

1.1 Unit description

Chemical ideas

This unit provides opportunities for students to develop the basic chemical skills of formulae writing, equation writing and calculating chemical quantities.

The study of energetics in chemistry is of theoretical and practical importance. In this unit students learn to define, measure and calculate enthalpy changes. They will see how a study of enthalpy changes can help chemists to understand chemical bonding.

The study of atomic structure introduces s, p, and d orbitals and shows how a more detailed understanding of electron configurations can account for the arrangement of elements in the periodic table.

The unit introduces the three types of strong chemical bonding (ionic, covalent and metallic).

Organic chemistry is also introduced, with students studying alkanes and alkenes.

How chemists work

Practical work measuring energy changes helps students to understand the ideas of uncertainty in measurements and evaluate their results in terms of systematic and random errors.

The study of atomic structure gives some insight into the types of evidence which scientists use to study electrons in atoms. This leads to an appreciation of one of the central features of chemistry which is the explanation of the properties of elements and the patterns in the periodic table in terms of atomic structure.

The role of instrumentation in analytical chemistry is illustrated by mass spectrometry.

Students are introduced to some of the evidence which will help them to understand the different kinds of chemical bonding.

Chemists set up theoretical models and gain insights by comparing real and ideal properties of chemicals. This is illustrated in the unit by the ionic model and the comparison of lattice energies calculated from theory with those determined with the help of Born-Haber cycles.

Throughout the unit students see the importance of chemical data and learn to select data from databases and use it to look for patterns and calculate other quantities.

The introduction to organic chemistry shows how chemists work safely with potentially hazardous chemicals by managing risks.

Chemistry in action

The uses of mass spectrometry illustrate the importance of sensitive methods of analysis in areas such as space research, medical research and diagnosis, in detecting drugs in sport and in environmental monitoring.

In this unit students learn how chemical insights can help to make the use of polymeric and other materials more sustainable. This involves analysis of the uses of energy, raw materials and other resources at each stage of the life cycle of products.

Core practicals

The following specification points are core practicals within this unit that students should complete:

1.3j

1.3k

1.4f

These practicals may appear in the written examination for Unit 1.

Use of examples**Examples in practicals**

Where 'e.g.' follows a type of experiment in the specification students are not expected to have carried out that specific experiment. However, they should be able to use data from that or similar experiments.

For instance in this unit, *1.4f ii Energetics*, the specification states:

simple enthalpy of combustion experiments using, e.g. a series of alcohols in a spirit burner.

Students should have carried out simple enthalpy of combustion reactions, but they may or may not have carried out these using alcohol in spirit burners.

In the unit test students could be given experimental data for this, or any other enthalpy of combustion reaction, and be expected to analyse and evaluate this data.

Examples in unit content

Where 'e.g.' follows a concept students are not expected to have been taught the particular example given in the specification. They should be able to illustrate their answer with an example of their choice.

For instance in this unit, *1.6.1f Ionic bonding*, the specification states:

recall trends in ionic radii down a group and for a set of isoelectronic ions, e.g. N^{3-} to Al^{3+} .

Students will be expected to recall the trends in ionic radii down a group, and for a set of isoelectronic ions, but they may or may not have done this from N^{3-} to Al^{3+} .

In the unit test students could be asked to recall the trends in ionic radii down a group. They could be asked this in reference to any group in the periodic table, either the one listed as an example or another group.

1.2 Assessment information

Unit 1 examination The examination will be 1 hour 30 minutes and have 80 marks. It will contain two sections – A and B.

Section A is an objective test section which will aim to cover a large proportion of the specification for this unit.

Section B contains a mixture of short-answer and extended answer questions. This will include questions on the analysis and evaluation of practical work.

Students may use a calculator.

Quality of written communication will be assessed in this examination through questions which are labelled with an asterisk (*). When answering these questions students should consider spelling, punctuation and grammar of their response, as well as the clarity of expression.

1.3 Formulae, equations and amount of substance

Application of ideas from this topic will be applied to all other units.

Students will be assessed on their ability to:

- a demonstrate an understanding of the terms *atom*, *element*, *ion*, *molecule*, *compound*, *empirical* and *molecular formulae*
- b write balanced equations (full and ionic) for simple reactions, including the use of state symbols
- c demonstrate an understanding of the terms *relative atomic mass*, *amount of substance*, *molar mass* and *parts per million (ppm)*, e.g. gases in the atmosphere, exhausts, water pollution
- d calculate the amount of substance in a solution of known concentration (excluding titration calculations at this stage), e.g. use data from the concentrations of the various species in blood samples to perform calculations in mol dm^{-3}
- e use chemical equations to calculate reacting masses and vice versa using the concepts of amount of substance and molar mass
- f use chemical equations to calculate volumes of gases and vice versa using the concepts of amount of substance and molar volume of gases, e.g. calculation of the mass or volume of CO_2 produced by combustion of a hydrocarbon (given a molar volume for the gas)
- g use chemical equations and experimental results to deduce percentage yields and atom economies in laboratory and industrial processes and understand why they are important
- h demonstrate an understanding of, and be able to perform, calculations using the Avogadro constant
- i analyse and evaluate the results obtained from finding a formula or confirming an equation by experiment, e.g. the reaction of lithium with water and deducing the equation from the amounts in moles of lithium and hydrogen

- j make a salt and calculate the percentage yield of product, e.g. preparation of a double salt (ammonium iron(II) sulfate from iron, ammonia and sulfuric acid)
- k carry out and interpret the results of simple test tube reactions, such as displacements, reactions of acids, precipitations, to relate the observations to the state symbols used in equations and to practise writing full and ionic equations.

1.4 Energetics

Students will be assessed on their ability to:

- a demonstrate an understanding of the term *enthalpy change*, ΔH
- b construct simple enthalpy level diagrams showing the enthalpy change
- c recall the sign of ΔH for exothermic and endothermic reactions, e.g. illustrated by the use of exo- and endothermic reactions in hot and cold packs
- d recall the definition of standard enthalpy changes of reaction, formation, combustion, neutralisation and atomisation and use experimental data to calculate energy transferred in a reaction and hence the enthalpy change of the reaction. This will be limited to experiments where substances are mixed in an insulated container and combustion experiments
- e recall Hess's Law and apply it to calculating enthalpy changes of reaction from data provided, selected from a table of data or obtained from experiments and understand why standard data is necessary to carry out calculations of this type
- f evaluate the results obtained from experiments using the expression:
$$\text{energy transferred in joules} = \text{mass} \times \text{specific heat capacity} \times \text{temperature change}$$
and comment on sources of error and assumptions made in the experiments. The following types of experiments should be performed:
 - i experiments in which substances are mixed in an insulated container and the temperature rise measured
 - ii simple enthalpy of combustion experiments using, e.g. a series of alcohols in a spirit burner
 - iii plan and carry out an experiment where the enthalpy change cannot be measured directly, e.g. the enthalpy change for the decomposition of calcium carbonate using the enthalpy changes of reaction of calcium carbonate and calcium oxide with hydrochloric acid
- g demonstrate an understanding of the terms *bond enthalpy* and *mean bond enthalpy*, and use bond enthalpies in Hess cycle calculations and recognise their limitations. Understand that bond enthalpy data gives some indication about which bond will break first in a reaction, how easy or difficult it is and therefore how rapidly a reaction will take place at room temperature.

1.5 Atomic structure and the periodic table

Students will be assessed on their ability to:

- a recall the definitions of relative atomic mass, relative isotopic mass and relative molecular mass and understand that they are measured relative to 1/12th the mass of a ^{12}C atom
- b demonstrate an understanding of the basic principles of a mass spectrometer and interpret data from a mass spectrometer to:
 - i deduce the isotopic composition of a sample of an element, e.g. polonium
 - ii deduce the relative atomic mass of an element
 - iii measure the relative molecular mass of a compound
- c describe some uses of mass spectrometers, e.g. in radioactive dating, in space research, in sport to detect use of anabolic steroids, in the pharmaceutical industry to provide an identifier for compounds synthesised for possible identification as drugs
- d recall and understand the definition of ionisation energies of gaseous atoms and that they are endothermic processes
- e recall that ideas about electronic structure developed from:
 - i an understanding that successive ionisation energies provide evidence for the existence of quantum shells and the group to which the element belongs
 - ii an understanding that the first ionisation energy of successive elements provides evidence for electron sub-shells
- f describe the shapes of electron density plots (or maps) for s and p orbitals
- g predict the electronic structure and configuration of atoms of the elements from hydrogen to krypton inclusive using $1s \dots$ notation and electron-in-boxes notation (recall electrons populate orbits singly before pairing up)
- h demonstrate an understanding that electronic structure determines the chemical properties of an element
- i recall that the periodic table is divided into blocks, such as s, p and d
- j represent data, in a graphical form, for elements 1 to 36 and use this to explain the meaning of the term *periodic property*

- k explain trends in the following properties of the element from periods 2 and 3 of the periodic table:
 - i melting temperature of the elements based on given data using the structure and the bonding between the atoms or molecules of the element
 - ii ionisation energy based on given data or recall of the shape of the plots of ionisation energy versus atomic number using ideas of electronic structure and the way that electron energy levels vary across the period.

1.6 Bonding

Students will be assessed on their ability to:

- 1 Ionic bonding
 - a recall and interpret evidence for the existence of ions, limited to physical properties of ionic compounds, electron density maps and the migration of ions, e.g. electrolysis of aqueous copper chromate(VI)
 - b describe the formation of ions in terms of electron loss or gain
 - c draw electron configuration diagrams of cations and anions using dots or crosses to represent electrons
 - d describe ionic crystals as giant lattices of ions
 - e describe ionic bonding as the result of strong net electrostatic attraction between ions
 - f recall trends in ionic radii down a group and for a set of isoelectronic ions, e.g. N^{3-} to Al^{3+}
 - g recall the stages involved in the formation of a solid ionic crystal from its elements and that this leads to a measure value for the lattice energy (students will not be expected to draw the full Born-Haber cycles)
 - h test the ionic model for ionic bonding of a particular compound by comparison of lattice energies obtained from the experimental values used in Born-Haber cycles, with provided values calculated from electrostatic theory
 - i explain the meaning of the term *polarisation* as applied to ions
 - j demonstrate an understanding that the polarising power of a cation depends on its radius and charge, and the polarisability of an anion depends on its size
 - k demonstrate an understanding that polarisation of anions by cations leads to some covalency in an ionic bond, based on evidence from the Born-Haber cycle
 - l use values calculated for standard heats of formation based on Born-Haber cycles to explain why particular ionic compounds exist, e.g. the relative stability of MgCl_2 over MgCl or MgCl_3 and NaCl over NaCl_2 .

2 Covalent bonding

- a demonstrate an understanding that covalent bonding is strong and arises from the electrostatic attraction between the nucleus and the electrons which are between the nuclei, based on the evidence:
 - i the physical properties of giant atomic structures
 - ii electron density maps for simple molecules
- b draw electron configuration diagrams for simple covalently bonded molecules, including those with multiple bonds and dative covalent bonds, using dots or crosses to represent electrons.

3 Metallic bonding

- a demonstrate an understanding that metals consist of giant lattices of metal ions in a sea of delocalised electrons
- b describe metallic bonding as the strong attraction between metal ions and the sea of delocalised electrons
- c use the models in 1.6.3a and 1.6.3b to interpret simple properties of metals, e.g. conductivity and melting temperatures.

1.7 Introductory organic chemistry

Related topics in Units 2, 4 and 5 will assume knowledge of this material.

Students will be assessed on their ability to:

1 Introduction

- a demonstrate an understanding that there are series of organic compounds characterised by a general formula and one or more functional groups
- b apply the rules of IUPAC nomenclature to compounds relevant to this specification and draw these compounds, as they are encountered in the specification, using structural, displayed and skeletal formulae
- c appreciate the difference between hazard and risk
- d demonstrate an understanding of the hazards associated with organic compounds and why it is necessary to carry out risk assessments when dealing with potentially hazardous materials. Suggest ways by which risks can be reduced and reactions can be carried out safely by:
 - i working on a smaller scale
 - ii taking specific precautions or using alternative techniques depending on the properties of the substances involved
 - iii carrying out the reaction using an alternative method that involves less hazardous substances.

2 Alkanes

- a state the general formula of alkanes and understand that they are saturated hydrocarbons which contain single bonds only
- b explain the existence of structural isomers using alkanes (up to C₅) as examples
- c know that alkanes are used as fuels and obtained from the fractional distillation, cracking and reformation of crude oil
- d discuss the reasons for developing alternative fuels in terms of sustainability and reducing emissions, including the emission of CO₂ and its relationship to climate change
- e describe the reactions of alkanes in terms of combustion and substitution by chlorine showing the mechanism of free radical substitution in terms of initiation, propagation and termination and using curly half-arrows in the mechanism to show the formation of free radicals in the initiation step using a single dot to represent the unpaired electron.

3 Alkenes

- a state the general formula of alkenes and understand that they are unsaturated hydrocarbons with a carbon-carbon double bond which consists of a σ and a π bond
- b explain E-Z isomerism (geometric/cis-trans isomerism) in terms of restricted rotation around a C=C double bond and the nature of the substituents on the carbon atoms
- c demonstrate an understanding of the E-Z naming system and why it is necessary to use this when the *cis*- and *trans*- naming system breaks down
- d describe the addition reactions of alkenes, limited to:
 - i the addition of hydrogen with a nickel catalyst to form an alkane
 - ii the addition of halogens to produce di-substituted halogenoalkanes
 - iii the addition of hydrogen halides to produce mono-substituted halogenoalkanes
 - iv oxidation of the double bond by potassium manganate(VII) to produce a diol
- e describe the mechanism (including diagrams), giving evidence where possible, of:
 - i the electrophilic addition of bromine and hydrogen bromide to ethene
 - ii the electrophilic addition of hydrogen bromide to propene
- f describe the test for the presence of C=C using bromine water and understand that the product is the addition of OH and Br
- g describe the addition polymerisation of alkenes and identify the repeat unit given the monomer, and vice versa
- h interpret given information about the uses of energy and resources over the life cycle of polymer products to show how the use of renewable resources, recycling and energy recovery can contribute to the more sustainable use of materials.

2.1 Unit description

Chemical ideas

This unit develops the treatment of chemical bonding by introducing intermediate types of bonding and by exploring the nature and effects of intermolecular forces.

Study of the periodic table is extended to cover the chemistry of groups 2 and 7. Ideas about redox reactions are applied in particular to the reactions of halogens and their compounds.

The unit develops a largely qualitative understanding of the ways in which chemists can control the rate, direction and extent of chemical change.

Organic chemistry in this unit covers alcohols and halogenoalkanes. The treatment is extended to explore the mechanisms of selected examples.

Students have to use formulae and balance equations and have an understanding of chemical quantities.

How chemists work

Electron-pair repulsion theory shows how chemists can make generalisations and use them to make predictions.

Chemists rationalise a great deal of information about chemical changes by using theory to categorise reagents and types of chemical change. This is illustrated by the use of inorganic and organic examples in this unit.

The use of models in chemistry is illustrated by the way in which the Maxwell-Boltzmann distribution and collision theory can account for the effects of temperature on the rates of chemical reactions.

The unit shows how chemists can study chemical changes on an atomic scale and propose mechanisms to account for their observations.

Chemistry in action

This unit shows the contribution that chemistry can make to a more sustainable economy by redeveloping manufacturing processes to make them more efficient, less hazardous and less polluting.

Insight into the mechanisms of chemical reactions can help to account for the damaging effects of some chemicals on the natural environment.

The study of spectroscopy gives further examples of the importance of accurate and sensitive methods of analysis which can be applied to study chemical changes but also to detect drugs such as alcohol.

The unit deals with issues regarding the environment, such as climate change, the effect of greenhouse gases, carbon footprints and other aspects of green chemistry. It ensures that students understand the underlying chemistry and can investigate ways to combat these issues.

Core practicals

The following specification points are core practicals within this unit that students should complete:

2.4d

2.5c

2.7.1g

2.7.2b

2.7.2c

2.7.2d

2.8f

2.10.1d

2.10.2c

2.10.2e

These practicals may appear in the written examination for Unit 2.

Use of examples**Examples in practicals**

Where 'e.g.' follows a type of experiment in the specification students are not expected to have carried out that specific experiment. However, they should be able to use data from that or similar experiments.

For instance in this unit, 2.7g ii *Properties down group 2*, the specification states:

simple acid-base titrations using a range of indicators, acids and alkalis, to calculate solution concentrations in g dm^{-3} and mol dm^{-3} , e.g. measuring the residual alkali present after skinning fruit with potassium hydroxide.

Students will be expected to have carried out simple acid-base titrations, but they may or may not have done this to measure the residual alkali present after skinning fruit.

In the unit test students could be given experimental data for this or any other acid-base titration, and be expected to analyse and evaluate this data.

Examples in unit content

Where 'e.g.' follows a concept students are not expected to have been taught the particular example given in the specification. They should be able to illustrate their answer with an example of their choice.

For instance in this unit, 2.10.2f *Halogenoalkanes*, the specification states:

discuss the uses of halogenoalkanes, e.g. as fire retardants and modern refrigerants.

Students will be expected to discuss the use of halogenoalkanes, but they may or may not have looked at their use as fire retardants or refrigerants.

In the unit test students could be asked to discuss some of the uses of halogenoalkanes. This could be those listed as examples or other uses.

2.2 Assessment information

Unit 2 examination The examination will be 1 hour 30 minutes and have 80 marks. It will contain three sections – A, B and C.

Section A is an objective test section which will aim to cover a large proportion of the specification for this unit.

Section B contains a mixture of short-answer and extended answer questions. This will include questions on the analysis and evaluation of practical work.

Section C will contain extended answer questions on contemporary contexts. This may contain stimulus materials on a scenario that students must read in order to answer the questions. It will focus on the chemistry behind the contexts and will not be a comprehension exercise.

Students may use a calculator.

Quality of written communication will be assessed in this examination through questions which are labelled with an asterisk (*). When answering these questions students should consider spelling, punctuation and grammar of their response, as well as the clarity of expression.

Questions on the analysis and evaluation of practical work will also be included in either Section B or C.

2.3 Shapes of molecules and ions

Students will be assessed on their ability to:

- a demonstrate an understanding of the use of electron-pair repulsion theory to interpret and predict the shapes of simple molecules and ions
- b recall and explain the shapes of BeCl_2 , BCl_3 , CH_4 , NH_3 , NH_4^+ , H_2O , CO_2 , gaseous PCl_5 and SF_6 and the simple organic molecules listed in Units 1 and 2
- c apply the electron-pair repulsion theory to predict the shapes of molecules and ions analogous to those in 2.3b
- d demonstrate an understanding of the terms *bond length* and *bond angle* and predict approximate bond angles in simple molecules and ions
- e discuss the different structures formed by carbon atoms, including graphite, diamond, fullerenes and carbon nanotubes, and the applications of these, e.g. the potential to use nanotubes as vehicles to carry drugs into cells.

2.4 Intermediate bonding and bond polarity

Students will be assessed on their ability to:

- a explain the meaning of the term *electronegativity* as applied to atoms in a covalent bond
- b recall that ionic and covalent bonding are the extremes of a continuum of bonding type and explain this in terms of electronegativity differences leading to bond polarity in bonds and molecules, and to ionic bonding if the electronegativity is large enough
- c distinguish between polar bonds and polar molecules and be able to predict whether or not a given molecule is likely to be polar
- d carry out experiments to determine the effect of an electrostatic force on jets of liquids and use the results to determine whether the molecules are polar or non-polar.

2.5 Intermolecular forces

Students will be assessed on their ability to:

- a demonstrate an understanding of the nature of intermolecular forces resulting from interactions between permanent dipoles, instantaneous dipoles and induced dipoles (London forces) and from the formation of hydrogen bonds
- b relate the physical properties of materials to the types of intermolecular force present, e.g.:
 - i the trends in boiling and melting temperatures of alkanes with increasing chain length
 - ii the effect of branching in the carbon chain on the boiling and melting temperatures of alkanes
 - iii the relatively low volatility (higher boiling temperatures) of alcohols compared to alkanes with a similar number of electrons
 - iv the trends in boiling temperatures of the hydrogen halides HF to HI
- c carry out experiments to study the solubility of simple molecules in different solvents
- d interpret given information about solvents and solubility to explain the choice of solvents in given contexts, discussing the factors that determine the solubility including:
 - i the solubility of ionic compounds in water in terms of the hydration of the ions
 - ii the water solubility of simple alcohols in terms of hydrogen bonding
 - iii the insolubility of compounds that cannot form hydrogen bonds with water molecules, e.g. polar molecules such as halogenoalkanes
 - iv the solubility in non-aqueous solvents of compounds which have similar intermolecular forces to those in the solvent.

2.6 Redox

Students will be assessed on their ability to:

- a demonstrate an understanding of:
 - i oxidation number — the rules for assigning oxidation numbers
 - ii oxidation and reduction as electron transfer
 - iii oxidation and reduction in terms of oxidation number changes
 - iv how oxidation number is a useful concept in terms of the classification of reactions as redox and as disproportionation

- b write ionic half-equations and use them to construct full ionic equations.

2.7 The periodic table — groups 2 and 7

Students will be assessed on their ability to:

1 Properties down group 2

- a explain the trend in the first ionisation energy down group 2
- b recall the reaction of the elements in group 2 with oxygen, chlorine and water
- c recall the reactions of the oxides of group 2 elements with water and dilute acid, and their hydroxides with dilute acid
- d recall the trends in solubility of the hydroxides and sulfates of group 2 elements
- e recall the trends in thermal stability of the nitrates and the carbonates of the elements in groups 1 and 2 and explain these in terms of size and charge of the cations involved
- f recall the characteristic flame colours formed by group 1 and 2 compounds and explain their origin in terms of electron transitions
- g describe and carry out the following:
 - i experiments to study the thermal decomposition of group 1 and 2 nitrates and carbonates
 - ii flame tests on compounds of group 1 and 2
 - iii simple acid-base titrations using a range of indicators, acids and alkalis, to calculate solution concentrations in g dm^{-3} and mol dm^{-3} , e.g. measuring the residual alkali present after skinning fruit with potassium hydroxide
- h demonstrate an understanding of how to minimise the sources of measurement uncertainty in volumetric analysis and estimate the overall uncertainty in the calculated result.

2 Inorganic chemistry of group 7 (limited to chlorine, bromine and iodine)

- a recall the characteristic physical properties of the elements limited to the appearance of solutions of the elements in water and hydrocarbon solvents
- b describe and carry out the following chemical reactions of halogens:
 - i oxidation reactions with metal and non-metallic elements and ions such as iron(II) and iron(III) ions in solution
 - ii disproportionation reactions with cold and hot alkali, e.g. hot potassium hydroxide with iodine to produce potassium iodate(V)
- c carry out an iodine/thiosulfate titration, including calculation of the results and evaluation of the procedures involved, e.g. determination of the purity of potassium iodate(V) by liberation of iodine and titration with standard sodium thiosulfate solution
- d describe and carry out the following reactions:
 - i potassium halides with concentrated sulfuric acid, halogens and silver nitrate solution
 - ii silver halides with sunlight and their solubilities in aqueous ammonia solution
 - iii hydrogen halides with ammonia and with water (to produce acids)
- e make predictions about fluorine and astatine and their compounds based on the trends in the physical and chemical properties of halogens.

2.8 Kinetics

Students will be assessed on their ability to:

- a recall the factors that influence the rate of chemical reaction, including concentration, temperature, pressure, surface area and catalysts
- b explain the changes in rate based on a qualitative understanding of collision theory
- c use, in a qualitative way, the Maxwell-Boltzmann model of the distribution of molecular energies to relate changes of concentration and temperature to the alteration in the rate of a reaction
- d demonstrate an understanding of the concept of activation energy and its qualitative relationship to the effect of temperature changes on the rate of reaction
- e demonstrate an understanding of the role of catalysts in providing alternative reaction routes of lower activation energy and draw the reaction profile of a catalysed reaction including the energy level of the intermediate formed with the catalyst
- f carry out simple experiments to demonstrate the factors that influence the rate of chemical reactions, e.g. the decomposition of hydrogen peroxide.

2.9 Chemical equilibria

Students will be assessed on their ability to:

- a demonstrate an understanding that chemical equilibria are dynamic
- b deduce the qualitative effects of changes of temperature, pressure and concentration on the position of equilibrium, e.g. extraction of methane from methane hydrate
- c interpret the results of simple experiments to demonstrate the effect of a change of temperature, pressure and concentration on a system at equilibrium, e.g.
 - i iodine(I) chloride reacting with chlorine to form iodine(III) chloride, or
 - ii $\text{N}_2\text{O}_4 \rightleftharpoons 2\text{NO}_2$.

2.10 Organic chemistry

Related topics in Units 4 and 5 will assume knowledge of this material.

Students will be assessed on their ability to:

1 Alcohols

- a give examples of, and recognise, molecules that contain the alcohol functional group
- b demonstrate an understanding of the nomenclature and corresponding structural, displayed and skeletal formulae of alcohols, and classify them as primary, secondary or tertiary
- c describe the following chemistry of alcohols:
 - i combustion
 - ii reaction with sodium
 - iii substitution reactions to form halogenoalkanes, including reaction with PCl_5 and its use as a qualitative test for the presence of the $-\text{OH}$ group
 - iv oxidation using potassium dichromate(VI) in dilute sulfuric acid on primary alcohols to produce aldehydes and carboxylic acids and on secondary alcohols to produce ketones
- d demonstrate an understanding of, and practise, the preparation of an organic liquid (reflux and distillation), e.g. oxidation of alcohols.

2 Halogenoalkanes

- a demonstrate an understanding of the nomenclature and corresponding structural, displayed and skeletal formulae for halogenoalkanes, including the distinction between primary, secondary and tertiary structures
- b interpret given data and observations comparing the reactions and reactivity of primary, secondary and tertiary compounds
- c carry out the preparation of an halogenoalkane from an alcohol and explain why a metal halide and concentrated sulfuric acid should not be used when making a bromoalkane or an iodoalkane

- d describe the typical behaviour of halogenoalkanes. This will be limited to treatment with:
 - i aqueous alkali, e.g. KOH (aq)
 - ii alcoholic potassium hydroxide
 - iii water containing dissolved silver nitrate
 - iv alcoholic ammonia
- e carry out the reactions described in 2.10.2d i, ii, iii
- f discuss the uses of halogenoalkanes, e.g. as fire retardants and modern refrigerants.

2.11 Mechanisms

Students will be assessed on their ability to:

- a classify reactions (including those in Unit 1) as addition, elimination, substitution, oxidation, reduction, hydrolysis or polymerisation
- b demonstrate an understanding of the concept of a reaction mechanism and that bond breaking can be homolytic or heterolytic and that the resulting species are either free radicals, electrophiles or nucleophiles
- c give definitions of the terms *free radical*, *electrophile* and *nucleophile*
- d demonstrate an understanding of why it is helpful to classify reagents
- e demonstrate an understanding of the link between bond polarity and the type of reaction mechanism a compound will undergo
- f describe the mechanisms of the substitution reactions of halogenoalkanes and recall those in 1.7.2e and 1.7.3e
- g demonstrate an understanding of how oxygen, O₂, and ozone, O₃, absorb UV radiation and explain the part played by emission of oxides of nitrogen, from aircraft, in the depletion of the ozone layer, including the free radical mechanism for the reaction and the fact that oxides act as catalysts.

2.12 Mass spectra and IR

Students will be assessed on their ability to:

- a interpret fragment ion peaks in the mass spectra of simple organic compounds, e.g. the difference between propanal and propanone
- b use infrared spectra, or data from infrared spectra, to deduce functional groups present in organic compounds and predict infrared absorptions, given wavenumber data, due to familiar functional groups. This will be limited to:
 - i C–H stretching absorptions in alkanes, alkenes and aldehydes
 - ii O–H stretching absorptions in alcohols and carboxylic acids
 - iii N–H stretching absorption in amines
 - iv C=O stretching absorptions in aldehydes and ketones
 - v C–X stretching absorption in halogenoalkanes
 - vi as an analytical tool to show the change in functional groups during the oxidation of an alcohol to a carbonyl
- c demonstrate an understanding that only molecules which change their polarity as they vibrate can absorb infrared radiation
- d demonstrate an understanding that H₂O, CO₂, CH₄ and NO molecules absorb IR radiation and are greenhouse gases, whilst O₂ and N₂ are not.

2.13 Green chemistry

Students will be assessed on their ability to:

- a demonstrate an understanding that the processes in the chemical industry are being reinvented to make them more sustainable ('greener') by:
 - i changing to renewable resources
 - ii finding alternatives to very hazardous chemicals
 - iii discovering catalysts for reactions with higher atom economies, e.g. the development of methods used to produce ethanoic acid based on catalysts of cobalt, rhodium and iridium
 - iv making more efficient use of energy, e.g. the use of microwave energy to heat reactions in the pharmaceutical industry
 - v reducing waste and preventing pollution of the environment
- b discuss the relative effects of different greenhouse gases as absorbers of IR and hence on global warming
- c discuss the difference between anthropogenic and natural climate change over hundreds of thousands of years
- d demonstrate understanding of the terms *carbon neutrality* and *carbon footprint*
- e apply the concept of carbon neutrality to different fuels, such as petrol, bio-ethanol and hydrogen
- f discuss and explain, including the mechanisms for the reactions, the science community's reasons for recommending that CFCs are no longer used due to their damaging effect on the ozone layer.

3.1 Unit description

Introduction

This unit contains a practical written examination that covers the content of Units 1 and 2. There is no specific content for this unit.

Development of practical skills, knowledge and understanding

Students are expected to develop experimental skills, and a knowledge and understanding of the necessary techniques, by carrying out a range of practicals while they study Units 1 and 2.

This unit will assess students' knowledge and understanding of practical procedures and techniques that they develop.

To prepare them for the assessment of this unit centres should provide opportunities for students to carry out practical activities, collect and analyse data, and draw conclusions.

Students should carry out at least five practicals in class. By completing these practicals students will be able to:

- follow and interpret experimental instructions, covering the full range of laboratory exercises set throughout the course, with minimal help from the teacher
- always work with interest and enthusiasm in the laboratory completing most laboratory exercises in the time allocated
- manipulate apparatus, use chemicals, carry out all common laboratory procedures and use data logging (where appropriate) with the highest level of skill that may be reasonably expected at this level
- work sensibly and safely in the laboratory paying due regard to health and safety requirements without the need for reminders from the teacher
- gain accurate and consistent results in quantitative exercises, make most of the expected observations in qualitative exercises and obtain products in preparations of high yield and purity.

How chemists work

Students should be given the opportunity to develop their practical skills for *How Science Works* by completing a range of different practicals that require a variety of different techniques.

Students' laboratory reports on their practical work should use appropriate scientific, technical and mathematical language, conventions and symbols in order to meet the requirements of *How Science Works*.

3.2 Assessment information

Unit 3 examination

This unit contains a practical written examination that covers the content of Units 1 and 2.

The practical written examination covers the following types of practicals:

- qualitative observations
- quantitative measurements
- preparations.

The examination will last 1 hour 15 minutes and have 50 marks. It will contain one section.

Students may use a calculator.

The quality of written communication will be assessed in the practical written examination. When answering these questions students will be assessed on their ability to organise and present information, ideas, descriptions and arguments clearly and logically, include the use of grammar, punctuation and spelling.

4.1 Unit description

Introduction

In this unit students make a quantitative study of chemical kinetics and take further their study of organic reaction mechanisms.

The topics of entropy and equilibria show how chemists are able to predict quantitatively the direction and extent of chemical change.

The organic chemistry in this unit covers carbonyl compounds, plus carboxylic acids and their derivatives.

Students are required to apply their knowledge gained in Units 1 and 2, to all aspects of this unit. This includes nomenclature, ideas of isomerism, bond polarity and bond enthalpy, reagents and reaction conditions, reaction types and mechanisms. Students are also expected to use formulae and balance equations and calculate chemical quantities.

How chemists work

Through practical work, students will learn about the methods used to measure reaction rates. They will collect data, analyse it and interpret the results. They then see how a knowledge of rate equations and other evidence can enable chemists to propose models to describe the mechanisms of reactions.

The study of entropy introduces students to the methods of thermodynamics and shows how chemists use formal, quantitative and abstract thinking to answer fundamental questions about the stability of chemicals and the direction of chemical change.

The unit tests the equilibrium law by showing the degree to which it can accurately predict changes during acid-base reactions, notably the changes to pH during titrations.

The historical development of theories explaining acids and bases shows how scientific ideas change as a result of new evidence and fresh thinking.

Chemistry in action

This unit shows how the principles of kinetics and thermodynamics can help to achieve optimal conditions for the manufacture of chemicals.

The study of buffer solutions shows the varied importance of equilibrium systems in living cells, in medicines, in foods and in the natural environment.

The two broad areas of application of chemistry are synthesis and analysis. In this unit synthesis is illustrated by reactions of carbonyl compounds (notably with cyanide ions) and the production of esters for use as solvents, flavourings and perfumes. The main analytical technique featured is nmr including coverage of magnetic resonance imaging.

Core practicals

The following specification points are core practicals within this unit that students should complete:

4.3c

4.3e

4.4g

4.8.2c

4.8.3d

4.8.4b

4.8.4c

These practicals may appear in the written examination for Unit 4.

Use of examples

Examples in practicals

Where 'e.g.' follows a type of experiment in the specification students are not expected to have carried out that specific experiment.

However they should be able to use data from that or similar experiments.

For instance in this unit, 4.3g *How fast? – rates*, the specification states:

investigate the activation energy of a reaction, e.g. oxidation of iodide ions by iodate(V).

Students will be expected to have investigated the activation energy of a reaction, but they may or may not have done this by the oxidation of iodide ions by iodate(V).

In the unit test students could be given experimental data for this or any other reaction, and be expected to use this data to evaluate or estimate the activation energy.

Examples in unit content

Where 'e.g.' follows a concept students are not expected to have been taught the particular example given in the specification. They should be able to illustrate their answer with an example of their choice.

For instance in this unit, 4.7m *Acid/base equilibria*, the specification states:

explain the importance of buffer solutions in biological environments, e.g. buffers in cells and in blood (H_2CO_3/HCO_3^-) and in foods to prevent deterioration due to pH change (caused by bacterial or fungal activity).

Students will be expected to explain the importance of buffer solutions in biological systems, but they may or may not have looked at buffers in cells and blood, or in food.

In the unit test students could be asked to illustrate the importance of buffer solutions with a biological example that they select themselves. This could be one listed as an example or it could be another example.

4.2 Assessment information

Unit 4 examination The examination will be 1 hour 40 minutes and have 90 marks. It will contain three sections – A, B and C.

Section A is an objective test section which will aim to cover a large proportion of the specification for this unit.

Section B contains a mixture of short-answer and extended answer questions.

Section C will contain data questions and will require students to select the necessary data from the data booklet. They will be provided with data from a laboratory experiment and asked a series of questions on it. The longer timing of the examination reflects the style of the questions for Section C.

Students will be able to show their full ability in Sections B and C as these will contain areas where they will be stretched and challenged.

Students may use a calculator.

Quality of written communication will be assessed in this examination through questions which are labelled with an asterisk (*). When answering these questions students should consider spelling, punctuation and grammar of their response, as well as the clarity of expression.

4.3 How fast? – rates

Knowledge of the concepts introduced in Unit 2, *Topic 2.8: Kinetics* will be assumed and extended in this topic.

Students will be assessed on their ability to:

- a demonstrate an understanding of the terms *rate of reaction*, *rate equation*, *order of reaction*, *rate constant*, *half-life*, *rate-determining step*, *activation energy*, *heterogeneous* and *homogenous catalyst*
- b select and describe a suitable experimental technique to obtain rate data for a given reaction, e.g. colorimetry, mass change and volume of gas evolved
- c investigate reactions which produce data that can be used to calculate the rate of the reaction, its half-life from concentration or volume against time graphs, e.g. a clock reaction
- d present and interpret the results of kinetic measurements in graphical form, including concentration-time and rate-concentration graphs
- e investigate the reaction of iodine with propanone in acid to obtain data for the order with respect to the reactants and the hydrogen ion and make predictions about molecules/ions involved in the rate-determining step and possible mechanism (details of the actual mechanism can be discussed at a later stage in this topic)
- f deduce from experimental data for reactions with zero, first and second order kinetics:
 - i half-life (the relationship between half-life and rate constant will be given if required)
 - ii order of reaction
 - iii rate equation
 - iv rate-determining step related to reaction mechanisms
 - v activation energy (by graphical methods only; the Arrhenius equation will be given if needed)
- g investigate the activation energy of a reaction, e.g. oxidation of iodide ions by iodate(V)

- h apply a knowledge of the rate equations for the hydrolysis of halogenoalkanes to deduce the mechanisms for primary and tertiary halogenoalkane hydrolysis and to deduce the mechanism for the reaction between propanone and iodine
- i demonstrate that the mechanisms proposed for the hydrolysis of halogenoalkanes are consistent with the experimentally determined orders of reactions, and that a proposed mechanism for the reaction between propanone and iodine is consistent with the data from the experiment in 4.3e
- j use kinetic data as evidence for S_N1 or S_N2 mechanisms in the nucleophilic substitution reactions of halogenoalkanes.

4.4 How far? – entropy

Students will be assessed on their ability to:

- a demonstrate an understanding that, since endothermic reactions can occur spontaneously at room temperature, enthalpy changes alone do not control whether reactions occur
- b demonstrate an understanding of entropy in terms of the random dispersal of molecules and of energy quanta between molecules
- c demonstrate an understanding that the entropy of a substance increases with temperature, that entropy increases as solid → liquid → gas and that perfect crystals at zero kelvin have zero entropy
- d demonstrate an understanding that the standard entropy of a substance depends mainly on its physical state but also on its complexity
- e demonstrate an understanding that reactions occur due to chance collisions, and that one possible ordered arrangement, e.g. in a crystalline solid, can be rearranged into many possible disordered arrangements, e.g. in a solution, so the probability of disorder is greater than order
- f interpret the natural direction of change as being in the direction of increasing total entropy (positive entropy change), e.g. gases spread spontaneously through a room
- g carry out experiments and relate the results to disorder and enthalpy changes including:
 - i dissolving a solid, e.g. adding ammonium nitrate crystals to water
 - ii gas evolution, e.g. reacting ethanoic acid with ammonium carbonate
 - iii exothermic reaction producing a solid, e.g. burning magnesium ribbon in air
 - iv endothermic reaction of two solids, e.g. mixing solid barium hydroxide, $\text{Ba(OH)}_2 \cdot 8\text{H}_2\text{O}$ with solid ammonium chloride
- h demonstrate an understanding that the entropy change in any reaction is made up of the entropy change in the system added to the entropy change in the surroundings, summarised by the expression:

$$\Delta S_{\text{total}} = \Delta S_{\text{system}} + \Delta S_{\text{surroundings}}$$

- i calculate the entropy change in the system for a reaction, ΔS_{system} , given entropy data
- j use the expression $\Delta S_{surroundings} = -\Delta H/T$ to calculate the entropy change in the surroundings and hence ΔS_{total}
- k demonstrate an understanding that the feasibility of a reaction depends on the balance between ΔS_{system} and $\Delta S_{surroundings}$, and that at higher temperatures the magnitude of $\Delta S_{surroundings}$ decreases and its contribution to ΔS_{total} is less. Reactions can occur as long as ΔS_{total} is positive even if one of the other entropy changes is negative
- l demonstrate an understanding of and distinguish between the concepts of thermodynamic stability and kinetic inertness
- m calculate ΔS_{system} and $\Delta S_{surroundings}$ for the reactions in 4.4g to show that endothermic reactions can occur spontaneously at room temperature
- n define the term *enthalpy of hydration* of an ion and use it and lattice energy to calculate the enthalpy of solution of an ionic compound
- o demonstrate an understanding of the factors that affect the values of enthalpy of hydration and the lattice energy of an ionic compound
- p use entropy and enthalpy of solution values to predict the solubility of ionic compounds.

4.5 Equilibria

Knowledge of the concepts introduced in Unit 2, *Topic 2.9: Chemical equilibria* will be assumed and extended in this topic.

Students will be assessed on their ability to:

- demonstrate an understanding of the term *dynamic equilibrium* as applied to states of matter, solutions and chemical reactions
- recall that many important industrial reactions are reversible
- use practical data to establish the idea that a relationship exists between the equilibrium concentrations of reactants and products which produces the equilibrium constant for a particular reaction, e.g. data on the hydrogen-iodine equilibrium
- calculate a value for the equilibrium constant for a reaction based on data from experiment, e.g. the reaction of ethanol and ethanoic acid (this can be used as an example of the use of ICT to present and analyse data), the equilibrium $\text{Fe}^{2+}(\text{aq}) + \text{Ag}^{+}(\text{aq}) \rightleftharpoons \text{Fe}^{3+}(\text{aq}) + \text{Ag}(\text{s})$ or the distribution of ammonia or iodine between two immiscible solvents
- construct expressions for K_c and K_p for homogeneous and heterogeneous systems, in terms of equilibrium concentrations or equilibrium partial pressures, perform simple calculations on K_c and K_p and work out the units of the equilibrium constants
- demonstrate an understanding that when ΔS_{total} increases the magnitude of the equilibrium constant increases since $\Delta S_{\text{total}} = R \ln K$
- apply knowledge of the value of equilibrium constants to predict the extent to which a reaction takes place
- relate the effect of a change in temperature on the value of ΔS_{total} .

4.6 Application of rates and equilibrium

Students will be assessed on their ability to:

- a demonstrate an understanding of how, if at all, and why a change in temperature, pressure or the presence of a catalyst affects the equilibrium constant and the equilibrium composition and recall the effects of changes of temperature and pressure on rate, e.g. the thermal decomposition of ammonium chloride, or the effect of temperature and pressure changes in the system $2\text{NO}_2 \rightleftharpoons \text{N}_2\text{O}_4$
- b use information on enthalpy change and entropy to justify the conditions used to obtain economic yields in industrial processes, and understand that in reality industrial processes cannot be in equilibrium since the products are removed, e.g. in the Haber process temperature affects the equilibrium yield and rate whereas pressure affects only the equilibrium yield (knowledge of industrial conditions are not required)
- c demonstrate an understanding of the steps taken in industry to maximise the atom economy of the process, e.g. recycling unreacted reagents or using an alternative reaction
- d demonstrate an understanding of the importance of being able to control reactions, through knowledge of equilibrium constants and entropy changes, the importance of controlling reactions to produce adequate yields under safe, economically viable conditions and why some reactions 'go' and some will never occur.

4.7 Acid/base equilibria

Students will be assessed on their ability to:

- a demonstrate an understanding that the theory about acidity developed in the 19th and 20th centuries from a substance with a sour taste to a substance which produces an excess of hydrogen ions in solution (Arrhenius theory) to the Brønsted-Lowry theory
- b demonstrate an understanding that a Brønsted-Lowry acid is a proton donor and a base a proton acceptor and that acid-base equilibria involve transfer of protons
- c demonstrate an understanding of the Brønsted-Lowry theory of acid-base behaviour, and use it to identify conjugate acid-base pairs
- d define the terms pH, K_a and K_w , pK_a and pK_w , and be able to carry out calculations relating the pH of strong acids and bases to their concentrations in mol dm^{-3}
- e demonstrate an understanding that weak acids and bases are only slightly dissociated in aqueous solution, and apply the equilibrium law to deduce the expressions for the equilibrium constants K_a and K_w
- f analyse the results obtained from the following experiments:
 - i measuring the pH of a variety of substances, e.g. equimolar solutions of strong and weak acids, strong and weak bases and salts
 - ii comparing the pH of a strong acid and a weak acid after dilution 10, 100 and 1000 times
- g analyse and evaluate the results obtained from experiments to determine K_a for a weak acid by measuring the pH of a solution containing a known mass of acid, and discuss the assumptions made in this calculation
- h calculate the pH of a solution of a weak acid based on data for concentration and K_a , and discuss the assumptions made in this calculation
- i measure the pH change during titrations and draw titration curves using different combinations of strong and weak monobasic acids and bases
- j use data about indicators, together with titration curves, to select a suitable indicator and the use of titrations in analysis

- k explain the action of buffer solutions and carry out calculations on the pH of buffer solutions, e.g. making buffer solutions and comparing the effect of adding acid or alkali on the pH of the buffer
- l use titration curves to show the buffer action and to determine K_a from the pH at the point where half the acid is neutralised
- m explain the importance of buffer solutions in biological environments, e.g. buffers in cells and in blood ($\text{H}_2\text{CO}_3/\text{HCO}_3^-$) and in foods to prevent deterioration due to pH change (caused by bacterial or fungal activity).

4.8 Further organic chemistry

Related topics in Unit 5 will assume knowledge of this material.

Students will be assessed on their ability to:

1 Chirality

- recall the meaning of structural and E-Z isomerism (geometric/cis-trans isomerism)
- demonstrate an understanding of the existence of optical isomerism resulting from chiral centre(s) in a molecule with asymmetric carbon atom(s) and understand optical isomers as object and non-superimposable mirror images
- recall optical activity as the ability of a single optical isomer to rotate the plane of polarisation of plane-polarised monochromatic light in molecules containing a single chiral centre and understand the nature of a racemic mixture
- use data on optical activity of reactants and products as evidence for proposed mechanisms, as in S_N1 and S_N2 and addition to carbonyl compounds.

2 Carbonyl compounds

- give examples of molecules that contain the aldehyde or ketone functional group
- explain the physical properties of aldehydes and ketones relating this to the lack of hydrogen bonding between molecules and their solubility in water in terms of hydrogen bonding with the water
- describe and carry out, where appropriate, the reactions of carbonyl compounds. This will be limited to:
 - oxidation with Fehling's or Benedict's solution, Tollens' reagent and acidified dichromate(VI) ions
 - reduction with lithium tetrahydridoaluminate (lithium aluminium hydride) in dry ether
 - nucleophilic addition of HCN in the presence of KCN, using curly arrows, relevant lone pairs, dipoles and evidence of optical activity to show the mechanism
 - the reaction with 2,4-dinitrophenylhydrazine and its use to detect the presence of a carbonyl group and to identify a carbonyl compound given data of the melting temperatures of derivatives
 - iodine in the presence of alkali.

3 Carboxylic acids

- a give some examples of molecules that contain the carboxylic acid functional group
- b explain the physical properties of carboxylic acids in relation to their boiling temperatures and solubility due to hydrogen bonding
- c describe the preparation of carboxylic acids to include oxidation of alcohols and carbonyl compounds and the hydrolysis of nitriles
- d describe and carry out, where appropriate, the reactions of carboxylic acids. This will be limited to:
 - i reduction with lithium tetrahydridoaluminate (lithium aluminium hydride) in dry ether (ethoxyethane)
 - ii neutralisation to produce salts, e.g. to determine the amount of citric acid in fruit
 - iii phosphorus(V) chloride (phosphorus pentachloride)
 - iv reactions with alcohols in the presence of an acid catalyst, e.g. the preparation of ethyl ethanoate as a solvent or as pineapple flavouring.

4 Carboxylic acid derivatives

- a demonstrate an understanding that these include acyl chlorides and esters and recognise their respective functional groups, giving examples of molecules containing these functional groups
- b describe and carry out, where appropriate, the reactions of acyl chlorides limited to their reaction with:
 - i water
 - ii alcohols
 - iii concentrated ammonia
 - iv amines
- c describe and carry out, where appropriate, the reactions of esters. This will be limited to:
 - i their hydrolysis with an acid
 - ii their hydrolysis with a base, e.g. to form soaps
 - iii their reaction with alcohols and acids to explain the process of trans-esterification and recall how it is applied to the manufacture of bio-diesel (as a potentially greener fuel) and low-fat spreads (replacing the hydrogenation of vegetable oils to produce margarine)
- d demonstrate an understanding of the importance of the formation of polyesters and describe their formation by condensation polymerisation of ethane-1,2-diol and benzene 1,4-dicarboxylic acid.

4.9 Spectroscopy and chromatography

Knowledge of the concepts introduced in Unit 2, *Topic 2.12: Mass Spectra and IR* will be assumed and extended in this topic.

Students will be assessed on their ability to:

- a explain the effect of different types of radiation on molecules and how the principles of this are used in chemical analysis and in reactions, limited to:
 - i infrared in analysis
 - ii microwaves for heating
 - iii radio waves in nmr
 - iv ultraviolet in initiation of reactions
- b explain the use of high resolution nmr spectra to identify the structure of a molecule:
 - i based on the different types of proton present from chemical shift values
 - ii by using the spin-spin coupling pattern to identify the number of protons adjacent to a given proton
 - iii the effect of radio waves on proton spin in nmr, limited to ^1H nuclei
 - iv the use of magnetic resonance imaging as a non-invasive technique, e.g. scanning for brain disorders, or the use of nmr to check the purity of a compound in the pharmaceutical industry
- c demonstrate an understanding of the use of IR spectra to follow the progress of a reaction involving change of functional groups, e.g. in the chemical industry to determine the extent of the reaction
- d interpret simple mass spectra to suggest possible structures of a simple compound from the m/e of the molecular ion and fragmentation patterns
- e describe the principles of gas chromatography and HPLC as used as methods of separation of mixtures, prior to further analysis (theory of R_f values not required), and also to determine if substances are present in industrial chemical processes.

5.1 Unit description

Introduction

In this unit the study of electrode potentials builds on the study of redox in Unit 2, including the concept of oxidation number and the use of redox half equations.

Students will study further chemistry related to redox and transition metals.

The organic chemistry section of this unit focuses on arenes and organic nitrogen compounds such as amines, amides, amino acids and proteins. Students are expected to use the knowledge and understanding of organic chemistry that they have gained over the whole International Advanced Level in Chemistry when covering the organic synthesis section.

This unit draws on all other units within the International Advanced Level in Chemistry and students are expected to use their prior knowledge when learning about these areas. Students will again encounter ideas of isomerism, bond polarity and bond enthalpy, reagents and reaction conditions, reaction types and mechanisms. Students are also expected to use formulae and balance equations, and calculate chemical quantities.

How chemists work

The study of chemical cells provides an opportunity to illustrate the impact on scientific thinking when it emerges that ideas developed in different contexts can be shown to be related to a major explanatory principle. In this unit, cell emfs and equilibrium constants are shown to be related to the fundamental criterion for the feasibility of a chemical reaction: the total entropy change.

The explanatory power of the energy-level model for electronic structures is further illustrated by showing how it can help to account for the existence and properties of transition metals. In this context there are opportunities to show the limitations of the models used at this level and to indicate the need for more sophisticated explanations.

Study of the structure of benzene is another example that shows how scientific models develop in response to new evidence. This links to further investigations of the models that chemists use to describe the mechanisms of organic reactions.

The study of catalysts touches on a 'frontier' area for current chemical research and development which is of theoretical and practical importance. This provides an opportunity to show how the scientific community reports and validates new knowledge.

Students have further opportunities to carry out quantitative analysis, to interpret complex data and assess the outcomes in terms of the principles of valid measurement. The topic of organic synthesis illustrates a selection of the techniques that chemists have developed to carry out reactions and purify products efficiently and safely.

Core practicals

The following specification points are core practicals within this unit that students should complete:

- 5.3.1d
- 5.3.1g
- 5.3.2g
- 5.3.2j
- 5.4.1d
- 5.4.1e
- 5.4.2b
- 5.4.2d
- 5.4.2i
- 5.4.3f

These practicals may appear in the written examination for Unit 5.

Use of examples

Examples in practicals

Where 'e.g.' follows a type of experiment in the specification students are not expected to have carried out that specific experiment. However they should be able to use data from that or similar experiments.

For instance in this unit, *5.3.1h i Application of redox equilibria*, the specification states:

demonstrate an understanding of the procedures of the redox titrations below (i and ii) and carry out a redox titration with one:

- i potassium manganate(VII), e.g. the estimation of iron in iron tablets.*

Students will be expected to have carried out a redox titration with potassium manganate(VII), but they may or may not have done this to estimate the amount of iron in iron tablets.

In the unit test students could be given experimental data for a potassium manganate(VII) titration, in any context, and be expected to analyse and evaluate this data.

Examples in unit content

Where 'e.g.' follows a concept students are not expected to have been taught the particular example given in the specification. They should be able to illustrate their answer with an example of their choice.

For instance in this unit, *5.4.2h Organic nitrogen compounds*:

amines, amides, amino acids and proteins, the specification states:

comment on the physical properties of polyamides and the solubility in water of the addition polymer poly(ethenol) in terms of hydrogen bonding, e.g. soluble laundry bags or liquid detergent capsules (liquid tabs).

Students will be expected to comment on the physical properties of polyamides and the solubility of poly(ethenol) in terms of hydrogen bonding, but they may or may not have looked at soluble laundry bags or liquid tabs.

In the unit test students could be asked to comment on the physical properties of this polyamide and the solubility of the addition polymer in terms of hydrogen bonding. This could be in the context of soluble laundry bags, or in another completely different context.

5.2 Assessment information

Unit 5 examination The examination will be 1 hour 40 minutes and have 90 marks. It will contain three sections – A, B and C.

Section A is an objective test section which will aim to cover a large proportion of the specification for this unit.

Section B contains a mixture of short-answer and extended answer questions. Questions on the analysis and evaluation of practical work will also be included in Section B.

Section C will contain extended answer questions on contemporary contexts. This may contain stimulus materials on a scenario that students must read in order to answer the questions. It will focus on the chemistry behind the contexts and will not be a comprehension exercise. The longer timing of the examination reflects the style of the questions for Section C.

Students will be able to show their full ability in Sections B and C as these will contain areas where they will be stretched and challenged.

Students may use a calculator.

The quality of written communication will be assessed in the context of this unit through questions which are labelled with an asterisk (*). When answering these questions students should consider spelling, punctuation and grammar of their response, as well as the clarity of expression.

5.3 Redox and the chemistry of the transition metals

Students will be assessed on their ability to:

1 Application of redox equilibria

- a demonstrate an understanding of the terms *oxidation number*, *redox*, *half-reactions* and use these to interpret reactions involving electron transfer
- b relate changes in oxidation number to reaction stoichiometry
- c recall the definition of standard electrode potential and standard hydrogen electrode and understand the need for a reference electrode
- d set up some simple cells and calculate values of $E_{\text{cell}}^{\ominus}$ from standard electrode potential values and use them to predict the thermodynamic feasibility and extent of reactions
- e demonstrate an understanding that $E_{\text{cell}}^{\ominus}$ is directly proportional to the total entropy change and to $\ln K$ for a reaction
- f demonstrate an understanding of why the predictions in 5.3.1d may not be borne out in practice due to kinetic effects and non-standard conditions
- g carry out and evaluate the results of an experiment involving the use of standard electrode potentials to predict the feasibility of a reaction, e.g. interchange of the oxidation states of vanadium or manganese
- h demonstrate an understanding of the procedures of the redox titrations below (i and ii) and carry out a redox titration with one:
 - i potassium manganate(VII), e.g. the estimation of iron in iron tablets
 - ii sodium thiosulfate and iodine, e.g. estimation of percentage of copper in an alloy
- i discuss the uncertainty of measurements and their implications for the validity of the final results
- j discuss the use of hydrogen and alcohol fuel cells as energy sources, including the source of the hydrogen and alcohol, e.g. used in space exploration, in electric cars
- k demonstrate an understanding of the principles of modern breathalysers based on an ethanol fuel cell and compare this to methods based on the use of IR and to the reduction of chromium compounds.

2 Transition metals and their chemistry

- a describe transition metals as those elements which form one or more stable ions which have incompletely filled d orbitals
- b derive the electronic configuration of the atoms of the d-block elements (Sc to Zn) and their simple ions from their atomic number
- c discuss the evidence for the electronic configurations of the elements Sc to Zn based on successive ionisation energies
- d recall that transition elements in general:
 - i show variable oxidation number in their compounds, e.g. redox reactions of vanadium
 - ii form coloured ions in solution
 - iii form complex ions involving monodentate and bidentate ligands
 - iv can act as catalysts both as the elements and as their compounds
- e recall the shapes of complex ions limited to linear $[\text{CuCl}_2]^-$, planar $[\text{Pt}(\text{NH}_3)_2\text{Cl}_2]$, tetrahedral $[\text{CrCl}_4]^-$ and octahedral $[\text{Cr}(\text{NH}_3)_6]^{3+}$, $[\text{Cu}(\text{H}_2\text{O})_6]^{2+}$ and other aqua complexes
- f use the chemistries of chromium and copper to illustrate and explain some properties of transition metals as follows:
 - i the formation of a range of compounds in which they are present in different oxidation states
 - ii the presence of dative covalent bonding in complex ions, including the aqua-ions
 - iii the colour or lack of colour of aqueous ions and other complex ions, resulting from the splitting of the energy levels of the d orbitals by ligands
 - iv simple ligand exchange reactions
 - v relate relative stability of complex ions to the entropy changes of ligand exchange reactions involving polydentate ligands (qualitatively only), e.g. EDTA
 - vi relate disproportionation reactions to standard electrode potentials and hence to E_{cell}^\ominus

- g carry out experiments to:
 - i investigate ligand exchange in copper complexes
 - ii study the redox chemistry of chromium in oxidation states Cr(VI), Cr(III) and Cr(II)
 - iii prepare a sample of a complex, e.g. chromium(II) ethanoate
- h recall that transition metals and their compounds are important as catalysts and that their activity may be associated with variable oxidation states of the elements or surface activity, e.g. catalytic converters in car exhausts
- i explain why the development of new catalysts is a priority area for chemical research today and, in this context, explain how the scientific community reports and validates new discoveries and explanations, e.g. the development of new catalysts for making ethanoic acid from methanol and carbon monoxide with a high atom economy (green chemistry)
- j carry out and interpret the reactions of transition metal ions with aqueous sodium hydroxide and aqueous ammonia, both in excess, limited to reactions with aqueous solutions of Cr(III), Mn(II), Fe(II), Fe(III), Ni(II), Cu(II), Zn(II)
- k write ionic equations to show the difference between amphoteric behaviour and ligand exchange in the reactions in 5.3.2g
- l discuss the uses of transition metals and/or their compounds, e.g. in polychromic sun glasses, chemotherapy drugs.

5.4 Organic chemistry – arenes, nitrogen compounds and synthesis

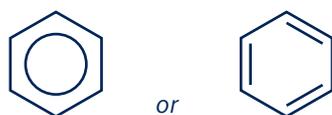
Knowledge of the common uses of organic compounds mentioned in this topic is expected.

Students will be assessed on their ability to:

1 Arenes: benzene

- a use thermochemical, x-ray diffraction and infrared data as evidence for the structure and stability of the benzene ring

Students may represent the structure of benzene as



as appropriate in equations and mechanisms

- b describe the following reactions of benzene, limited to:
- i combustion to form a smoky flame
- treatment with:
- ii bromine
 - iii concentrated nitric and sulfuric acids
 - iv fuming sulfuric acid
 - v halogenoalkanes and acyl chlorides with aluminium chloride as catalyst (Friedel-Crafts reaction)
 - vi addition reactions with hydrogen
- c describe the mechanism of the electrophilic substitution reactions of benzene in halogenation, nitration and Friedel-Crafts reactions including the formation of the electrophile
- d carry out the reactions in 5.4.1b where appropriate (using methylbenzene or methoxybenzene)
- e carry out the reaction of phenol with bromine water and dilute nitric acid and use these results to illustrate the activation of the benzene ring.

2 Organic nitrogen compounds: amines, amides, amino acids and proteins

- a give examples of:
- molecules that contain amine and amide functional groups
 - amino acids
- b describe and carry out, where appropriate (using butylamine and phenylamine), reactions to investigate the typical behaviour of primary amines. This will be limited to:
- characteristic smell
 - miscibility with water as a result of hydrogen bonding and the alkaline nature of the resulting solution
 - formation of salts
 - complex ion formation with copper(II) ions
 - treatment with ethanoyl chloride and halogenoalkanes, e.g. making paracetamol
- c describe the reduction of aromatic nitro-compounds using tin and concentrated hydrochloric acid to form amines
- d describe and carry out, where appropriate, the reaction of aromatic amines with nitrous acid to form benzenediazonium ions followed by a coupling reaction with phenol to form a dye
- e recall the synthesis of amides using acyl chlorides
- f describe:
- condensation polymerisation for the formation of polyesters such as terylene and polyamides such as nylon and Kevlar
 - addition polymerisation including poly(propenamide) and poly(ethenol)
- g draw the structural formulae of the repeat units of the polymers in 5.4.2f
- h comment on the physical properties of polyamides and the solubility in water of the addition polymer poly(ethenol) in terms of hydrogen bonding, e.g. soluble laundry bags or liquid detergent capsules (liquid tabs)

- i describe and carry out, where appropriate, experiments to investigate the characteristic behaviour of amino acids. This is limited to:
 - i acidity and basicity and the formation of zwitterions
 - ii separation and identification by chromatography
 - iii effect of aqueous solutions on plane-polarised monochromatic light
 - iv formation of peptide groups in proteins by condensation polymerisation
 - v reaction with ninhydrin.

3 Organic synthesis

- a give examples to illustrate the importance of organic synthesis in research for the production of useful products
- b explain why sensitive methods of chemical analysis are important when planning and monitoring organic syntheses
- c deduce the empirical formulae, molecular formulae and structural formulae from data drawn from combustion analysis, elemental percentage composition, characteristic reactions of functional groups, infrared spectra, mass spectra and nuclear magnetic resonance
- d use knowledge of organic chemistry contained in this specifications to solve problems such as:
 - i predicting the properties of unfamiliar compounds containing one or more of the functional groups included in the specification, and explain these predictions
 - ii planning reaction schemes of up to four steps, recalling familiar reactions and using unfamiliar reactions given sufficient information
 - iii selecting suitable practical procedures for carrying out reactions involving compounds with functional groups included in the specification
 - iv identifying appropriate control measures to reduce risk during a synthesis based upon data of hazards
 - v understanding why, in the synthesis of stereo-specific drugs, it is important to understand the mechanism of the reaction and how this can help to plan the synthesis
- e explain why the pharmaceutical industry has adopted combinatorial chemistry in drug research, including passing reactants over reagents on polymer supports

- f describe and carry out, where appropriate, the preparation of a compound, e.g. cholesteryl benzoate (a liquid crystal) and of methyl 3-nitrobenzoate, requiring some of the following techniques:
- i refluxing
 - ii purification by washing, e.g. with water and sodium carbonate solution
 - iii solvent extraction
 - iv recrystallisation
 - v drying
 - vi distillation
 - vii steam distillation
 - viii melting temperature determination
 - ix boiling temperature determination.

6.1 Unit description

Introduction

This unit contains a practical written examination that covers the content of Units 4 and 5. There is no specific content for this unit.

Development of practical skills, knowledge and understanding

Students are expected to develop experimental skills, and a knowledge and understanding of the necessary techniques, by carrying out a range of practicals while they study Units 4 and 5.

This unit will assess students' knowledge and understanding of practical procedures and techniques that they develop.

To prepare them for the assessment of this unit centres should provide opportunities for students to carry out practical activities, collect and analyse data, and draw conclusions.

By completing these practicals students will be able to:

- follow and interpret experimental instructions, covering the full range of laboratory exercises set throughout the course, with minimal help from the teacher
- always work with interest and enthusiasm in the laboratory completing most laboratory exercises in the time allocated
- manipulate apparatus, use chemicals, carry out all common laboratory procedures and use data logging (where appropriate) with the highest level of skill that may be reasonably expected at this level
- work sensibly and safely in the laboratory paying due regard to health and safety requirements without the need for reminders from the teacher
- gain accurate and consistent results in quantitative exercises, make most of the expected observations in qualitative exercises and obtain products in preparations of high yield and purity.

These practical activities should cover a range of different topic areas and require the use of a variety of practical techniques.

How chemists work

Students should be given the opportunity to develop their practical skills for *How Science Works* by completing a range of different practicals that require a variety of different techniques.

Students' laboratory reports on their practical work should use appropriate scientific, technical and mathematical language, conventions and symbols in order to meet the requirements of *How Science Works*.

6.2 Assessment information

Unit 6 examination

This unit contains a practical written examination that covers the content of Units 4 and 5.

The practical written examination covers the following types of practicals:

- qualitative observations
- quantitative measurements
- preparations.

The examination will last 1 hour 15 minutes and have 50 marks. It will contain one section.

Students may use a calculator.

The quality of written communication will be assessed in the practical written examination. When answering these questions students will be assessed on their ability to organise and present information, ideas, descriptions and arguments clearly and logically, including the use of grammar, punctuation and spelling.