AQA Chemistry A-level

Physical Chemistry I
Definitions

Definitions and Concepts for AQA Chemistry A-level
Physical Chemistry I

1.1: Atomic Structure

Acceleration: Second stage of TOF spectrometry. The positively charged ions are accelerated by an electric field so that they have the same kinetic energy.

Atom: The smallest part of an element that can exist. All substances are made up of atoms.

Atomic nucleus: Positively charged object composed of protons and neutrons at the centre of every atom with one or more electrons orbiting it.

Atomic number: The number of protons in the nucleus.

Electron: Negatively charged subatomic particle which orbit the nucleus at various energy levels. Relative mass of 1/2000.

Electron configuration: The distribution of electrons of an atom in orbitals.
E.g. Ca: $1s^22s^22p^63s^23p^64s^2$.

Electron impact ionisation: Method of ionisation in TOF spectrometry. The sample is vaporised and an electron gun fires high energy electrons at it, causing an electron to be knocked off each particle to produce 1+ ions.

Electrospray ionisation: Method of ionisation in TOF spectrometry. The sample is dissolved and pushed through a fine nozzle at a high pressure. A high voltage is applied to it causing each particle to gain an H^+ ion. The sample is then turned into a gas.

First ionisation energy: : The energy required to remove 1 mole of electrons from 1 moles of gaseous atoms to form 1 mole of gaseous 1+ ions. E.g. $O(g) \rightarrow O^+ (g) + e^-$.

Ion detection: Fourth stage of TOF spectrometry. The negatively charged plate detects charged particles and a mass spectrum is produced.

Ion drift: Third stage of TOF spectrometry. The ions enter a region with no electric field, so they drift through it. The lighter the ion, the faster they will drift.

Ionisation: First stage of TOF spectrometry. The sample can be ionised by electrospray ionisation or electron impact ionisation.

Isotope: Atoms of the same element with the same number of protons but a different number of neutrons. E.g. ^{35}Cl and ^{37}Cl.

Mass number: The total number of protons and neutrons in the nucleus.

Mass spectrometer: A mass spectrometer gives accurate information about relative isotopic mass and also about the relative abundance of isotopes.

Mass spectrometry: Mass spectrometry can be used to identify elements and determine relative molecular mass.

Neutron: Neutral subatomic particle present in the nucleus of the atom. Relative mass of 1.

Nuclear charge: Total charge of all the protons in the nucleus. It has the same value as the atomic number. Increases as you go across the periodic table.

Proton: Positively charged subatomic particle present in the nucleus of the atom. Relative mass of 1.

Second ionisation energy: The energy required to remove 1 mole of electrons from 1 moles of gaseous 1+ ions to form 1 moles of gaseous 2+ ions. E.g. $O^-(g) \rightarrow O^{2+}(g) + e^-$.

Sub-shells (orbitals): Electron shells are divided up into sub-shells which have slightly different energy levels. The sub-shells have different numbers of orbitals which can each hold up to two electrons. Types of sub-shell: s, p, d and f.

Time of Flight (TOF) spectrometer: A method of mass spectrometry where an ions mass-to-charge ratio is determined by a time of flight measurement. Consists of four stages: ionisation, acceleration, ion drift and detection.

1.2: Amount of Substance

Atom economy: The measure of the amount of starting materials that end up as useful products.

$$\text{Percentage atom economy} = \frac{\text{Molecular mass of desired product}}{\text{Sum of molecular masses of all reactants}} \times 100$$

Avogadro's constant: The number of atoms, molecules or ions in one mole of a given substance.

Concentration: The amount of substance per unit volume. Units given in g/dm^3 or mol/dm^3.

Empirical formula: The smallest whole number ratio of atoms of each element in a compound.

Limiting reactant: The reactant that is completely used up since it limits the amount of products formed.

Mole: The mass of a substance containing the same number of units as there are atoms in exactly 12 g of carbon-12.

Molecular formula: The actual ratio of atoms of each element present in a compound.

Percentage by mass: A value representing the concentration of an element in a compound or a component in a mixture.

$$\text{Percentage by mass} = \frac{\text{Mass of desired component}}{\text{Total mass of the mixture}} \times 100$$

Percentage yield: The percentage ratio of the actual yield of product from a reaction compared with the theoretical yield.

$$\text{Percentage yield} = \frac{\text{Actual yield}}{\text{Theoretical Yield}} \times 100$$

Relative atomic mass: The average mass of an atom of an element compared to 1/12th the mass of an atom of carbon-12.

Relative molecular mass: The average mass of one molecule of an element or compound compared to 1/12th the mass of an atom of carbon-12.

1.3: Bonding

Co-ordinate bond: A co-ordinate (dative covalent) bond contains a shared pair of electrons with both electrons supplied by one atom.

Covalent bond: A shared pair of electrons between two non-metals.

Dipole: Difference in charge between the two atoms of a covalent bond caused by a shift in electron density in the bond due to the electronegativity difference between elements participating in bonding.

Electron pair repulsion: Repulsion that exists between electron pairs due to the negatively charged electrons. This repulsion means electron pairs position themselves as far apart from each other as possible around the central metal atom.

Electronegativity: The power of an atom to attract the electron density in a covalent bond towards itself.

Electrostatic forces: The strong forces of attraction between oppositely charged ions.

Hydrogen bonding: An interaction between a hydrogen atom and an electronegative atom, commonly nitrogen, fluorine or oxygen. The slightly positive hydrogen is attracted to the lone pair on the electronegative atom. Hydrogen bonds are stronger than van der Waals and dipole-dipole forces but weaker than ionic and covalent bonds.

Intermolecular forces: The forces which exist between molecules. The strength of the intermolecular forces impact physical properties like boiling/melting point.

Ion: An atom or molecule with an electric charge due to the loss or gain of electrons.

Ionic bond: A metal atom loses electron(s) to form a positively charged ion and a non-metal atom gains these electron(s) to form a negatively charged ion. An ionic bond is formed between the oppositely charged ions.

Ionic compound: Chemical compound formed of ions, held together by strong electrostatic forces.

Lattice: A repeating regular arrangement of atoms/ions/molecules. This arrangement occurs in crystal structures.

Macromolecular crystal structure: Giant covalent structures. Macromolecules have very high melting points because many strong covalent bonds have to be broken. Examples include diamond and graphite.

Metallic bond: The bonds present in metals between the positive metal ions and negatively charged electrons.

Permanent dipole-dipole forces: When molecules with polar covalent bonds interact with dipoles in other molecules dipole-dipole intermolecular forces are produced between the molecules. These intermolecular forces are generally stronger than van der Waals forces but weaker than hydrogen bonding.

Polar bond: A covalent bond between two atoms in which the electrons in the bond are unevenly distributed. This causes a slight charge difference, inducing a dipole in the molecule.

Simple molecular crystal structure: Structures in which the atoms are joined by strong covalent bonds. Weak intermolecular forces mean simple molecules have low melting and boiling points.

Van der Waals: Also known as induced dipole–dipole, dispersion and London forces, van der Waals forces exist between all molecules. They arise due to fluctuations of electron density within a nonpolar molecule. These fluctuations may temporarily cause an uneven electron distribution, producing an instantaneous dipole. This dipole can induce a dipole in another molecule, and so on.

VSEPR theory: Valence shell electron pair repulsion theory is used to deduce the geometry of molecules. Pairs of electrons in the outer shell of atoms arrange themselves as far apart as possible to minimise repulsion. Lone pair–lone pair repulsion is greater than lone pair–bond pair repulsion, which is greater than bond pair–bond pair repulsion.

1.4: Energetics

Calorimetry: The process of measuring the amount of energy absorbed or released during a chemical reaction.

Endothermic reaction: An endothermic reaction is one that takes in energy from the surroundings so the temperature of the surroundings decreases. In an endothermic reaction, the energy needed to break existing bonds is greater than the energy released from forming new bonds.

Enthalpy change (ΔH): The heat energy change measured under conditions of constant pressure.

Exothermic reaction: An exothermic reaction is one that transfers energy to the surroundings so the temperature of the surroundings increases. In an exothermic reaction, the energy released from forming new bonds is greater than the energy needed to break existing bonds.

Hess's law: The enthalpy change of a reaction is independent of the route taken.

Mean bond enthalpy: The enthalpy change when one mole of a specified covalent bond is broken averaged out across the range of compounds.

Molar enthalpy change: The enthalpy change per mole of substance.

Standard conditions: 100 kPa and a stated temperature (generally 298K).

Standard enthalpy of combustion (Δ_cH$^\ominus$): The enthalpy change when one mole of a substance is burned in excess oxygen under standard conditions.

Standard enthalpy of formation (Δ_fH$^\ominus$): The enthalpy change when one mole of a substance in its standard state under standard conditions is formed from its elements under standard conditions.

1.5: Kinetics

Activation energy: The minimum amount of energy for particles to collide with for a successful reaction to take place.

Catalyst: A substance that increases the rate of a reaction without being changed in chemical composition or amount. They work by providing an alternative reaction pathway with a lower activation energy.

Collision theory: Reactions can only occur when collisions take place between particles having sufficient energy.

Effect of concentration on reaction rate: As the concentration of reactants increases, the reacting particles get closer together meaning they will collide more often. As a result, there will be a higher rate of successful collisions and a faster rate of reaction.

Effect of pressure on reaction rate: As the pressure of gaseous reactants increases, the reacting particles get closer together meaning they will collide more often. As a result, there will be a higher rate of successful collisions and a faster rate of reaction.

Effect of temperature on reaction rate: Increasing the temperature means the particles will have more kinetic energy and so will move faster. If the molecules are moving faster they will collide more often and, since they've gained kinetic energy, a larger proportion of the particles will have at least the activation energy. For both these reasons the rate of reaction increases.

Maxwell-Boltzmann distribution: Shows the distribution of the molecular energies in a gas at a constant temperature. The area under the curve indicates the total number of particles present. Example distribution:
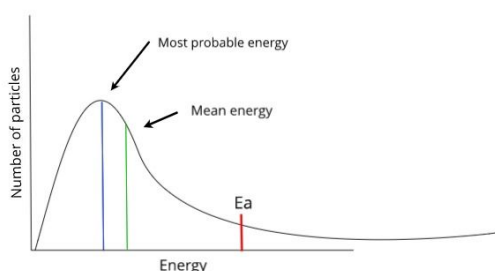
Rate of reaction: The measure of the amount of product formed or reactant used over time. The units of rate of reaction may be given as g/s, cm^3/s or mol/s.

1.6: Chemical Equilibria, Le Chatelier's Principle and K_C

Catalyst: A substance that increases the rate of a reaction without being changed in chemical composition or amount. They work by providing an alternative reaction pathway with a lower activation energy.

Closed system: A system where there is only heat exchange occurring between the system and its surroundings. No matter can enter or exit the system.

Dynamic equilibrium: Dynamic equilibrium is reached when the rate of the forward reaction of a reversible reaction equals the rate of the backward reaction. The concentrations of the reactants and products remain constant.

Effect of changing concentration on equilibrium: If the concentration of a reactant increases, more products will be formed to re-establish the equilibrium.

Effect of changing pressure on equilibrium: If pressure is increased, the position of equilibrium shifts towards the side with the fewest number of molecules. If the pressure is decreased, the position of equilibrium shifts towards the side with the greatest number of molecules.

Effect of changing temperature on equilibrium: If the temperature of a system in equilibrium is increased, there will be an increase in the relative amount of products for an endothermic reaction and a decrease for an exothermic reaction.

Equilibrium constant (K_C): A value that expresses the relationship between the concentration of products and reactants present at equilibrium in a reversible reaction.

Heterogeneous system: A system where not all the chemicals are in the same phase.

Homogeneous system: A system where all the chemicals are in the same phase.

Le Chatelier's principle: If a reaction at equilibrium is subjected to a change in concentration, temperature or pressure, the position of equilibrium will move to counteract the change.
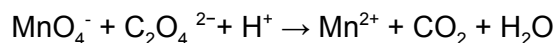
Reversible reaction: Reactions in which the products from the reaction can react together to form the original reactants. The direction of reversible reactions can be changed by changing the conditions.
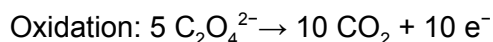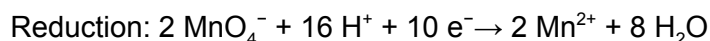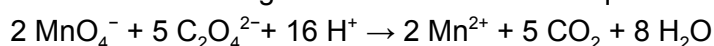
1.7: Oxidation, Reduction and Redox Equations

Half equation: A full redox equation can be split into two half-equations, one involving oxidation and the other involving reduction. This concept is useful for balancing complex redox reactions, such as:

$$MnO_4^- + C_2O_4^{\,2-} + H^+ \rightarrow Mn^{2+} + CO_2 + H_2O$$

can be split into:

Reduction: $2\ MnO_4^- + 16\ H^+ + 10\ e^- \rightarrow 2\ Mn^{2+} + 8\ H_2O$

Oxidation: $5\ C_2O_4^{2-} \rightarrow 10\ CO_2 + 10\ e^-$

And combined to give the balanced redox equation:
$2\ MnO_4^- + 5\ C_2O_4^{2-} + 16\ H^+ \rightarrow 2\ Mn^{2+} + 5\ CO_2 + 8\ H_2O$

Oxidation: Process involving the loss of electrons. Results in an increase in oxidation number.

Oxidation state: The charge of an ion or a theoretical charge of an atom in a covalently bonded compound assuming the bond becomes ionic.

Oxidising agent: Electron acceptors. The elements/compounds which accept electrons causing itself to be reduced.

Redox reaction: A reaction in which both reduction and oxidation are occurring simultaneously.

Reducing agent: Electron donors. The elements/compounds which donate electrons causing itself to be oxidised.

Reduction: Process involving the gain of electrons. Results in a decrease in oxidation number.