SECTION 8

AMOUNT OF SUBSTANCE AND ITS UNIT, THE MOLE

Suppose a chemist wishes to carry out the chemical reaction of adding bromine to hexene to give dibromohexane, $C_6H_{12} + Br_2 \rightarrow C_6H_{12}Br_2$, starting with a known amount of hexene. How does the chemist know how much bromine is needed? The chemical equation tells you that one molecule of dibromine is needed for each molecule of hexene. But the very large numbers of molecules required for reactions on a practicable scale cannot be counted. If the mass of hexene is known how could the mass of bromine required be calculated? This section tells how this type of question is answered. It requires the introduction of a new quantity specific to chemistry , *amount of substance*, and

Amount of substance: symbol *n*, a quantity fundamental to chemistry. Atoms and molecules are much too small or light to be counted or weighed individually in the laboratory. The chemist therefore needs a unit to specify the quantity **amount of substance** of an appropriate magnitude (size) for laboratory or industrial scale work. The chosen unit is the **mole**.

Mole: symbol mol, the unit of the quantity amount of substance. The **mole** is defined as the amount of substance of a system which contains as many elementary entities as there are atoms in 12 grams of carbon-12 (i.e. carbon consisting only of the isotope ^{12}C).

12 g is an easily measurable mass. When the mole is used, the elementary entities must be specified and may be atoms, molecules, ions, electrons, other particles or specified groups of such particles.

It follows from this definition of the mole that *x* moles of dihydrogen (H_2,) will contain exactly the same number of dihydrogen molecules as there are dioxygen molecules (O_2) in *x* moles of dioxygen or water molecules (H_2O) in *x* moles of water. Thus it follows from the chemical equation

$$2H_2 + O_2 \rightarrow 2H_2O$$

that 2 moles of dihydrogen react with 1 mole of dioxygen to give 2 moles of water, i.e. the chemical equation is also a simple way of expressing the reaction of measurable amounts of substances as well as of individual molecules. Thus the chemical equation (*page 2-2*)

$$C_2H_6 + {}^7/_2O_2 \rightarrow 2CO_2 + 3H_2O$$

is quite satisfactory when the reaction coefficients refer to amounts measured in moles.

Molar mass: symbol *M*, the mass per mole of substance (the substance being defined by its chemical formula). (Molar means per mole in this context.) The mass of any substance is proportional to the amount of that substance and the proportionality constant is its molar mass;
$m = Mn$. [e.g. for water m = 18 g when n = 1 mol; 18 g = $M(H_2O)$ x 1 mol;

$$M(H_2O) = 18\ \text{g}/(1\ \text{mol}) = 18\ \text{g mol}^{-1}.]$$

This is usually written as $m = nM$. (i.e. mass of substance is the amount in moles multiplied by the mass per one mole). Commonly used units are grams per mole [e.g. $M(^{12}C)$ = 12 g mol^{-1}]. The molar mass of the atoms of each element in units of grams per mole (g mol^{-1}) is given in the periodic table immediately under the symbol for the element. The molar mass of any substance defined by its chemical formula is the sum of the molar masses of all of its constituent atoms.

$$[\text{ e.g. } M(H_2O) = 2M(H) + M(O) = (2 \text{ x } 1.01 + 16.00)\ \text{g mol}^{-1} = 18.02\ \text{g mol}^{-1}\ ]$$

The amount of substance is normally obtained by weighing, (i.e. by measuring its mass using a balance), and converting the mass of the sample to the amount of the sample in moles by rearranging the equation $m = nM$ to give $n = \dfrac{m}{M}$.

[e.g. What is the amount of copper of 20.0 g of the metal?

$$n(\text{Cu}) = \frac{m(\text{Cu})}{M(\text{Cu})} = \frac{20.0\ \text{g}}{63.5\ \text{g mol}^{-1}} = 0.3150\ \text{mol}].$$

For a liquid the volume might be measured and this converted to amount in moles by using both the density and the molar mass of the substance.

[e.g. What is the amount of tetrachloromethane in a 20.0 cm^3 sample? $\rho(CCl_4)$ = 1.584 g cm^{-3}; $M(CCl_4)$ = 153.8 g mol^{-1}. Convert from volume to mass using the density,

$$m(\text{CCl}_4) = \rho(\text{CCl}_4)V(\text{CCl}_4),$$

and then to amount using the molar mass,

$$n(\text{CCl}_4) = \frac{m(\text{CCl}_4)}{M(\text{CCl}_4)} = \frac{\rho(\text{CCl}_4)V(\text{CCl}_4)}{M(\text{CCl}_4)} \quad \{\text{by replacing } m(\text{CCl}_4) \text{ by } \rho(\text{CCl}_4)V(\text{CCl}_4)\}$$

$$= \frac{1.584\ \text{g cm}^{-3} \times 20.0\ \text{cm}^3}{153.8\ \text{g mol}^{-1}} = 0.206\ \text{mol} \ ]$$

Stoichiometry: The quantitative relationship between the amounts of reactants consumed and products formed in a chemical reaction as expressed by its balanced chemical equation. The general chemical equation

$$a\text{A} + b\text{B} \rightarrow c\text{C} + d\text{D}$$

implies that *a* moles of substance A react with *b* moles of substance B to produce *c* moles of substance C and *d* moles of substance D.

[e.g. What amount of copper oxide could be formed from 20.0 g of copper in the reaction

$$4\text{Cu} + \text{O}_2 \rightarrow 2\text{Cu}_2\text{O}$$

From the stoichiometry of the equations, $\dfrac{n(\text{Cu}_2\text{O})}{n(\text{Cu})}$ = 2/4 = 0.5

Therefore $n(Cu_2O) = 0.5n(Cu)$ = 0.5 x 0.3150 mol = 0.1575 mol

What is the mass of the Cu_2O formed?

$m(Cu_2O) = n(Cu_2O)M(Cu_2O)$ = 0.1575 mol x (2 x 63.5 + 16.0) g mol^{-1}

= 0.1575 mol x 143 g mol^{-1} = 22.5 g]

The most useful expression for the stoichiometry of the above general chemical equation is

$$\frac{n(\text{A})}{a} = \frac{n(\text{B})}{b} = \frac{n(\text{C})}{c} = \frac{n(\text{D})}{d}$$

This equation and $n = \dfrac{m}{M}$ are two of the most important equations used in practical quantitative chemistry.

Avogadro Constant: Symbol N_A or *L*, the number (of entities) per mole. From many varied measurements its value has been determined as 6.022 x 10^{23} mol^{-1}.

Atomic mass constant: Symbol m_u, One twelfth of the mass of one atom of ^{12}C.
Also sometimes called **unified atomic mass unit**, symbol u, previously amu.

Thus $m_u = \dfrac{{}^1/_{12} \times 12\ \text{g mol}^{-1}}{N_A} = \dfrac{1\ \text{g mol}^{-1}}{6.022 \times 10^{23}\ \text{mol}^{-1}}$ = 1.667 x 10^{-24} g

Relative atomic mass: Symbol A_r, mean mass of one atom of an element (i.e. taking into account the relative natural abundance of the isotopes) relative to (i.e. divided by) m_μ. With the exception of the heaviest elements which have been formed from different radioactive isotopes, in general the relative amounts of the different isotopes of an element is independent of its source [e.g. chlorine, A_r(Cl) = 35.45, consists naturally of 75.5% ^{35}Cl and 24.5% ^{37}Cl].

Note that the relative atomic mass has no units because it is the ratio of two masses. Most reference books and periodic tables simply give A_r values for the elements. From a practical viewpoint it is most important to realise that the numerical value of the molar mass M(E) is equal to A_r(E) when the units of molar mass are g mol^{-1} .

Atomic weight: An older term for mean molar mass of an element, M(E), but sometimes used for relative atomic mass, A_r(E).

Relative molecular mass: Symbol M_r, the mass of one molecule of the substance relative to m_μ. It is simply the sum of all the A_r values of the atoms in the molecule.

Instead of stating the relative molecular mass of a large molecule is, for example, 20,000, biochemists often say the molecular mass is 20 000 daltons or 20 000 Da or 20 kDa. The **dalton** is just another (friendlier) name for the unified atomic mass constant, m_μ, and is not a unit in the sense of the gram (or the second, or the mole, or the metre) because its value depends on the Avogadro constant, an experimentally derived quantity. The dalton is never used in chemical calculations.

Molecular weight: An older term for molar mass, but sometimes used for relative molecular mass.

The term "relative molecular mass" is also used for an ionic substance or for substances which do not exist as discrete molecules, such as MgO or SiO_2 [e.g. M_r(MgO) = 40]. The formula given with the symbol M_r makes it quite clear what is meant. Some authors try and avoid this problem by using the term "relative formula mass". But this is somewhat unsatisfactory because formulae are concepts and do not have mass!

EXERCISES

Determine the amount of substance in the given masses of the following compounds. (Molar masses for the elements in grams per mole are given in the periodic table.)

1. *Example*: 25.2 g of NaCl

   Answer: $n = m/M$ $M(\text{NaCl}) = (23.0 + 35.5)\text{ g mol}^{-1} = 58.5\text{ g mol}^{-1}$

   $$n(\text{NaCl}) = \frac{25.2\text{ g}}{58.5\text{ g mol}^{-1}} = 0.431\text{ mol}$$

   In words this equation says the amount of sodium chloride is 0.431 moles.

2. 23 g of KNO_3 3. 75 kg of C_6H_6 4. 33 μg of $C_3H_7CO_2C_5H_{11}$ (odour of banana)

Determine the masses of the given amounts of the following compounds.

5. 45 mol of graphite (C) 6. 8.2 mol of Al_2O_3 7. 5.3 mmol of $PtCl_4$

Determine the mass of the product that would be formed from the given mass of reactant in the following reactions.

8. Carbon monoxide from 24 g of methane in the steam reforming of natural gas

$$CH_4 + H_2O \rightarrow CO + 3H_2$$

9. Iron from 24 kg of magnetite, Fe_3O_4, in steel making

$$Fe_3O_4 + 4C \rightarrow 3Fe + 4CO$$

10. Sulfuric acid from 100 t of sulfur in the manufacture of sulfuric acid

$$S_8 + 12O_2 + 8H_2O \rightarrow 8H_2SO_4$$

11. Acetic acid from 500 L of ethanol ($\rho = 0.785$ g cm^{-3}), in making vinegar

$$CH_3CH_2OH + O_2 \rightarrow CH_3CO_2H + H_2O$$