1 Basic Chemical Terms

Elementary Particles of Matter, Substances, Elements, Compounds

Substance is a specific kind of matter, which exhibits stable physical characteristics at definite conditions. All substances are built up by atoms.

Atom is the smallest electrically neutral particle, which still keeps the chemical characteristics (quality) of the corresponding element. It consists from a positively charged nucleus and negatively charged electron shell. The arrangement of electrons in the shell influences the chemical characteristics of an atom.

Molecule is the smallest part of a pure substance, which still keeps the chemical characteristics of this substance. It is electroneutral, characterized by a specific composition (nature and number of the present atoms) and structure (their mutual arrangement in space, kind of bonds). Di- or polyatomic molecules of one type of chemical element have homoatomic composition (they contain one kind of atoms e.g. H_2, O_2, N_2, Cl_2). Molecules of compounds have heteroatomic composition, e.g. HCl, H_2O etc. In some substances (e.g. solid substances with crystal structure), the individual molecules are not identifiable. In this case, we formally appoint the smallest part of the substance (the smallest numerical ratio of atoms), the composition of which still describes the composition of the whole substance, and we call it **formula unit** (e.g. a pair of ions Na^+ and F^- in sodium fluoride, carbon atom in diamond, Si atom and two O atoms in silicon dioxide etc.). From this formula unit (the repeating part) the name of the substance is derived.

According to the composition are distinguished chemically pure substances and mixtures (homogeneous, colloid, and heterogeneous). In the nature, substances occur usually in the form of mixtures.

A chemically pure substance (chemical individual) consists of identical particles with stable characteristic properties (boiling point and melting point, density, refractive index, specific rotation etc.). We distinguish two groups of chemically pure substances – elements and compounds.

An element is a chemically pure substance consisting of atoms with the same proton/atomic number. If the element is formed by atoms with the same mass number, it is called **nuclide**. Atoms of the given element can be non-combined (noble gases), form molecules (gaseous oxygen O_2), or they are combined altogether to form more complex structures (covalent bonds – diamond, metal bonds – metals, covalent bonds and van der Waals forces – graphite).

A compound is a chemically pure substance consisting of two or more different atoms. The atoms can be arranged in isolated molecules (gaseous carbon dioxide) or they can form more complex structures (crystalline structures – sodium chloride).

A mixture (dispersion system) consists of several different, chemically pure substances. The mixture can be homogeneous (formed by only one phase – air, solutions), colloid (e.g. egg white in water) or heterogeneous (more phases physically separated from each other – water with sand).

Expressing the Amount of Substance and Their Structural Elements

The amount of any substance (chemical element, compound, mixture) can be expressed in several ways: mass (*m*), volume (*V*) or the number of basic structural particles (atoms, ions, molecules).

Atomic and Molecular Mass

Mass (*m*) is an additive quantity, which does not depend on the temperature and pressure. The mass of the structural particles can be expressed in common mass units (kg, g). The **absolute mass of an atom** (the value of its resting mass) is very small, about 10^{-27}–10^{-25} kg. Thus, the absolute quantities are impractical for everyday use. Mass can be more conveniently expressed by comparing to standard (object with a mass similar to the mass of these particles). This standard was stated during the last correction in 1961 to be the atom of a carbon nuclide ^{12}C. Exactly 1/12 of the mass of this atom $m(^{12}C)$ was determined as an accessory unit. It is the unified **atomic mass unit** (symbol **u**); in biochemistry and molecular biology, it is more often called **dalton** (symbol **Da**). The value of its mass is called the **atomic mass constant** (symbol $\boldsymbol{m_u}$).

$$m_u = 1/12\ m(^{12}C) = 1.660\ 56 \times 10^{-27}\ kg = 1\ u$$

The absolute atomic masses are not as important from the chemical point of view as the ratio (the relative amount), under which the atoms react with each other. Therefore, we most frequently use the relative (proportional) expression of mass (related to the 1/12 of the mass of the carbon nuclide ^{12}C).

The relative atomic mass ($\boldsymbol{A_r}$) is a dimensionless number representing how many times the mass of a given atom (X) is higher than the atomic mass constant m_u. It is given by the ratio between the (absolute) mass of one atom m(X) in kg to the atomic mass constant m_u in kg.

For the given element X it is accepted that:

$$A_r(X) = \frac{m(X)}{m_u}$$

The relative molecular mass ($\boldsymbol{M_r}$) is sum of the relative atomic masses of all atoms present in the molecule. It is equal to the ratio of the molecular mass m(XY) in kg to the atomic mass constant m_u in kg.

Volume

Volume, as the expression of the amount of substances, is most frequently used in case of liquids or gases. It is additive quantity only in case of ideal systems in gaseous state, where the individual particles do not affect each other. The effect of temperature and pressure on the volume is very significant.

Avogadro's law is of great importance for calculations of ideal gas volume: at the same pressure and temperature, equal volumes of different gases contain the same number of particles. In simplified calculations, the gaseous substances will be assumed to be ideal.

Substance Amount

The substance amount (*n*) is the quantity related to the number of particles (*N*). If we used one molecule (ion, atom) in calculations as the unit for quantity of a substance, we would deal with very large numbers. Therefore in chemistry is used one **mole** as the basic unit of the substance amount. It contains exactly the same number of elementary entities (molecules, atoms, ions, electrons) as there are atoms in exactly 12 g of the carbon nuclide ^{12}C. This number is expressed by the **Avogadro's constant** $\boldsymbol{N_A = 6.022 \times 10^{23}\ \mathrm{mol^{-1}}}$.

The substance amount (n) is then calculated as

$$n = \frac{N}{N_A}$$

The mole is one of the seven SI base units. When the mol is used, the kind of elementary entities must be always specified.

Molar Quantities

Quantities related to the mole are called **molar** (mass, volume, charge).

The molar mass (*M*) is the (absolute) mass of 6.022×10^{23} particles, e.g. 1 mole of a given substance expressed in **g mol^{-1}**. It can be calculated by multiplying the absolute mass of an atom or molecule by the Avogadro's constant:

$$M = m_x N_A$$

where m_x is a mass of one atom or molecule.

Because the atomic mass can be expressed as the product of the relative atomic mass and atomic mass unit, it follows that $M = A_r \times u \times N_A$, which after substitution gives:

$$M = A_r \times 1.66 \times 10^{-27} \times 6.022 \times 10^{23}\ \mathrm{kg\ mol^{-1}} = A_r \times 1.66 \times 10^{-24} \times 6.022 \times 10^{23}\ \mathrm{g\ mol^{-1}}$$

Because the product $1.66 \times 10^{-24} \times 6.022 \times 10^{23}$ is approximately equal to one, it implies that the mass of one mole of substance ***M* is numerically equal to the relative atomic or molecular mass**, **but it is expressed in grams**.

If we know the mass of a substance containing a certain number of moles of this substance, the molar mass is expressed by the equation:

$$M = \frac{m}{n}$$

The molar volume of a gas (V_M) is the volume of one mole of an ideal gas under given conditions. It is equal to **22.4 l mol^{-1}** at temperature 0 °C and pressure 101.3 kPa (1 atm). It is calculated by dividing the volume of a gas (V) by the quantity of a substance (n):

$$V_M = \frac{V}{n}$$

The molar charge is the electric charge of one mole of charged particles with one elementary charge and it is the product of the elementary charge and the Avogadro's constant N_A. **The elementary charge** is the smallest possible charge of a particle (the absolute quantity of the charge of an electron or proton) and it is equal to **1.602×10^{-19} C** (coulombs). Then the charge of one mole of particles with one elementary charge is **Faraday's constant *F*** = $1.602 \times 10^{-19}\ \mathrm{C} \times 6.022 \times 10^{23}$ = **96 485 C mol^{-1}**.