
Fundamentals

1.2 Measurement, units, and nomenclature

- SI units are based on seven base units; other units are derived from these and are called derived units.
- Bond lengths are conveniently measured in picometres ($1 \text{ pm} = 1 \times 10^{-12} \text{ m}$).
- Temperature can be measured in degrees Celsius or in kelvin. The kelvin scale is the international standard in science and is called the thermodynamic temperature scale or the absolute temperature scale.
- Many compounds have both a common name and a systematic IUPAC name.

1.3 Atoms and the mole

- Elements contain atoms that all have the same number of protons.
- Compounds are made up of atoms of more than one element; the atoms are bonded together in molecules or in extended network structures.
- A simple classical model of the atom consists of a tiny dense positively charged nucleus surrounded by electrons.
- The atomic number Z of an element is the number of protons in an atom. The mass number is the total number of protons and neutrons in an atom.
- Many elements have more than one isotope. Isotopes are atoms of an element that contain different numbers of neutrons in their nuclei. An isotope can be represented by an atomic symbol showing the mass number and atomic number.
- A mole (1 mol) of a substance is the amount of substance that contains as many formula units (atoms, molecules, groups of ions, etc.) as there are in exactly 12 g of ^{12}C . The number of formula units in a mole is $6.022 \times 10^{23} \text{ mol}^{-1}$, N_A , the Avogadro constant.

- The empirical formula of a substance gives the *ratio* of the numbers of different types of atom in the substance; the molecular formula gives the actual number of different types of atom in a molecule.

1.4 Chemical equations

- A balanced equation is one with equal numbers of each type of atom on either side of the equation. It is a balance sheet of where each atom starts and where it ends up. For an ionic equation, the total charge on either side of the equation must be the same.
- The relationship between the amounts of reactants and products is called the stoichiometry of the reaction. It allows you to calculate the masses that react exactly and the masses of the products formed.
- The percentage yield of a reaction tells you what percentage of the theoretical yield is actually obtained.
- An ionic equation shows only the ions that take part in the reaction, plus any non-ionic substances involved. Spectator ions are not included.
- Oxidation is loss of electrons or increase in oxidation state. Reduction is gain of electrons or decrease in oxidation state.
- Redox reactions can be formally represented by two half equations, one for oxidation and the other for reduction.
- Systematic names for inorganic compounds tell you which elements are present, in what combination and in what oxidation states.
- For organic compounds, oxidation levels are more useful than oxidation states.

1.5 Working out how much you have

- The molarity of a solution is the amount (in moles) of solute dissolved in 1 dm³ of solution.
- The amount (in **mol**) of solute (n) dissolved in a volume (V) of solution (in **dm⁻³**) is given by:
$$n = c \times V$$
, where c is the concentration of the solution in **mol dm⁻³**.
- Volumetric analysis involves accurate measurements of volumes of solutions.
- Gravimetric analysis involves accurate measurements of mass.

1.6 Energy changes in chemical reactions

- An exothermic reaction gives out energy and heats the surroundings; an endothermic reaction takes in energy and cools the surroundings.
- The enthalpy change, ΔH , for a reaction is the heat transferred between the reacting system and the surroundings *at constant pressure*; the value of ΔH is negative for an exothermic reaction and positive for an endothermic reaction.
- The standard enthalpy change of reaction, $\Delta_r H^\ominus_{298}$ is the enthalpy change for a reaction at 1 bar and 298 K with all components in their standard states.
- A thermochemical equation links an enthalpy change to the molar amounts in a balanced equation for the reaction.
- Bond breaking is an endothermic process; bond formation is an exothermic process.

1.7 States of matter and phase changes

- There are three common states of matter: solid; liquid; and gas.
- The three states of matter are phases. Within any state, there may be more than one phase.
- The kinetic-molecular model for the structure of matter explains macroscopic properties in terms of the arrangement and motion of the molecules.
- Transitions between states of matter are called phase changes.
- The enthalpy changes accompanying phase changes are called enthalpy changes of state. Values refer to 1 mol of the substance.
- Melting (fusion), vaporization, and sublimation all involve the breaking of intermolecular attractions and are endothermic processes. The reverse processes, freezing, condensation, and reverse sublimation, respectively, involve the formation of intermolecular interactions and are exothermic processes.
- $$\Delta_{\text{fus}}H^\ominus = -\Delta_{\text{freezing}}H^\ominus$$
$$\Delta_{\text{vap}}H^\ominus = -\Delta_{\text{cond}}H^\ominus$$
$$\Delta_{\text{sub}}H^\ominus = -\Delta_{\text{reverse sub}}H^\ominus$$

1.8 Non-covalent interactions

- Non-covalent interactions include interactions between molecules, between ions and molecules, and between ionic groups within molecules.

- London dispersion interactions are present in all molecules and in monatomic gases. They arise from the electrostatic attraction between an instantaneous dipole in a molecule and an induced dipole in an adjacent molecule.
- Other types of interactions include:
 - dipole–dipole interactions;
 - dipole–induced dipole interactions;
 - ion–dipole interactions;
 - hydrogen bonds;
 - ion–ion interactions.
- These types of interactions are summarized in Table 1.10 (p.56).

1.9 Chemical equilibrium: how far has a reaction gone?

- A chemical equilibrium is a dynamic equilibrium in which the forward and reverse reactions are taking place at the same rate, so concentrations remain constant.
- Le Chatelier’s principle summarizes the effects of external changes on an equilibrium: when an external change is made to a system in dynamic equilibrium, the system responds to minimize the effect of the change.
- Equilibrium constants can be expressed in terms of concentrations, K_c , or, for gaseous reactions, in terms of partial pressures, K_p , where $K_p = K_c(RT)^{\Delta n}$.
- Table 1.13 summarizes the effect of changing conditions on the composition of equilibrium mixtures and on equilibrium constants. Remember that K_c and K_p are constant unless the temperature changes. Note that catalysts do not affect the position of equilibrium or the equilibrium constant. They increase the *rates* of both the forward and reverse reactions so that the same position of equilibrium is reached—but it is reached more quickly.

Table 1.13 The effect of changing conditions on the composition of equilibrium mixtures and equilibrium constants

Change in	Composition	K_c or K_p
Concentration	Changes	Unchanged
Partial pressure	Changes	Unchanged
Total pressure	May change	Unchanged
Temperature	Changes	Changes
Catalyst	Unchanged	Unchanged

Learning outcomes

By the end of this chapter, you should be able to do the following.

- Understand and be able to use IUPAC base units and derived units
- Describe the structure of an atom in terms of protons, neutrons, and electrons
- Understand the terms mass number and atomic number and write atomic symbols for chemical elements
- Describe how a simple mass spectrometer can be used to show the isotopic composition of an element
- Understand and use the terms: relative atomic mass (A_r); relative formula (or molecular) mass (M_r); Avogadro constant (N_A); the mole (mol) as a unit of amount of substance
- Work out the empirical formula of a compound from its elemental composition and understand the relationship between empirical formula and molecular formula
- Write a balanced equation for a reaction, including state symbols, and use it to calculate reacting masses
- Work out the yield of a chemical reaction
- Write ionic equations
- Understand and use the terms redox, oxidation and reduction, oxidizing agent, and reducing agent
- Write half equations for a redox reaction and use them to construct a balanced overall equation for the reaction
- Assign oxidation states and use changes of oxidation state to decide what has been oxidized and what reduced in a redox reaction
- Perform calculations involving concentrations of compounds in solution
- Understand the techniques of volumetric analysis and gravimetric analysis and be able to carry out relevant calculations
- Understand what is meant by the terms: exothermic; endothermic; enthalpy change of a reaction; standard conditions; and thermochemical equation

- Draw an enthalpy level diagram and relate enthalpy changes to bond-breaking and bond-formation processes
- Describe the states of matter and phase changes in terms of a kinetic-molecular model of matter
- Recognize different types of non-covalent (intermolecular) interactions
- Understand that chemical equilibrium is a dynamic equilibrium and use Le Chatelier's principle to predict the effect of changes on the position of equilibrium
- Write expression for the equilibrium constants, K_c and K_p , and carry out simple calculations.