Unit 2 - Atoms, Moles & Stoichiometry

Relative Masses

Relative atomic mass - the weighted average mass of an atom of an element compared with 1/12 of the mass of an atom of carbon-12.

Relative isotopic mass - the mass of an atom of an isotope as compared to 1/12 of the mass of an atom of carbon-12.

Relative molecular mass - the weighted average mass of one molecule of an element or compound compared with 1/12 of the mass of an atom of carbon-12

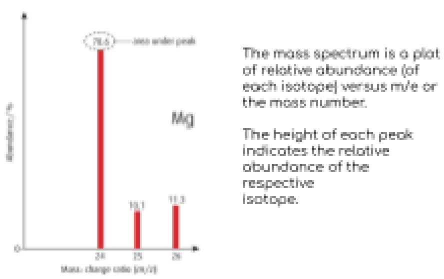
Relative formula mass - the weighted average mass of one unit of a substance compared with 1/12 of the mass of an atom of carbon-12

The Mole and Avogadro's Constant

1 mole is the amount of any substance containing as many particles as there are carbon atoms in exactly 12g of carbon-12. One mole of any substance will always contain exactly the same number of particles. Avogadro's Constant is the number of particles in one mole of any substance. This is equal to 6.02×10^{23}.
Therefore:

Number of particles = Avogadro's constant x moles

Relative Atomic Mass



A mass spectrometer is an analytical machine used to calculate the relative atomic mass of an atom by comparing it with the mass of a 12C atom.
∟ It is also used to calculate the relative abundance of different isotopes of any element.

To calculate relative isotopic mass from a mass spectrometer graph like this, take the percentage abundance and multiply it by the corresponding m/e, and divide it by 100:

$(78.6 \times 24) + (10.1 \times 25) + (11.3 \times 26) = 2432.7$
$2432.7 / 100 = 24.33$

Molecular Ions

Molecules also give peaks in their mass spectrum. For example, the mass spectrum of chlorine gaseous molecule includes both peaks of its isotopes and peaks of its molecular form (molecular ions).

Empirical and Molecular Formulae

Empirical formula - the simplest whole number ratio of atoms of each element in a compound

Molecular formula - the actual number of atoms of each element in a compound

Calculating the empirical formula from mass

1) Divide the mass (or percentage by mass) of each element making up the compound by its molecular mass (Mr of the element) to get a molar ratio.
2) Divide each number in the ratio by the smallest number to get the simplest ratio of elements
3) If the ratio contains decimal numbers, multiply them out to obtain whole numbers (e.g. something is 1.5, multiply everything by 2)

Calculating the empirical formula from combustion data

If the compound contains only carbon and hydrogen:
1) Divide the mass of CO_2 produced by 44 to find the number of moles of CO_2 (44 is the Mr of CO_2). this will get you the amount of carbon in the compound
2) Divide the mass of water produced by 18 to find the number of moles of water (18 is the Mr of H_2O). Since one mole of water contains 2 moles of hydrogen, double the number of moles of water to find the number of moles of hydrogen in the compound.
3) Divide the number of moles of hydrogen and carbon by the smallest value to find the simplest molar ratio.

Example:
A sample is durned in oxygen. 0.069g of CO_2 and 0.0113g of H_2O is produced. What is the empirical formula of the sample burned?
Moles of C: (0.069 / 44) = 0.00157
Moles of H: (0.0113 / 18) x 2 = 0.00126

of C to H = 1.25 : 1
ical formula ratio = 5 : 4 = C_5H_4

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If the compound contains other elements:

1) Use the mass of CO_2 to calculate the number of moles of carbon atoms then use this to calculate the mass of carbon present.
2) Use the mass of H_2O to calculate the number of moles of hydrogen atoms, then use this to calculate the mass of hydrogen present
3) Ass the masses of carbon and hydrogen and compare them to the initial mass of the compound. If there is no difference, the compound is a hydrocarbon and you can move on to the next step. If there IS a difference, assume that this is due to oxygen (unless told otherwise). Calculate the mass of oxygen present and use this to calculate the number of moles of oxygen atoms.
4) Divide the moles of each element by the smallest value to obtain the empirical formula.

Calculating the Molecular Formula

Calculate the relative formula mass of the empirical formula, then divide the relative formula mass of the compound by the calculated value. This will show how many times larger the molecular formula is than the empirical formula.

Example:
A compound has the empirical formula HO and the relative formula mass 34. What is the molecular formula?
Empirical formula mass: 16 + 1 = 17
34 / 17 = 2 so the molecular formula is H_2O_2

<u>Reacting Masses and Volumes</u>

When completing calculations, quantities should be given to the <u>same number of significant figures</u> as the least accurate measured quantity. So if the values are given to 2 significant figures, then the answer should also be given to 2 significant figures.

Calculations involving reacting masses

<u>Molar mass</u> is the mass per mole of a substance and can be calculated by adding the relative atomic masses of all the atoms in a formula. To calculate the number of moles using mass and molar mass:

Number of moles = mass (g) / molar mass

<u>Calculations involving volumes of gases</u>

At the same temperature and pressure, one mole of any gas will occupy the same volume. At room temperature and pressure, this is 24 dm^3. This does not mean that these gases will have the same mass. The number of moles of a gas at room temperature and pressure can be calculated, where V = volume:

Moles of gas = Volume (dm^3) / 24

<u>Calculations involving concentration and volumes of solutions</u>

Concentration is the amount of solute dissolved in a given volume of solution. The number of moles can be calculated from concentration and volume:

Number of moles = concentration (mol dm^3) x volume (dm^3)

Stoichiometry - the proportions of reactants and products. A balanced chemical equation can be used to find the stoichiometry of a reaction.

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