

4.2 Covalent Bonding

Single Covalent Bonds

- Involves the sharing of one or more pairs of electrons so that each atom in the molecule achieves an inert gas configuration
- The two electrons in a hydrogen molecule (H_2) are shared between the two atoms to form a molecule
- When one pair of electrons is shared the resulting bond is known as a single covalent bond

Lewis Structures

- In the Lewis structure all the valence electrons are shown
- **Single Covalent Bonds:**
- **Multiple Covalent Bonds:**
 - o In atoms some compounds can share more than one pair of electrons to achieve an inert gas configuration

Co-Ordinate (Dative) Bonds

- The electrons in the shared pair may originate from the same atom

Bond Length and Bond Strength

- The strength of attraction that the two nuclei have for the shared electrons affects both the length and strength of the bond
- Double bonds are generally much stronger and shorter than single bonds
- Triple bonds are generally much stronger and shorter than double bonds

Bond Polarity

- In diatomic molecules containing the same element the electron pair will be shared equally as both atoms exert an identical attraction
- When the atoms are different, the more electronegative atom exerts a greater attraction for the electron pair
- One end of the molecule will thus be more electron rich than the other end, resulting in a polar bond
- The bigger the difference in electronegativity values, the more polar the bond

5.2- ΔH Calculations

Calculation of Enthalpy Changes

- The heat involved in changing the temperature of any substance can be calculated from the equation: *Heat energy (Q) = Mass (m) x Specific Heat Capacity (c) x Temperature Change (ΔT)*
- The specific heat capacity of water is $4.18\text{kJkg}^{-1}\text{K}^{-1}$, that is, it requires 4.18 kilojoules of energy to raise the temperature of one kilogram of water by one kelvin

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5.6 Spontaneity of a Reaction

Possible Combinations for Free Energy Change

Type	ΔH^θ	ΔS^θ	$T\Delta S^\theta$	$\Delta H^\theta - T\Delta S^\theta$	ΔG^θ
1	0	+	+	0 - +	-
2	0	-	-	0 - -	+
3	-	+	+	- - +	-
4	+	-	-	+ - -	+
5	+	+	+	+ - +	-or+
6	-	-	-	- - -	+ or -

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6.1- Rates of Reaction and Collision Theory

Rate of Reaction

- Chemical kinetics is the study of the factors affecting the rate of a chemical reaction
- **Reaction Rate:** the increase in the concentration of one of the products per unit time or the decrease in the concentration of one of the reactants per unit time ($\text{mol dm}^{-3} \text{ s}^{-1}$)
- The change in concentration can be measured by using any property that differs between the reactants and the products
- When the concentration of the reactant/product is graphed, the rate at any given moment in time is the gradient of the graph at that point in time
- Rates of reaction usually decrease with time as the reactants are used up

Maxwell-Boltzmann Distribution

- The moving particles in a liquid or gas do not all travel with the same velocity
- The faster they move the more kinetic energy they possess
- The Maxwell-Boltzmann Distribution illustrates the distribution of the kinetic energies of particles
- As the temperature increases the area under the curve does not change as the total number of particles remains constant
- However more particles have a higher average kinetic energy which leads to a broadening of the curve
- The peak of the curve shifts to the right and decreases in height

Collision Theory

- For a reaction to occur three conditions must be met
 - o The particles must collide
 - o They must collide with the appropriate geometry or orientation so that the respective parts of the particles come into contact with each other
 - o They must collide with sufficient energy to bring about the reaction
- **Activation Energy:** the minimum amount of energy required for a reaction to occur
- Any factor which either increases the frequency of the collisions or increases the energy with which they collide will make the reaction go faster

9.1 Redox Reactions

Definitions of Oxidation and Reduction

- **Oxidation:** the loss of one or more electrons from a substance
- **Reduction:** the gain of one or more electrons
- Since the processes involve the transfer of electrons oxidation and reduction must occur simultaneously
 - o Such reactions are known as redox reactions

Rules for Determining Oxidation Numbers

- Useful tools to identify which species have been oxidised and which reduced
1. In an ionic compound between two elements the oxidation number of each element is equal to the charge carried by the ion
 - a. NaCl : $\text{Na} = +1$, $\text{Cl} = -1$
 2. For covalent compounds assume the compound is ionic with the more electronegative element forming the negative ion
 - a. CCl_4 : $\text{C} = +4$, $\text{Cl} = -1$
 3. The algebraic sum of all oxidation numbers in a compound is equal to zero
 - a. CCl_4 : $\text{C} = +4$, $4 \times \text{Cl} = -4$
 4. The algebraic sum of all the oxidation numbers in an ion is equal to the charge on the ion
 - a. SO_4^{2-} : $\text{S} = +6$, $4 \times \text{O} = -8$
 5. Elements not combined with other elements have an oxidation number of zero
 - a. $\text{O}_2 = 0$
 6. Oxygen when combined always has an oxidation number of -2 except in peroxides (H_2O_2) where it is -1
 7. Hydrogen when combined always has an oxidation number of +1 except in metal hydrides (NaH) where it is -1
- Many elements show different oxidation numbers in different compounds
 - When elements show more than one oxidation state the oxidation number is represented by using Roman numerals when naming the compound

Oxidation and Reduction in Terms of Oxidation Numbers

- When an element is oxidised its oxidation number increases
- When an element is reduced its oxidation number decreases
- The change in oxidation number will be equal to the number of electrons involved in the half equations
- Reactions where an element is uncombined on one side of the equation and combined on the other side must be redox reactions since there must be a change in oxidation number

Oxidizing Agents and Reducing Agents

- A substance that readily oxidizes other substances is known as an oxidizing agent

- Oxidizing agents readily accept electrons
- Reducing agents readily donate electrons

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9.2 Reactivity Series

Reactivity

- Reactivity with water decreases down group 1
- In all of these reactions the metal is losing electrons
 - o It is being oxidized and in the process it is acting as a reducing agent
- A reactivity series of reducing agents can be deduced by considering the reactivity of metals with water and acids
- The more readily the metal loses its outer electrons the more reactive it is
- Metals higher in the series can displace metal ions lower in the series from the solution
- The series can be extended for oxidizing agents, the most reactive oxidising agent will be the species that gains electrons the most readily
- Oxidising agents lower in the series gain electrons from species higher in the series

Simple Voltaic Cells

- A half-cell is simply a metal in contact with an aqueous solution of its own ions
- Voltaic cells consist of two half-cells, connected together to enable the electrons transferred during the redox reaction to produce energy in the form of electricity
- Connected by an external wire and a salt bridge which allows free movement of ions
- The electrons will flow from the metal which is higher in the reactivity series to the one which is lower
- The voltage produced by a voltaic cell depends on the relative difference between the two metals in the reactivity series
 - o The greater the difference the greater the voltage produced
- In a voltaic cell:
 - o The anode is the negative electrode where oxidation occurs
 - o The cathode is the positive electrode where reduction occurs

10.2 Properties of Different Functional Groups

Boiling Points

- As the carbon chain gets longer the mass of the molecules increases and the van der Waals forces increase
- The boiling point hence increases as the carbon chain gets longer
- When branching occurs the molecules become more spherical in shape which reduces the contact surface area between them and lowers the boiling point
- Volatility of the compounds follows the same pattern
- Lower members of the alkanes are all gases as the attractive forces are weak and the next few members are volatile liquids
- As the carbon chain increases in length the alcohols have lower volatility

Solubility in Water

- Depends on the functional group and on the chain length
- Lower members of alcohols, amines, aldehydes, ketones and carboxylic acids are all water soluble
- As carbon chain length increases solubility in water decreases
- Compounds with non-polar functional groups such as alkanes and alkenes do not dissolve in water but are soluble in other non-polar solvents

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10.4 Alkanes

Low Reactivity of Alkanes

- The relatively strong C-C and C-H bonds and the low polarity of alkanes tends to be quite unreactive
- Only readily undergo combustion reactions with oxygen and substitution reactions in ultraviolet light

Combustion

- Alkanes are hydrocarbons and only hydrocarbons burn in a plentiful supply of oxygen to give carbon dioxide and water
- $C_xH_y + (x + y/4)O_2 \rightarrow xCO_2 + y/2H_2O$
- This reaction is exothermic and much use is made of the alkanes as fuels
- If there is an insufficient supply of oxygen then incomplete combustion occurs and carbon monoxide and carbon are also produced as products

Substitution Reactions

- Alkanes can react with chlorine (or other halogens) in the presence of ultraviolet light to form hydrogen chloride and a substituted alkane
- $CH_4 + Cl_2 \xrightarrow{UV} CH_3Cl + HCl$

Mechanism of Chlorination of Methane

- When chemical bonds break they may break heterolytically or homolytically
 - o Heterolytic fission: both of the shared electrons go to one of the atoms resulting in a negative and a positive ion
 - o Homolytic fission: each of the two atoms forming the bond retains one of the shared electrons resulting in the formation of two free radicals
- $Cl_2 \rightarrow Cl\cdot + Cl\cdot$ This step is called initiation
- Free radicals contain an unpaired electron and are highly reactive
- When the chlorine free radicals come into contact with a methane molecule they combine with a hydrogen atom to produce hydrogen chloride and a methyl radical
- $H_3C-H + Cl\cdot \rightarrow H_3C\cdot + HCl$
- Since a new radical is produced this stage is called propagation
- The methyl radical is also highly reactive and reacts with a chlorine molecule to form the product and regenerate another chlorine radical
- This is a further propagation step and enables a chain reaction to occur as the process can repeat itself
- $CH_3\cdot + Cl_2 \rightarrow CH_3Cl + Cl\cdot$
- Termination occurs when two radicals react together
- $Cl\cdot + Cl\cdot \rightarrow Cl_2$
- Further substitution can occur when chlorine radicals react with the substituted products
- The substitution can continue even further to produce trichloromethane and then tetrachloromethane
- The overall mechanism is called free radical substitution

10.5 Alkenes

Addition Reactions

- The C=C bond accounts for the relative reactivity of alkenes compared to alkanes
- Most important reactions are addition reactions
- Reactive molecules are able to add across the double bond
- Double bond is unsaturated and the product is said to be saturated
- $CZ_2CZ_2 + XY \rightarrow CZ_2XCZ_2Y$
- To produce an alcohol from an alkene a sulfuric acid catalyst is required

Uses of Addition Reactions

Bromination

- Pure bromine is red liquid but has distinct yellow/orange colour in solution
- When added to an alkene the product is colourless
- The decolourisation of bromine solution provides a useful test to indicate the presence of an alkene group

Hydration

- Ethene is an important product formed during the cracking of oil
- Although ethanol can be made from the fermentation of starch and sugars
- Much industrial ethanol is formed from the addition of steam to ethene

Hydrogenation

- The addition of hydrogen to unsaturated vegetable oils is used industrially to make margarine
- Hydrogenation reduces the number of double bonds in the polyunsaturated vegetable oils present in the margarine which causes it to become a solid at room temperature

Addition Polymerisation

- Under certain conditions ethene can undergo addition reactions with itself to form a long chain polymer containing many thousands of carbon atoms
- $n(CH_2CH_2) \rightarrow -(CH_2CH_2)_n$
- These addition reactions can be extended to other substituted alkenes to give a wide variety of different addition polymers

10.12- Stereoisomerism

- **Structural Isomers:** share the same molecular formula but have different structural formulas
- **Stereoisomers:** have the same structural formula but differ in their spatial arrangement
 - o Two types of stereoisomerism:
 - Geometrical Isomerism
 - Optical Isomerism

Geometrical Isomerism

- Occurs when rotation about a bond is restricted or prevented
- The classic examples of geometric isomers occur with asymmetric non-cyclic alkenes
- A *cis*- isomer is one in which the substituents are on the same side of the double bond
- In a *trans*- isomer the substituents are on opposite sides of the double bond
 - o *Cis*-: $\text{H}_3\text{CHC}=\text{CHCH}_3$
 - o *Trans*-: $\text{HH}_3\text{CC}=\text{CHCH}_3$
- When there is a single bond between two carbon atoms free rotation about the bond is possible
- However, the double bond in an alkene is made up of a σ and a π bond
- The π bond is formed from the combination of two p orbitals, one from each of the carbon atoms
- These two p orbitals must be in the same plane to combine
- Rotating the bond would cause the π bond to break so no rotation is possible
- *Cis*- and *trans*- isomerism will always occur in alkenes when the two groups attached to each of the two carbon atoms are different
- Geometrical isomerism can also occur in disubstituted cycloalkanes
 - o The rotation is restricted because the C-C single bond is part of a ring system

Physical and Chemical Properties of Geometrical Isomers

- The chemical properties of geometric isomers tend to be similar but their physical properties are different
- Sometimes there can be a marked difference in both chemical and physical properties which tends to occur when there is some sort of chemical interaction between the substituents

Optical Isomerism

- Optical isomerism is shown by all compounds that contain at least one asymmetric or chiral carbon atom within the molecule
- A chiral carbon is one that contains four different atoms or groups bonded to it
- The two isomers are known as enantiomers and are mirror images of each other
- The two different isomers are optically active with plane polarised light
- Normal light consists of electromagnetic radiation which vibrates in all planes
- When it is passed through a polarizing filter the waves only vibrate in one plane and the light is said to be plane polarized
- The two enantiomers both rotate the plane of plane polarised light
- One of the enantiomers rotates it to the left and the other rotates it by the same amount to the right
- Enantiomers have identical physical properties