

# Chemistry

## Singapore-Cambridge General Certificate of Education Advanced Level Higher 3 (2021) (Syllabus 9813)

### CONTENTS

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	<i>Page</i>
INTRODUCTION	2
AIMS	2
PRACTICES OF SCIENCE	2
CURRICULUM FRAMEWORK	4
ASSESSMENT OBJECTIVES	5
SCHEME OF ASSESSMENT	6
ADDITIONAL INFORMATION	6
SUBJECT CONTENT	7
SUMMARY OF KEY QUANTITIES AND UNITS	13
MATHEMATICAL REQUIREMENTS	15
GLOSSARY OF TERMS	16
REFERENCES	18
DATA BOOKLET	19
PERIODIC TABLE	38

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The Common Last Topics for 9813 H3 Chemistry is An Introduction to the Chemistry of Transition Elements as highlighted in yellow in the 9729 H2 Chemistry syllabus and will not be examined in 2021 A-Level national examination.



## INTRODUCTION

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The H3 Chemistry syllabus has been designed to build on and extend the knowledge, understanding and skills acquired from the H2 Chemistry syllabus. It caters to students of strong ability and keen interest in chemistry, and is designed with an emphasis on independent and self-directed learning. The H3 Chemistry syllabus provides greater depth and rigour in the subject for students pursuing further studies in chemistry-related fields.

Students should simultaneously offer H2 Chemistry, and will be assumed to have knowledge and understanding of chemistry at H2 level.

## AIMS

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The aims of a course based on this syllabus should be to:

- 1 provide students with an experience that deepens their knowledge and skills in chemistry, and foster attitudes necessary for further studies in related fields
- 2 develop in students the appreciation of the practice, value and rigour of chemistry as a discipline
- 3 develop in students the skills to analyse chemical issues, and to apply relevant concepts and techniques to solve problems.

## PRACTICES OF SCIENCE

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Science as a discipline is more than the acquisition of a body of knowledge (e.g. scientific facts, concepts, laws, and theories); it is a way of knowing and doing. It includes an understanding of the nature of scientific knowledge and how this knowledge is generated, established and communicated. Scientists rely on a set of established procedures and practices associated with scientific inquiry to gather evidence and test their ideas on how the natural world works. However, there is no single method and the real process of science is often complex and iterative, following many different paths. While science is powerful, generating knowledge that forms the basis for many technological feats and innovations, it has limitations.

The *Practices of Science* are explicitly articulated in this syllabus to allow teachers to embed them as learning objectives in their lessons. Students' understanding of the nature and limitations of science and scientific inquiry are developed effectively when the practices are taught in the context of relevant science content. Attitudes relevant to science such as inquisitiveness, concern for accuracy and precision, objectivity, integrity and perseverance should be emphasised in the teaching of these practices where appropriate. For example, students learning science should be introduced to the use of technology as an aid in practical work or as a tool for the interpretation of experimental and theoretical results.

The *Practices of Science* comprise three components:

### 1 Understanding the Nature of Scientific Knowledge

- 1.1 Understand that science is an evidence-based, model-building enterprise concerned with the natural world
- 1.2 Understand that the use of both logic and creativity is required in the generation of scientific knowledge
- 1.3 Recognise that scientific knowledge is generated from consensus within the community of scientists through a process of critical debate and peer review
- 1.4 Understand that scientific knowledge is reliable and durable, yet subject to revision in the light of new evidence

## 2 Demonstrating Science Inquiry Skills

- 2.1. Identify scientific problems, observe phenomena and pose scientific questions/hypotheses
- 2.2 Plan and conduct investigations by selecting the appropriate experimental procedures, apparatus and materials, with due regard for accuracy, precision and safety
- 2.3 Obtain, organise and represent data in an appropriate manner
- 2.4 Analyse and interpret data
- 2.5 Construct explanations based on evidence and justify these explanations through reasoning and logical argument
- 2.6 Use appropriate models<sup>1</sup> to explain concepts, solve problems and make predictions
- 2.7 Make decisions based on evaluation of evidence, processes, claims and conclusions
- 2.8 Communicate scientific findings and information using appropriate language and terminology

## 3 Relating Science and Society

- 3.1. Recognise that the application of scientific knowledge to problem solving could be influenced by other considerations such as economic, social, environmental and ethical factors
- 3.2 Demonstrate an understanding of the benefits and risks associated with the application of science to society
- 3.3 Use scientific principles and reasoning to understand, analyse and evaluate real-world systems as well as to generate solutions for problem solving

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<sup>1</sup> A model is a representation of an idea, an object, a process or a system that is used to describe and explain phenomena that cannot be experienced directly. Models exist in different forms, from the concrete, such as physical scale models, to the abstract, such as diagrams or mathematical expressions. The use of models involves the understanding that all models contain approximations and assumptions limiting their validity and predictive power.

# CURRICULUM FRAMEWORK

The curriculum framework for H3 Chemistry builds on the framework for H2 Chemistry as illustrated in Fig. 1.

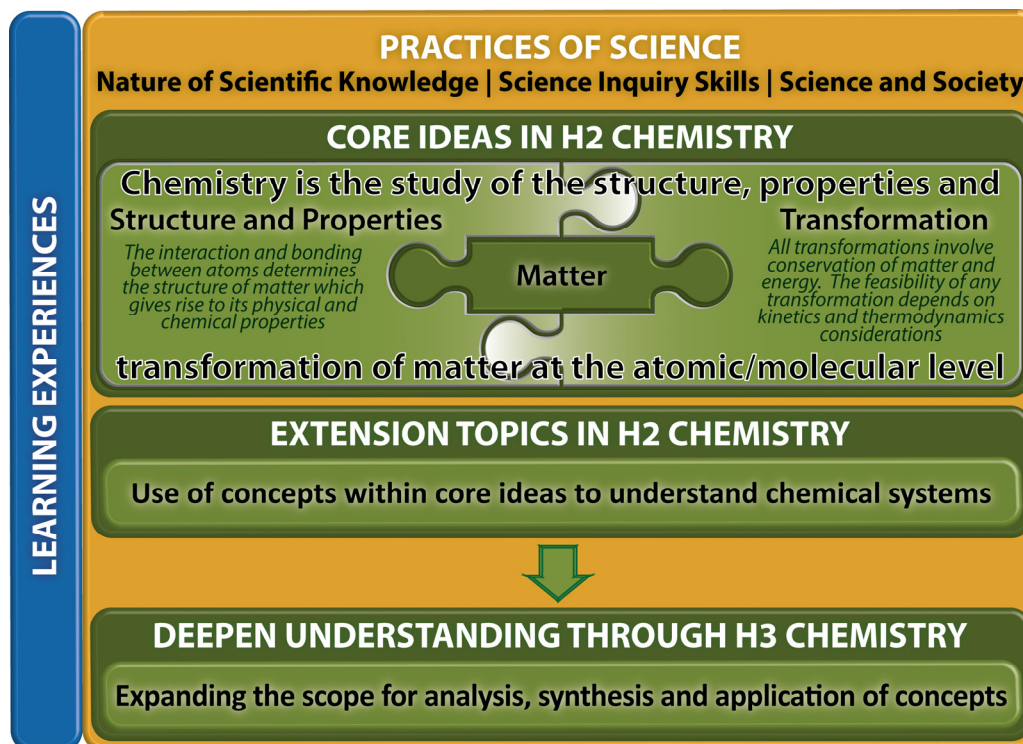


Fig. 1: H3 Chemistry Curriculum Framework

## 1. Content Topics

The content topics in the H3 Chemistry are organised into two levels underpinned by the *Practices of Science*:

- Core ideas and Extension topics in H2 Chemistry. These are elaborated in the corresponding H2 Chemistry syllabus.
- Additional content in H3 Chemistry. Two content areas *Spectroscopic Techniques* and *Further Organic Mechanisms* are included to deepen the understanding of the core ideas by expanding the scope for analysis, synthesis and application of concepts.

## 2 Practices of Science

The *Practices of Science* are common to the natural sciences of physics, chemistry and biology. These practices highlight the ways of thinking and doing that are inherent in the scientific approach, with the aim of equipping students with the understanding, skills, and attitudes shared by the scientific disciplines, including an appropriate approach to ethical issues.

## 3 Learning Experiences

The *Learning Experiences*<sup>2</sup> refer to a range of learning opportunities selected by teachers to link the chemistry content with the *Core Ideas* and the *Practices of Science* to enhance students' learning of the concepts. Rather than being mandatory, teachers are encouraged to incorporate learning experiences that match the interests and abilities of their students and provide opportunities to illustrate and exemplify the *Practices of Science*, where appropriate. Real-world contexts can help illustrate the concepts in chemistry and their applications. Experimental activities and ICT tools can also be used to build students' understanding.

<sup>2</sup> The *Learning Experiences* can be found in the Teaching and Learning Syllabus.

## ASSESSMENT OBJECTIVES

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The *Assessment Objectives* listed below reflect those parts of the *Aims and Practices of Science* that will be assessed.

### A Knowledge with understanding

Candidates should be able to demonstrate knowledge and understanding in relation to:

- 1 scientific phenomena, facts, laws, definitions, concepts and theories
- 2 scientific vocabulary, terminology and conventions (including symbols, quantities and units)
- 3 scientific instruments and apparatus, including techniques of operation and aspects of safety
- 4 scientific quantities and their determination
- 5 scientific and technological applications with their social, economic and environmental implications.

The syllabus content defines the factual knowledge that candidates may be required to recall and explain. Questions testing these objectives will often begin with one of the following words: *define, state, name, describe, explain or outline* (see the *Glossary of Terms*).

### B Handling, applying and evaluating information

Candidates should be able (in words or by using symbolic, graphical and numerical forms of presentation) to:

- 1 locate, select, organise and present information from a variety of sources
- 2 handle information, distinguishing the relevant from the extraneous
- 3 manipulate numerical and other data and translate information from one form to another
- 4 analyse and evaluate information so as to identify patterns, report trends and conclusions, and draw inferences
- 5 present reasoned explanations for phenomena, patterns and relationships
- 6 apply knowledge, including principles, to novel situations
- 7 bring together knowledge, principles, concepts and skills from different areas of chemistry, and apply them in a particular context
- 8 evaluate information and hypotheses
9. construct arguments to support hypotheses or to justify a course of action
- 10 demonstrate an awareness of the limitations of chemistry theories and models.

These *Assessment Objectives* cannot be precisely specified in the syllabus content because questions testing such skills may be based on information which is unfamiliar to the candidate. In answering such questions, candidates are required to use principles and concepts that are within the syllabus and apply them in a logical, reasoned or deductive manner to a novel situation. Questions testing these objectives will often begin with one of the following words: *predict, suggest, construct, calculate or determine* (see the *Glossary of Terms*).

## SCHEME OF ASSESSMENT

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Candidates will take a 2 h 30 min paper (100 marks total). This paper consists of two sections and will include questions that require candidates to integrate knowledge and understanding from different sections in the syllabus.

### Section A (60 marks)

This section will consist of a variable number of compulsory free response questions including 1 or 2 stimulus-based questions. The stimulus-based question(s) constitute(s) 15–20 marks for this paper.

### Section B (40 marks)

Candidates will be required to answer **two** out of three free response questions. Each question will carry 20 marks.

### Weighting of Assessment Objectives

Assessment Objectives		Weighting (%)
A	Knowledge with understanding	25
B	Handling, applying and evaluating information	75

## ADDITIONAL INFORMATION

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### Data Booklet

A *Data Booklet* is available for use in the theory papers. The booklet is reprinted at the end of this syllabus document.

### Nomenclature

Candidates will be expected to be familiar with the nomenclature used in the syllabus. The proposals in '*Signs, Symbols and Systematics*' (The Association for Science Education Companion to 16–19 Science, 2000) will generally be adopted although the traditional names sulfate, sulfite, nitrate, nitrite, sulfurous and nitrous acids will be used in question papers. Sulfur (and all compounds of sulfur) will be spelt with f (not with ph) in question papers, however candidates can use either spelling in their answers.

### Units and significant figures

Candidates should be aware that misuse of units and/or significant figures, i.e. failure to quote units where necessary, the inclusion of units in quantities defined as ratios or quoting answers to an inappropriate number of significant figures, is liable to be penalised.

# SUBJECT CONTENT

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## Preamble

Students who offer H3 Chemistry should have a strong foundation in H2 Chemistry, through the three core ideas of matter, structure and properties, and transformation, as well as through the extension topics of chemistry of aqueous solutions, organic chemistry, electrochemistry and chemistry of the transition elements.

The syllabus for H3 Chemistry builds on that for H2 Chemistry, and includes the whole of the H2 Chemistry syllabus. Only content that is not already part of the H2 Chemistry syllabus is specifically set out here.

The H3 Chemistry syllabus introduces additional content in two areas, namely *Spectroscopic Techniques* and *Further Organic Mechanisms*. The additional content has been selected to highlight basic principles in chemistry and to strengthen the focus on applications. The topics chosen as extensions to the H2 syllabus expand the scope for students to engage in solving challenging problems, while allowing a deeper appreciation of the unity, cohesion and beauty of the discipline of chemistry.

With this expanded scope, students who offer H3 Chemistry are expected to tackle more sophisticated problems than students who only offer H2 Chemistry.

## 1. SPECTROSCOPIC TECHNIQUES

### 1.1 Basic Principles of Spectroscopy

#### Content

- Molecular orbital theory
- Electromagnetic spectrum
- Quantisation of energy
- Energy level transitions

#### Learning Outcomes

Candidates should be able to:

- (a) understand basic molecular orbital (MO) theory, involving
  - (i) atomic and molecular orbitals
  - (ii) bonding, anti-bonding and non-bonding orbitals
  - (iii) molecular orbitals with  $\sigma$  and  $\pi$  symmetry
- (b) understand that molecular orbitals represent discrete electronic energy levels in molecules  
[see also e(ii)]
- (c) apply linear combination of atomic orbitals (LCAO) principles to obtain the shape and relative energies of molecular orbitals in the following:
  - (i) simple homonuclear diatomic molecules such as  $H_2$ ,  $O_2$ , and  $F_2$
  - (ii) benzene and linear polyenes (molecular orbitals of  $\pi$  symmetry only)
 [quantitative treatment of LCAO is **not** required]
- (d) construct and interpret molecular orbital diagrams, and identify the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) for the following:
  - (i) simple homonuclear diatomic molecules such as  $H_2$ ,  $O_2$ , and  $F_2$
  - (ii) benzene and linear polyenes (molecular orbitals of  $\pi$  symmetry only)
 [knowledge of orbital mixing between orbitals of the same symmetry is **not** required]

- (e) understand the following in relation to the fundamental principles of spectroscopy:
- (i) properties of electromagnetic radiation
    - the electromagnetic spectrum (with range of wavelengths for different types of radiation used in spectroscopy)
    - the photon as a discrete packet (quantum) of electromagnetic energy
    - the relationship between wavelength, frequency and speed of light, including the use of the equation,  $E = hf$
  - (ii) the quantisation of energy in relation to
    - electronic, vibrational and rotational energy levels
    - nuclear energy levels in applied magnetic field
  - (iii) energy level transitions associated with the absorption and emission of photons with energy matching the energy gap

## 1.2 Ultraviolet/visible Spectroscopy

### Content

- Electronic transitions
- Chromophores
- Molar absorptivity and the Beer–Lambert law

### Learning Outcomes

Candidates should be able to:

- (a) explain that ultraviolet/visible absorption in organic molecules requires electronic transitions ( $\sigma \rightarrow \sigma^*$ ,  $n \rightarrow \sigma^*$ ,  $\pi \rightarrow \pi^*$ ,  $n \rightarrow \pi^*$  transitions; forbidden and allowed transitions) between energy levels in chromophores which contain a double or triple bond, a delocalised system, or a lone pair of electrons [detailed knowledge of instrumentation is **not** required]
- (b) predict whether a given organic molecule will absorb in the ultraviolet/visible region by identifying the chromophore
- (c) explain qualitatively how increasing conjugation in an organic molecule decreases the gap between energy levels and hence shifts the absorption towards longer wavelength
- (d) use the Beer–Lambert law, absorbance =  $\lg(I_0/I) = \epsilon cl$ , where  $\epsilon$  is taken merely as a constant characteristic of the substance concerned, to calculate the concentration of a given species (either organic or inorganic) in solution
- (e) apply ultraviolet/visible spectroscopy to quantitative analysis of a given species (either organic or inorganic) in solution



### 1.3 Infra-red (IR) Spectroscopy

#### Content

- molecular vibrations: stretching and bending
- characteristic IR absorptions

#### Learning Outcomes

Candidates should be able to:

- explain the origin of IR spectroscopy in simple molecules in terms of
  - stretching vibrations
  - bending vibrations
 [detailed knowledge of instrumentation is **not** required]
- predict the number of IR absorptions for a given simple molecule (e.g. CO<sub>2</sub> or SO<sub>2</sub>), and identify the molecular vibrations which give rise to them
- identify characteristic IR absorptions in the IR spectrum of a compound which may contain different functional groups  
[Absorptions of common functional groups will be provided in the *Data Booklet*.]
- suggest structures for a compound from its IR spectrum
- predict the characteristic IR absorptions that will be present in the IR spectrum of a compound, given its structure

### 1.4 Nuclear Magnetic Resonance (NMR) Spectroscopy

#### Content

- nuclear spin and energy absorption
- chemical shift:  $\delta$  scale, internal reference, electronegativity effects, anisotropic effects, hydrogen bonding
- calculation of peak area and proton counting
- spin-spin splitting

#### Learning Outcomes

Candidates should be able to:

- outline the basic principles of NMR with reference to
  - nuclear spin
  - the process of absorption of energy
 [quantitative calculations of transitional energy are **not** required; detailed knowledge of instrumentation is **not** required]

- (b) understand the following features and use them in the interpretation and prediction of  $^1\text{H}$  NMR spectra:
- chemical shift
  - deuterated solvents in the identification of labile protons
  - the number of  $^1\text{H}$  NMR signals: equivalent and non-equivalent protons
  - peak area (integration) and proton counting
  - spin-spin splitting: first order spin-spin coupling; multiplicity
- (c) explain the use of the  $\delta$  scale with tetramethylsilane (TMS) as the reference
- (d) explain the factors affecting chemical shift
- electronegativity: inductive effect of substituents, including shielding and deshielding effects
  - anisotropic effects
  - hydrogen bonding

## 1.5 Mass Spectrometry

### Content

- ionisation, fragmentation and mass/charge ratio
- interpretation of spectra: molecular ion peak, isotopic abundance, fragment ions

### Learning Outcomes

Candidates should be able to:

- (a) outline the basic principles of mass spectrometry, with reference to
- ionisation and fragmentation
  - mass/charge ratio,  $m/z$
- [detailed knowledge of instrumentation is **not** required]
- (b) understand the following features and use them in the interpretation and prediction of mass spectra:
- molecular ion peak
  - isotopic abundances including the use of (M+1) peak caused by  $^{13}\text{C}$  and (M+2) and (M+4) peaks for the identification of halogen compounds
  - major fragment ions
- [fragment ions obtained from rearrangements are **not** included]

## 2. FURTHER ORGANIC MECHANISMS

### 2.1 Molecular Stereochemistry

#### Content

- stereochemical projection
- isomerism: conformational, *cis-trans*, enantiomerism, diastereomerism

#### Learning Outcomes

Candidates should be able to:

- (a) (i) use stereochemical projections, including Newman projections, to represent molecules  
 (ii) interpret stereochemical projections of molecules  
 [knowledge of Fischer projections is **not** required]
- (b) apply their understanding of the following types of isomerism to explain the stereochemistry of molecules, including saturated ring systems:
- (i) conformational isomerism, including energy barriers to rotation and interconversion
- (ii) *cis-trans* isomerism, including *E, Z* nomenclature
- (iii) enantiomerism and diastereomerism:
- *R, S* configuration
  - optical activity
  - optical purity as the excess of one enantiomer, including calculation of optical purity by the

$$\text{equation: optical purity} = \frac{[\alpha]_{\text{obs}}}{[\alpha]_{\text{pure material}}} \times 100\%$$

### 2.2 Basic Physical Organic Chemistry

#### Content

- kinetic and thermodynamic control: the Hammond postulate, the Bell–Evans–Polanyi principle
- calculations involving activation energy and enthalpy change of reaction

#### Learning Outcomes

Candidates should be able to:

- (a) understand and apply the following concepts involving kinetic control and thermodynamic control to the study of reaction mechanisms:
- (i) the Hammond postulate: relationship between the transition state and the nearest stable species
- (ii) the Bell–Evans–Polanyi principle
- relationship between activation energy and enthalpy change of reaction
  - quantitative calculations based on  $E_a = A + B\Delta H_r$

## 2.3 Nucleophilic Substitution

### Content

- mechanism: nature of nucleophiles and leaving group,  $S_N1$ ,  $S_N2$
- kinetics of mechanisms: energy profile, rate law, simple rate equations, orders of reaction, rate constants, stereochemistry, substituent effects
- competition between  $S_N1$  and  $S_N2$

### Learning Outcomes

Candidates should be able to:

- explain how the relative rate of nucleophilic substitution is affected by the nature of the
  - nucleophile
  - leaving group
  - substituents
- describe and compare the mechanisms and kinetics of  $S_N1$  and  $S_N2$  reactions, in terms of
  - the energy profile and rate law, including steady state approximation in  $S_N1$  [mathematical treatment of steady state is **not** required]
  - stereochemistry, including ion pair interactions in  $S_N1$
  - substituent effects
- explain the factors affecting competition between  $S_N1$  and  $S_N2$  mechanisms [solvent effects are **not** required]

## 2.4 Elimination

### Content

- mechanism: syn-/anti-elimination, stereoselectivity, regioselectivity, E1, E2
- kinetics of mechanisms: energy profile, rate law, regioselectivity
- E2/ $S_N2$  competition: substrate effects, base effects

### Learning Outcomes

Candidates should be able to:

- understand and apply the following concepts to the study of elimination reactions:
  - syn- and anti-elimination; and its effect on stereoselectivity
  - regioselectivity: Zaitsev (thermodynamic) and Hofmann (kinetic) product(s)
- describe and compare the mechanisms and kinetics of E1 and E2 reactions, in terms of
  - the energy profile and rate law
  - regioselectivity
- explain the E2/ $S_N2$  competition, in terms of
  - substrate effects
  - base effects

## SUMMARY OF KEY QUANTITIES AND UNITS

The following list illustrates the symbols and units that will be used in question papers. The list is not exhaustive.

<b>Quantity</b>	<b>Usual symbols</b>	<b>Unit</b>
<b>Base quantities</b>		
amount of substance	$n$	mol
electric current	$I$	A
length	$l$	m
mass	$m$	kg, g
thermodynamic temperature	$T$	K
time	$t$	s
<b>Other quantities</b>		
acid dissociation constant	$K_a$	$\text{mol dm}^{-3}$
atomic mass	$m_a$	g, kg
Avogadro constant	$L$	$\text{mol}^{-1}$
base dissociation constant	$K_b$	$\text{mol dm}^{-3}$
bond energy	–	$\text{kJ mol}^{-1}$
charge on the electron	$e$	C
chemical shift	$\delta$	–
concentration	$c$	$\text{mol dm}^{-3}$
density	$\rho$	$\text{kg m}^{-3}$ , $\text{g dm}^{-3}$ , $\text{g cm}^{-3}$
electric potential difference	$V$	V
electromotive force	$E$	V
electron affinity	–	$\text{kJ mol}^{-1}$
enthalpy change of reaction	$\Delta H$	J, kJ
equilibrium constant	$K$ , $K_p$ , $K_c$	as appropriate
Faraday constant	$F$	$\text{C mol}^{-1}$
frequency	$\nu$ , $f$	Hz
half-life	$T_{1/2}$ , $t_{1/2}$	s
ionic product, solubility product	$K$ , $K_{sp}$	as appropriate
ionic product of water	$K_w$	$\text{mol}^2 \text{dm}^{-6}$
ionisation energy	$I$	$\text{kJ mol}^{-1}$
lattice energy	–	$\text{kJ mol}^{-1}$
molar absorption coefficient	$\epsilon$	$\text{mol}^{-1} \text{dm}^3 \text{cm}^{-1}$
molar gas constant	$R$	$\text{J K}^{-1} \text{mol}^{-1}$
molar mass	$M$	$\text{g mol}^{-1}$
mole fraction	$x$	–
molecular mass	$m$	g, kg
neutron number	$N$	–
nucleon number	$A$	–
number of molecules	$N$	–
number of molecules per unit volume	$n$	$\text{m}^{-3}$

<b>Quantity</b>	<b>Usual symbols</b>	<b>Unit</b>
order of reaction	$n, m$	–
partition coefficient	$K$	–
Planck constant	$h$	J s
pH	pH	–
pressure	$p$	Pa
proton number	$Z$	–
rate constant	$k$	as appropriate
relative $\left\{ \begin{array}{l} \text{atomic} \\ \text{isotopic} \end{array} \right\}$ mass	$A_r$	–
relative molecular mass	$M_r$	–
specific rotation	$[\alpha]$	–
speed of electromagnetic waves	$c$	$\text{m s}^{-1}$
(standard) $\left\{ \begin{array}{l} \text{electrode} \\ \text{redox} \end{array} \right\}$ potential	$(E^\ominus)E$	V
standard enthalpy change of reaction	$\Delta H^\ominus$	$\text{J mol}^{-1}, \text{kJ mol}^{-1}$
standard entropy change of reaction	$\Delta S^\ominus$	$\text{J K}^{-1} \text{mol}^{-1}, \text{kJ K}^{-1} \text{mol}^{-1}$
standard Gibbs free energy change of reaction	$\Delta G^\ominus$	$\text{J mol}^{-1}, \text{kJ mol}^{-1}$
temperature	$\theta, t$	$^\circ\text{C}$
volume	$V, v$	$\text{m}^3, \text{dm}^3$
wavelength	$\lambda$	m, mm, nm

## MATHEMATICAL REQUIREMENTS

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It is assumed that candidates will be competent in the techniques described below.

Make calculations involving addition, subtraction, multiplication and division of quantities.

Make approximate evaluations of numerical expressions.

Express small fractions as percentages, and vice versa.

Calculate an arithmetic mean.

Transform decimal notation to power of ten notation (standard form).

Use calculators to evaluate logarithms (for pH calculations), squares, square roots, and reciprocals.

Change the subject of an equation. (Most such equations involve only the simpler operations but may include positive and negative indices and square roots.)

Substitute physical quantities into an equation using consistent units so as to calculate one quantity. Check the dimensional consistency of such calculations, e.g. the units of a rate constant  $k$ .

Solve simple algebraic equations.

Comprehend and use the symbols/notations  $<$ ,  $>$ ,  $\approx$ ,  $/$ ,  $\Delta$ ,  $\equiv$ ,  $\bar{x}$  (or  $\langle x \rangle$ ).

Test tabulated pairs of values for direct proportionality by a graphical method or by constancy of ratio.

Select appropriate variables and scales for plotting a graph, especially to obtain a linear graph of the form  $y = mx + c$ .

Determine and interpret the slope and intercept of a linear graph.

Choose by inspection a straight line that will serve as the 'least bad' linear model for a set of data presented graphically.

Understand (i) the slope of a tangent to a curve as a measure of rate of change, (ii) the 'area' below a curve where the area has physical significance, e.g. Boltzmann distribution curves.

Comprehend how to handle numerical work so that significant figures are neither lost unnecessarily nor used beyond what is justified.

Estimate orders of magnitude.

Formulate simple algebraic equations as mathematical models, e.g. construct a rate equation, and identify failures of such models.

### Calculators

Any calculator used must be on the Singapore Examinations and Assessment Board list of approved calculators.

## GLOSSARY OF TERMS

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It is hoped that the glossary (which is relevant only to science subjects) will prove helpful to candidates as a guide, i.e. it is neither exhaustive nor definitive. The glossary has been deliberately kept brief not only with respect to the number of terms included but also to the descriptions of their meanings. Candidates should appreciate that the meaning of a term must depend in part on its context.

1. *Define (the term(s)...) is intended literally, only a formal statement or equivalent paraphrase being required.*
2. *What do you understand by/What is meant by (the term(s)...) normally implies that a definition should be given, together with some relevant comment on the significance or context of the term(s) concerned, especially where two or more terms are included in the question. The amount of supplementary comment intended should be interpreted in the light of the indicated mark value.*
3. *State implies a concise answer with little or no supporting argument, e.g. a numerical answer that can be obtained 'by inspection'.*
4. *List requires a number of points, generally each of one word, with no elaboration. Where a given number of points is specified, this should not be exceeded.*
5. *Explain may imply reasoning or some reference to theory, depending on the context.*
6. *Describe requires candidates to state in words (using diagrams where appropriate) the main points of the topic. It is often used with reference either to particular phenomena or to particular experiments. In the former instance, the term usually implies that the answer should include reference to (visual) observations associated with the phenomena.*  
*In other contexts, describe and give an account of should be interpreted more generally, i.e. the candidate has greater discretion about the nature and the organisation of the material to be included in the answer. Describe and explain may be coupled in a similar way to state and explain.*
7. *Discuss requires candidates to give a critical account of the points involved in the topic.*
8. *Outline implies brevity, i.e. restricting the answer to giving essentials.*
9. *Predict implies that the candidate is not expected to produce the required answer by recall but by making a logical connection between other pieces of information. Such information may be wholly given in the question or may depend on answers extracted in an early part of the question.*
10. *Deduce is used in a similar way as predict except that some supporting statement is required, e.g. reference to a law/principle, or the necessary reasoning is to be included in the answer.*
11. *Comment is intended as an open-ended instruction, inviting candidates to recall or infer points of interest relevant to the context of the question, taking account of the number of marks available.*
12. *Suggest is used in two main contexts, i.e. either to imply that there is no unique answer (e.g. in chemistry, two or more substances may satisfy the given conditions describing an 'unknown'), or to imply that candidates are expected to apply their general knowledge to a 'novel' situation, one that may be formally 'not in the syllabus'.*
13. *Find is a general term that may variously be interpreted as calculate, measure, determine etc.*
14. *Calculate is used when a numerical answer is required. In general, working should be shown, especially where two or more steps are involved.*
15. *Measure implies that the quantity concerned can be directly obtained from a suitable measuring instrument, e.g. length, using a rule, or angle, using a protractor.*



16. *Determine* often implies that the quantity concerned cannot be measured directly but is obtained by calculation, substituting measured or known values of other quantities into a standard formula, e.g. relative molecular mass.
17. *Estimate* implies a reasoned order of magnitude statement or calculation of the quantity concerned, making such simplifying assumptions as may be necessary about points of principle and about the values of quantities not otherwise included in the question.
18. *Sketch*, when applied to graph work, implies that the shape and/or position of the curve need only be qualitatively correct, but candidates should be aware that, depending on the context, some quantitative aspects may be looked for, e.g. passing through the origin, having an intercept, asymptote or discontinuity at a particular value.

In diagrams, sketch implies that a simple, freehand drawing is acceptable: nevertheless, care should be taken over proportions and the clear exposition of important details.

19. *Construct* is often used in relation to chemical equations where a candidate is expected to write a balanced equation, not by factual recall but by analogy or by using information in the question.
20. *Compare* requires candidates to provide both the similarities and differences between things or concepts.
21. *Classify* requires candidates to group things based on common characteristics.
22. *Recognise* is often used to identify facts, characteristics or concepts that are critical (relevant/appropriate) to the understanding of a situation, event, process or phenomenon.

## REFERENCES

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Teachers and students may find reference to the following books helpful.

A Primer to Mechanism in Organic Chemistry by P Sykes, published by Longman Scientific & Technical

Advanced Organic Chemistry (5th Edition) by F A Carey and R J Sundberg, published by Springer

Introduction to Spectroscopy (5th Edition) by D L Pavia, G M Lampman, G S Kriz and J A Vyvyan, published by Cengage Learning

IR Spectroscopy: An Introduction by H Günzler and H Gremlich, published by Wiley-VCH

March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure (7th Edition) by M Smith, published by Wiley

Modern Physical Organic Chemistry by E V Anslyn and D A Dougherty, published by University Science

NMR Spectroscopy: Basic Principles, Concepts and Applications in Chemistry (3rd Edition) by H Günther, published by Wiley-VCH

Organic Mechanisms: Reactions, Stereochemistry and Synthesis (English edition) by R Bruckner, M Harmata and K Beifuss, published by Springer

Organic Spectroscopy by L D S Yadav, published by Kluwer

Organic Synthesis: The Disconnection Approach (2nd Edition) by S Warren and P Wyatt, published by Wiley

Oxford Chemistry Primers: Foundations of Organic Chemistry by M Hornby and J Peach, published by Oxford University Press

Oxford Chemistry Primers: Structure and Reactivity in Organic Chemistry by H Maskill, published by Oxford University Press

Oxford Chemistry Primers: Mechanisms of Organic Chemistry by H Maskill, published by Oxford University Press

Perspectives on Structure and Mechanism in Organic Chemistry (2nd Edition) by F A Carroll, published by Wiley

The Art of Writing Reasonable Organic Reaction Mechanisms (2nd Edition) by R B Grossman, published by Springer

UV Spectroscopy: Techniques, Instrumentation and Data handling by B J Clark, T Frost and M A Russell, published by Chapman & Hall

Teachers are encouraged to choose texts for class use which they feel will be of interest to their students and will support their own teaching style.

# Data Booklet

for

**Chemistry**  
**(Advanced Level)**

For use from 2017 in all papers, except practical examinations,  
for the 9729 H2 Chemistry and H3 Chemistry syllabuses.

For use from 2018 in all papers, for the 8873 H1 Chemistry syllabuses.

**Contents: Tables of Chemical data**

- 1 Important values, constants and standards
- 2 Ionisation energies (1st, 2nd, 3rd and 4th) of selected elements in  $\text{kJ mol}^{-1}$
- 3 Bond energies
- 4 Standard electrode potential and redox potentials,  $E^\ominus$  at 298 K (25 °C)
- 5 Atomic and ionic radii
- 6 Typical proton ( $^1\text{H}$ ) chemical shift values ( $\delta$ ) relative to TMS = 0
- 7 Characteristic infra-red absorption frequencies for some selected bonds
- 8 The orientating effect of groups in aromatic substitution reactions
- 9 Qualitative Analysis Notes
- 10 The Periodic Table of Elements

**1 Important values, constants and standards**

molar gas constant	$R = 8.31 \text{ J K}^{-1} \text{ mol}^{-1}$
the Faraday constant	$F = 9.65 \times 10^4 \text{ C mol}^{-1}$
the Avogadro constant	$L = 6.02 \times 10^{23} \text{ mol}^{-1}$
the Planck constant	$h = 6.63 \times 10^{-34} \text{ J s}$
speed of light in a vacuum	$c = 3.00 \times 10^8 \text{ m s}^{-1}$
rest mass of proton, ${}^1_1\text{H}$	$m_p = 1.67 \times 10^{-27} \text{ kg}$
rest mass of neutron, ${}^1_0\text{n}$	$m_n = 1.67 \times 10^{-27} \text{ kg}$
rest mass of electron, ${}^0_{-1}\text{e}$	$m_e = 9.11 \times 10^{-31} \text{ kg}$
electronic charge	$e = -1.60 \times 10^{-19} \text{ C}$
molar volume of gas	$V_m = 22.7 \text{ dm}^3 \text{ mol}^{-1}$ at s.t.p. $V_m = 24 \text{ dm}^3 \text{ mol}^{-1}$ at r.t.p. (where s.t.p. is expressed as $10^5 \text{ Pa}$ [1 bar] and $273 \text{ K}$ [ $0 \text{ }^\circ\text{C}$ ], r.t.p. is expressed as $101325 \text{ Pa}$ [1 atm] and $293 \text{ K}$ [ $20 \text{ }^\circ\text{C}$ ])
ionic product of water	$K_w = 1.00 \times 10^{-14} \text{ mol}^2 \text{ dm}^{-6}$ (at $298 \text{ K}$ [ $25 \text{ }^\circ\text{C}$ ])
specific heat capacity of water	$= 4.18 \text{ kJ kg}^{-1} \text{ K}^{-1}$ (= $4.18 \text{ J g}^{-1} \text{ K}^{-1}$ )

**2 Ionisation energies (1st, 2nd, 3rd and 4th) of selected elements, in kJ mol<sup>-1</sup>**

	Proton Number	First	Second	Third	Fourth
H	1	1310	–	–	–
He	2	2370	5250	–	–
Li	3	519	7300	11800	–
Be	4	900	1760	14800	21000
B	5	799	2420	3660	25000
C	6	1090	2350	4610	6220
N	7	1400	2860	4590	7480
O	8	1310	3390	5320	7450
F	9	1680	3370	6040	8410
Ne	10	2080	3950	6150	9290
Na	11	494	4560	6940	9540
Mg	12	736	1450	7740	10500
Al	13	577	1820	2740	11600
Si	14	786	1580	3230	4360
P	15	1060	1900	2920	4960
S	16	1000	2260	3390	4540
Cl	17	1260	2300	3850	5150
Ar	18	1520	2660	3950	5770
K	19	418	3070	4600	5860
Ca	20	590	1150	4940	6480
Sc	21	632	1240	2390	7110
Ti	22	661	1310	2720	4170
V	23	648	1370	2870	4600
Cr	24	653	1590	2990	4770
Mn	25	716	1510	3250	5190
Fe	26	762	1560	2960	5400
Co	27	757	1640	3230	5100
Ni	28	736	1750	3390	5400
Cu	29	745	1960	3350	5690

## 9813 CHEMISTRY GCE ADVANCED LEVEL H3 SYLLABUS (2021)

	Proton Number	First	Second	Third	Fourth
Zn	30	908	1730	3828	5980
Ga	31	577	1980	2960	6190
Ge	32	762	1540	3300	4390
Br	35	1140	2080	3460	4850
Rb	37	403	2632	3900	5080
Sr	38	548	1060	4120	5440
Ag	47	731	2074	3361	–
Sn	50	707	1410	2940	3930
I	53	1010	1840	3200	4030
Cs	55	376	2420	3300	–
Ba	56	502	966	3390	–
Pb	82	716	1450	3080	4080

**3 Bond energies****3(a) Bond energies in diatomic molecules (these are exact values)****Homonuclear**

Bond	Energy/kJ mol <sup>-1</sup>
H—H	436
D—D	442
N≡N	944
O=O	496
F—F	158
Cl—Cl	244
Br—Br	193
I—I	151

**Heteronuclear**

Bond	Energy/kJ mol <sup>-1</sup>
H—F	562
H—Cl	431
H—Br	366
H—I	299
C≡O	1077



**3(b) Bond energies in polyatomic molecules (these are average values)****Homonuclear**

Bond	Energy/kJ mol <sup>-1</sup>
C—C	350
C=C	610
C≡C	840
C $\equiv\equiv$ C (benzene)	520
N—N	160
N=N	410
O—O	150
Si—Si	222
P—P	200
S—S	264

**Heteronuclear**

Bond	Energy/kJ mol <sup>-1</sup>
C—H	410
C—F	485
C—Cl	340
C—Br	280
C—I	240
C—N	305
C=N	610
C≡N	890
C—O	360
C=O	740
C=O in CO <sub>2</sub>	805
N—H	390
N—Cl	310
O—H	460
Si—Cl	359
Si—H	320
Si—O (in SiO <sub>2</sub> (s))	460
Si=O (in SiO <sub>2</sub> (g))	640
P—H	320
P—Cl	330
P—O	340
P=O	540
S—H	347
S—Cl	250
S—O	360
S=O	500

**4 Standard electrode potential and redox potentials,  $E^\ominus$  at 298 K (25 °C)**

For ease of reference, two tabulations are given:

- (a) an extended list in alphabetical order;  
 (b) a shorter list in decreasing order of magnitude, i.e. a redox series.

**4(a)  $E^\ominus$  in alphabetical order**

Electrode reaction	$E^\ominus / \text{V}$
$\text{Ag}^+ + \text{e}^- \rightleftharpoons \text{Ag}$	+0.80
$\text{Al}^{3+} + 3\text{e}^- \rightleftharpoons \text{Al}$	-1.66
$\text{Ba}^{2+} + 2\text{e}^- \rightleftharpoons \text{Ba}$	-2.90
$\text{Br}_2 + 2\text{e}^- \rightleftharpoons 2\text{Br}^-$	+1.07
$\text{Ca}^{2+} + 2\text{e}^- \rightleftharpoons \text{Ca}$	-2.87
$\text{Cl}_2 + 2\text{e}^- \rightleftharpoons 2\text{Cl}^-$	+1.36
$2\text{HOCl} + 2\text{H}^+ + 2\text{e}^- \rightleftharpoons \text{Cl}_2 + 2\text{H}_2\text{O}$	+1.64
$\text{ClO}^- + \text{H}_2\text{O} + 2\text{e}^- \rightleftharpoons \text{Cl}^- + 2\text{OH}^-$	+0.81
$\text{Co}^{2+} + 2\text{e}^- \rightleftharpoons \text{Co}$	-0.28
$\text{Co}^{3+} + \text{e}^- \rightleftharpoons \text{Co}^{2+}$	+1.89
$[\text{Co}(\text{NH}_3)_6]^{2+} + 2\text{e}^- \rightleftharpoons \text{Co} + 6\text{NH}_3$	-0.43
$\text{Cr}^{2+} + 2\text{e}^- \rightleftharpoons \text{Cr}$	-0.91
$\text{Cr}^{3+} + 3\text{e}^- \rightleftharpoons \text{Cr}$	-0.74
$\text{Cr}^{3+} + \text{e}^- \rightleftharpoons \text{Cr}^{2+}$	-0.41
$\text{Cr}_2\text{O}_7^{2-} + 14\text{H}^+ + 6\text{e}^- \rightleftharpoons 2\text{Cr}^{3+} + 7\text{H}_2\text{O}$	+1.33
$\text{Cu}^+ + \text{e}^- \rightleftharpoons \text{Cu}$	+0.52
$\text{Cu}^{2+} + 2\text{e}^- \rightleftharpoons \text{Cu}$	+0.34
$\text{Cu}^{2+} + \text{e}^- \rightleftharpoons \text{Cu}^+$	+0.15
$[\text{Cu}(\text{NH}_3)_4]^{2+} + 2\text{e}^- \rightleftharpoons \text{Cu} + 4\text{NH}_3$	-0.05
$\text{F}_2 + 2\text{e}^- \rightleftharpoons 2\text{F}^-$	+2.87
$\text{Fe}^{2+} + 2\text{e}^- \rightleftharpoons \text{Fe}$	-0.44
$\text{Fe}^{3+} + 3\text{e}^- \rightleftharpoons \text{Fe}$	-0.04

Electrode reaction	$E^{\ominus} / \text{V}$
$\text{Fe}^{3+} + \text{e}^{-} \rightleftharpoons \text{Fe}^{2+}$	+0.77
$[\text{Fe}(\text{CN})_6]^{3-} + \text{e}^{-} \rightleftharpoons [\text{Fe}(\text{CN})_6]^{4-}$	+0.36
$\text{Fe}(\text{OH})_3 + \text{e}^{-} \rightleftharpoons \text{Fe}(\text{OH})_2 + \text{OH}^{-}$	-0.56
$2\text{H}^{+} + 2\text{e}^{-} \rightleftharpoons \text{H}_2$	0.00
$\text{I}_2 + 2\text{e}^{-} \rightleftharpoons 2\text{I}^{-}$	+0.54
$\text{K}^{+} + \text{e}^{-} \rightleftharpoons \text{K}$	-2.92
$\text{Li}^{+} + \text{e}^{-} \rightleftharpoons \text{Li}$	-3.04
$\text{Mg}^{2+} + 2\text{e}^{-} \rightleftharpoons \text{Mg}$	-2.38
$\text{Mn}^{2+} + 2\text{e}^{-} \rightleftharpoons \text{Mn}$	-1.18
$\text{Mn}^{3+} + \text{e}^{-} \rightleftharpoons \text{Mn}^{2+}$	+1.54
$\text{MnO}_2 + 4\text{H}^{+} + 2\text{e}^{-} \rightleftharpoons \text{Mn}^{2+} + 2\text{H}_2\text{O}$	+1.23
$\text{MnO}_4^{-} + \text{e}^{-} \rightleftharpoons \text{MnO}_4^{2-}$	+0.56
$\text{MnO}_4^{-} + 4\text{H}^{+} + 3\text{e}^{-} \rightleftharpoons \text{MnO}_2 + 2\text{H}_2\text{O}$	+1.67
$\text{MnO}_4^{-} + 8\text{H}^{+} + 5\text{e}^{-} \rightleftharpoons \text{Mn}^{2+} + 4\text{H}_2\text{O}$	+1.52
$\text{NO}_3^{-} + 2\text{H}^{+} + \text{e}^{-} \rightleftharpoons \text{NO}_2 + \text{H}_2\text{O}$	+0.81
$\text{NO}_3^{-} + 3\text{H}^{+} + 2\text{e}^{-} \rightleftharpoons \text{HNO}_2 + \text{H}_2\text{O}$	+0.94
$\text{NO}_3^{-} + 10\text{H}^{+} + 8\text{e}^{-} \rightleftharpoons \text{NH}_4^{+} + 3\text{H}_2\text{O}$	+0.87
$\text{Na}^{+} + \text{e}^{-} \rightleftharpoons \text{Na}$	-2.71
$\text{Ni}^{2+} + 2\text{e}^{-} \rightleftharpoons \text{Ni}$	-0.25
$[\text{Ni}(\text{NH}_3)_6]^{2+} + 2\text{e}^{-} \rightleftharpoons \text{Ni} + 6\text{NH}_3$	-0.51
$\text{H}_2\text{O}_2 + 2\text{H}^{+} + 2\text{e}^{-} \rightleftharpoons 2\text{H}_2\text{O}$	+1.77
$\text{HO}_2^{-} + \text{H}_2\text{O} + 2\text{e}^{-} \rightleftharpoons 3\text{OH}^{-}$	+0.88
$\text{O}_2 + 4\text{H}^{+} + 4\text{e}^{-} \rightleftharpoons 2\text{H}_2\text{O}$	+1.23
$\text{O}_2 + 2\text{H}_2\text{O} + 4\text{e}^{-} \rightleftharpoons 4\text{OH}^{-}$	+0.40
$\text{O}_2 + 2\text{H}^{+} + 2\text{e}^{-} \rightleftharpoons \text{H}_2\text{O}_2$	+0.68

Electrode reaction	$E^{\ominus} / \text{V}$
$\text{O}_2 + \text{H}_2\text{O} + 2\text{e}^- \rightleftharpoons \text{HO}_2^- + \text{OH}^-$	-0.08
$2\text{H}_2\text{O} + 2\text{e}^- \rightleftharpoons \text{H}_2 + 2\text{OH}^-$	-0.83
$\text{Pb}^{2+} + 2\text{e}^- \rightleftharpoons \text{Pb}$	-0.13
$\text{Pb}^{4+} + 2\text{e}^- \rightleftharpoons \text{Pb}^{2+}$	+1.69
$\text{PbO}_2 + 4\text{H}^+ + 2\text{e}^- \rightleftharpoons \text{Pb}^{2+} + 2\text{H}_2\text{O}$	+1.47
$\text{SO}_4^{2-} + 4\text{H}^+ + 2\text{e}^- \rightleftharpoons \text{SO}_2 + 2\text{H}_2\text{O}$	+0.17
$\text{S}_2\text{O}_8^{2-} + 2\text{e}^- \rightleftharpoons 2\text{SO}_4^{2-}$	+2.01
$\text{S}_4\text{O}_6^{2-} + 2\text{e}^- \rightleftharpoons 2\text{S}_2\text{O}_3^{2-}$	+0.09
$\text{Sn}^{2+} + 2\text{e}^- \rightleftharpoons \text{Sn}$	-0.14
$\text{Sn}^{4+} + 2\text{e}^- \rightleftharpoons \text{Sn}^{2+}$	+0.15
$\text{V}^{2+} + 2\text{e}^- \rightleftharpoons \text{V}$	-1.20
$\text{V}^{3+} + \text{e}^- \rightleftharpoons \text{V}^{2+}$	-0.26
$\text{VO}^{2+} + 2\text{H}^+ + \text{e}^- \rightleftharpoons \text{V}^{3+} + \text{H}_2\text{O}$	+0.34
$\text{VO}_2^+ + 2\text{H}^+ + \text{e}^- \rightleftharpoons \text{VO}^{2+} + \text{H}_2\text{O}$	+1.00
$\text{VO}_3^- + 4\text{H}^+ + \text{e}^- \rightleftharpoons \text{VO}^{2+} + 2\text{H}_2\text{O}$	+1.00
$\text{Zn}^{2+} + 2\text{e}^- \rightleftharpoons \text{Zn}$	-0.76

All ionic states refer to aqueous ions but other state symbols have been omitted.

**4(b)  $E^\ominus$  in decreasing order of oxidising power**

(a selection only – see also the extended alphabetical list on the previous pages)

Electrode reaction	$E^\ominus / \text{V}$
$\text{F}_2 + 2\text{e}^- \rightleftharpoons 2\text{F}^-$	+2.87
$\text{S}_2\text{O}_8^{2-} + 2\text{e}^- \rightleftharpoons 2\text{SO}_4^{2-}$	+2.01
$\text{H}_2\text{O}_2 + 2\text{H}^+ + 2\text{e}^- \rightleftharpoons 2\text{H}_2\text{O}$	+1.77
$\text{MnO}_4^- + 8\text{H}^+ + 5\text{e}^- \rightleftharpoons \text{Mn}^{2+} + 4\text{H}_2\text{O}$	+1.52
$\text{PbO}_2 + 4\text{H}^+ + 2\text{e}^- \rightleftharpoons \text{Pb}^{2+} + 2\text{H}_2\text{O}$	+1.47
$\text{Cl}_2 + 2\text{e}^- \rightleftharpoons 2\text{Cl}^-$	+1.36
$\text{Cr}_2\text{O}_7^{2-} + 14\text{H}^+ + 6\text{e}^- \rightleftharpoons 2\text{Cr}^{3+} + 7\text{H}_2\text{O}$	+1.33
$\text{O}_2 + 4\text{H}^+ + 4\text{e}^- \rightleftharpoons 2\text{H}_2\text{O}$	+1.23
$\text{Br}_2 + 2\text{e}^- \rightleftharpoons 2\text{Br}^-$	+1.07
$\text{NO}_3^- + 10\text{H}^+ + 8\text{e}^- \rightleftharpoons \text{NH}_4^+ + 3\text{H}_2\text{O}$	+0.87
$\text{ClO}^- + \text{H}_2\text{O} + 2\text{e}^- \rightleftharpoons \text{Cl}^- + 2\text{OH}^-$	+0.81
$\text{NO}_3^- + 2\text{H}^+ + \text{e}^- \rightleftharpoons \text{NO}_2 + \text{H}_2\text{O}$	+0.81
$\text{Ag}^+ + \text{e}^- \rightleftharpoons \text{Ag}$	+0.80
$\text{Fe}^{3+} + \text{e}^- \rightleftharpoons \text{Fe}^{2+}$	+0.77
$\text{I}_2 + 2\text{e}^- \rightleftharpoons 2\text{I}^-$	+0.54
$\text{O}_2 + 2\text{H}_2\text{O} + 4\text{e}^- \rightleftharpoons 4\text{OH}^-$	+0.40
$\text{Cu}^{2+} + 2\text{e}^- \rightleftharpoons \text{Cu}$	+0.34
$\text{SO}_4^{2-} + 4\text{H}^+ + 2\text{e}^- \rightleftharpoons \text{SO}_2 + 2\text{H}_2\text{O}$	+0.17
$\text{Sn}^{4+} + 2\text{e}^- \rightleftharpoons \text{Sn}^{2+}$	+0.15
$\text{S}_4\text{O}_6^{2-} + 2\text{e}^- \rightleftharpoons 2\text{S}_2\text{O}_3^{2-}$	+0.09
$2\text{H}^+ + 2\text{e}^- \rightleftharpoons \text{H}_2$	0.00
$\text{Pb}^{2+} + 2\text{e}^- \rightleftharpoons \text{Pb}$	-0.13
$\text{Sn}^{2+} + 2\text{e}^- \rightleftharpoons \text{Sn}$	-0.14

Electrode reaction	$E^\ominus / \text{V}$
$\text{Fe}^{2+} + 2\text{e}^- \rightleftharpoons \text{Fe}$	-0.44
$\text{Zn}^{2+} + 2\text{e}^- \rightleftharpoons \text{Zn}$	-0.76
$2\text{H}_2\text{O} + 2\text{e}^- \rightleftharpoons \text{H}_2 + 2\text{OH}^-$	-0.83
$\text{V}^{2+} + 2\text{e}^- \rightleftharpoons \text{V}$	-1.20
$\text{Mg}^{2+} + 2\text{e}^- \rightleftharpoons \text{Mg}$	-2.38
$\text{Ca}^{2+} + 2\text{e}^- \rightleftharpoons \text{Ca}$	-2.87
$\text{K}^+ + \text{e}^- \rightleftharpoons \text{K}$	-2.92

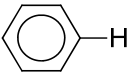
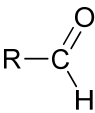
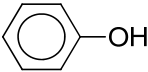
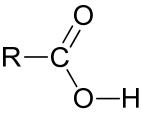
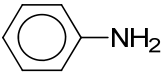
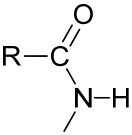
**5 Atomic and ionic radii**

(a) Period 1	atomic/nm		ionic/nm			
single covalent	H	0.037	H <sup>-</sup>	0.208		
van der Waals	He	0.140				
(b) Period 2						
metallic	Li	0.152	Li <sup>+</sup>	0.060		
	Be	0.112	Be <sup>2+</sup>	0.031		
single covalent	B	0.080	B <sup>3+</sup>	0.020		
	C	0.077	C <sup>4+</sup>	0.015	C <sup>4-</sup>	0.260
	N	0.074		N <sup>3-</sup>	0.171	
	O	0.073		O <sup>2-</sup>	0.140	
	F	0.072		F <sup>-</sup>	0.136	
van der Waals	Ne	0.160				
(c) Period 3						
metallic	Na	0.186	Na <sup>+</sup>	0.095		
	Mg	0.160	Mg <sup>2+</sup>	0.065		
	Al	0.143	Al <sup>3+</sup>	0.050		
single covalent	Si	0.117	Si <sup>4+</sup>	0.041		
	P	0.110		P <sup>3-</sup>	0.212	
	S	0.104		S <sup>2-</sup>	0.184	
	Cl	0.099		Cl <sup>-</sup>	0.181	
van der Waals	Ar	0.190				
(d) Group 2						
metallic	Be	0.112	Be <sup>2+</sup>	0.031		
	Mg	0.160	Mg <sup>2+</sup>	0.065		
	Ca	0.197	Ca <sup>2+</sup>	0.099		
	Sr	0.215	Sr <sup>2+</sup>	0.113		
	Ba	0.217	Ba <sup>2+</sup>	0.135		
	Ra	0.220	Ra <sup>2+</sup>	0.140		

(e) Group 14		atomic/nm		ionic/nm	
single covalent	C	0.077			
	Si	0.117	Si <sup>4+</sup>	0.041	
	Ge	0.122	Ge <sup>2+</sup>	0.093	
metallic	Sn	0.162	Sn <sup>2+</sup>	0.112	
	Pb	0.175	Pb <sup>2+</sup>	0.120	
(f) Group 17					
single covalent	F	0.072		F <sup>-</sup>	0.136
	Cl	0.099		Cl <sup>-</sup>	0.181
	Br	0.114		Br <sup>-</sup>	0.195
	I	0.133		I <sup>-</sup>	0.216
	At	0.140			
(g) First row d block elements					
metallic	Sc	0.164		Sc <sup>3+</sup>	0.075
	Ti	0.146	Ti <sup>2+</sup>	0.086	Ti <sup>3+</sup> 0.067
	V	0.135	V <sup>2+</sup>	0.079	V <sup>3+</sup> 0.064
	Cr	0.129	Cr <sup>2+</sup>	0.073	Cr <sup>3+</sup> 0.062
	Mn	0.132	Mn <sup>2+</sup>	0.083	Mn <sup>3+</sup> 0.058
	Fe	0.126	Fe <sup>2+</sup>	0.061	Fe <sup>3+</sup> 0.055
	Co	0.125	Co <sup>2+</sup>	0.065	Co <sup>3+</sup> 0.055
	Ni	0.124	Ni <sup>2+</sup>	0.069	Ni <sup>3+</sup> 0.056
	Cu	0.128	Cu <sup>2+</sup>	0.073	
	Zn	0.135	Zn <sup>2+</sup>	0.074	



6 Typical proton ( $^1\text{H}$ ) chemical shift values ( $\delta$ ) relative to TMS = 0

Type of proton	Environment of proton	Example structures	Chemical Shift range ( $\delta$ )
C–H	alkane	$-\text{CH}_3$ , $-\text{CH}_2-$ , $\text{CH}-$	0.9–1.7
	alkyl next to C=O	$\text{CH}_3-\text{C}=\text{O}$ , $-\text{CH}_2-\text{C}=\text{O}$ , $\text{CH}-\text{C}=\text{O}$	2.2–3.0
	alkyl next to aromatic ring	$\text{CH}_3-\text{Ar}$ , $-\text{CH}_2-\text{Ar}$ , $\text{CH}-\text{Ar}$	2.3–3.0
	alkyl next to electronegative atom	$\text{CH}_3-\text{O}$ , $-\text{CH}_2-\text{O}$ , $-\text{CH}_2-\text{Cl}$ , $\text{CH}-\text{Br}$	3.2–4.0
	attached to alkyne	$\equiv\text{C}-\text{H}$	1.8–3.1
	attached to alkene	$=\text{CH}_2$ , $=\text{CH}-$	4.5–6.0
	attached to aromatic ring		6.0–9.0
	aldehyde		9.3–10.5
O–H (see note below)	alcohol	$\text{RO}-\text{H}$	0.5–6.0
	phenol		4.5–7.0
	carboxylic acid		9.0–13.0
N–H (see note below)	alkyl amine	$\text{R}-\text{NH}-$	1.0–5.0
	aryl amine		3.0–6.0
	amide		5.0–12.0

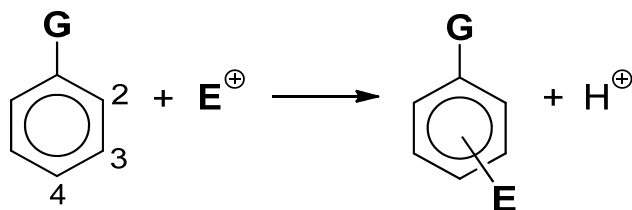
Note:  $\delta$  values for  $-\text{O}-\text{H}$  and  $-\text{N}-\text{H}$  protons can vary depending on solvent and concentration.

## 7 Characteristic infra-red absorption frequencies for some selected bonds

Bond	Functional groups containing the bond	Absorption range (in wavenumbers) / $\text{cm}^{-1}$	Appearance of peak ( <i>s</i> = strong, <i>w</i> = weak)
C–Cl	chloroalkanes	700–800	<b>s</b>
C–O	alcohol ether ester carboxylic acids	970–1260 1000–1310 1050–1330 1210–1440	<b>s</b> <b>s</b> <b>s</b> <b>s</b>
C=C	aromatic alkenes	1475–1625 1635–1690	<b>s</b> <b>w</b>
C=O	amides ketones and aldehydes carboxylic acids esters	1640–1690 1670–1740 1680–1730 1710–1750	<b>s</b> <b>s</b> <b>s</b> <b>s</b>
C≡C	alkynes	2150–2250	<b>w</b> unless conjugated
C≡N	nitriles	2200–2250	<b>w</b>
C–H	alkanes, CH <sub>2</sub> –H alkenes/arenes, =C–H	2850–2950 3000–3100	<b>s</b> <b>w</b>
N–H	amines, amides	3300–3500	<b>w</b>
O–H	carboxylic acid, RCO <sub>2</sub> –H H-bonded alcohol/phenol, RO–H free alcohol, RO–H	2500–3000 3200–3600 3580–3650	<b>s</b> and very broad <b>s</b> <b>s</b> and sharp

## 8 The orientating effect of groups in aromatic substitution reactions

The position of the incoming group, **E**, is determined by the nature of the group, **G**, already bonded to the ring, and not by the nature of the incoming group **E**.



<b>G</b>	<ul style="list-style-type: none"> <li>–alkyl</li> <li>–OH or –OR</li> <li>–NH<sub>2</sub>, –NHR or –NR<sub>2</sub></li> <li>–NHCOR</li> </ul>	–Cl, –Br, –I	<ul style="list-style-type: none"> <li>–CHO, –COR</li> <li>–CO<sub>2</sub>H, –CO<sub>2</sub>R</li> <li>–NH<sub>3</sub><sup>+</sup></li> <li>–NO<sub>2</sub>, –CN</li> </ul>
<b>Reactivity of ring (compared to benzene)</b>	Activated	Deactivated	Deactivated
<b>Position of E (relative to position of G)</b>	2- and/or 4-	2- and/or 4-	3-

**9 Qualitative Analysis Notes**

[ppt. = precipitate]

**9(a) Reactions of aqueous cations**

cation	reaction with	
	NaOH(aq)	NH <sub>3</sub> (aq)
aluminium, Al <sup>3+</sup> (aq)	white ppt. soluble in excess	white ppt. insoluble in excess
ammonium, NH <sub>4</sub> <sup>+</sup> (aq)	ammonia produced on heating	–
barium, Ba <sup>2+</sup> (aq)	no ppt. (if reagents are pure)	no ppt.
calcium, Ca <sup>2+</sup> (aq)	white ppt. with high [Ca <sup>2+</sup> (aq)]	no ppt.
chromium(III), Cr <sup>3+</sup> (aq)	grey-green ppt. soluble in excess giving dark green solution	grey-green ppt. insoluble in excess
copper(II), Cu <sup>2+</sup> (aq),	pale blue ppt. insoluble in excess	blue ppt. soluble in excess giving dark blue solution
iron(II), Fe <sup>2+</sup> (aq)	green ppt., turning brown on contact with air insoluble in excess	green ppt., turning brown on contact with air insoluble in excess
iron(III), Fe <sup>3+</sup> (aq)	red-brown ppt. insoluble in excess	red-brown ppt. insoluble in excess
magnesium, Mg <sup>2+</sup> (aq)	white ppt. insoluble in excess	white ppt. insoluble in excess
manganese(II), Mn <sup>2+</sup> (aq)	off-white ppt., rapidly turning brown on contact with air insoluble in excess	off-white ppt., rapidly turning brown on contact with air insoluble in excess
zinc, Zn <sup>2+</sup> (aq)	white ppt. soluble in excess	white ppt. soluble in excess

**9(b) Reactions of anions**

<i>anion</i>	<i>reaction</i>
carbonate, $\text{CO}_3^{2-}$	$\text{CO}_2$ liberated by dilute acids
chloride, $\text{Cl}^-(\text{aq})$	gives white ppt. with $\text{Ag}^+(\text{aq})$ (soluble in $\text{NH}_3(\text{aq})$ )
bromide, $\text{Br}^-(\text{aq})$	gives pale cream ppt. with $\text{Ag}^+(\text{aq})$ (partially soluble in $\text{NH}_3(\text{aq})$ )
iodide, $\text{I}^-(\text{aq})$	gives yellow ppt. with $\text{Ag}^+(\text{aq})$ (insoluble in $\text{NH}_3(\text{aq})$ )
nitrate, $\text{NO}_3^-(\text{aq})$	$\text{NH}_3$ liberated on heating with $\text{OH}^-(\text{aq})$ and <i>Al</i> foil
nitrite, $\text{NO}_2^-(\text{aq})$	$\text{NH}_3$ liberated on heating with $\text{OH}^-(\text{aq})$ and <i>Al</i> foil; $\text{NO}$ liberated by dilute acids (colourless $\text{NO} \rightarrow$ (pale) brown $\text{NO}_2$ in air)
sulfate, $\text{SO}_4^{2-}(\text{aq})$	gives white ppt. with $\text{Ba}^{2+}(\text{aq})$ (insoluble in excess dilute strong acids)
sulfite, $\text{SO}_3^{2-}(\text{aq})$	$\text{SO}_2$ liberated with dilute acids; gives white ppt. with $\text{Ba}^{2+}(\text{aq})$ (soluble in dilute strong acids)

**9(c) Tests for gases**

<i>gas</i>	<i>test and test result</i>
ammonia, $\text{NH}_3$	turns damp red litmus paper blue
carbon dioxide, $\text{CO}_2$	gives a white ppt. with limewater (ppt. dissolves with excess $\text{CO}_2$ )
chlorine, $\text{Cl}_2$	bleaches damp litmus paper
hydrogen, $\text{H}_2$	“pops” with a lighted splint
oxygen, $\text{O}_2$	relights a glowing splint
sulfur dioxide, $\text{SO}_2$	turns aqueous acidified potassium manganate(VII) from purple to colourless

**9(d) Colour of halogens**

<i>halogen</i>	<i>colour of element</i>	<i>colour in aqueous solution</i>	<i>colour in hexane</i>
chlorine, $\text{Cl}_2$	greenish yellow gas	pale yellow	pale yellow
bromine, $\text{Br}_2$	reddish brown gas / liquid	orange	orange-red
iodine, $\text{I}_2$	black solid / purple gas	brown	purple

## 10 The Periodic Table of Elements

Group																				
1	2											13	14	15	16	17	18			
		<b>Key</b>										1 H hydrogen 1.0								2 He helium 4.0
		atomic number atomic symbol name relative atomic mass												5 B boron 10.8	6 C carbon 12.0	7 N nitrogen 14.0	8 O oxygen 16.0	9 F fluorine 19.0	10 Ne neon 20.2	
3 Li lithium 6.9	4 Be beryllium 9.0											13 Al aluminium 27.0	14 Si silicon 28.1	15 P phosphorus 31.0	16 S sulfur 32.1	17 Cl chlorine 35.5	18 Ar argon 39.9			
11 Na sodium 23.0	12 Mg magnesium 24.3	3	4	5	6	7	8	9	10	11	12	31 Ga gallium 69.7	32 Ge germanium 72.6	33 As arsenic 74.9	34 Se selenium 79.0	35 Br bromine 79.9	36 Kr krypton 83.8			
19 K potassium 39.1	20 Ca calcium 40.1	21 Sc scandium 45.0	22 Ti titanium 47.9	23 V vanadium 50.9	24 Cr chromium 52.0	25 Mn manganese 54.9	26 Fe iron 55.8	27 Co cobalt 58.9	28 Ni nickel 58.7	29 Cu copper 63.5	30 Zn zinc 65.4	49 In indium 114.8	50 Sn tin 118.7	51 Sb antimony 121.8	52 Te tellurium 127.6	53 I iodine 126.9	54 Xe xenon 131.3			
37 Rb rubidium 85.5	38 Sr strontium 87.6	39 Y yttrium 88.9	40 Zr zirconium 91.2	41 Nb niobium 92.9	42 Mo molybdenum 95.9	43 Tc technetium –	44 Ru ruthenium 101.1	45 Rh rhodium 102.9	46 Pd palladium 106.4	47 Ag silver 107.9	48 Cd cadmium 112.4	81 Tl thallium 204.4	82 Pb lead 207.2	83 Bi bismuth 209.0	84 Po polonium –	85 At astatine –	86 Rn radon –			
55 Cs caesium 132.9	56 Ba barium 137.3	57–71 lanthanoids	72 Hf hafnium 178.5	73 Ta tantalum 180.9	74 W tungsten 183.8	75 Re rhenium 186.2	76 Os osmium 190.2	77 Ir iridium 192.2	78 Pt platinum 195.1	79 Au gold 197.0	80 Hg mercury 200.6	114 Fl flerovium –	116 Lv livermorium –	118 Og oganesson –	119 Uue unbinilium –	120 Uuo unbinilium –	121 Uuq unbinilium –			
87 Fr francium –	88 Ra radium –	89–103 actinoids	104 Rf rutherfordium –	105 Db dubnium –	106 Sg seaborgium –	107 Bh bohrium –	108 Hs hassium –	109 Mt meitnerium –	110 Ds darmstadtium –	111 Rg roentgenium –	112 Cn copernicium –	114 Fl flerovium –	116 Lv livermorium –	118 Og oganesson –	119 Uue unbinilium –	120 Uuo unbinilium –	121 Uuq unbinilium –			

lanthanoids	57 La lanthanum 138.9	58 Ce cerium 140.1	59 Pr praseodymium 140.9	60 Nd neodymium 144.2	61 Pm promethium –	62 Sm samarium 150.4	63 Eu europium 152.0	64 Gd gadolinium 157.3	65 Tb terbium 158.9	66 Dy dysprosium 162.5	67 Ho holmium 164.9	68 Er erbium 167.3	69 Tm thulium 168.9	70 Yb ytterbium 173.1	71 Lu lutetium 175.0
	actinoids	89 Ac actinium –	90 Th thorium 232.0	91 Pa protactinium 231.0	92 U uranium 238.0	93 Np neptunium –	94 Pu plutonium –	95 Am americium –	96 Cm curium –	97 Bk berkelium –	98 Cf californium –	99 Es einsteinium –	100 Fm fermium –	101 Md mendelevium –	102 No nobelium –