HNO_3

1 H	1(1.008) =	1.008 amu
1 N	1(14.01) =	14.01 amu
3 O	3(16.00) =	48.00 amu
Total		63.018 amu; correct SF = 63.02 amu

Mole Concept

Question: Which has more number of atoms? 1 g of He or 1 g of Au?

Answer: He – it will take many more atoms of helium to weigh 1 g because the mass of He atom is about 4 amu (or grams for convenience) per atom, whereas Au is 197g per atom.

In chemical reactions atoms undergo rearrangement to form new compounds. There is also no loss of matter (Law of Conservation of Matter). So we have to account for ALL atoms. To calculate how many atoms will be completely going from one rearrangement to another, we need to be able to count them.

Avogadro, an Italian chemist, was the first one to calculate a number using mass of protons and carbon -12 isotope that could be useful for such calculations.

Mole Concept (mol)

- Mole is a measurement given to a certain number of atoms.
- 1 mol of substance has 6.022×10^{23} number of atoms
- 1 mol is like 1 dozen – a conversion factor:
  - 1 mol of people are 6.022×10^{23} of people
  - 1 mol of pencils are 6.022×10^{23} number of pencils
  - 1 mol of stars are 6.022×10^{23} number of stars
- The mass of 1 mol of a substance is the mass number of the substance.
- Example:

1 mol C = 12.01 g of C = 6.022×10^{23} atoms of C

1 mol Fe = 55.847 g Fe = 6.022×10^{23} atoms of Fe

Atomic Mass

- Units of mass on the periodic table are reported as g/mol.
- Nitrogen is 14.007g/mol – there are 14.007 g of N in every mol of N
- Sodium is 22.989 g/mol – there are 22.989 g of Na in every mol of Na
- For majority of calculations we don't use the number of atoms as they cannot be counted. It is easier to work in grams.
- Remember – mols is a unit but it cannot be measured by any instrument; it has to be converted to grams to be measured.
- The number of atoms are important because all reactions take place at atomic level and according to the conservation of mass no atoms are destroyed – only rearranged. Mol is an easy way to work with atoms without working in exponents.

Molar Mass

- Atomic mass is obtained from the periodic table – the mass numbers given are what is used.
- Molar mass (and formula mass) is the addition of the mass of ALL the atoms in the formula.
- Example: as before calculate the mass of calcium hydroxide. Use the same numbers and method, but instead of using amu – use g/mol.

Calcium hydroxide, $Ca(OH)_2$

1 Ca	1(40.08) =	40.08 g/mol
2 O	2(16.00) =	32.00 g/mol
2 H	2(1.008) =	2.016 g/mol
Total		74.096 g/mol; correct SF = 74.10 g/mol

Solved Examples

- You have to be able to covert number of atoms to mols, mols to grams and all possible combinations.
- These calculations are done similar to unit conversion as in chapter 1; i.e. dimensional analysis.

Example:

A sample of nitric acid, HNO_3, contains 0.253 mol HNO_3. How many grams is this?

First, find the molar mass of HNO_3:

1 H	1(1.008) = 1.008	
1 N	1(14.01) = 14.01	
3 O	3(16.00) = 48.00	
Total		63.018 g/mol

$$\frac{0.253\ mol}{} \ x \ \frac{63.02\ g}{1\ mol} = 15.94406 \text{ g} = 15.9 \text{ g/mol}$$

Calcite is a mineral composed of calcium carbonate, $CaCO_3$. A sample of calcite composed of pure calcium carbonate weighs 23.6 g. How many moles of calcium carbonate is this?

First, find the molar mass of $CaCO_3$:

1 Ca	1(40.08) =	40.08
1 C	1(12.01) =	12.01
3 O	3(16.00) =	48.00
		100.09

2 decimal places
100.09 g/mol

Next, find the number of moles in 23.6 g:

$$23.6 \text{ g} \times \frac{1 \text{ mole}}{100.09 \text{ g}} \qquad = 2.35787791 \times 10^{-1} \text{ g}$$

$$= 2.36 \times 10^{-1} \text{ g or } 0.236 \text{ g}$$

(3 significant figures)

The average daily requirement of the essential amino acid leucine, $C_6H_{14}O_2N$, is 2.2 g for an adult. What is the average daily requirement of leucine in moles?

First, find the molar mass of leucine:

6 C	6(12.01) =	72.06
2 O	2(16.00) =	32.00
1 N	1(14.01) =	14.01
14 H	14(1.008) =	14.112
		132.182

2 decimal places

132.18 g/mol

Next, find the number of moles in 2.2 g:

$$2.2\ \text{g} \times \frac{1\ \text{mole}}{132.18\ \text{g}} = 1.6643 \times 10^{-2}\ \text{mol} = 1.7 \times 10^{-2}\ \text{mol} \quad \text{or} \quad 0.017\ \text{mol}$$

(2 significant figures)

The daily requirement of chromium in the human diet is 1.0×10^{-6} g. How many atoms of chromium does this represent?

First, find the molar mass of Cr:

1 Cr 1(51.996) = 51.996

Now, convert 1.0×10^{-6} grams to moles:

$$1.0 \times 10^{-6}\ \text{g} \times \frac{1\,\text{mol}}{51.996\ \text{g}} \times \frac{6.022 \times 10^{23}\ \text{atoms}}{1\,\text{mol}}$$

$= 1.158166 \times 10^{16}$ atoms

1.2×10^{16} atoms

(2 significant figures)

Mass Percents

- Mass percent of compounds is the mass percent of each element in that compound.
- Find the total mass of the compound and find the mass of each of the elements in the compound.

$$\% \; mass\ of\ an\ element = \frac{mols\ of\ element\ x\ at.mass\ of\ element}{molar\ mass\ of\ the\ compound} \text{ x } 100\%$$

e.g. in Na_2CO_3 – there are 2 mols of sodium, 1 mol of carbon and 3 mols of oxygen.

Lead(II) chromate, $PbCrO_4$, is used as a paint pigment (chrome yellow). What is the percentage composition of lead(II) chromate?

First, find the molar mass of $PbCrO_4$:

1 Pb	1(207.2) =	207.2
1 Cr	1(51.996) =	51.996
4 O	4(16.00) =	64.00
		323.196

(1 decimal place)

323.2 g/mol

Now, convert each to percent composition:

$$\text{Pb}: \quad \frac{207.2\ \text{g}}{323.20\ \text{g}} \times 100\% = 64.11\%$$

$$\text{Cr}: \quad \frac{51.996\ \text{g}}{323.20\ \text{g}} \times 100\% = 16.09\%$$

$$\text{O}: \quad \frac{64.00\ \text{g}}{323.20\ \text{g}} \times 100\% = 19.80\%$$

Check:
64.11 + 16.09 + 19.80 = 100.00

The chemical name of table sugar is sucrose, $C_{12}H_{22}O_{11}$. How many grams of carbon are in 68.1 g of sucrose?

First, find the molar mass of $C_{12}H_{22}O_{11}$:

12 C	12(12.01) =	144.12	
11 O	11(16.00) =	176.00	
22 H	22(1.008) =	22.176	(2 decimal places)
		342.296	342.30 g/mol

Now, find the mass of carbon in 68.1 g sucrose:

$$68.1\,\text{g sucrose} \times \frac{144.12\,\text{g carbon}}{342.30\,\text{g sucrose}} = 28.7\,\text{g carbon}$$

(3 significant figures)

What is the percent water in copper(II) sulfate pentahydrate, $CuSO_4 \cdot 5\ H_2O$?

1 Cu	(1)63.55 g = 63.55 g	
1 S	(1)32.07 g = 32.07 g	
4 O	(4)16.00 g = 64.00 g	
		159.62 g/mol

2 H	(2)1.01 = 2.02 g	
1 O	(1)16.00 =16.00 g	
		18.02 g/mol

Formula Mass = 159.62 + 5(18.02) = 249.72 g/mol

Divide the mass of water in one mole of the hydrate by the molar mass of the hydrate and multiply this fraction by 100.

$$\text{percent hydration} = \frac{(5\ x\ 18.02)}{249.72}\ x\ 100\% = 36.08\%$$

More Examples: Converting Mass, Moles and Atoms

Example 1: Determine the number of moles in 85.00 grams of sodium chlorate, $NaClO_3$

$$85.00\text{ g }NaClO_3 \times \frac{1\text{ mole }NaClO_3}{106.44\text{ g }NaClO_3} = 0.7986\text{ mol }NaClO_3$$

Example 2: Determine the number of molecules in 4.6 moles of ethanol, C_2H_5OH. (1 mole = 6.022×10^{23})

$$4.6\text{ mol }C_2H_5OH \times \frac{6.02 \times 10^{23}\text{ molecules }C_2H_5OH}{1\text{mol }C_2H_5OH} = 2.8 \times 10^{24}\text{ molecules}$$

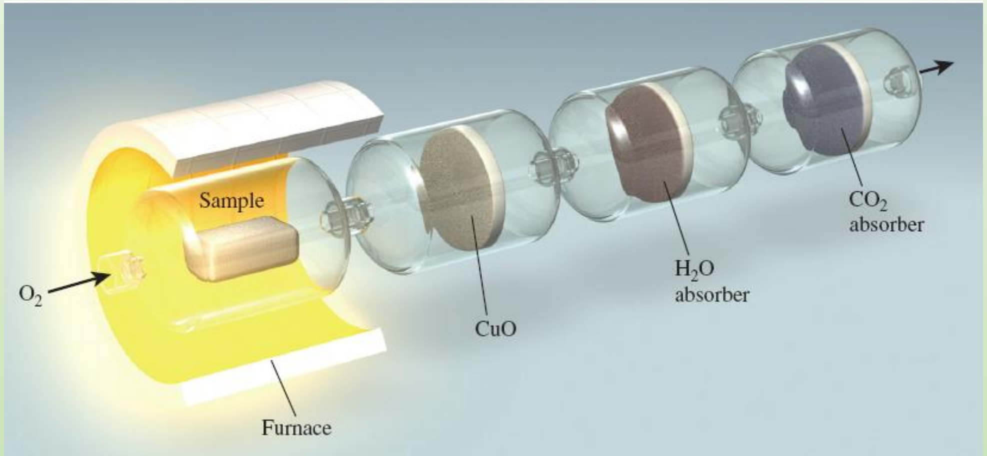
Example 3: (continued from 2) Determine how many H atoms are in 4.6 moles of ethanol.

- Begin with the answer to the last problem

$$2.8 \times 10^{24}\text{ molecules }C_2H_5OH \times \frac{6\text{ H atoms}}{1\text{ molecule }C_2H_5OH} = 1.7 \times 10^{25}\text{ atoms H}$$

Combustion Analysis

- Analysis of organic compounds (C,H, N, S and sometimes O) are carried using an apparatus like the one below



- The sample is combusted (burned in oxygen) and the products, carbon dioxide and water and other oxides are collected and weighed.
- The percent of elements can then be calculated followed by calculation of the empirical formula.

Empirical Formula

The formula of a substance written with the smallest integer subscripts.

The empirical formula for N_2O_4 is NO_2.

The empirical formula for H_2O_2 is HO.

Determining the Empirical Formula

Beginning with percent composition:

- Assume exactly 100 g so percentages convert directly to grams.
- Convert grams to moles for each element.
- Round off the resulting mole ratios to obtain whole numbers.
- Divide each mole amount by the smallest mole amount to get mol ratio.

If the result is not a whole number:

- Multiply each mole amount by a factor to make whole numbers.

For example:

- If the decimal portion is 0.5, multiply by 2.
- If the decimal portion is 0.33 or 0.67, multiply by 3.
- If the decimal portion is 0.25 or 0.75, multiply by 4.

To get the molecular formula divide the molecular weight by the mass of the empirical formula. Multiply the empirical formula with that number obtained.

Benzene is composed of 92.3% carbon and 7.7% hydrogen. What is the empirical formula of benzene? Its molecular weight is 78.1 amu. What is its molecular formula?

$$92.3 \text{ g C} \frac{1 \text{ mol C}}{12.01 \text{ g C}} = 7.685 \text{ mol C} \qquad \frac{7.685}{7.64} = 1$$

$$7.7 \text{ g H} \frac{1 \text{ mol H}}{1.008 \text{ g H}} = 7.64 \text{ mol H} \qquad \frac{7.64}{7.64} = 1$$

Empirical formula: CH

$$\text{Empirical formula weight} = 13.02 \text{ amu}$$

$$\frac{78.1}{13.02} = 6$$

Molecular formula: C_6H_6

Sodium pyrophosphate is used in detergent preparations. It is composed of 34.5% Na, 23.3% P, and 42.1% O. What is its empirical formula?

Step 1

$$34.5\,\text{g Na}\,\frac{1\,\text{mol Na}}{22.99\,\text{g Na}} = 1.501\,\text{mol Na}$$

$$23.3\,\text{g P}\,\frac{1\,\text{mol P}}{30.97\,\text{g P}} = 0.7523\,\text{mol P}$$

$$42.1\,\text{g O}\,\frac{1\,\text{mol O}}{16.00\,\text{g O}} = 2.631\,\text{mol O}$$

Step 2

$1.501\,\text{mol Na}$ $\quad \frac{1.501}{0.7523} = 2.00 \quad \times 2 = 4$

$0.7523\,\text{mol P}$ $\quad \frac{0.7523}{0.7523} = 1.00 \quad \times 2 = 2$

$2.631\,\text{mol O}$ $\quad \frac{2.631}{0.7523} = 3.50 \quad \times 2 = 7$

Empirical formula

$Na_4P_2O_7$

Hexamethylene is one of the materials used to produce a type of nylon. It is composed of 62.1% C, 13.8% H, and 24.1% N. Its molecular weight is 116 amu. What is its molecular formula?

Step 1

$$62.1\,g\,C \frac{1\,mol\,C}{12.01\,g\,C} = 5.171\,mol\,C$$

$$13.8\,g\,H \frac{1\,mol\,H}{1.008\,g\,H} = 13.69\,mol\,H$$

$$24.1\,g\,N \frac{1\,mol\,N}{14.01\,g\,N} = 1.720\,mol\,H$$

Step 2

$$5.171\,mol\,C \qquad \frac{5.171}{1.720} = 3$$

$$13.69\,mol\,H \qquad \frac{13.69}{1.720} = 8$$

$$1.720\,mol\,H \qquad \frac{1.720}{1.720} = 1$$

Step 3

Empirical formula

C_3H_8N

Step 4

Find the formula weight of the empirical formula C_3H_8N.

3(12.01) + 8(1.008) + 1(14.01) = 58.104 amu

$$n = \frac{116}{58.10} = 2$$

Molecular formula: $C_6H_{16}N_2$

Key Words and Concepts

- Formula mass
- Mole concept
- Avogadro’s number
- Mass percents
- Elemental analysis