

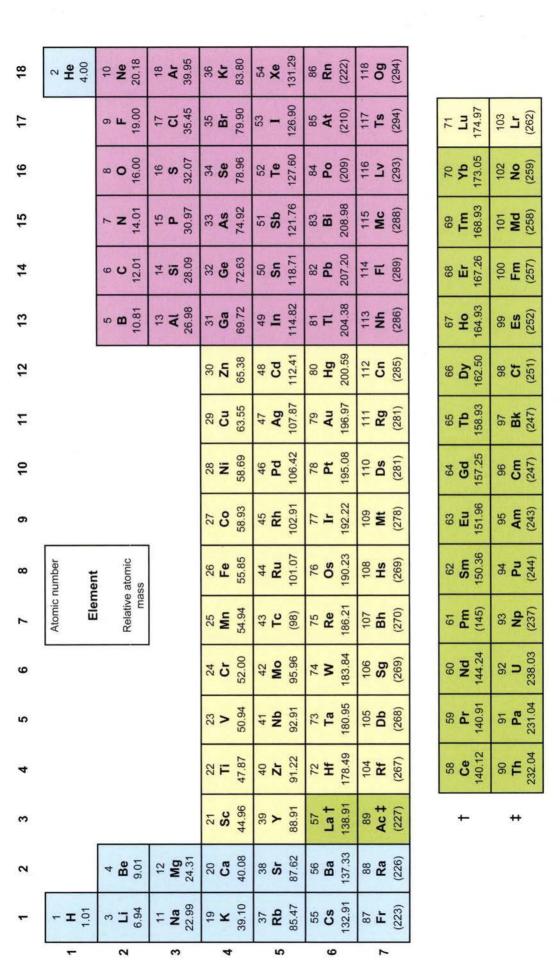
## Chemistry

for the IB Diploma Programme

? Pearson

3<sup>rd</sup> Edition

CATRIN BROWN MIKE FORD OLIVER CANNING ANDREAS ECONOMOU GARTH IRWIN



# Chemistry for the IB Diploma Programme

Catrin Brown, Mike Ford, Oliver Canning, Andreas Economou and Garth Irwin

Published by Pearson Education Limited, 80 Strand, London, WC2R ORL.

www.pearson.com/international-schools

Copies of official specifications for all Pearson Edexcel qualifications may be found on the website:

https://qualifications.pearson.com

Text © Pearson Education Limited [2023]
Development edited by Sarah Ryan
Copy edited by Katharine Godfrey Smith
Proofread by Sarah Ryan
Indexed by Georgie Bowden
Designed by Pearson Education Limited
Typeset by Tech-Set Itd
Picture research by Integra
Original illustrations © Pearson Education Limited 2023
Cover design © Pearson Education Limited 2023

The rights of Catrin Brown, Mike Ford, Oliver Canning, Andreas Economou, and Garth Irwin to be identified as the authors of this work has been asserted by them in accordance with the Copyright, Designs and Patents Act 1988.

First published 2023

25 24 23 10 9 8 7 6 5 4 3 2 1

British Library Cataloguing in Publication Data

A catalogue record for this book is available from the British Library

ISBN 978 1 29242 772 0

Copyright notice

All rights reserved. No part of this publication may be reproduced in any form or by any means (including photocopying or storing it in any medium by electronic means and whether or not transiently or incidentally to some other use of this publication) without the written permission of the copyright owner, except in accordance with the provisions of the Copyright, Designs and Patents Act 1988 or under the terms of a licence issued by the Copyright Licensing Agency, 5th Floor, Shackleton House, 4 Battlebridge Lane, London, SE1 2HX (<a href="https://www.cla.co.uk">www.cla.co.uk</a>). Applications for the copyright owner's written permission should be addressed to the publisher.

Printed in Slovakia by Neografia

#### Acknowledgements

The authors and publisher would like to thank the following individuals and organisations for permission to reproduce photographs, illustrations, and text:

Text extracts relating to the IB syllabus and assessment have been reproduced from IBO documents. Our thanks go to the International Baccalaureate for permission to reproduce its copyright.



The "In cooperation with IB" logo signifies the content in this textbook has been reviewed by the IB to ensure it fully aligns with current IB curriculum and offers high-quality guidance and support for IB teaching and learning.

 $\textbf{KEY} \ (t-top, c-center, b-bottom, l-left, r-right)$ 

#### Images:

123RF: Yhelfman 205, Glevalex 257t, Emzet70 422, Aliaksandr Mazurkevich 525r, Aleksandr Rado 582, Federico Rostagno 642; **Alamy Stock Photo**: Phil Degginger 11, 351, US Navy Photo 12, Wladimir Bulgar/Science Photo Library 21, 819l, The Picture Art Collection 31, Hank Morgan/Rainbow/RGB Ventures/SuperStock 34, The Book Worm 36, David Taylor 52l, 52r, World History Archive 88t, Sciencephotos 99, Anne Gilbert 110b, Photo Researchers/Science History Images 179, 485, Gina Rodgers 220, Science Photo Library 242, 517, 852, Steffen Trumpf 273, Oxford Science Archive/Heritage Images/The Print Collector 291, Artem Evdokimov 350t, Peter Cripps 350b, Steve Dunwell/Agefotostock 359r, Richard lawrence wade 366b, Pete Titmuss 391l, Science History Images 394r, GS UK/Greenshoots Communications 439, Kevin Schafer 484, Er Degginger 488b, Jim West 497, 561, Mark Waugh 524r, North Wind Picture Archives 548, SpaceX 572, ALFRED PASIEKA/Science Photo Library 616, Marwan Naamani/ dpa/Alamy Live News 641b, Imaginechina Limited 643, Aerial-photos.com 761tl, Jan Eickhoff/Colouria Media 816, PBH Images 818b, Zoonar/Kudrin Ruslan 842l, Molekuul 844l,864b, ScotStock 856, Akademie 865c, GL Archive 884br, Charlie Newham 893; Catrin Brown: Catrin Brown 117, 193, 214, 346bl, 683, 728, 751; Fliegende Blätter: Fliegende Blätter 883t; Getty Images: DigitalGlobe/Maxar 549, Kororokerokero/iStock/ Getty Images Plus 612t, Dave G Kelly/Moment 651, IgorSPb/iStock 824, SONGPHOL THESAKIT/Moment 906t, Imagenavi 923; Microsoft Corporation: Used by the permission from Microsoft © Microsoft Corporation 450, 579; Pearson Education: Coleman Yuen 241tr; Science Photo Library: Julien Ordan 4, Greg Dimijian 6, Sheila Terry 9, Charles D. Winters 10t, 10b, 13bl, 13br, 128, 429r, 487tl, 487b, 627, 638, 693t, 697, 722, 738cl, 754, 757, 802, Andrew Lambert Photography 13c, 16, 60, 76, 95, 101, 130, 157l, 157r, 294t, 305l, 305r, 306, 307t, 307b, 308, 310, 324, 332t, 332l, 333, 361, 365l, 365r, 490J, 588, 636, 681c, 696, 718, 736, 753, 761cr, 762, 779t, 780, 836, 837, 864, 883b, 889r, Martyn F. Chillmaid 18b, 91, 187, 241b, 290, 424, 438, 463, 487tr, 490r, 491r, 493, 581, 612b, 671, 677, 738b, 749, 779c, 842b, 886, George Bernard 19, Adam Hart-davis 20, 313t, Ian Cuming 28, Physics Dept., Imperial College 30, 56, Patrick Landmann 40,

James King-Holmes 46, Kenneth Eward/Biografx 51, 452, David A. Hardy 53, Dr Juerg Alean 55, Laguna Design 61, 162, 340, Giphotostock 111, 519l, 519r, 885, Mikkel Juul Jensen 115, Karsten Schneider 120, Oxford Science Archive 121, Edward Kinsman 122, 176, Martin Shields 127l, 127r, Spencer Sutton 133, Clive Freeman 146, 245, Alfred Pasieka 148, 201r, 211b, 294b, Millard h. Sharp 149, Susumu Nishinaga 153, 199t, Chris Knapton 155, Turtle Rock Scientific 156, 229, Science Photo Library 170, 292, 293b, 305c, 491l, 681r, 682, 738tl, Hagley Museum and Archive 174, Carlos Clarivan 188, Victor Habbick Visions 202t, Eye of Science 204, 282, Molekuul 219, European space agency/nasa, c. Gunn 254, Dr Jeremy Burgess 264, Juan Gaertner 275t, Pascal Goetgheluck 276, Steve Gschmeissner 278, 692, Tek Image 288, 390r, Dorling Kindersley 293r, 323, Noaa 313b, Equinox Graphics 325, 891b, Ramon Andrade 3dciencia 346bc, 346br, 390l, Prof. K.Seddon & Dr. T.Evans, Queen's University Belfast 369l, 369r, 370l, 370r, 703, Leonard Lessin 374, St. Bartholomew's Hospital 377, Du Cane Medical Imaging Ltd 395, Biosym Technologies, Inc 420, Turtle Rock Scientific/Science Source 429t, John Durham 435, David Hay Jones 459, 50 474, Ray Ellis 496, Ed Dlugokencky, Noaa/Gml 5011, Simon Fraser/Mauna Loa Observatory 501r, Tony Craddock 503, Nasa/ Ssai Edward Winstead 507, Volker Steger 511, Phil Degginger 516bl, 516br, Conceptual Images 516t, Crown Copyright/Health & Safety Laboratory 589, Philippe Plailly 600, US Department of Energy 606, Editorial Image 646, 687, Paul Kent, National Center for Computational Sciences, Ornl/Jorge Sofo, Penn State University 666, W K Fletcher 668, Simon Fraser 678, Trevor Clifford Photography 690, 861, Bob Gibbons 693b, Monica Schroeder 694t, Gustoimages 694b, 717, Geoff Kidd 707, Andre Seale/Vwpics 721, Saturn Stills 725, Cordelia Molloy 742, Doug Martin 761tr, Steve Horrell 769, Mikkel Juul Jensen 770, Maximilian Stock Ltd 776, Ashley Cooper 794, Nasa 821bl, Nasa's Goddard Space Flight Center 821br, Steve Allen 855, Stephen a. Skirius 865t, Clive Freeman/Biosym Technologies 873, Jean-loup Charmet 880, Library of Congress, Rare Book and Special Collections Division 884tl, Microscopy Australia, University of Sydney 889l, Microgen Images 890, Peggy Greb/Us Department of Agriculture 891t, Wladimir Bulgar 892; Shutterstock: Romix Image xiv, Production Perig 2, Studio Light and Shade 18t, Pixel-Shot 41, Artem Onoprienko 50, Huseyin Eren Obuz 88b, Susan Santa Maria 109, Rabbitmindphoto 110t, 564, Krakenimages.com 137, GlennV 165, AptTone 199b, Juancat 211t, Marcin Wos 257b, Karynav 262, Vadim Ratnikov 270r, 270l, ABCDstock 271, Exopixel 274, Larina Marina 275b, Alba\_alioth 281, Irina Flamingo 284, Leonori 358, Tatjana Baibakova 359c, LightField Studios 391r, LnP images 394l, SJ Travel Photo and Video 426l, DimaBerlin 426r, Sararwut Jaimassiri 432, Pitsanu suanlim 488t, XXLPhoto 505, Sean Pavone 524l, Shutterstock 525l, Torychemistry 557, Pattani Studio 565, Mipan 591t, Vetpathologist 591b, Gigra 624, BORDOMARS 625, Evgeniyqw 628, FoodAndPhoto 641t, Ron Zmiri 658, Albert Russ 755, ANGHI 766, Everett Collection 767, Scharfsinn 803, Alisia Luther 807, Dashtik 818t, Jason Patrick Ross 819r, Dimbar76 821cr, Love Employee 822, Jitchanamont 835, StudioMolekuul 844r, Milatas 929; The Royal Swedish Academy of Sciences: @Airi Iliste/The Royal Swedish Academy of Sciences 2011:

#### Text:

Amedeo Avogadro: Amedeo Avogadro 553; American Association of Physics Teachers: Richard Feynman (1969) The Physics Teacher Vol. 7, issue 6, 1969, pp. 313-320, @ American Association of Physics Teachers 29, 884; Eldredge & brother: Houston, Edwin James. The Elements of Chemistry: For the Use of Schools, Academies, and Colleges. United States: Eldredge & brother, 1883. 114; Hachette Book Group: Feynman, R. P., Sands, M., Leighton, R. B. (2011). The Feynman Lectures on Physics Vol. I: The New Millennium Edition: Mainly Mechanics, Radiation, and Heat. United Kingdom: Basic Books. 423; HarperCollins: Heisenberg, W. (1962). Physics and philosophy; the revolution in modern science. United Kingdom: Harper & Row. 886; Hebrew University of Jerusalem: Einstein, Albert, 1879-1955. (1950). Out of My Later Years. New York: Philosophical Library 894; Henri Poincaré: Henri Poincaré, 1854-1912. 289; International Baccalaureate Organization: © International Baccalaureate Organization, 2005-2022 86; John Wiley & Sons, Inc: Cheng, X., Corey, E. J. (1989). The Logic of Chemical Synthesis. United Kingdom: Wiley. 889; Lindau Nobel Laureate Meetings: Kroto S W. 2014 May 12. Sir Harold Kroto (2011) - Créativité Sans Frontières <a href="https://www.mediatheque.lindau.nobel.org/">https://www.mediatheque.lindau.nobel.org/</a> videos/31303/creeativitee-sans-frontires-2011/meeting-2011>. Accessed 2022 Aug 2. 879; Louis Pasteur: Louis Pasteur 885; MIT Press: Feynman, R. P. (1967). The Character of Physical Law. United Kingdom: MIT Press. 885; NASA: NASA 501; Nature Publishing Group: Molina, M., Rowland, F. Stratospheric sink for chlorofluoromethanes: chlorine atom-catalysed destruction of ozone. Nature 249, 810–812 (1974). https://doi.org/10.1038/249810a0 823; Oxford University Press: Warner, D. o. C. J., Anastas, I. C. B. P., Warner, J. C., Anastas, P. T. (1998). Green Chemistry: theory and practice. United Kingdom: Oxford University Press. 872; Penguin Random House: Bronowski, J. (2011). The Ascent of Man. United Kingdom: Ebury Publishing. 879; Philosophical Library: Planck, M., Laue, M. v. (1949). Scientific Autobiography: And Other Papers. United States: Philosophical Library. 884; Random House: Bronowski, J. (2011). The ascent of man. Random House. 31; Richard L. Apodaca: Richard L. Apodaca 904; Samuel Taylor Coleridge: Taylor Coleridge, Samuel, The Rime of the Ancient Mariner, 1834. 166; The George Washington University: The George Washington University 904; Werner Heisenberg: Quote from Werner Heisenberg 31.



MIX
Paper from
responsible sources
FSC™ C128612

## **Contents**

Syllabus roadmap	vii
Authors' introduction to the third edition	viii
Introduction to 'Skills in the study of chemistry'	xiv

#### Structure

All the second s	
Structure 1 Models of the particulate nature of matter	4
Structure 1.1 Introduction to the particulate nature of matter	6
Structure 1.1.1 - Elements, compounds and mixtures	7
Structure 1.1.2 - The kinetic molecular theory	14
Structure 1.1.3 - Kinetic energy and temperature	20
Structure 1.2 The nuclear atom	28
Structure 1.2.1 – The atomic model	29
Structure 1.2.2 – Isotopes	39
Structure 1.2.3 – Mass spectra HL	42
Structure 1.3 Electron configurations	50
Structure 1.3.1 and 1.3.2 - Emission spectra	51
Structure 1.3.3, 1.3.4 and 1.3.5 - Electron configuration	58
Structure 1.3.6 and 1.3.7 – Ionization energies HL	73
Structure 1.4 Counting particles by mass: The mole	88
Structure 1.4.1 - The mole as the unit of amount	89
Structure 1.4.2 - Relative atomic mass and relative formula mass	93
Structure 1.4.3 – Molar mass	96
Structure 1.4.4 - Empirical and molecular formulas	99
Structure 1.4.5 – Molar concentration	107
Structure 1.4.6 – Avogadro's Law	113
Structure 1.5 Ideal gases	120
Structure 1.5.1 – The ideal gas model	121
Structure 1.5.2 - Real gases	124
Structure 1.5.3 and 1.5.4 – The ideal gas laws	126
Structure 2 Models of bonding and structure	146
Structure 2.1 The ionic model	148
Structure 2.1.1 and 2.1.2 - The ionic bond	150
Structure 2.1.3 - Ionic structures and properties	161
Structure 2.2 The covalent model	174
Structure 2.2.1 - Covalent bonding, the octet rule and Lewis formulas	176
Structure 2.2.2 - Single, double and triple covalent bonds	182
Structure 2.2.3 – Coordination bonds	186
Structure 2.2.4 - The Valence Shell Electron Pair Repulsion (VSEPR) model	188
Structure 2.2.5 – Bond polarity	193
Structure 2.2.6 - Molecular polarity	196
Structure 2.2.7 - Covalent network structures	198
Structure 2.2.8 and 2.2.9 – Intermolecular forces	206
Structure 2.2.10 - Intermolecular forces and chromatography	216
Structure 2.2.11 – Resonance structures HL	219
Structure 2.2.12 - Benzene HL	222
Structure 2.2.13 - Molecules with an expanded octet HL	227

Structure 2.2.14 – Formal charge  Structure 2.2.15 – Sigma and pi bonds  Structure 2.2.16 – Hybridization  HL  Structure 2.3 The metallic model  Structure 2.3.1 and 2.3.2 – The metallic bond  Structure 2.3.3 – Transition elements  HL  Structure 2.4 From models to materials  Structure 2.4.1 – The bonding triangle  Structure 2.4.2 – Application of the bonding triangle  Structure 2.4.3 – Alloys  Structure 2.4.4 – Polymers	233 237 239 <b>254</b> 255 260 <b>264</b> 265 268 271 273
Structure 2.4.5 – Addition polymers Structure 2.4.6 – Condensation polymers  HL	276 280
Structure 3 Classification of matter	288
Structure 3.1 The periodic table: Classification of elements  Structure 3.1.1 – Periods, groups and blocks  Structure 3.1.2 – Periodicity and electron configuration  Structure 3.1.3 – Periodicity in properties of elements  Structure 3.1.4 – Periodicity in reactivity  Structure 3.1.5 – Metal and non-metal oxides  Structure 3.1.6 – Oxidation states  Structure 3.1.7 – Discontinuities in patterns of first ionization energy  Structure 3.1.8 – Characteristic properties of transition elements  Structure 3.1.9 – Variable oxidation states  Structure 3.1.10 – Coloured complexes  HL  Structure 3.2 Functional groups: Classification of organic compounds  Structure 3.2.1 – Structural representations of organic compounds  Structure 3.2.2 – Functional groups and classes of compounds  Structure 3.2.3 and 3.2.4 – Homologous series  Structure 3.2.5 – IUPAC nomenclature  Structure 3.2.6 – Structural isomers  Structure 3.2.7 – Stereoisomers  HL  Structure 3.2.9 – Infrared spectroscopy  HL  Structure 3.2.10 and 3.2.11 – Nuclear magnetic resonance spectroscopy  Structure 3.2.12 – Combining analytical techniques  HL  Reactivity	290 291 295 297 304 309 315 320 321 326 328 340 342 348 352 355 361 368 380 385 HL 393 405
Reactivity 1 What drives chemical reactions?	422
Reactivity 1.1 Measuring enthalpy changes  Reactivity 1.1.1 – Chemical reactions involve heat transfers  Reactivity 1.1.2 – Endothermic and exothermic reactions  Reactivity 1.1.3 – Energetic stability and the direction of change  Reactivity 1.1.4 – Measuring enthalpy changes  Reactivity 1.2 Energy cycles in reactions  Reactivity 1.2.1 – Bond enthalpy  Reactivity 1.2.2 – Hess's law  Reactivity 1.2.3 – Standard enthalpy changes of combustion and formation	424 425 428 430 434 452 454 460

Reactivity 1.2.4 – Calculating enthalpy changes HL  Reactivity 1.2.5 – Born–Haber cycles HL	467 472
Reactivity 1.3 Energy from fuels  Reactivity 1.3.1 – Combustion reactions  Reactivity 1.3.2 – Incomplete combustion of organic compounds  Reactivity 1.3.3 – Fossil fuels  Reactivity 1.3.4 – Biofuels  Reactivity 1.3.5 – Fuel cells	484 486 491 494 504
Reactivity 1.4 Entropy and spontaneity Reactivity 1.4.1 – Entropy Reactivity 1.4.2 – Gibbs energy Reactivity 1.4.3 – $\Delta G$ and spontaneity Reactivity 1.4.4 – $\Delta G$ and equilibrium	516 518 523 531 534
Reactivity 2 How much, how fast and how far?	546
Reactivity 2.1 How much? The amount of chemical change Reactivity 2.1.1 – Chemical equations Reactivity 2.1.2 – Using mole ratios in equations Reactivity 2.1.3 – The limiting reactant and theoretical yield Reactivity 2.1.4 – Percentage yield Reactivity 2.1.5 – Atom economy  Reactivity 2.2 How fast? The rate of chemical change Reactivity 2.2.1 – Rate of reaction Reactivity 2.2.2 – Collision theory Reactivity 2.2.3, 2.2.4 and 2.2.5 – Factors that influence the rate of reaction Reactivity 2.2.6, 2.2.7 and 2.2.8 – Reaction mechanisms	548 549 553 563 566 568 574 575 584 588 596
Reactivity 2.2.9 and 2.2.10 – Rate equations HL  Reactivity 2.2.11 – The rate constant, k HL  Reactivity 2.2.12 and 2.2.13 – The Arrhenius equation HL	600 612 613
Reactivity 2.3 How far? The extent of chemical change Reactivity 2.3.1 – Dynamic equilibrium Reactivity 2.3.2 and 2.3.3 – Equilibrium law Reactivity 2.3.4 – Le Châtelier's principle Reactivity 2.3.5 – The reaction quotient, Q HL Reactivity 2.3.6 – Quantifying the composition of equilibrium HL Reactivity 2.3.7 – Measuring the position of equilibrium HL	626 627 632 637 648 650 657
Reactivity 3 What are the mechanisms of chemical change?	668
Reactivity 3.1 Proton transfer reactions  Reactivity 3.1.1 and 3.1.2. – Brønsted-Lowry acids and bases Reactivity 3.1.3 – Amphiprotic species Reactivity 3.1.4 – The pH scale Reactivity 3.1.5 – The ion product constant of water Reactivity 3.1.6 – Strong and weak acids and bases Reactivity 3.1.7 – Neutralization reactions Reactivity 3.1.8 – pH curves Reactivity 3.1.9 – The pOH scale  HL  Reactivity 3.1.10 and 3.1.11 – Acid and base dissociation constants  HL  Reactivity 3.1.12 – pH of salt solutions	670 671 677 680 685 688 693 697 701 704 712

A PROPERTY OF THE

Reactivity 3.1.13 – pH curves revisited HL	715
Reactivity 3.1.14 and 3.1.15 - Acid-base indicators HL	719
Reactivity 3.1.16 - Buffer solutions HL	722
Reactivity 3.1.17 – Buffer composition and pH HL	726
Reactivity 3.2 Electron transfer reactions	738
Reactivity 3.2.1 - Redox reactions	739
Reactivity 3.2.2 - Half-equations	748
Reactivity 3.2.3 - Trends in ease of oxidation and reduction of elements	755
Reactivity 3.2.4 - Oxidation of metals by acids	759
Reactivity 3.2.5 - Comparing voltaic and electrochemical cells	761 762
Reactivity 3.2.6 - Primary (voltaic) cells	770
Reactivity 3.2.7 - Secondary (rechargeable) cells  Reactivity 3.2.8 - Electrolytic cells	774
Reactivity 3.2.9 – Oxidation of functional groups in organic compounds	779
Reactivity 3.2.10 - Reduction of functional groups in organic compounds	785
Reactivity 3.2.11 - Reduction of unsaturated compounds	787
Reactivity 3.2.12 - The standard hydrogen electrode HL	789
Reactivity 3.2.13 - Standard electrode potentials HL	794
Reactivity 3.2.14 - Electrode potentials and Gibbs energy changes HL	799
Reactivity 3.2.15 - Electrolysis of aqueous solutions HL	802
Reactivity 3.2.16 - Electroplating HL	808
Reactivity 3.3 Electron sharing reactions	818
Reactivity 3.3.1 - Radicals	819
Reactivity 3.3.2 - Homolytic fission	822
Reactivity 3.3.3 - Radical substitution reactions of alkanes	825
Reactivity 3.4 Electron-pair sharing reactions	830
Reactivity 3.4.1 – Nucleophiles	831 832
Reactivity 3.4.2 – Nucleophilic substitution reactions Reactivity 3.4.3 – Heterolytic fission	834
Reactivity 3.4.4 – Electrophiles	836
Reactivity 3.4.5 – Electrophilic addition of alkenes	837
Reactivity 3.4.6 and 3.4.7 – Lewis acids and Lewis bases	841
Reactivity 3.4.8 - Complex ions HL	843
Reactivity 3.4.9 and 3.4.10 - S <sub>N</sub> 1 and S <sub>N</sub> 2 nucleophilic substitution mechanisms HL	847
Reactivity 3.4.11 - Electrophilic substitution mechanism HL	854
Reactivity 3.4.12 - Addition of hydrogen halides to asymmetrical alkenes HL	860
Reactivity 3.4.13 - Electrophilic substitution of benzene HL	863
Green Chemistry	874
Theory of Knowledge in chemistry	878
Internal Assessment	897
Skills in the study of chemistry	907
Strategies for success	918
Extended Essay	922
Index	930

### Syllabus roadmap

The aim of the syllabus is to integrate concepts, topic content and the Nature of Science through inquiry. Students and teachers are encouraged to personalize their approach to the syllabus according to their circumstances and interests.

	Skills in the stu	dy of chemistry		
Structure Structure refers to the nature of matter from simple to more complex forms		Reactivity  Reactivity refers to how and why  chemical reactions occur		
Struct	ure determines reactivity, v	which in turn tra	nsforms structure	
Structure 1  Models of the particulate nature of	Structure 1.1 – Introduction to the particulate nature of matter	Reactivity 1 What drives chemical reactions?	Reactivity 1.1 – Measuring enthalpy changes	
matter	Structure 1.2 – The nuclear atom	reactions:	Reactivity 1.2 – Energy cycles in reactions	
	Structure 1.3 – Electron configurations		Reactivity 1.3 – Energy from fuels	
	Structure 1.4 – Counting particles by mass: The mole		Reactivity 1.4 – Entropy and spontaneity (Additional higher level	
	Structure 1.5 – Ideal gases			
Structure 2 Models of bonding and	Models of model How much,	Reactivity 2.1 – How much? The amount of chemical change		
structure	Structure 2.2 – The covalent model	how fast and how far?	Reactivity 2.2 – How fast? The rate of chemical change	
	Structure 2.3 – The metallic model		Reactivity 2.3 – How far? The extent of chemical	
100	Structure 2.4 – From models to materials		change	
Structure 3 Classification of matter	Structure 3.1 – The periodic table: Classification of elements	Reactivity 3 What are the mechanisms	Reactivity 3.1 – Proton transfer reactions	
of matter	Structure 3.2 – Functional groups: Classification of organic compounds	of chemical change?	Reactivity 3.2 – Electron transfer reactions	
		7	Reactivity 3.3 – Electron sharing reactions	
			Reactivity 3.4 – Electron- pair sharing reactions	

#### Authors' introduction to the third edition

Welcome to your study of IB Diploma Programme chemistry. This is the third edition of Pearson's highly successful Higher Level (HL) chemistry book, first published in 2009. It has been completely rewritten to match the specifications of the new IB chemistry curriculum for first assessments in 2025 and gives thorough coverage of the entire course content. While there is much new and updated material, we have kept and refined the features that made the previous editions so successful. We are delighted to share our enthusiasm for learning chemistry in the IB programme with you!

#### Content

This book covers the entire HL course. It is divided into the two main themes, **Structure** and **Reactivity**, which in turn are divided into six topics, Structure 1–3 and Reactivity 1–3. Separate chapters cover each sub-topic within each topic. For example, the Structure 1.1 chapter deals with 'Introduction to the particulate nature of matter'.

The syllabus is presented as a sequence of numbered Understandings, which are shown as three-part boxes. We have given the relevant Understanding from the subject guide at the start of each section within a chapter under a brief header. The Table of Contents shows the full list of these Understanding headers, so you can see what is covered in each chapter.

For example:

Syllabus header

## Structure 1.4.2 – Relative atomic mass and relative formula mass

Outcomes of Content learning and teaching statement Structure 1.4.2 - Masses of atoms are compared on a scale relative to 12C and are expressed as relative atomic mass (A,) and relative formula mass (M,) Determine relative formula masses  $M_r$  from relative atomic masses  $A_r$ . Structure 3.1 - Atoms increase in mass as Relative atomic mass and relative formula their position descends in the periodic table. mass have no units. What properties might be related to this The values of relative atomic masses given to trend? two decimal places in the data booklet should be used in calculations. Guidance on Linking the coverage Questions expected

The Understandings are presented in the same sequence as in the subject guide, so that common Standard Level (SL) and HL content is covered first, followed by HL only material. The transition from SL to HL content is shown by icons as follows.

#### HL

Individual icons to identify HL material such as exercises and practice questions can also be found throughout the book.

The text covers the course content using plain language, with all scientific terms explained and shown in bold as they are first introduced. It follows SI notation, and IUPAC nomenclature and definitions throughout. We have been careful also to apply the same terminology you will see in IB examinations in all worked examples and questions.

#### Conceptual approach

The syllabus emphasizes a conceptual approach, where the two main themes of chemistry, Structure and Reactivity, are shown to be interdependent. There is no suggested sequence for the coverage of the topics, and many different routes through the syllabus are possible. What is important though, is that the relationships between the different topics are recognized, which leads to an increasing depth of understanding.

There are two features, **Guiding Questions** and **Linking Questions**, which are incorporated into each topic in the syllabus. These are designed to help promote the conceptual approach, and we have emphasized them in the text as follows.

#### **Guiding Question**



#### **Guiding Question**

How do the nuclei of atoms differ?

Each chapter starts with the Guiding Question for the sub-topic from the IB chemistry subject guide. This is followed by a brief consideration of the question itself, which sets the context for the topic and how it relates to your previous knowledge. It is expected that by the end of the chapter you will be able to answer the Guiding Question more fully.

#### Guiding Question revisited



#### **Guiding Question revisited**

How do we quantify matter on the atomic scale?

At the end of each chapter, the Guiding Question is revisited, and can now be answered with significantly more detail and understanding. It is presented as a bulleted list of the material covered, that may help serve as a checklist of your learning at the end of each chapter. The Guiding Question revisited bulleted lists are available as downloadable PDFs from the eBook to help you with revision.

Reactivity 3.2 – How can oxidation states be used to analyze redox reactions?



#### **Linking Questions**

Linking Questions are given in many of the Understandings. Linking Questions have a number which indicates a link from the current chapter to another sub-topic, to Tools or to the Nature of Science (NOS). These questions are designed as prompts to help you build a grasp of unifying concepts and to stimulate further learning. Linking Question boxes can be found in the margin next to the content they link to (see example on the left).

By their very nature, the Linking Questions make reference to different parts of the course, some of which you may not have studied yet. As the questions can be asked in either direction, you may choose to consider them as part of the study of either or both of the linked topics. You will again find that you are able to answer the question more fully as your knowledge and understanding increase.

The Linking Questions are designed to lead to a thoughtful response. For this reason, we have given brief answers alongside the questions in the text, and hope these stimulate further consideration of the question.

#### The Nature of Science

Throughout the course you are encouraged to think about the nature of scientific knowledge and the scientific process as it applies to chemistry. Examples are given of the evolution of chemical theories as new information is gained, the use of models to conceptualize our understanding, and the ways in which experimental work is enhanced by modern technologies. Ethical considerations, environmental impacts, the importance of objectivity, and the responsibilities regarding scientists' code of conduct are also considered here. The emphasis is not on learning any of these examples, but on appreciating the broader conceptual themes in context. We have included several NOS examples in each chapter, and hope you will come up with your own as you keep these ideas at the forefront of your learning.

#### Key to feature boxes

You will find different coloured feature boxes interspersed throughout each chapter. These are used to enhance your learning and how it applies to real world examples, as explained below.



#### **Nature of Science**

As mentioned this is an overarching theme in the course. Throughout the book you will find NOS themes and questions emerging across different topics. We hope they help you to develop your skills in scientific literacy.



#### **Nature of Science**

Magnetism was used in navigation long before it was explained scientifically. Historically, technology emerged before science. Materials were often used practically long before there was an understanding of why they possessed their properties.

In today's world, the reverse is often the case, with scientific understanding leading to technological developments, which in turn drive further developments in scientific ideas.



#### Global context

The impact of the study of chemistry is global, and includes environmental, political and socio-economic considerations. Examples of this are given to help you to see the importance of chemistry in an international context. These examples also illustrate some of the innovative and cutting-edge aspects of research in chemistry.



A different unit of concentration is known as **ppm**, parts per million. It denotes one part per 10<sup>6</sup> parts of the whole solution, and is useful in describing very low concentrations. This unit is widely used in reporting levels of pollutants in air, water, soil and food. For example, in the USA the FDA has set a maximum permissible level of 1 part of methylmercury in a million parts of seafood (1 ppm).



#### Skills in the study of chemistry

These boxes indicate links to the Skills section of the course, including ideas for lab work and experiments that will support your learning and help you prepare for the Internal Assessment. These link to further resources in the eBook (look out for the grey icon).



#### Theory of Knowledge

These questions, which are mostly from the Theory of Knowledge (TOK) guide, stimulate thought and consideration of knowledge issues as they arise in context. The questions are open-ended and will help trigger critical thinking and discussion.



#### **Key fact**

These key facts are drawn out of the main text and highlighted in bold. These boxes will help you to identify the core learning points within each section. They also act as a quick summary for review.



#### Hint for success

These give hints on how to approach questions, and suggest approaches that examiners like to see. They also identify common pitfalls in understanding, and omissions made in answering questions.

#### Challenge yourself

These boxes contain probing questions that encourage you to think about the topic in more depth, and may take you beyond the syllabus content. They are designed to be challenging and to make you think.

#### Challenge yourself

The components of a mixture can usually be separated by physical means.
 What might be the challenges of trying to separate the metals from an alloy?



Using spectra to confirm the structure of a compound. Full details of how to carry out this experiment with a worksheet are available in the eBook.



How might developments in scientific knowledge trigger political controversies or controversies in other areas of knowledge?



At equilibrium the rate of the forward reaction is equal to the rate of the backward reaction.



Note the definition of bond enthalpy indicates that all the species have to be in the gaseous state.



#### Interesting fact

These give background information that will add to your wider knowledge of the topic and make links with other topics and subjects. Aspects such as historic notes on the life of scientists and origins of names are included here.



Gilbert Lewis (1875–1946), responsible for the electron-pair theory of the covalent bond, was nominated 41 times for the Nobel Prize in Chemistry without winning. In 1946, he was found dead in his laboratory where he had been working with the toxic compound hydrogen cyanide.

Towards the end of the book, there are chapters on Green Chemistry, TOK as it relates to chemistry, the Internal Assessment, the Extended Essay and Strategies for success in IB chemistry.

#### Questions

There are three types of question in this book.

#### Worked examples with solutions

Worked examples appear at intervals in the text and are used to illustrate the concepts covered.

They are followed by the solution, which shows the thinking and the steps used in solving the problem.

#### Worked example

Identify the species with 19 protons, 20 neutrons and 18 electrons.

#### Solution

- the number of protons tells us the atomic number, Z = 19, and so the element is potassium, K
- the mass number = p + n = 19 + 20 = 39:  $_{19}^{39}$ K
- the charge = p e = 19 18 = +1 as there is one extra proton:  $^{39}_{19}K^+$

#### 2. Exercises

These questions are found throughout the text, usually at the end of each Understanding. They allow you to apply your knowledge and test your understanding of what you have just been reading. The answers to these, together with worked solutions, are accessed via icons on the first page of each chapter in the eBook. Exercise answers can also be found at the back of the eBook.

#### **Exercise**

**Q1.** Explain why the relative atomic mass of tellurium is greater than the relative atomic mass of iodine, even though iodine has a greater atomic number.

#### 3. Practice questions

These questions are found at the end of each chapter. They are mostly taken from previous years' IB exam papers. The markschemes used by examiners when marking these questions are accessed via icons in the eBook on the first page of each chapter. Questions which are based on the Understandings for SL are given first, followed by questions which include HL only material. HL questions are clearly marked.

#### **Practice questions**

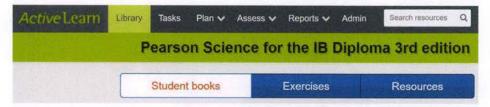
7. HL The transition element gold, Au, is used in electrical circuits due to its high electrical conductivity.

Explain why transition elements are generally better electrical conductors than s and p block metals. (2)

(Total 2 marks)

#### eBook

In your eBook you will find more information on the Skills section of the course including detailed suggestions for lab work. You will also find links to videos. In addition, there are auto-marked quizzes in the Exercises tab of your eBook account (see screenshot below).



We hope you enjoy your study of IB chemistry from this textbook.

Catrin Brown, Mike Ford, Oliver Canning, Andreas Economou and Garth Irwin

#### Introduction to skills in the study of chemistry

"I hear and I forget, I see and I remember, I do and I understand"

Chemistry is an experimental science and its progress continues to be based on the scientific method. The study of chemistry in the IB programme reflects this in the emphasis it places on laboratory work. This approach will help you to understand concepts, learn some practical skills and give you opportunities to explore further through investigations. It is also often the best part about studying chemistry!

The syllabus roadmap on page vii has 'Skills in the study of chemistry' at the top. This unit is a summary of experimental skills and techniques that should be experienced during the course, including the application of technology and mathematics. It is not intended that these 'Tools' are covered as separate content, but should be integrated into the study of all topics. The 'Skills in the study of chemistry' chapter towards the back of this book includes tables that summarize the details of this unit with references to where in the syllabus content the Tools may be suitably included. There are also many links to experimental work and resources available in the ebook.

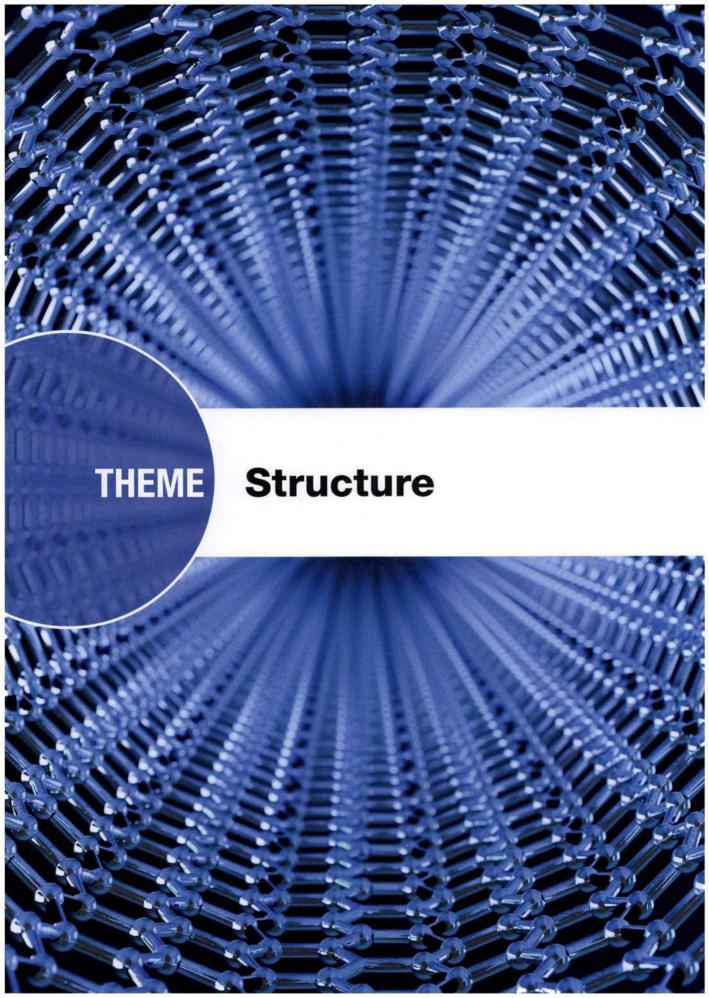


#### **Nature of Science**

The scientific method consists of systematic observation, the formulation and testing of hypotheses, and the collection of data for analysis and evaluation. Central to this process is a consideration of the limits of the usefulness of the data obtained. The interpretation of results must take into account the precision and accuracy of the measurements, the amount and limitations of data collected and the reproducibility of the results. Effective communication of the results must include this information.

The choice of apparatus for measurement in the laboratory determines the precision of the data collected. Here a pipette is used to deliver a single drop of liquid.





▼ View of graphene with 3D rendering. Graphene is a relatively modern structure, usually composed of a single layer of carbon atoms. It is considered to be the world's thinnest, strongest and most conductive material, of both electricity and heat. Understanding the structure of graphene has helped develop its applications in many fields such as energy generation, sensors, medical equipment and composite materials.

#### Structure

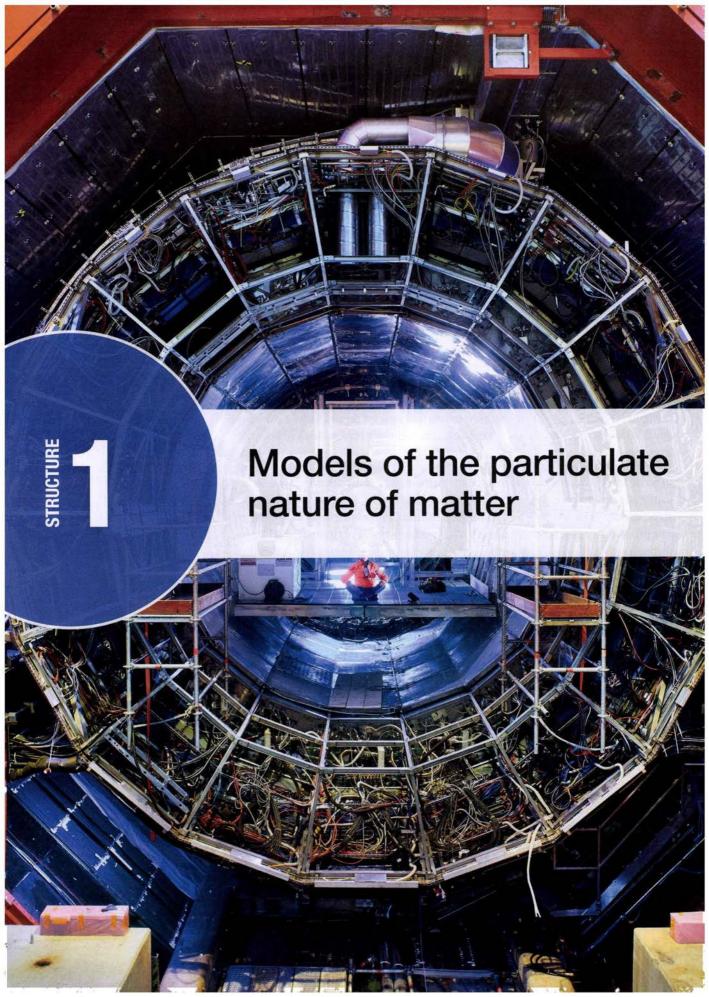
Structure refers to the nature of matter. Chemists seek to understand the way in which fundamental particles, the building blocks of all chemical structure, combine to form every chemical structure that exists – from single atoms to the most complex compounds. An understanding of structure leads to the ability to explain and predict chemical properties, as studied in our second theme, *Reactivity*.

A major challenge in the study of structure is that the fundamental particles are too small for us to observe directly. Even the most advanced technology gives us only limited information on the nature and behaviour of these particles. As a result, since the early days of chemical exploration, scientists have used models to help explain and predict the nature of matter. Over time, these models have developed and changed in the light of increasingly detailed observations and new evidence. As we explore the applications of these models, we must also consider their limitations and how they may continue to evolve.

In Structure 1 we consider evidence for the particulate nature of matter. From an exploration of the properties of sub-atomic particles, we build an understanding of the structure of atoms and how they characterize the unique properties of each element. The problem of scale, how we quantify what we cannot observe directly, is addressed through an introduction to the mole as the unit of amount in chemistry. A detailed study of electron configurations helps us to recognize why atoms of different elements differ in their tendency to attract electrons. This leads to descriptions of the models of different chemical bonds – ionic, covalent and metallic – in Structure 2. The organization of elements in the periodic table, as studied in Structure 3, suggests patterns in elements' properties. This gives predictive power to the types of bonds that they will form. As atoms associate through bond formation, the products have different properties, giving rise to an infinite variety of structures. Chemists have developed clear terminology to communicate about chemical structure, and in Structure 3 we are introduced to the IUPAC (International Union of Pure and Applied Chemistry) system of nomenclature, and learn how compounds are given unambiguous and internationally agreed names.

Our understanding of structure has developed alongside advances in technology and has led to many innovations in materials science. Many modern materials, such as breathable fabrics and biodegradable plastics, and compounds such as therapeutic drugs, are designed for specific functions. You need look no further than your smart phone or clothing to realize how much our lives are influenced by these products. And yet, despite their extraordinary variety and complexity, every chemical structure is based on associations between a relatively small number of different atoms.

Structure determines reactivity, which in turn transforms structure.



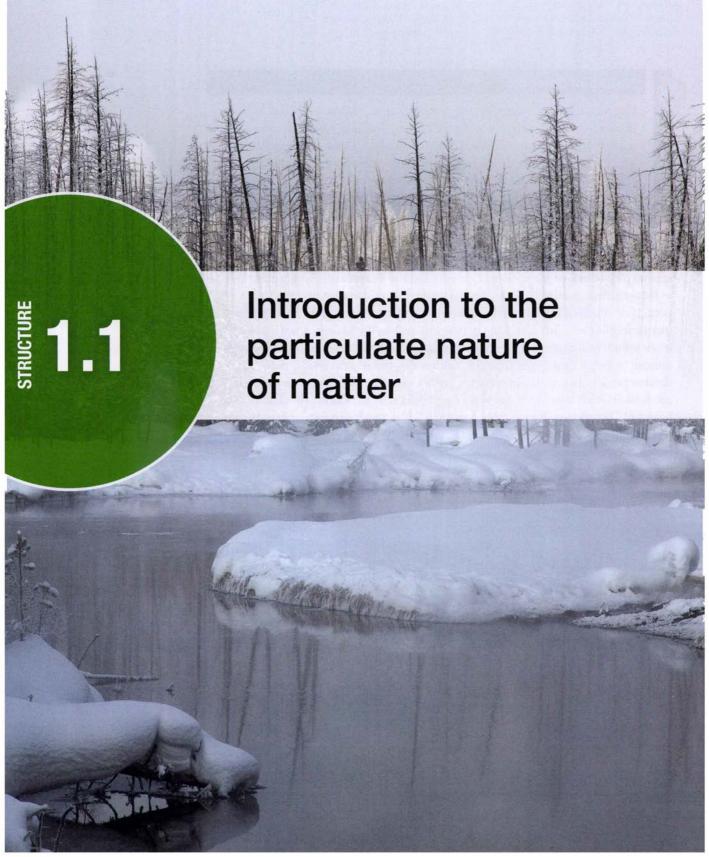
■ Inside the empty skeleton of the ALICE detector at CERN (the European particle physics laboratory) near Geneva, Switzerland. ALICE (A Large Ion Collider Experiment) is a detector built around the Large Hadron Collider (LHC). The LHC is the world's largest and most powerful particle collider. Beams of ions are accelerated to collide head-on. The collision energy creates new particles that decay into other particles. The LHC energies have allowed the study of exotic materials like quark-gluon plasma, a form of quark matter. CERN announced the Higgs boson discovery on 4 July 2012.



#### **Nature of Science**

Progress in science often follows technological developments. The discovery of the Higgs boson was due to the use of particle accelerators, detectors and sophisticated computers. Such technological advances are only possible with international collaboration between scientists. Scientists communicate and collaborate throughout the world. CERN is run by over 20 member states, and many non-European countries are involved in different ways.

One of the earliest questions philosophers asked concerned the divisibility of matter. Could a piece of material be divided again and again continually into smaller and smaller pieces as Aristotle proposed, or would a limit be reached, a single particle, as Democritus argued? The latter idea has generally stood the test of time. This particulate model of matter enables us to explain many aspects of the behaviour of matter despite these particles being not directly visible. We have no proof that matter is not infinitely divisible, but we do have evidence that it becomes increasingly more difficult to divide it into smaller pieces. The limiting factor is the energy required to divide a particle. Experimental evidence for this has come from work with particle accelerators, such as at CERN, referenced in the photo at the start of the chapter, where beams of ions undergo high-energy collisions, which produce new particles. We are still learning about how the world is made up of fundamental particles. The Higgs boson, a key elementary particle, was only discovered as recently as 2012 although its existence had been predicted by scientific models in 1964.



Yellowstone National Park, Wyoming, USA, with mist rising on a cold winter morning from waters warmed by thermal springs. Matter can exist in the solid, liquid and gaseous states. The difference in physical properties of the three states is explained by kinetic molecular theory.





#### **Guiding Question**

How can we model the particulate nature of matter?

All things are made from atoms. This is one of the most important ideas that the human race has learned about the universe. Atoms are everywhere and they make up everything. You are surrounded by atoms – they make up the foods you eat, the liquids you drink and the fragrances you smell. Atoms make up you! To understand the world and how it changes, you need to understand atoms.

Atoms are the smallest particle of an element and so are fundamental to chemistry. As they are too small ever to be seen directly by a human eye, scientists have developed a series of models to explain the physical and chemical properties of materials. We can understand many aspects of the world simply by considering how these particles move and interact with each other. This particulate model of matter, which includes atoms, molecules and ions, provides a very strong foundation for our chemical understanding and is a good place to start our explorations.



#### **Nature of Science**

Scientists construct models as artificial representations of natural phenomena. All models have limitations that need to be considered in their application.

## Structure 1.1.1 – Elements, compounds and mixtures

Structure 1.1.1 – Elements are the primary constituents of matter, which cannot be chemically broken down into simpler substances.

Compounds consist of atoms of different elements chemically bonded together in a fixed ratio.

Mixtures contain more than one element or compound in no fixed ratio, which are not chemically bonded and so can be separated by physical methods.

Distinguish between the properties of elements, compounds and mixtures.

Solvation, filtration, recrystallization, evaporation, distillation and paper chromatography should be covered.

The differences between homogeneous and heterogeneous mixtures should be understood.

Tool 1 – What factors are considered in choosing a method to separate the components of a mixture?

Tool 1 – How can the products of a reaction be purified?

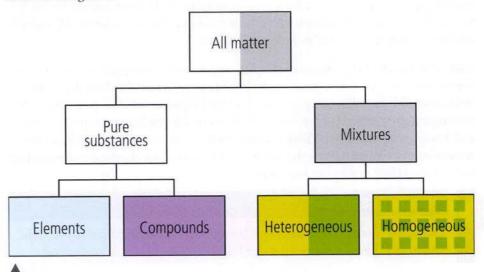
Structure 2.2 – How do intermolecular forces influence the type of mixture that forms between two substances?

Structure 2.3 – Why are alloys generally considered to be mixtures, even though they often contain metallic bonding?

## Matter can be classified into elements, compounds and mixtures

#### Classifying matter

Matter is present in an infinite number of different forms. The first step to understanding the chemistry of all these substances is an effective classification system. We start with a basic chemical distinction: some matter is made of pure substances, and some is made from mixtures. The chapter will follow the classification outlined in Figure 1.



**S1.1 Figure 1** Matter can be classified into pure substances and mixtures. Pure substances can be elements or compounds. Mixtures can be homogeneous or heterogeneous.

## Elements are the primary constituents of matter, which cannot be chemically broken down into simpler substances

All languages are based on an alphabet of a limited number of characters. The 26 letters of the English alphabet, for example, can be combined in different ways to form the estimated 600 000 words in the language. In a similar way, the substances known as chemical elements can combine to form the material of our universe. Elements are the primary constituents of matter. They cannot be chemically broken down into simpler substances. The near infinite number of different chemical substances in our world are made from only about 100 known elements.

In Structure 2.1 we will learn about atomic structure, and how each element is made up of a particular type of atom. Atoms of the same element all have the same number of protons in the atomic nucleus and the same number of electrons. The distinct makeup of an element's atoms gives each element its individual properties. An atom is the smallest particle of an element to show the characteristic properties of that element.

An element is a pure chemical substance composed of atoms with the same number of protons in the atomic nucleus.

An atom is the smallest particle of an element to show the characteristic properties of that element.



a

Œ

Gallat of Iron 10

ret of Iron OC

VO

OT)

The number of elements is open to change as new ones can be invented or discovered. It takes time for an element's existence to be confirmed by IUPAC so in the interim, a provisional systematic three-letter symbol is used. Latin abbreviations represent the atomic number. The letters u(un) = 1, b(bi) = 2, t(tri) = 3and so on are used. The element of atomic number 118 now known as oganesson (Og) was previously known as ununoctium or uuo.

Pictographic symbols used at the beginning of the 18th century to represent chemical elements and compounds. They are similar to those of the ancient alchemists. As more elements were discovered during the 18th century, attempts to devise a chemical nomenclature led to the modern alphabetic notational system. This system was devised by the Swedish chemist Berzelius and introduced in 1814.

3

0 0 0

@ 10

Each element is denoted by a chemical symbol and some examples are given below.

Name of element	Symbol	
carbon	С	
fluorine	F	
potassium	K	
calcium	Ca	
mercury	Hg	
tungsten	W	

You will notice that often the letter or letters used to represent the elements are derived from its English name, but in some cases, they derive from other languages. For example, Hg for mercury comes from Latin, whereas W for tungsten has its origin in European dialects. These symbols are all accepted and used internationally, which allows for effective global communication between chemists. A complete list of the names of the elements and their symbols is given in Section 6 of the data booklet.

1

Chemistry is a very exact subject, and it is important to be careful in distinguishing between upper and lower case letters.

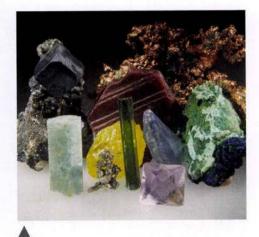
Cobalt (Co) is a metallic element whereas carbon monoxide (CO) is a poisonous gas.

## Compounds consist of atoms of different elements chemically bonded together in a fixed ratio

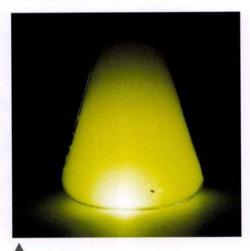
Some elements, such as nitrogen and gold, are found in **native** form, uncombined with other elements in nature. But more commonly, elements exist in chemical combinations with other elements, as **chemical compounds**. Compounds consist of atoms of different elements chemically bonded together in a fixed ratio. The physical and chemical properties of compounds are completely different from those of their component elements.

Sodium chloride, for example, is a white crystalline solid that is added to improve the taste of food, whereas sodium is a dangerously reactive metal that reacts violently with water, and chlorine is a toxic gas.

The **chemical formula** of a compound uses a combination of chemical symbols of its constituent elements. A subscript is used to show the number of atoms of each element in a unit of the compound. Some examples are given below. (The reasons for the different ratios of elements in compounds will become clearer after we have studied atomic structure and bonding in Structure 2.)



Assorted minerals, including elements such as sulfur and silver, and compounds such as  $Al_2O_3$  (sapphire) and  $CaF_2$  (fluorite). Most minerals are impure and exist as mixtures of different elements and compounds.



Sodium, Na, reacts violently with chlorine, Cl<sub>2</sub>, to produce white crystals of the compound sodium chloride, NaCl.

2Na(s) + Cl<sub>2</sub>(g) → 2NaCl(s)

The properties of the compound are completely different from those of its component elements.

A compound is a substance made by chemically combining two or more elements in a fixed ratio of atoms. The physical and chemical properties of a compound are different from those of its constituent elements.



Name of compound	Chemical formula	Name of compound	Chemical formula
sodium chloride	NaCl	methane	CH <sub>4</sub>
magnesium hydroxide	Mg(OH) <sub>2</sub>	ammonia	NH <sub>3</sub>
copper sulfate	CuSO <sub>4</sub>	glucose	C <sub>6</sub> H <sub>12</sub> O <sub>6</sub>
water	H <sub>2</sub> O	sulfuric acid	H <sub>2</sub> SO <sub>4</sub>

## Mixtures contain more than one element or compound in no fixed ratio

Chemistry is primarily concerned with understanding the structure and reactivities of pure substances but dealing with mixtures is a practical reality. Although there are a countable number of pure substances, the elements and compounds, which all have distinctive names, there is an infinite number of mixtures. The composition of any one mixture can vary continuously – the relative amounts of ice cream, milk and flavourings in a milkshake can vary depending on the taste of the person preparing the drink. Names for all the mixtures we could make do not exist.

Air is described as a **mixture** of gases because the separate components – different elements and compounds – are interspersed with each other, but not chemically combined. The gases nitrogen and oxygen when mixed in air, for example, have the same properties as they do when they are in pure samples. Substances burn in air because they react with the oxygen in the same way that they react with pure oxygen. As substances can be mixed in any proportion, mixtures, in contrast to compounds, do not have a fixed composition and cannot be represented by a chemical formula. The composition of air for example varies widely around the world due to the presence of different pollutants.

Air is an example of a **homogeneous mixture**, as it has uniform composition and properties throughout. A solution of salt in water and a metal alloy such as bronze, which is a mixture of copper and tin, are also homogeneous. To form a homogeneous mixture, the inter-particle attraction within the different components must be similar in nature to those between the components in the mixture. Explanations of the different particle interactions are given in Structure 2.2.

Mixture	Component 1	Particle interaction 1	Component 2	Particle interaction 2	Interaction in mixture
air	N <sub>2</sub>	dispersion forces	O <sub>2</sub>	dispersion forces	dispersion forces
bronze	Cu	metallic bonding	Sn	metallic bonding	metallic bonding
salt water	NaCl	ionic	H <sub>2</sub> O	hydrogen bonding	ion-dipole

Making alloys at a steel mill. Alloys are formed by mixing two molten metals that can then form a mixture of uniform composition. There is no chemical reaction between the metallic elements as the metallic bonding present in the individual metals and the alloys is non-directional and not significantly disrupted by the mixing process. Metallic bonding is explored more fully in Structure 2.3.

ток

Our classification systems are embedded in the language we use. To what extent do the classification systems we use affect the knowledge we obtain? To what extent do the names and labels that we use help or hinder the acquisition of knowledge?



A mixture contains more than one element or compound in no fixed ratio, which are not chemically bonded. The components of a mixture can be separated by physical methods.



Structure 2.3 – Why are alloys generally considered to be mixtures, even though they often contain metallic bonding?

#### Challenge yourself

1. If you add 10 cm3 of water to 10 cm3 of water, you get 20 cm3 of water. Similarly, if you add 10 cm<sup>3</sup> of ethanol to 10 cm<sup>3</sup> of ethanol you get 20 cm<sup>3</sup> of ethanol. Explain why the volume of the solution formed between 10 cm<sup>3</sup> of water and 10 cm<sup>3</sup> ethanol is less than 20 cm<sup>3</sup>.

Structure 2.2 - How do intermolecular forces influence the type of mixture that forms between two substances?

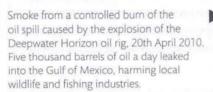


A heterogeneous mixture, by contrast, such as water and oil, has a non-uniform composition, and its properties are not the same throughout. The interactions between the components of a heterogeneous mixture are different in nature. The water molecules interact by hydrogen bonding and the oil molecules by dispersion forces, as discussed in Structure 2.2.

It is usually possible to see the separate components in a heterogeneous mixture but not in a homogeneous mixture.

Ocean oil spills can occur when oil is extracted or transported. They cause widespread damage to the environment and can have a major impact on local industries such as fishing and tourism. Efforts to reduce the impact of the spill include the use of dispersants, which break up the oil into smaller droplets, allowing it to mix better

with water.





#### Challenge yourself

2. Does a mixture have the same classification at all scales?

The components in a mixture can be relatively easy to separate if they have a distinct physical property. The technique chosen will depend on this distinct property.

Mixture	Difference in property of components	Technique used
sand and salt	solubility in water	solution and filtration
salt and water	boiling point	distillation
iron and sulfur	magnetism	response to a magnet
pigments in food colouring	adsorption to solid phase	paper chromatography



The required product of a chemical reaction similarly needs to be separated from the reaction mixture, which also contains unreacted reactants and other unwanted products. It is a practical challenge to both maximize the yield and the purity, as some product can be removed with the impurities during the purification process.



Filtration is the process where a solid is separated from a liquid or gas using a membrane. The solid is collected on the membrane as the residue, and the filtrate containing the solute passes through. Sand and salt have different solubilities in water so can be separated by adding water which dissolves the salt - an example of solvation. The resulting mixture can be filtered with the insoluble sand removed as the residue leaving the salt water solution as the filtrate. The water can be separated from the salt by evaporation, which allows the salt crystals to form (crystallization).

Filtration apparatus



Tool 1 - What factors are considered in choosing a method to separate the components of a mixture?



Tool 1 - How can the products of a reaction be purified?



Preparation of Agl precipitate from aqueous solutions. Full details of how to carry out this experiment with a worksheet are available in the eBook.

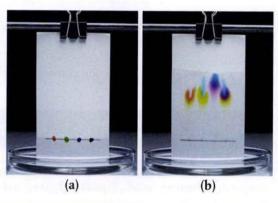


Distillation apparatus

Distillation is used to separate a solvent from a solute. The solvent has a lower boiling point than the solute and so is collected as a gas and passes into the condensing tube, which is surrounded by cold flowing water. The gas is condensed in the beaker at the bottom. This method can be used to separate water from seawater, for example.

In paper chromatography, small spots of solutions containing the samples being tested are placed on the baseline. The paper is suspended to ensure that it is saturated (a). The different components have different affinities for the water in the paper (the solvent) and so separate as the solvent moves up the paper (b). This method can be used to investigate the different pigments in food colouring.

into the pure solvent collected



Paper chromatography apparatus

#### **Exercise**

Q1. Identify the homogeneous mixture.

A water and oil

B sand and water

C salt and water

D sand and salt

Q2. Identify the correct descriptions about mixtures.

I. The components can be elements or compounds.

II. All components must be in the same state.

III. The components retain their individual properties.

A I and II only

B I and III only

C II and III only

D I, II and III

Q3. Identify the homogeneous mixtures.

I. gold

II. bronze

III. steel

A I and II only

B I and III only

C II and III only

D I, II and III

- Q4. (a) River water needs to be purified to make it safe to drink. The water passes through a grid and is then left in a tank where other impurities are removed as they fall to the bottom in a process known as sedimentation. Suggest why pollutants such as fertilizers are not removed in this process.
  - (b) Drinking water can be obtained from seawater by distillation. Explain the disadvantages of using distillation to obtain large amounts of drinking water.
- **Q5.** A layer of oil paint is left to dry in the air and it hardens. Suggest what causes the oil to harden.
- **Q6.** Metal coins are made from different metals. The composition of a 20-cent and a 50-cent euro coin is given below.

	Mass/g			
Coin	Copper	Aluminium	Zinc	Tin
20 cent	5.11	0.287	0.287	0.057
50 cent	6.94	0.39	0.39	0.080

Compare the chemical compositions of the two coins.

#### Structure 1.1.2 - The kinetic molecular theory

Structure 1.1.2 – The kinetic molecular theory is a model to explain physical properties of matter (solids, liquids and gases) and changes of state.

Distinguish the different states of matter.

Use state symbols (s, l, g and aq) in chemical equations.

Names of the changes of state should be covered: melting, freezing, vaporization (evaporation and boiling), condensation, sublimation and deposition.

Structure 2.4 – Why are some substances solid while others are fluid under standard conditions?

Structure 2 (all), Reactivity 1.2 – Why are some changes of state endothermic and some exothermic?

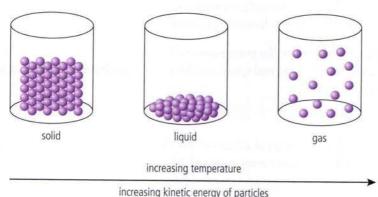
## The kinetic molecular theory explains physical properties

If you were hit with a bucket of solid water (ice), you could be seriously injured, but the same mass of liquid water would only be annoying. Gaseous water (steam) could

also be harmful but for different reasons. These three samples are all made from the same particles: water molecules,  $H_2O$ . The difference in physical properties of the three states is explained by **kinetic molecular theory**.

## Matter exists in different states as determined by the temperature and the pressure

From our common experience, we know that all matter (elements, compounds, and mixtures) can exist in different forms depending on the temperature and pressure. Liquid water changes into a solid form, such as ice, hail, or snow, as the temperature drops, and it becomes a gas, steam, at higher temperatures. These different forms are known as the **states of matter** and are characterized by the different energies of the particles.



Solid	Liquid	Gas
<ul> <li>particles closely packed</li> </ul>	particles more spaced	particles fully spread out
• inter-particle forces strong, particles vibrate in position	inter-particle forces weaker, particles can slide over each other	inter-particle forces negligible, particles move freely
<ul> <li>fixed shape</li> </ul>	no fixed shape	no fixed shape
<ul> <li>fixed volume</li> </ul>	fixed volume	no fixed volume

This is known as the kinetic molecular theory of matter as the three states are distinguished by the way the particles move. The temperature of the system is directly related to the average kinetic energy of the particles and the state of matter at a given temperature and pressure is determined by the strength of **inter-particle forces** that exist between the particles relative to this average kinetic energy. If the inter-particle forces are sufficiently strong to keep the particles in position at a given temperature and pressure, the substance will be a solid. If not, it will be a liquid or a gas. The different inter-particle forces are explored more fully in Structure 2.

#### Challenge yourself

**3.** What evidence based on simple observations can you think of that supports the idea that water is made from discrete particles?

**51.1 Figure 2** Representation of the arrangement of the particles of the same substance in the solid, liquid, and gas states.

i

A fourth state of matter, plasma, exists only at conditions of very high temperatures and pressures, such as those commonly found in stars such as our Sun.



Depending on the chemical nature of the substance, matter may exist as atoms such as Ar(g), as molecules such as H<sub>2</sub>O(l), or as ions such as Na<sup>+</sup> and Cl<sup>-</sup> in aqueous solution NaCl(aq). The term **particle** is therefore used as an inclusive term that is applied in this text to any or all of these entities of matter.

Temperature is a measure of the average kinetic energy of the particles of a substance.



#### Worked example

Which of the following has the highest average kinetic energy?

A He at 100°C

B H<sub>2</sub> at 200 °C

C O2 at 300°C

D H<sub>2</sub>O at 400°C

#### Structure 2.4 – Why

are some substances solid while others are fluid under standard conditions?



#### Solution

**D** The substance at the highest temperature has the highest average kinetic energy.

Liquids and gases are both referred to as **fluids**, as they have the ability to flow. In the case of liquids, it means that they take the shape of their container. **Diffusion**, the process by which the particles of a substance spread out more evenly, occurs as a result of their random movements. It occurs predominantly in these two fluid states.

Kinetic energy  $(E_k)$  refers to the energy associated with movement or motion. It is determined by the mass (m) and speed or velocity (v) of a substance, according to the relationship:

$$E_{\rm k} = \frac{1}{2} \, m v^2$$

As the average kinetic energy of all particles at the same temperature is the same, there is an inverse relationship between mass and velocity:

$$E_{k} = \frac{1}{2} m_{1} v_{1}^{2} = \frac{1}{2} m_{2} v_{2}^{2}$$
$$\frac{m_{1}}{m_{2}} = \frac{v_{2}^{2}}{v_{1}^{2}}$$

Particles with smaller mass therefore diffuse more quickly than those with greater mass, at the same temperature.

**State symbols** are used to show the states of the reactants and products taking part in a reaction. These are abbreviations, which are given in parenthesis after each term in an equation, as shown below.

State	Symbol	Example
solid	(s)	Fe(s)
liquid	(1)	Br <sub>2</sub> (l)
gas	(g)	O <sub>2</sub> (g)
aqueous	(aq)	H <sub>2</sub> SO <sub>4</sub> (aq)

For example:

$$2Na(s) + 2H_2O(l) \rightarrow 2NaOH(aq) + H_2(g)$$

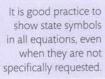
Sodium hydroxide, NaOH, is produced during this reaction in aqueous solution.

Solutions more generally are mixtures of two components. The less abundant component is the **solute** and the more abundant is the **solvent**. The solute can be solid, liquid or gas but the solvent is generally a liquid. Solutions in water are particularly important and are given the state symbol (aq).





Bromine liquid, Br<sub>2</sub>(I), has been placed in the lower gas jar only, and its vapour has diffused to fill both jars. Bromine vaporizes readily at room temperature and its distinctive colour allows the diffusion to be observed.





#### Matter changes state reversibly

As the movement or kinetic energy of the particles increases with temperature, they will overcome the inter-particle forces and change state. This occurs at a fixed temperature and pressure for each substance. A solid (X(s)) changes to a liquid at a defined **melting point** and a liquid (Y(l)) changes to a gas at its **boiling point**.

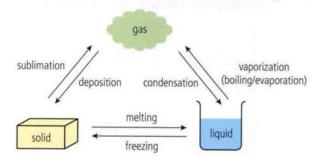
These changes can be reversed when the substance is cooled: a liquid freezes and becomes solid at the same temperature as the solid melts.

A gas or vapour condenses at the same temperature as the liquid boils.

The reversibility of these changes can be represented by reversible arrows as shown in the table.

Change of state		Change of state		Reversible equation
melting	$X(s) \longrightarrow X(l)$	freezing	$X(l) \rightarrow X(s)$	$X(s) \rightleftharpoons X(l)$
boiling	$Y(l) \rightarrow Y(g)$	condensing	$Y(g) \rightarrow Y(l)$	$Y(l) \rightleftharpoons Y(g)$

Some substances can also change directly between the solid and gaseous states.



**Sublimation** is the direct inter-conversion of a solid to a gas without going through the liquid state. It is characteristic of some substances such as iodine, carbon dioxide and ammonium chloride.

**Deposition** is the reverse of sublimation and occurs when a gas changes directly to a solid. It occurs when snow and frost are formed.



a

The temperature of a state change can be presented from both perspectives:
melting point = freezing point;
boiling point =

condensation point.

**S1.1 Figure 3** The different state changes between the solid, liquid and gaseous states.



and iodine. Full details of how to carry out this experiment with a worksheet are available in the eBook.

Sublimation of iron

Ice crystals, known as hair ice, formed by deposition on dead wood in a forest on Vancouver Island. Canada A liquid can change to gas by two processes: **evaporation** and **boiling**. Boiling occurs at a fixed temperature for a given pressure, when bubbles of gas form throughout the liquid. Evaporation, by contrast, occurs only at the surface and takes place over a range of temperatures below the boiling point.

More precisely, the boiling point is the temperature at which the vapour pressure is equal to the



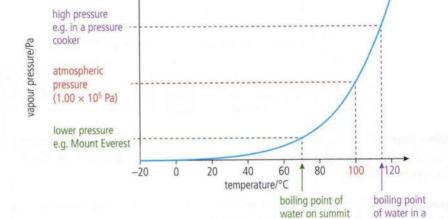
The heat of the Sun enables all the water to evaporate from the clothes.

external pressure. As a liquid is heated, more particles enter the vapour state and the vapour pressure increases. When the vapour pressure reaches the external atmospheric pressure the liquid boils. When the external pressure is lower, the vapour pressure needed to boil is reduced and so boiling occurs at a lower temperature.

The relationship between temperature and vapour pressure and the influence of external pressure on the boiling point is demonstrated in Figure 4.

**\$1.1 Figure 4** Graph showing the boiling point of water at three different pressures.

A pressure cooker is a sealed container in which a high pressure can be generated. This raises the boiling point of water, allowing cooking time to decrease. Conversely, at altitude, where the atmospheric pressure is lower, the boiling point of water is reduced so it takes much longer to cook food.





■ A butane gas camping stove. Butane, C<sub>4</sub>H<sub>10</sub>, is stored as a liquid because the high pressure in the canister raises its boiling point. When the valve is opened the release of pressure causes the butane to boil, releasing a gas that can be burned.

pressure cooker

of Mount Everest

#### Challenge yourself

**4.** Propane (C₃H₀) and butane (C₄H₁₀) are both commonly used in portable heating devices. Their boiling points are butane −1 °C and propane −42 °C. Suggest why butane is less suitable for use in very cold climates.



 Macrophotograph of freezedried instant coffee granules.



Freeze-drying is used to preserve food and some pharmaceuticals. It differs from standard methods of dehydration as the energy needed to evaporate water is produced by the sublimation of ice. The substance to be preserved is first frozen. and then warmed gently at very low pressure which causes the ice to change directly to water vapour. The process is slow but has the significant advantage that the composition of the material, and so also its flavour, are largely conserved. The freeze-dried product is stored in a moisturefree package that excludes oxygen, and can be reconstituted by the addition of water.

#### **Exercise**

- **Q7.** A mixture of two gases, X and Y, which both have strong but distinct smells, is released. From across the room the smell of X is detected more quickly than the smell of Y. What can you deduce about X and Y?
- **Q8.** Use the kinetic theory to explain whether you would expect the rate of diffusion in a liquid to increase or decrease as the temperature is increased.
- **Q9.** Which is the correct descriptor for the movement of particles in the solid, liquid and gaseous states?

	Solid	Liquid	Gas
A vibrational movement in one dimension		vibrational movement in two dimensions	vibrational movement in three dimensions
В	no movement, fixed in position	only vibrational movement	free movement in all dimensions
C	free movement in all dimensions	free movement in all dimensions	free movement in all dimensions
D	vibrational movement	limited movement in all dimensions	free movement in all dimensions

- **Q10.** A closed flask contains a pure substance, a brown liquid that is at its boiling point.
  - (a) Explain what you are likely to observe in the flask.
  - **(b)** Distinguish between the inter-particle distances and the average speeds of the particles in the two states present.
- **Q11.** A beaker containing solid carbon dioxide is placed in a fume cupboard at room temperature. The carbon dioxide becomes gaseous. Which process describes this change of state?
  - A boiling
- B condensation
- C evaporation
- D sublimation
- **Q12.** Water exists in three states: ice, liquid water or steam. Which transition can occur over a range of temperatures at constant pressure?
  - A freezing
- B melting
- C evaporation
- D boiling

a

At night, as the temperature is lowered, the rate of condensation increases. As the air temperature drops below its saturation point, known as the dew point, condensed water called dew forms. The temperature of the dew point depends on the atmospheric pressure and the water content of the air - that is, the relative humidity.

- **Q13.** A liquid is placed in an open dish. Which change increases the rate of evaporation?
  - I. increased temperature of the liquid
  - II. increased depth of the liquid
  - III. increased surface area of the liquid
  - A Land II
- B I and III
- C II and III
- D I. II and III
- **Q14.** During very cold weather, snow often gradually disappears without melting. Explain how this is possible.

#### Structure 1.1.3 - Kinetic energy and temperature

Structure 1.1.3 – Temperature (T) in kelvin (K) is a measure of average kinetic energy  $(E_k)$  of particles.

Interpret observable changes in physical properties and temperature during changes of state. Convert between values in the Celsius and Kelvin scales.

The kelvin (K) is the SI unit of temperature and has the same incremental value as the Celsius degree (°C).

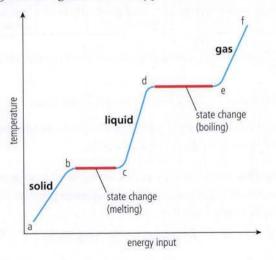
Reactivity 2.2 – What is the graphical distribution of kinetic energy values of particles in a sample at a fixed temperature?

Reactivity 2.2 – What must happen to particles for a chemical reaction to occur?

#### Temperature is constant during changes of state

#### Matter changes state when it is heated

Simple experiments can be done to monitor the temperature change while a substance is heated and changes state. Figure 5 shows a typical result.



**S1.1 Figure 5** Temperature change versus energy input at fixed pressure as a solid substance is heated. The flat regions shown in red are where a change of state is occurring. Heat energy is used to overcome the inter-particle forces.

The heat curve of water. Full details of how to carry out this experiment with a worksheet are available in the eBook.







Ice cubes melting in a beaker of water. Heat from the surroundings breaks some inter-particle forces between the water molecules in the ice. In Structure 2.2.8, we will see that the inter-particle forces in ice are hydrogen bonds.

The graph can be interpreted as follows:

- a–b As the solid is heated, the vibrational energy of its particles increases and so the temperature increases.
- b—c This is the melting point. The vibrations are sufficiently energetic for the particles to move away from their fixed positions and form a liquid. Energy added during this stage is used to break the inter-particle forces, not to raise the kinetic energy, so the temperature remains constant.
- c–d As the liquid is heated, the particles gain kinetic energy and so the temperature increases.
- d-e This is the boiling point. There is now sufficient energy to break all of the inter-particle forces and form a gas. Note that this state change needs more energy than melting, as all the inter-particle forces must be broken. The temperature remains constant as the kinetic energy does not increase during this stage. Bubbles of gas are visible through the volume of the liquid.
- e—f As the gas is heated under pressure, the kinetic energy of its particles continues to rise, as does the temperature.

Melting (b to c) and boiling (d to e) are endothermic processes as energy is needed to separate the particles. The reverse processes, freezing (c to b) and condensation (e to d), are exothermic. Energy is given out as the inter-particle forces bring the particles closer together. Energy changes are explored in Reactivity 1.2.

### Challenge yourself

**5**. Which physical properties determine the gradient of the lines for the different states in Figure 5?



### **Nature of Science**

Scientists analyse their observations looking for patterns, trends or discrepancies. You may have noticed that the volume decreases as ice melts and its density increases. This is unusual as density generally decreases as a solid melts. This discrepancy is explained in Structure 2.2.8.

### Temperature in kelvin is known as the absolute temperature

The movement or kinetic energy of the particles of a substance depends on the temperature. If the temperature of a substance is decreased, the average kinetic energy of the particles also decreases. Absolute zero  $(-273\,^{\circ}\text{C})$  is the lowest possible temperature attainable as this is the temperature at which all movement stops.

The kelvin is the SI unit of temperature. The absolute temperature is directly proportional to the average kinetic energy of its particles. A temperature increase of  $1\,^\circ\text{C}$  is also an increase of  $1\,^\kappa\text{C}$ . This facilitates conversions between the two scales.



Geothermal hot spring, Hveragerdi, Iceland. The geothermal spring provides sufficient energy to separate the water molecules and turn water into steam.



Structure 2 (all), Reactivity 1.2 - Why are some changes of state endothermic and some exothermic?



The Celsius scale of temperature is defined relative to the boiling and freezing points of water. The original scale, developed by the Swedish astronomer Anders Celsius, made the boiling point of water zero and the freezing point 100. The modern scale reverses this with the boiling point of water 100°C and the melting point of ice as 0°C. The original scale may now seem absurd, but the modern scale is just as arbitrary.

An increase of temperature  $\Delta T = 1 \text{ K} = 1 ^{\circ}\text{C}$ . More generally  $T(\text{K}) = T(^{\circ}\text{C}) + 273.15$ The kelvin is the SI unit of temperature.

William Thomson (1824-1907), who became known as Lord Kelvin later in life, completed most of his work at the University of Glasgow, Scotland. His concept of the absolute temperature scale followed from his recognition of the relationship between heat energy and the ability to do work. The existence of a minimum possible temperature at which no heat can be extracted from the system and so no work done, led him to the definition of absolute zero in 1848. This in turn led to the formulation of the laws of thermodynamics. Kelvin is considered one of the great scientists of the 19th century, and is buried next to Isaac Newton in London.

Reactivity 2.2 - What is the graphical distribution of kinetic energy values of particles in a sample at a fixed temperature?

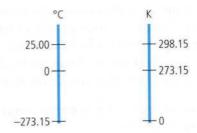
Reactivity 2.2 – What must happen to particles for a chemical reaction to occur?



Temperature can be converted from Celsius to the Kelvin scale by the relation:

$$T(K) = T(^{\circ}C) + 273.15$$
 therefore  $T(^{\circ}C) = T(K) - 273.15$ 

temperature (K) = temperature (°C) + 273.15

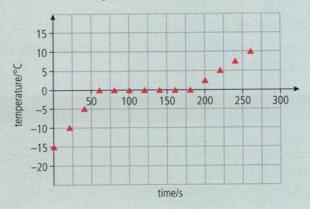


\$1.1 Figure 6 The Celsius and Kelvin scales of temperature.

Although we can only relate the average kinetic energy to the temperature, there are many particles in a sample each with a different kinetic energy. The total kinetic energy is conserved in particle collisions, but the kinetic energy of individual particles changes upon each collision. We can however predict the statistical distribution of energies in a sample at a particular temperature, known as the Maxwell–Boltzmann distribution. This distribution will also help us understand the effect of temperature on rates of reaction. To react, particles must collide with sufficient kinetic energy known as the activation energy. Both these points are explored in Reactivity 2.2.

#### **Exercise**

Q15. A solid is heated and the temperature is measured every 20 seconds.



- (a) Identify the solid.
- (b) Describe how the particles in the solid are moving in the interval 0–60 s.
- (c) Describe how the particles are moving in the interval after  $180\,\mathrm{s}$ .
- (d) Explain why the temperature does not change in the interval 60–180 s.
- (e) Use the graph to predict the temperature after the material has been heated for 600 s.
- **(f)** Use the graph to predict the temperature after 1200 s. Comment on the validity of your prediction.

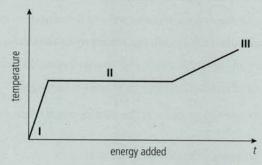
Q16. Which of the following shows the correct Celsius temperature for the given kelvin temperature?

	Kelvin scale	Celsius scale
A	0	273
В	50	323
C	283	110
D	323	50

- Q17. Which of the following occurs at the freezing point when a liquid is converted to a solid?
  - I. kinetic energy of the particles decreases
  - II. separation between the particles decreases
  - A I only
- B II only C I and II
- D neither I nor II
- Q18. Two objects made from different masses of iron have the same temperature. Which of the following is the correct comparison of the average kinetic energy and the total energy of the atoms in the objects?

	Average kinetic energy of the atoms	Total energy of the atoms
A	greater in an object of larger mass	same
В	less in an object of larger mass	same
C	same	greater in an object of larger mass
D	same	less in an object of larger mass

Q19. A substance is heated. The graph shows how the temperature changes with the heat energy added.



In which region of the graph must the solid state be present?

- AI
- BII
- C III
- D None
- Q20. Explain why a burn to the skin caused by boiling water is less harmful than a burn caused by the same amount of steam produced as the water boils.



### **Guiding Question revisited**

How can we model the particulate nature of matter?

In this chapter we have used a particulate model to show:

- All matter is made up from small particles.
- An element is a pure chemical substance composed of the same type of atoms.
- Compounds consist of atoms of different elements chemically bonded together in a fixed ratio.
- Mixtures are made from particles of one substance interspersed between particles of at least one other substance. If this mixing is uniform, it is a homogeneous mixture. If it is not uniform, it is heterogeneous.
- The different states of matter are characterized by the movement and arrangement of the particles.
- Changes of state require energy changes as energy is needed to separate particles and is given out when particles come together.

### **Practice questions**

- Which statements are correct?
   I. Solids have a fixed shape because the particles can only vibrate about a fixed point.
   II. Liquids can flow because the particles can move freely.
   III. Gases are less dense because the interactions between the particles are very weak.
   A I and II B I and III C II and III D I, II and III
- 2. The temperature of a gas is reduced. Which of the following statements is true?
  - A The molecules collide with the walls of the container less frequently.
  - B The molecules collide with each other more frequently.
  - C The time of contact between the molecules and the wall is reduced.
  - D The time of contact between molecules is increased.
- 3. Which of the following occurs at the melting point when a solid is converted to a liquid?
  - I. kinetic energy of the particles increases
  - II. separation between the particles increases
  - A I only B II only C I and II D neither I nor II
- **4.** Identify the change(s) that occur at the boiling point when a liquid is converted to a gas.
  - I. kinetic energy of the particles increases
  - II. separation between the particles increases
  - A I only B II only C I and II D neither I nor II

5. A substance is heated at a constant rate.

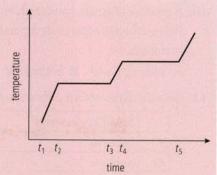
During which interval does the energy of the substance increase the most?



$$\mathbf{B}$$
  $t_2$  to  $t_3$ 

$$C t_3 to t_4$$

 $D t_4 to t_5$ 



**6.** An ice cube of mass 10.0 g with a temperature of 0 °C is placed into a glass containing 90 cm<sup>3</sup> of water at 10 °C.

After 5 minutes some of the ice has melted. What is the temperature of the ice remaining?

B 0.5°C

C 2.0°C

D 5°C

7. Identify the pair of substances that can form a homogeneous mixture.

A olive oil and vinegar

B sand and water

C carbon dioxide and water

D salt and pepper

8. Identify the equation that represents sublimation.

A 
$$I_2(g) \rightarrow 2I(g)$$

**B** 
$$I_2(s) \rightarrow I_2(g)$$

C 
$$I_2(s) + I^-(aq) \rightarrow I_3^-(aq)$$

**D** 
$$2Al(s) + 3I_2(s) \rightarrow 2AlI_3(s)$$

9. Which descriptions are consistent with the diagram?

	Diagram	Description
I.	0 0 0	A compound in the gaseous state.
II.	0000	A compound in the liquid state.
III.	*************	A heterogeneous mixture in the solid state.

A I and II only

B I and III only

C II and III only

D I, II and III

10. A mixture of ethanol and methanol can be separated by fractional distillation. This method of separation depends on the difference of which property of the two alcohols?

A melting point B boiling point

C solubility

D density

11. The solubilities of four different substances in water and ethanol are given.

9.0	Solubility in water	Solubility in ethanol
P	insoluble	insoluble
Q	insoluble	soluble
R	soluble	insoluble
S	soluble	soluble

Some mixtures can be separated by solvation and filtration using water or ethanol as solvents.

Method I uses water as the solvent.

Method II uses ethanol as the solvent.

Which substances can be separated from each other using both methods?

A Pand S

B Q and S

C R and S

D Q and P

12. Classify the following mixtures as homogeneous or heterogeneous:

(a) smoke

(b) sugar and water

(c) steel

(3)

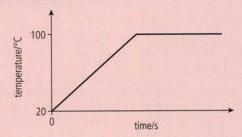
(2)

(Total 3 marks)

- 13. During very cold weather, snow often gradually disappears without melting. Explain how this is possible.
- 14. (a) Describe two differences, in terms of particle structure, between a gas and a liquid.

(b) The temperature of a gas is a measure of the average kinetic energy of the gas particles. Suggest why the average kinetic energy is specified. (2)

(c) A sample of water was heated. The graph shows how the temperature of the water varied with time.



(i) State why the temperature initially increases.

(1)

(ii) State why the temperature remains constant at 100 °C.

(2)

(Total 7 marks)

15. (a) The physical properties of some halogens are shown in the table.

Element	Molecular formula	Melting point/°C	Boiling point/°C
fluorine	F <sub>2</sub>	-220	-188
chlorine	Cl <sub>2</sub>	-101	-35
bromine	Br <sub>2</sub>		58.8
iodine	$I_2$	114	184

Predict the melting point of bromine.

(1)

- **(b)** Describe the trend in the boiling points of the halogens down the group.
- (1)

(c) Predict the physical state of iodine at 200 °C.

- (1)
- (d) A simplified diagram of the structure for bromine is shown.



- (i) Suggest the state of bromine with this structure and justify your answer. (2)
- (ii) Describe the changes that occur to this arrangement when bromine is heated. (2)
- (iii) Describe the changes that occur when bromine reacts. (1)
- (iv) Use the kinetic theory to explain the effect of an increase in temperature on the rate of diffusion of bromine. (1)

(Total 9 marks)

The nuclear atom

The atomic nucleus is at the centre of the atom. The number of protons in the nucleus gives the atom its identity.





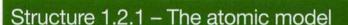
### **Guiding Question**

How do the nuclei of atoms differ?

We saw in Structure 1.1 that all matter is built from no more than about 100 elements. The smallest amount of an element that can exist is an atom, which is the smallest particle of an element to show the element's characteristic properties. It is amazing that particles as small as the atom can have such a huge impact on the universe. Almost all explanations in chemistry refer to the atom, either individually or in the groups we call molecules.

In this chapter we will explore the structure of atoms in more detail. Although the word 'atom' means uncuttable, the atom can be split into smaller subatomic particles. All atoms are made from the same basic ingredients: protons, neutrons and electrons, but differ in their composition. If you look at the periodic table, you will see that each element has an atomic number. This was originally used to give the relative position of the element in the table. For example, the first element, hydrogen, has an atomic number of 1. We now know that this number is more fundamental than just a ranking. The atomic number is the defining property of an element as it is the number of protons in the nucleus of the atom.

Although the nucleus is only a small part of the atom, you can think of it as the atom's control centre. As an atom has a neutral charge, the number of protons also determines the number of electrons. The number of protons gives an atom its identity and the number of electrons determines its chemical properties. The mass of an element's atoms can vary due to a difference in the number of neutrons in the nucleus. but this has little impact on the chemistry of the atom. The number of neutrons does, however, affect some physical properties, including the nuclear stability.



Structure 1.2.1 - Atoms contain a positively charged, dense nucleus composed of protons and neutrons (nucleons). Negatively charged electrons occupy the space outside the nucleus.

Use the nuclear symbol  $\binom{A}{Z}X$ ) to deduce the number of protons, neutrons and electrons in atoms and ions.

Relative masses and charges of the subatomic particles should be known; actual values are given in the data booklet. The mass of the electron can be considered negligible.

Structure 1.3 - What determines the different chemical properties of atoms?

Structure 3.1 - How does the atomic number relate to the position of an element in the periodic table?



TOK

Richard Feynman: ... if all of scientific knowledge were to be destroyed, and only one sentence passed on to the next generation of creatures. what statement would contain the most information in the fewest words? I believe it is the atomic hypothesis... that all things are made of atoms." Are the models and theories that scientists create accurate descriptions of the natural world, or are

they primarily useful interpretations for prediction, explanation, and control of the natural world?

### Atoms contain a positively charged, dense nucleus

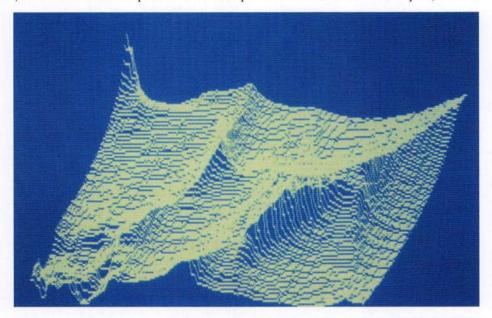
### Dalton's model of the atom

One of the first great achievements of chemistry was to show that all matter is built from about 100 **elements**. As mentioned in Structure 1.1, the elements are substances which cannot be broken down into simpler components by chemical reactions. Different elements have different chemical properties but gold foil, for example, reacts in essentially the same way as a single piece of gold dust. Indeed, if the gold dust is cut into smaller and smaller pieces, the chemical properties would remain the same until we reached an **atom**. The atom is the smallest unit of an element. There are only 92 elements which occur naturally on Earth, and they are made up of only 92 different types of atom. (This statement will be qualified when isotopes are discussed later in the chapter.)

The word 'atom' comes from the Greek words for 'not able to be cut'.



Scanning tunnelling microscope (STM) image of the surface of pure gold. STM imaging records the surface structure at the level of the individual atoms. Gold exists in many forms, but all the forms contain the same type of atoms. The 'rolling hills' structure seen here is the result of changes in the surface energy as the gold cooled from its molten state.





### **Nature of Science**

The idea that matter is made up of elements and atoms dates back to the 4th century BCE. This was speculative as there was little evidence to support the idea. Scientists adopt a sceptical attitude to claims and evaluate them using evidence. A significant development for chemistry came with the publication of Robert Boyle's *Sceptical Chymist* in 1661 which emphasized the need for scientific knowledge to be justified by evidence from practical investigations. Boyle was the first person to propose the modern concept of an element as a substance which cannot be changed into anything simpler.

The modern idea of the atom dates from the beginning of the 19th century. John Dalton noticed that the elements hydrogen and oxygen always combined in fixed proportions. To explain this observation, he proposed that:

- all matter is composed of tiny indivisible particles called atoms
- · atoms cannot be created or destroyed
- · atoms of the same element are alike in every way
- · atoms of different elements are different
- · atoms can combine together in small numbers to form molecules.

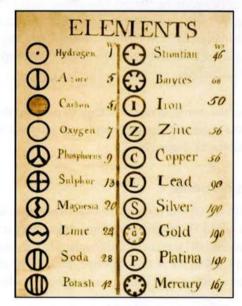
Using this model, we can understand how elements react together to make **compounds**. The compound water, for example, is formed when two hydrogen atoms combine with one oxygen atom to produce one water molecule. If we repeat the reaction on a larger scale with  $2 \times 6.02 \times 10^{23}$  atoms of hydrogen and  $6.02 \times 10^{23}$  atoms of oxygen, then  $6.02 \times 10^{23}$  molecules of water will be formed. This leads to the conclusion (see Structure 1.4) that  $2.02\,\mathrm{g}$  of hydrogen will react with  $16.00\,\mathrm{g}$  of oxygen to form  $18.02\,\mathrm{g}$  of water. This is one of the observations Dalton was trying to explain.



### **Nature of Science**

Dalton was a man of regular habits. 'For fifty-seven years... he measured the rainfall, the temperature... Of all that mass of data, nothing whatever came. But of the one searching, almost childlike, question about the weights that enter the construction of simple molecules — out of that came modern atomic theory. That is the essence of science: ask an impertinent question: and you are on the way to the pertinent answer.' (J. Bronowski).

Dalton was the first person to assign chemical symbols to the different elements.



### Challenge yourself

It is now known that some of these substances are not elements but compounds.
 Lime, for example, is a compound of calcium and oxygen. Find any other examples of compounds in this list, and explain why the component elements had not been extracted at this time.

Following Dalton's example, you can write the formation of water using modern notation:

$$2H + O \rightarrow H_2O$$

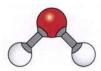
But what are atoms really like? It can be useful to think of them as hard spheres (Figure 1), but this tells us little about how the atoms of different elements differ. To understand this, it is necessary to probe deeper.

ток

'What we observe is not nature itself but nature exposed to our mode of questioning.' (Werner Heisenberg).

How does the knowledge we gain about the natural world depend on the questions we ask and the experiments we perform?

John Dalton's symbols for the elements.



S1.2 Figure 1 A model of a water molecule made from two hydrogen atoms and one oxygen atom. Dalton's picture of the atom as a hard ball is the basis behind the molecular models we use today.

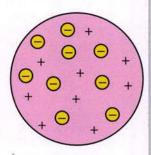
### **Nature of Science**

Dalton's atomic theory was not accepted when it was first proposed. Many scientists considered it as nothing more than a useful fiction which should not be taken too seriously. Over time, as the supporting evidence grew, this changed to its widespread acceptance. These revolutions in understanding, or 'paradigm shifts', are characteristic of the evolution of scientific thinking.

One of the barriers to the acceptance of Dalton's model of the atom was opposition from leading scientists such as Kelvin. In what ways can influential individuals help or hinder the development of scientific knowledge?

Atoms contain electrons

The first indication that atoms were destructible came at the end of the 19th century when the British scientist J. J. Thomson discovered that different metals produce a stream of negatively charged particles when a high voltage is applied across two electrodes. As these particles, which we now know as **electrons**, were the same regardless of the metal, he suggested that they are part of the make-up of all atoms.



### **Nature of Science**

The properties of electrons, or cathode rays as they were first called, could only be investigated once powerful vacuum pumps had been invented – and once advances had been made in the use and understanding of electricity and magnetism. Improved instrumentation and new technology are often the drivers for new discoveries.

**S1.2 Figure 2** Thomson's 'plum pudding' model of the atom. The negatively charged electrons (yellow) are positioned in a positively charged sponge-like substance (pink).

As Thomson knew that the atom had no net charge, he pictured the atom as a 'plum pudding', with the negatively charged electrons positioned in a positively charged sponge-like substance (Figure 2).

### Atoms contain a nucleus

Ernest Rutherford (1871–1937) and his research team working at Manchester University in England, tested Thomson's model by firing alpha particles at a piece of gold foil. If Thomson's model was correct, the alpha particles should either pass straight through or get stuck in the positive 'sponge'. Most of the alpha particles did indeed pass straight through, but a very small number were repelled.

When Rutherford's team reported that they had seen a small number of alpha particles deflected by small angles, he asked them to see if any of the alpha particles had bounced back. This was a very unusual suggestion to make at the time, with little logical justification. What is the role of intuition in the pursuit of scientific knowledge?

The large number of undeflected particles led Rutherford to the conclusion that the atom is mainly empty space. Large deflections occur when the positively charged alpha particles collide with, and are repelled by, a positively charged nucleus. The fact that only a small number of alpha particles bounce back suggests that the nucleus is very small.



TOK

### **Nature of Science**

Our knowledge of the nuclear atom came from Rutherford's experiments with the relatively newly discovered alpha particles. Progress in science often follows technological developments that allow new experimental techniques.



### **Nature of Science**

Rutherford used his model of a positively charged nucleus to derive an equation for the scattering pattern of the alpha particles. His derivation assumed that only electrostatic repulsive forces acted between the positive gold nucleus and the positive alpha particles. All models have limitations which need to be considered in their application.

### Challenge yourself

2. The derivation of the Rutherford formula is based on the assumption that only electrostatic forces need to be considered during the scattering process. Suggest why the experimental results deviate from this model for high-energy alpha particles.

### Subatomic particles

A hundred years or so after Dalton first proposed his model, further experiments showed that the nucleus of an atom is made up of **protons** and **neutrons**, collectively called **nucleons**. Protons and neutrons have almost the same mass and together account for most of the mass of the atom. Electrons, which have a charge equal and opposite to that of the proton, have generally negligible mass and occupy the space in the atom outside of the nucleus.

The absolute masses and charges of these fundamental particles are given in Section 2 of the data booklet and this table gives their relative masses and charges. Note that relative quantities are ratios and so have no units.

Subatomic particle	Relative mass	Relative charge
proton	1	+1
electron	0.0005	-1
neutron	1	0



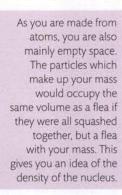
You should know the relative masses and charges of the subatomic particles. Actual values are given in the data booklet. The mass of the electron can generally be considered to be negligible.

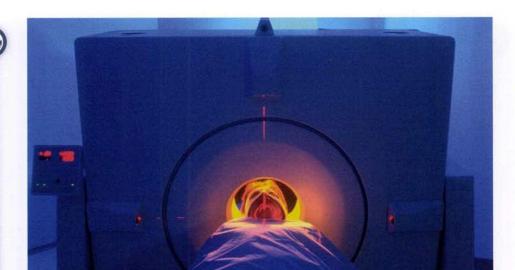


### **Nature of Science**

The description of subatomic particles given here is sufficient to understand chemistry but it is incomplete. Although the electron is indeed a fundamental particle, we now know that protons and neutrons are both themselves made up of more fundamental particles called quarks. We also know that all particles have anti-particles. The positron is the anti-particle of an electron; it has the same mass but has an equal and opposite positive charge. When particles and anti-particles collide, they destroy each other and release energy in the form of high-energy **photons** called gamma rays. Our treatment of subatomic particles is in line with the principle of Occam's razor, which states that theories should be as simple as possible while maximizing explanatory power.

PET (positron-emission tomography) scanners give three-dimensional images of tracer concentration in the body, and can be used to detect cancers. The patient is injected with a tracer compound labelled with a positron-emitting isotope. The positrons collide with electrons after travelling a short distance (≈1 mm) within the body. Both particles are destroyed, and two photons are produced. The protons can be collected by the detectors surrounding the patient, and used to generate an image.





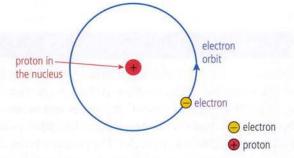
A patient undergoing a positron-emission tomography (PET) brain scan. A radioactive tracer is injected into the patient's bloodstream, which is then absorbed by active tissues of the brain. The PET scanner detects photons emitted by the tracer and produces 'slice' images.

### Challenge yourself

**3.** Construct an equation for the collision of an electron and a positron to give two photons and explain why it is balanced.

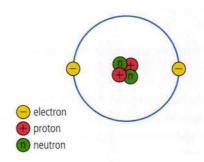
### Bohr model of the hydrogen atom

The Danish physicist Niels Bohr pictured the hydrogen atom as a small 'solar system', with an electron moving in an orbit (energy level) around the positively charged nucleus of one proton (Figure 3). The electrostatic force of attraction between the oppositely charged subatomic particles prevents the electron from leaving the atom. The nuclear radius is  $10^{-15}$  m and the atomic radius  $10^{-10}$  m, so most of the volume of the atom is empty space.



**\$1.2 Figure 3** The Bohr model of the simplest atom. Only one proton and one electron make up the hydrogen atom. Most of the volume of the atom is empty – the only occupant is the single negatively charged electron. It is useful to think of the electron orbiting the nucleus in a similar way to the planets orbiting the Sun. The absence of a neutron is significant – it would be essentially redundant as there is only one proton.

The existence of neutrally charged neutrons is crucial for the stability of nuclei of elements that have more than one proton (Figure 4). Without the neutrons, the positively charged protons would mutually repel each other and the nucleus would fall apart.

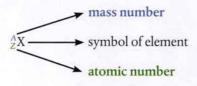


### Atomic number and mass number

We are now in a position to understand how the atoms of different elements differ. They are all made from the same basic ingredients, the subatomic particles. The only difference is the recipe – how many of each of these subatomic particles are present in the atoms of different elements. If you look at the periodic table, you will see that the elements are each given a number which describes their relative position in the table. This is their **atomic number**. We now know that the atomic number, represented by Z, is the defining property of an element as it tells us something about the structure of the atoms of the element. The atomic number is defined as the number of protons in the atom.

As an atom has no overall charge, the positive charge of the protons must be balanced by the negative charge of the electrons. Therefore the atomic number is also equal to the number of electrons in an atom.

The electron has such a very small mass that it is essentially ignored in mass calculations. The mass of an atom depends on the number of protons and neutrons only. The **mass number**, given the symbol **A**, is defined as the number of protons plus the number of neutrons in an atom. An atom is identified in the following way:

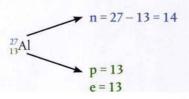


We can use these numbers to find the composition of any atom.

number of protons (p) = number of electrons = Z

number of neutrons (n) = mass number – number of protons = A - Z

Consider an atom of aluminium:



An aluminium atom has 13 protons and 13 electrons. An atom of gold on the other hand has 79 protons and 79 electrons. Can you find gold in the periodic table? The periodic table arranges the elements in order of their atomic number as discussed in Structure 3.1.

■ S1.2 Figure 4 The Bohr model of a helium atom. The two neutrons allow the two protons, which repel each other, to stay in the nucleus. A strong nuclear force acts between all the nucleons which is larger than the repulsive electrostatic forces that act between the protons.

None of these TOK subatomic particles can be (or ever will be) directly observed. What assumptions

are made when we interpret indirect evidence gained through the use of technology?

The atomic number is defined as the number of protons in the nucleus.

Make sure you have a precise understanding of the terms. The atomic number, for example, is defined in terms of the number of protons, not electrons.

The mass number (A) is the number of protons plus the number of neutrons in an atom. It is sometimes called the nucleon number.

Build an atom PhET activity. Full details on how to carry out this activity with a worksheet are available in the eBook.

> Structure 3.1 - How does the atomic number relate to the position of an element in the periodic table?

A





### Challenge yourself

- **4.** Explain why the 13 protons in aluminium stay in the nucleus despite their mutual repulsion.
- **5.** Experiments show the nuclear radius R depends on the mass number A according to the expression:  $R = 1.2 \times 10^{-15} A^{\frac{1}{3}}$ . Deduce an expression for the density of a nucleus and comment on your result.

### Worked example

Identify the subatomic particles present in an atom of <sup>226</sup>Ra.

### Solution

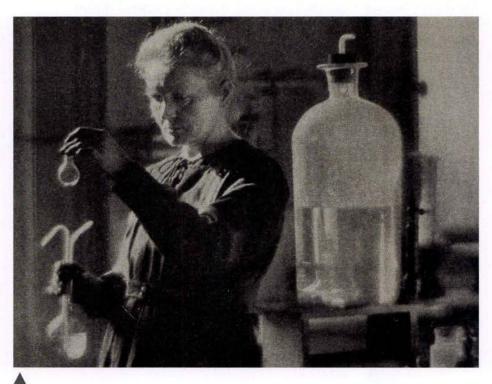
The number identifying the atom is the atomic number. We can find the atomic number from the data booklet (Section 6).

We have Z = 88 and A = 226

number of protons (p) = 88

number of electrons (e) = 88

number of neutrons (n) = 226 - 88 = 138

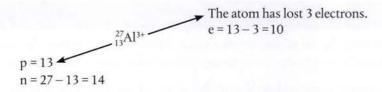


The element radium was first discovered by the Polish–French scientist Marie Curie. She is the only person to win Nobel Prizes in both Physics and Chemistry. The Curies were a remarkable family for scientific honours – Marie shared her first prize with her husband Pierre, and her daughter Irène shared hers with her husband Frédéric. All the Curies' prizes were for work on radioactivity.

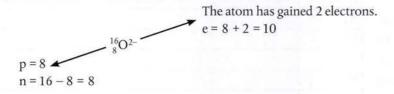
### lons

The atomic number is defined in terms of the number of protons because it is a fixed characteristic of the element. The number of protons identifies the element in the same way your fingerprints identify you. The number of protons and neutrons never changes during a chemical reaction. It is the electrons which are responsible for chemical change. Structure 2.1 examines how atoms can lose or gain electrons to form **ions**. When the number of protons in a particle is no longer balanced by the number of electrons, the particle has a non-zero charge. When an atom loses electrons, it forms a positive ion or **cation**, as the number of protons is now greater than the number of electrons. Negative ions or **anions** are formed when atoms gain electrons. The magnitude of the charge depends on the number of electrons lost or gained. The loss or gain of electrons makes a very big difference to the chemical properties. You swallow sodium ions, Na<sup>+</sup>, every time you eat table salt, whereas (as covered in Structure 3.1) sodium atoms, Na, are dangerously reactive.

An aluminium ion is formed when the atom loses three electrons. There is no change in the atomic or mass numbers of an ion because the number of protons and neutrons remains the same.



Oxygen forms the oxide ion when its atoms gain two electrons.



### Worked example

Most nutrient elements in food are present in the form of ions. The calcium ion  $^{40}$ Ca $^{2+}$ , for example, is essential for healthy teeth and bones. Identify the subatomic particles present in the ion.

#### Solution

We can find the atomic number from the data booklet (Section 6). We have Z = 20 and A = 40:

- number of protons (p) = 20
- number of neutrons (n) = 40 20 = 20

As the ion has a positive charge of 2+ there are two more protons than electrons:

• number of electrons = 20 - 2 = 18



When an atom loses electrons, a positive ion is formed and when an atom gains electrons, a negative ion is formed. Positive ions are called cations and negative ions are called anions.



Structure 1.3 – What determines the different chemical properties of atoms?

### Worked example

Identify the species with 19 protons, 20 neutrons and 18 electrons.

### Solution

- the number of protons tells us the atomic number, Z = 19, and so the element is potassium, K
- the mass number = p + n = 19 + 20 = 39:  $_{19}^{39}$ K
- the charge = p e = 19 18 = +1 as there is one extra proton:  ${}_{19}^{39}K^+$

### Challenge yourself

**6.** We generally make the approximation that the mass of an ion is the same as that of the corresponding atom. To how many significant figures is this approximation valid for the H<sup>+</sup> ion?

### Exercise

- **Q1.** Explain why the relative atomic mass of tellurium is greater than the relative atomic mass of iodine, even though iodine has a greater atomic number.
- **Q2.** Use the periodic table to identify the subatomic particles present in the following species.

Species	No. of protons	No. of neutrons	No. of electrons
<sup>7</sup> Li			
<sup>1</sup> H			
14C	The second second		SIEN MAN
19F-			
<sup>56</sup> Fe <sup>3+</sup>		N PERSONAL PROPERTY.	

**Q3.** Isoelectronic species have the same number of electrons. Identify the following isoelectronic species by giving the correct symbol and charge. You will need a periodic table.

The first one has been done as an example.

Species	No. of protons	No. of neutrons	No. of electrons
<sup>40</sup> Ca <sup>2+</sup>	20	20	18
	18	22	18
	19	20	18
THE LINE	17	18	18

- **Q4.** What is the difference between two neutral atoms represented by the symbols  ${}^{14}_{6}\text{C}$  and  ${}^{14}_{7}\text{N}$ ?
  - I. the number of neutrons II. the number of protons
  - III. the number of electrons
  - A I and II only B I and III only C II and III only D I, II and III

### Structure 1.2.2 - Isotopes

### Structure 1.2.2 – Isotopes are atoms of the same element with different numbers of neutrons.

Perform calculations involving non-integer relative atomic masses and abundance of isotopes from given data.

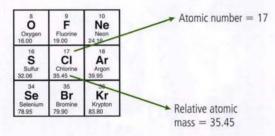
Differences in the physical properties of isotopes should be understood.

Specific examples of isotopes need not be learned.

Nature of Science, Reactivity 3.4 – How can isotope tracers provide evidence for a reaction mechanism?

## Isotopes are atoms of the same element with different numbers of neutrons

Find chlorine in the periodic table. There are two numbers associated with the element, as shown below.



How can an element have a fractional relative atomic mass if protons and neutrons each have a relative mass of 1? One reason is that atoms of the same element with different mass numbers exist, and the relative atomic mass given in the periodic table is an average value.

To have different mass numbers, the atoms must have different numbers of neutrons — all the atoms have the same number of protons as they are all chlorine atoms. Atoms of the same element with different numbers of neutrons are called **isotopes**.

The isotopes show the same chemical properties, as a difference in the number of neutrons makes no difference to how atoms react and so they occupy the same place in the periodic table.

Chlorine exists as two isotopes,  $\frac{35}{17}\text{Cl}$  and  $\frac{37}{17}\text{Cl}$ . The average relative mass of the isotopes is, however, not 36, but 35.45. This value is closer to 35 as there are more  $\frac{35}{17}\text{Cl}$  atoms in nature – it is the more *abundant* isotope. In a sample of 1000 chlorine atoms, there are 775 atoms of  $\frac{35}{17}\text{Cl}$  and 225 atoms of the heavier isotope,  $\frac{37}{17}\text{Cl}$ .

To work out the average mass of one atom, we first have to calculate the total mass of the thousand atoms:

total mass = 
$$(775 \times 35) + (225 \times 37) = 35450$$
  
relative average mass =  $\frac{\text{(total mass)}}{\text{(number of atoms)}} = \frac{35450}{1000} = 35.45$ 



Modelling isotopic abundance. Full details on how to carry out this experiment with a worksheet are available in the eBook.



Isotopes are atoms of the same element with different mass numbers.



The word 'isotope' derives from the Greek for 'same place'. As isotopes are atoms of the same element, they occupy the same place in the periodic table.

A common error is to misunderstand the meaning of 'physical property'. A difference in the number of neutrons is not a different physical property. A physical property of a substance can be measured without changing the chemical composition of the substance. Density and boiling point are examples of physical properties.

Uranium consists of two natural isotopes: mostly U-238 and less than 1% U-235. The fuel used in nuclear power stations is U-235; its content needs to be increased to around 3-5% of the overall mixture to make a controlled nuclear fission reaction feasible. The enrichment can be carried out by gas diffusion, by heating solid uranium hexafluoride (UF6). The UF<sub>6</sub> molecules containing U-235 are lighter and diffuse faster through the pipelines and filters, producing a UF<sub>6</sub> gas that is enriched with U-235.

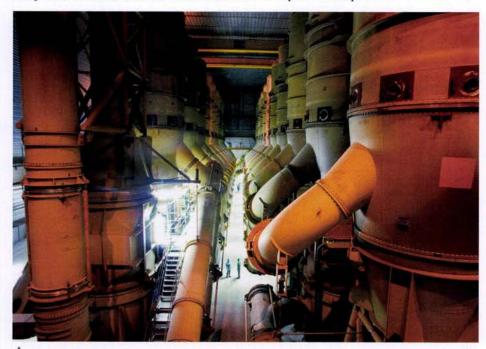
Nature of Science, Reactivity 3.4 - How can isotope tracers provide evidence for a reaction mechanism?



The two isotopes are both atoms of chlorine with 17 protons and 17 electrons.

- $\begin{bmatrix} \frac{35}{17} \text{Cl} \\ \text{number of neutrons} = 35 17 = 18 \end{bmatrix}$
- $\frac{37}{17}$ Cl number of neutrons = 37 17 = 20

Although both isotopes essentially have the same chemical properties, the difference in mass does lead to different physical properties such as boiling and melting points. As explained in Structure 1.1, heavier particles move more slowly at a given temperature and these differences can be used to separate isotopes.



Gas diffusion machinery in southern France used to enrich uranium for use in nuclear reactors.

### Challenge yourself

Suggest why isotope nuclear enrichment plants based on gaseous diffusion are so large.



The stability of a nucleus depends on the balance between the number of protons and neutrons. A nucleus which contains either too many or too few neutrons to be stable is radioactive and changes to a more stable nucleus by giving out radiation. As these **radioisotopes** behave chemically in the same way as nonradioactive isotopes, they can be used as tracers to follow the movement of elements or compounds in complex processes such as living systems. The radioisotopes can be located because the radioactivity they emit can be detected. Radioactive isotopes can also provide evidence for the reaction mechanisms explored in Reactivity 3.4.



Human activities have caused increased atmospheric nitrogen pollution, mainly nitrogen oxides and ammonia. This nitrogen is eventually taken up by plants, increasing plant growth. Evidence for this comes from experiments using tracer isotopes of nitrogen  $\binom{15}{7}N$  to follow the nitrogen through the air and plants.



Evidence for increased nitrogen pollution comes from experiments using tracer isotopes of nitrogen  $\binom{15}{7}$ N) in plants.

### Challenge yourself

**8.** Use the periodic table in the data booklet to identify an element with an atomic number of less than 80 which has no stable isotopes.

### **Exercise**

- **Q5.** State two physical properties other than boiling point and melting point that would differ for the two isotopes of chlorine.
- **Q6.** Identify the particles which account for the existence of isotopes.
  - A electrons
- B nucleons
- C neutrons
- **D** protons
- Q7. Which of the following species contains more electrons than neutrons?
  - $A^{2}H$
- B 11 B
- C 16 O2-
- **D** 19 F
- Q8. Which of the following gives the correct composition of the <sup>71</sup>Ga<sup>+</sup> ion?

Protons	Neutrons	Electrons
31	71	30
31	40	30
31	40	32
32	40	31

**Q9.** Chromium has an atomic number of 24. The mass numbers of its four stable isotopes are 50, 52, 53 and 54.

Identify the correct statements about the isotopes.

- I. All the isotopes have the same chemical properties.
- II. All the isotopes have nuclei containing 24 protons.
- III. One of the isotopes has 54 neutrons.
- A I and II only B I and III only C II and III only D I, II and III
- Q10. Identify the atoms which are isotopes.

	Mass number	Atomic number
W	52	24
X	53	25
Y	53	24
Z	52	25

- A Wand Z
- B X and Y
- C Wand Y
- D Y and Z
- **Q11.** The relative atomic mass of silicon is 28.09. Comment on the claim that no atom of silicon exists with this relative mass.
- Q12. Deduce the composition of a nucleus of boron-11, 11/8.

	Protons	Neutrons
A	5	11
В	11	5
C	6	5
D	5	6

- **Q13.** What is the same for an atom of phosphorus-26 and an atom of phosphorus-27?
  - A atomic number and mass number
  - B number of protons and electrons
  - C number of neutrons and electrons
  - D number of protons and neutrons

HL

### Structure 1.2.3 - Mass spectra

Structure 1.2.3 – Mass spectra are used to determine the relative atomic masses of elements from their isotopic composition.

Interpret mass spectra in terms of identity and relative abundance of isotopes.

The operational details of the mass spectrometer will not be assessed.

Structure 3.2 – How does the fragmentation pattern of a compound in the mass spectrometer help in the determination of its structure?

# Mass spectra are used to determine the relative atomic masses of elements from their isotopic composition

## The mass spectrometer can measure the mass and abundance of isotopes

The masses of the different isotopes and their relative abundance can be measured using a mass spectrometer.

The element to be tested is first vaporized so that individual atoms can be analysed. The atoms are then ionized by high-energy electrons which knock out an electron to produce a positively charged ion:

$$X(g) + e^- \rightarrow X^+(g) + 2e^-$$

The positively charged ions are attracted to a negatively charged plate and deflected by a magnetic field placed at right angles to their path. The amount of deflection is inversely proportional to their  $\mathbf{mass/charge}$  (m/z) ratio. This is equivalent to the mass when the ions have a single positive charge. Single-charge ions with smaller mass are deflected more than heavier ions with the same charge.

If a compound is analysed in a mass spectrometer, the electron collisions during the ionization step are so energetic that they can cause the molecule to break up into different fragments. The resulting **fragmentation pattern** provides useful evidence about the structure of the compound. A chemist pieces together the fragments to form a picture of the complete molecule, in the same way that archaeologists find clues about the past from the pieces of artefacts discovered in the ground. Fragmentation patterns are explored more fully in Structure 3.2.

### The relative atomic mass of an element

The mass of a hydrogen atom is  $1.67 \times 10^{-24} g$  and that of a carbon atom is  $1.99 \times 10^{-23} g$ . As the masses of all elements are in the range  $10^{-24}$  to  $10^{-22} g$ , and as these numbers are beyond our direct experience, it makes more sense to use relative values. The mass needs to be recorded relative to some agreed standard. As carbon is a very common element which is easy to transport and store because it is a solid, its isotope,  $^{12}C$ , was chosen as the standard in 1961. This is discussed in Structure 1.4 and  $^{12}C$  is given a relative mass of exactly 12, as shown below.

Element	Symbol	Relative atomic mass
carbon	C	12.011
chlorine	Cl	35.453
hydrogen	Н	1.008
iron	Fe	55.845
Standard isotope	Symbol	Relative atomic mass
carbon-12	<sup>12</sup> C	12.000



Structure 3.2 - How does the fragmentation pattern of a compound in the mass spectrometer help in the determination of its structure?



You will not be assessed on the operational details of the mass spectrometer but you should include the positive charge when identifying the ions in a mass spectrum.



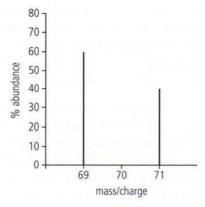
The relative atomic mass of an element (A<sub>r</sub>) is the average mass of an atom of the element, taking into account all its isotopes and their relative abundance, compared to one atom of carbon-12.

Carbon-12 is the most abundant isotope of carbon but carbon-13 and carbon-14 also exist. This explains why the average value for the element is greater than 12.

### Mass spectra

The results of the analysis by a mass spectrometer are presented in the form of a **mass spectrum**. As discussed earlier, the mass spectrometer measures the mass/charge ratio of the deflected particles and this is displayed on the horizontal axis using the carbon-12 scale. In most cases the charge of the ion is +1 so the horizontal axis generally also gives the mass. The relative abundance of the ions corresponding to different isotopes is shown on the vertical axis.

The mass spectrum of gallium in Figure 5 shows that in a sample of 100 atoms, 60 have a mass of 69 and 40 have a mass of 71. We can use this information to calculate the relative atomic mass of the element.



**S1.2 Figure 5** Mass spectrum for gallium. The number of lines indicates the number of isotopes (two in this case), the value on the x-axis indicates their mass numbers (69 and 71) and the y-axis shows the percentage abundance.

total mass of 100 atoms = 
$$(60 \times 69) + (40 \times 71) = 6980$$

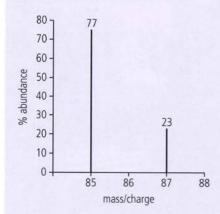
relative average mass = 
$$\frac{\text{total mass}}{\text{number of atoms}} = \frac{6980}{100} = 69.80$$

### Challenge yourself

Suggest how the mass spectrum of gallium changes if the kinetic energy of the electrons used in ionizing the sample in a mass spectrometer is significantly increased.

### Worked example

Deduce the relative atomic mass of the element rubidium from the data given in the graph.



#### Solution

Consider a sample of 100 atoms.

total mass of 100 atoms = 
$$(85 \times 77) + (87 \times 23) = 8546$$

relative atomic mass = average mass of atom = 
$$\frac{\text{total mass}}{\text{number of atoms}} = \frac{8546}{100} = 85.46$$

### Worked example

Boron exists as two isotopes,  $^{10}$ B and  $^{11}$ B.  $^{10}$ B is used as a control for nuclear reactors. Use your periodic table to find the abundances of the two isotopes.

#### Solution

Consider a sample of 100 atoms.

Let x atoms be  $^{10}$ B atoms. The remaining atoms are  $^{11}$ B.

number of <sup>11</sup>B atoms = 100 - x

total mass of 100 atoms = 
$$[x \times 10] + [(100 - x) \times 11] = 10x + 1100 - 11x = 1100 - x$$

average mass = 
$$\frac{\text{total mass}}{\text{number of atoms}} = \frac{1100 - x}{100}$$

From the periodic table, the relative atomic mass of boron = 10.81.

$$10.81 = \frac{1100 - x}{100}$$

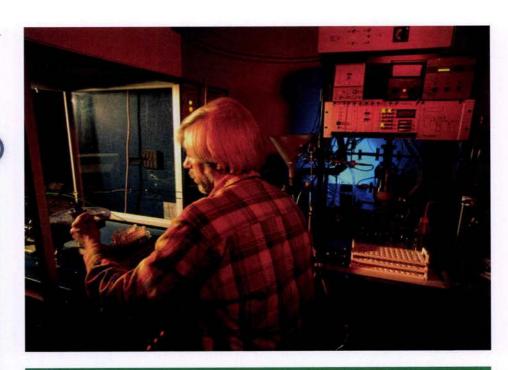
$$1081 = 1100 - x$$

$$x = 1100 - 1081 = 19$$

The abundances are  ${}^{10}B = 19\%$  and  ${}^{11}B = (100 - 19) = 81\%$ 

A mass spectrometer used in radiocarbon dating. The ratio of radioactive <sup>14</sup>C to stable <sup>12</sup>C is related to the time since the death of the animal or plant being investigated.

Carbon-14 has eight neutrons, which is too many to be stable. It can reduce the neutron-to-proton ratio by radioactive decay. The relative abundance of carbon-14 present in living plants is constant as the carbon atoms are continually replenished from the carbon present in atmospheric carbon dioxide. When organisms die, however, no more carbon-14 is absorbed and the levels of carbon-14 fall as they decay. As this process occurs at a regular rate, it can be used to date carbon-containing materials.



### **Exercise**

Q14. A sample of chromium has the following isotopic composition by mass.

Isotope	<sup>50</sup> Cr	<sup>52</sup> Cr	<sup>53</sup> Cr	<sup>54</sup> Cr	
Relative abundance / %	4.31	83.76	9.55	2.38	

Calculate the relative atomic mass of chromium based on these data, giving your answer to two decimal places.

- **Q15.** Use the periodic table to find the percentage abundance of neon-20, if neon has only one other isotope, neon-22.
- **Q16.** Magnesium has three stable isotopes: <sup>24</sup>Mg, <sup>25</sup>Mg, and <sup>26</sup>Mg. The lightest isotope has an abundance of 78.90%. Calculate the percentage abundance of the other isotopes.
- **Q17.** The relative abundances of the two isotopes of chlorine are shown in this table:

Isotope		Relative abundance		
	35Cl	75%		
	<sup>37</sup> Cl	25%		

Use this information to deduce the mass spectrum of chlorine gas, Cl<sub>2</sub>.



In 1911, a 40 kg meteorite fell in Egypt. Isotopic and chemical analyses of oxygen extracted from this meteorite showed a different relative atomic mass to that of oxygen normally found on Earth. The relative atomic mass value did however match measurements made of the Martian atmosphere by the Viking landing in 1976. This provides strong evidence that the meteorite had originated from Mars.

### Challenge yourself

Oxygen atoms in water molecules from two different samples in an ice core were analysed.

	Sample 1		Sample 2	
isotope	<sup>16</sup> O	18O	16O	18O
relative abundance / %	99.759	0.241	99.757	0.243

Determine the relative mass of oxygen in the two samples and identify which sample originated from higher historic temperatures.

**11.** Bromine is a mixture of two isotopes with mass numbers 79 and 81. They are naturally present in equal amounts.

The relative abundances of the two isotopes of chlorine are  $^{35}$ Cl (75%) and  $^{37}$ Cl (25%).

Calculate the percentage of naturally occurring CH<sub>2</sub>BrCl molecules with a relative molecular mass of 128.

You can assume that the carbon atoms have a mass number of 12 and the hydrogen atoms have a mass number of 1.

HL end



### **Guiding Question revisited**

How do the nuclei of atoms differ?

In this chapter we explored the structure of the atom and how the nuclei of atoms differ.

- All atoms are made up of protons, neutrons and electrons.
- The protons and neutrons, which contribute most of the mass of the atom, are
  in a small dense nucleus surrounded by electrons which occupy most of the
  volume of the atom.
- The atomic number gives the atom its identity. This is the number of protons in the nucleus. In a neutral atom this is also the number of electrons.
- The mass number is the number of nucleons: the number of protons and neutrons in the nucleons.
- Evidence shows that most elements have more than one isotope: atoms with the same number of protons but a different number of neutrons.
- The relative atomic mass, which is the average mass of an atom, can be determined from the relative abundance of its isotopes.

### HL

- The mass of individual atomic masses can be measured by a mass spectrometer.
- A mass spectrum shows the relative abundance of the different isotopes of an element.

HL end



### **Practice questions**

1.	Which statements ab	out the isotop	es of chlorine	, 35 Cl and	1 37 Cl, are correct?
----	---------------------	----------------	----------------	-------------	-----------------------

I. They have the same chemical properties.

II. They have the same atomic number.

III. They have the same physical properties.

A I and II only

B I and III only

C II and III only

D I, II and III

2. Which statement about the numbers of protons, electrons and neutrons in an atom is always correct?

A The number of neutrons minus the number of electrons is zero.

**B** The number of protons plus the number of neutrons equals the number of electrons.

C The number of protons equals the number of electrons.

D The number of neutrons equals the number of protons.

3. Which quantities are the same for all atoms of chlorine?

I. number of protons

II. number of neutrons

III. number of electrons

A I and II only

B I and III only

C II and III only

D I. II and III

**4.** How many electrons does the ion  ${}_{15}^{31}P^{3-}$  contain?

A 12

B 15

C 16

D 18

**4.** Deduce the number of elementary particles present in the  $^{55}_{25}Mn^{2+}$  ion. (3)

(Total 3 marks)

6. A sample of iron has the following isotopic composition by mass.

Isotope	<sup>54</sup> Fe	<sup>56</sup> Fe	<sup>57</sup> Fe
Relative abundance / %	5.95	91.88	2.17

Calculate the relative atomic mass of iron based on these data, giving your answer to two decimal places.

(Total 2 marks)

(2)

(1)

7. (a) Explain why the relative atomic mass of cobalt is greater than the relative atomic mass of nickel, even though the atomic number of nickel is greater than the atomic number of cobalt. (1)

**(b)** Deduce the numbers of protons and electrons in the Co<sup>2+</sup> ion.

(Total 2 marks)

8. The table below refers to a sample of silicon.

Mass number of isotope	28	29	30	
Relative abundance / %	92.18	4.70	3.12	F.

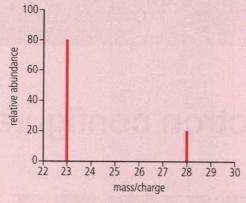
- (a) Explain why atoms of an element can have different mass numbers. (1)
- **(b)** Compare the chemical properties of the four isotopes and justify your answer.
- (c) HL Identify the instrument used to collect these data. (1)
- (d) Calculate the relative atomic mass of this sample of silicon. (2)

(Total 5 marks)

(1)

HL

**9.** What is the relative atomic mass of an element with the following mass spectrum?



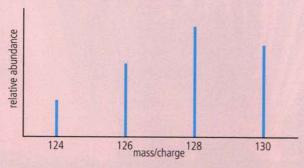
A 24

B 25

C 26

D 27

10. The mass spectrum of an element is shown below.



(a) Identify the element and justify your answer.

(2)

**(b)** Estimate the percentage of the total mass of the element due to neutrons.

(2)

(Total 4 marks)

HL end



The dazzling colours observed during a firework display are a result of electrons moving between different energy states.

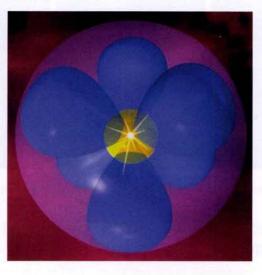




### **Guiding Question**

How can we model the energy states of electrons in atoms?

The chemical behaviour of an atom is determined by its electron configuration. As we cannot look inside the atom directly, we have to look elsewhere for evidence of how the electrons are arranged. The analysis of light emitted from an atom gives us valuable information about the electron configuration within it. It shows that an electron can exist only in certain discrete energy states. This cannot be understood with reference to our everyday experience and demands a new perspective. The notion of particles following fixed trajectories does not apply to the microscopic world of the atom. We can only give a probability description of electron behaviour and use quantum theory to adopt a wave description of the electron. The possible positions of an electron are spread out in space in the same way as a wave spreads through space. We will see how the energy states of electrons are best explained in terms of atomic orbitals. These are regions in space where an electron is likely to be found. Within one atom, there are an infinite number of orbitals of different shapes, sizes and energies. These ideas are revolutionary. As Niels Bohr, one of the principal scientists involved in the development of quantum theory said, 'Anyone who is not shocked by quantum theory has not understood it'.



Electrons occupy atomic orbitals of different energy states. The atomic orbitals in an atom of neon, Ne, are represented here. The nucleus is shown by a flash of light and the 1s orbital as a yellow sphere. The 2s orbital is shown as a pink sphere, and the 2p orbitals as blue lobes.

### Structure 1.3.1 and 1.3.2 - Emission spectra

Structure 1.3.1 – Emission spectra are produced by atoms emitting photons when electrons in excited states return to lower energy levels.

Qualitatively describe the relationship between colour, wavelength, frequency and energy across the electromagnetic spectrum.

Distinguish between a continuous and a line spectrum.

Details of the electromagnetic spectrum are given in the data booklet.

### Structure 1.3.2 – The line emission spectrum of hydrogen provides evidence for the existence of electrons in discrete energy levels, which converge at higher energies.

Describe the emission spectrum of the hydrogen atom, including the relationships between the lines and energy transitions to the first, second and third energy levels.

The names of the different series in the hydrogen emission spectrum will not be assessed.

Inquiry 2 – In the study of emission spectra from gaseous elements and from light, what qualitative and quantitative data can be collected from instruments such as gas discharge tubes and prisms?

Nature of Science, Structure 1.2 – How do emission spectra provide evidence for the existence of different elements?

## Atoms of different elements give out light of distinctive colours

Atoms of different elements give out light of a distinctive colour when an electric discharge is passed through a vapour of the element. Similarly, metals can be identified by the colour of the flame produced when their compounds are heated in a Bunsen burner. Analysis of the light emitted by different atoms gives us insights into the electron configurations within the atom.

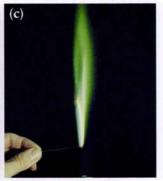
Flame tests on the compounds of (a) sodium, (b) potassium and (c) copper.

Flame colours can be used to identify unknown compounds. Full details of how to carry out a flame test experiment with a worksheet are available in the eBook.







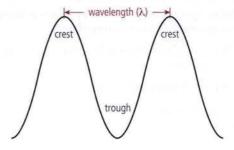


To interpret these results, we must consider the nature of electromagnetic radiation.

## Electromagnetic radiation is emitted in different forms of differing energies

Electromagnetic radiation comes in different forms of differing energy. The visible light we need to see the world is only a small part of the full spectrum, which ranges from low-energy radio waves to high-energy gamma ( $\gamma$ ) rays. All electromagnetic waves travel at the same **speed** (c) but can be distinguished by their different **wavelengths** ( $\lambda$ ) (Figure 1).

**S1.3 Figure 1** Snapshot of a wave at a given instant. The distance between successive crests or peaks is called the wavelength (λ).



Different colours of visible light have different wavelengths; red light, for example, has a longer wavelength than blue light. The full electromagnetic spectrum is given in Section 5 of the data booklet.

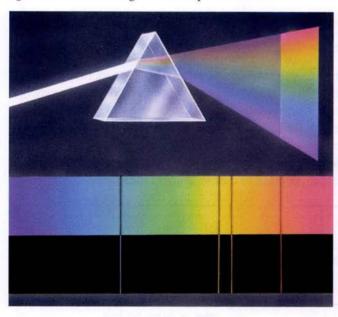
The number of waves that pass a particular point in 1s is called the **frequency** (f); the shorter the wavelength, the higher the frequency. Blue light has a higher frequency than red light.

The precise relation is:

$$c = f\lambda$$

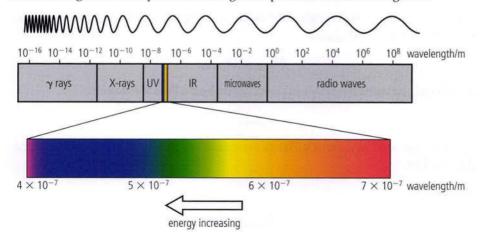
where *c* is the speed of light.

White light is a mixture of light waves of differing wavelengths or colours. We see this when sunlight passes through a prism to produce a **continuous spectrum** or when light is scattered through water droplets in the air.



A continuous spectrum is produced when white light is passed through a prism. The different colours merge smoothly into one another. The two spectra below the illustration of the prism show (top) a continuous spectrum with a series of discrete absorption lines, and (bottom) a line emission spectrum. Details of the absorption spectrum will not be assessed.

As well as visible light, atoms emit infrared (IR) radiation, which has a longer wavelength than red light, and ultraviolet radiation, which has a shorter wavelength than violet light. The complete electromagnetic spectrum is shown in Figure 2.



i

All electromagnetic waves travel at the same speed,  $c = 3.00 \times 10^8 \, \text{m s}^{-1}$ . This is the cosmic speed limit as, according to Einstein's Theory of Relativity, nothing in the universe can travel faster than this in a vacuum.

a

The distance between two successive crests (or troughs) is called the wavelength ( $\lambda$ ). The frequency (f) of the wave is the number of waves that pass a point in one second. The wavelength and frequency are related by the equation  $c = f \lambda$  where c is the speed of light.

\$1.3 Figure 2 The changing wavelength (in m) of electromagnetic radiation through the spectrum is shown by the trace across the top. At the short wavelength end (on the left) of the spectrum are gamma rays, X-rays, and ultraviolet light. In the centre of the spectrum are wavelengths that the human eye can see, known as visible light. Visible light comprises light of different wavelengths, energies, and colours. At the longer wavelength end of the spectrum (on the right) are infrared radiation, microwaves, and radio waves. The visible spectrum gives us only a small window to see the world.

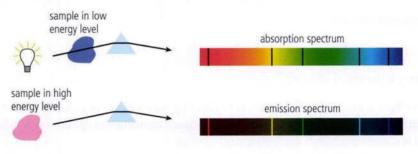
Electromagnetic waves allow energy to be transferred across the universe. They also carry information. Low-energy radio waves are used in radar and television, for example, and higher energy gamma rays are used as medical tracers. The precision with which we view the world is limited by the wavelengths of the colours we can see. This is why we will never be able to see an atom directly; it is too small to interact with the relatively long waves of visible light. What are the implications of this for human knowledge?

**S1.3 Figure 4** Emission spectra are the result of electrons falling from an excited state  $E_2$  to a lower energy level  $E_1$ .

- A continuous spectrum shows an unbroken sequence of frequencies, such as the spectrum of visible light.
- A line emission spectrum has only certain frequencies of light because it is produced by excited atoms and ions as they fall back to a lower energy level.

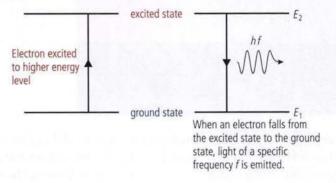
## An emission spectrum is produced when an atom moves from a higher to a lower energy level

When electromagnetic radiation is passed through a collection of atoms, some of the radiation is absorbed and used to excite the atoms from a lower energy level to a higher energy level. A spectrometer analyses the transmitted radiation relative to the incident radiation and an absorption spectrum is produced (Figure 3).



**\$1.3 Figure 3** The origin of absorption and emission spectra. An absorption spectrum shows the radiation absorbed as atoms move from a lower to a higher energy level. An emission spectrum is produced when an atom moves from a higher to a lower level.

Gases produce a characteristic **emission line spectrum** when they are heated to a high temperature or if a high voltage is applied. Atoms are excited into a higher energy level, which is unstable, so the electron soon falls back to the **ground state**. The energy the electron gives out when it falls into lower levels is in the form of electromagnetic radiation. One packet of energy, a **photon**, is released for each electron transition (Figure 4). Photons of ultraviolet light have more energy than photons of infrared light. The energy of the photon is proportional to the frequency of the radiation.



The energy of the photon of light emitted ( $E_{photon}$ ) is equal to the energy change of the electron in the atom ( $\Delta E_{electron}$ ):

$$\Delta E_{\rm electron} = E_{\rm photon}$$

It is also related to the frequency of the radiation by the Planck equation:

$$E_{\rm photon} = hf$$

This equation and the value of h (Planck's constant) are given in Sections 1 and 2 of the data booklet.

This leads to:

$$\Delta E_{\text{electron}} = hf$$

This is a very significant equation because it shows that line spectra allow us to glimpse inside the atom. The atoms emit photons of certain energies, which give lines of certain frequencies because the electron can only occupy certain energy levels. You can think of the energy levels as a staircase. The electron cannot change its energy in a continuous way, in the same way that you cannot stand between steps; it can only change its energy by discrete amounts. This energy of the atom is said to be **quantized**. The line spectrum is crucial evidence for quantization: if the energy were not quantized, the emission spectrum would be continuous.



#### **Nature of Science**

The idea that you can think of electromagnetic waves as a stream of photons, or quanta, is one aspect of quantum theory. The theory has implications for human knowledge and technology. The key idea is that energy can only be transferred in discrete amounts or quanta. Quantum theory shows us that our everyday experience cannot be transferred to the microscopic world of the atom. It has led to great technological breakthroughs such as the modern computer. It has been estimated that 30% of the gross national product of the USA depends on the application of quantum theory. Our scientific understanding has led to many technological developments. These new technologies in turn drive developments in science. The implications of quantum theory for the electron are discussed in more detail later (page 60). Note that 'discrete' has a different meaning to 'discreet'.

As different elements have different line spectra, they can be used like barcodes to identify unknown elements. They give us valuable information about the electron configurations of different atoms.

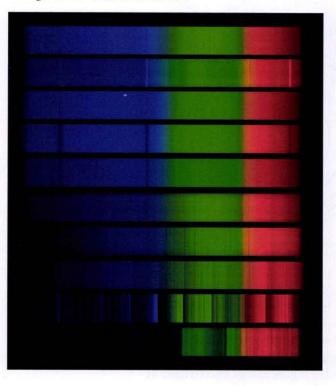


Diagram of the spectra of stars, showing a set of dark absorption lines, which indicate the presence of certain elements, such as hydrogen and helium, in the outer atmosphere of the star.



The words 'discrete' meaning 'separate', and 'discreet' meaning 'unobtrusive' both come from the Latin word 'discretus' for 'to keep separate'.



When asked to distinguish between a line spectrum and a continuous spectrum, references should be made to discrete or continuous energy levels and to specific colours, wavelengths or frequencies.



Elements discovered from their line spectra and named from their flame colours include rubidium (red), caesium (sky blue), thallium (green), and indium (indigo). Emission spectroscopy was a key tool in the discovery of new elements.



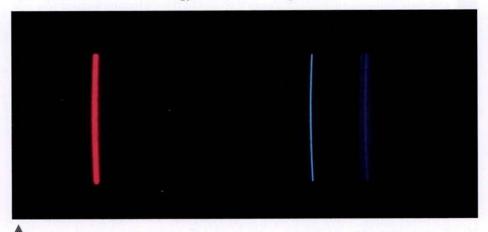
Nature of Science, Structure 1.2 – How do emission spectra provide evidence for the existence of different elements?



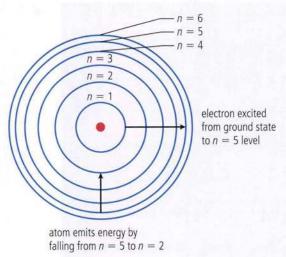
The elemental composition of stars can be determined by analysing their spectra. The gases that surround the center of a star absorb some wavelengths of the star's emitted radiation, producing dark absorption lines in the spectrum. These dark bands can be used to identify the elements present. The Sun's spectrum shows dark lines that represent absorbed radiation due to the presence of hydrogen and helium.

## The line emission spectrum of hydrogen provides evidence for discrete energy levels

As discussed earlier, a line emission spectrum provides evidence for the electrons in an atom occupying discrete energy levels. A simple picture of the hydrogen atom was considered in Structure 1.2 with the electron orbiting the nucleus in a circular energy level. Niels Bohr proposed that an electron moves into an orbit further from the nucleus (a higher energy level) when an atom absorbs energy. This energy is given out in the form of electromagnetic radiation when the electron falls back from a higher to a lower energy level. In any sample of hydrogen many transitions can occur with each line corresponding to a particular transition. Visible light is produced when the electron falls to the second energy level (n = 2; see Figure 5).

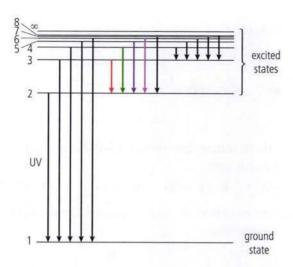


Visible emission spectrum of hydrogen. The energy of lines increases from left to right. They converge at higher energies. Similar series are found in the UV and IR regions.



**S1.3 Figure 5** An electron is excited from the ground state to a higher energy level. If the unstable electron then falls to a lower n = 2 energy level, visible light is emitted.

The transitions to the first energy level (n = 1) correspond to the highest energy change and are in the ultraviolet region of the spectrum. Infrared radiation is produced when an electron falls to the third or higher energy levels (Figure 6).



**S1.3 Figure 6** Energy levels of the hydrogen atom showing the transitions. The transition  $1 \to \infty$  corresponds to ionization:

$$H(g) \rightarrow H^{+}(g) + e^{-}$$

HL This is discussed in more detail later.

The pattern of the lines in Figure 6 gives us a picture of the energy levels in the atom. The lines converge at higher energies because the energy levels inside the atoms are closer together. When an electron is at the highest energy  $n = \infty$ , it is no longer in the atom and the atom has been ionized. The energy needed to remove an electron from the ground state of one mole of gaseous atoms, ions, or molecules is called the **ionization energy**. Ionization energies can also be used to support this model of the atom (see page 74).

#### **Exercise**

- Q1. Emission spectra provide evidence for:
  - A the existence of neutrons
  - **B** the existence of isotopes
  - C the existence of atomic energy levels
  - D the nuclear model of the atom
- **Q2.** The diagram shows the lowest five electron energy levels in the hydrogen atom.

$$n = \frac{1}{2}$$

$$n=3$$

$$n=2$$

Deduce how many different frequencies in the visible emission spectrum of atomic hydrogen would arise as a result of electron transitions between these levels.

A 3

B 4

C 6

D 10

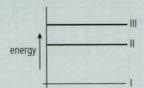


Emission spectra can be observed using discharge tubes of different gases and a spectroscope. The colours and relative intensities of the lines should be observed. The wavelengths can be measured.



Inquiry 2 – In the study of emission spectra from gaseous elements and from light, what qualitative and quantitative data can be collected from instruments such as gas discharge tubes and prisms?

Q3. The diagram shows three energy levels of an atom.



(a) Identify the transition that corresponds to the emission of light with the shortest wavelength.

 $A I \rightarrow II$ 

 $\mathbf{B} \quad \text{II} \to \text{III}$ 

C  $III \rightarrow I$ 

D III → II

**(b)** Identify the emission line spectra that results from transitions between these energy levels.

increasing frequency

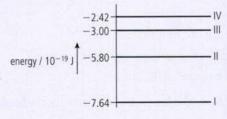
D

increasing frequency

**Q4.** The visible emission spectrum for hydrogen includes a red line with a wavelength of 657 nm corresponding to the transition  $3 \rightarrow 2$ . State if the transition from  $4 \rightarrow 2$  corresponds to a higher or lower wavelength and justify your answer.

# Challenge yourself

1. One of the wavelengths in the emission spectrum of helium occurs at 588 nm. Some energy levels of the helium atom are shown. The energies of the levels are given in joules. Identify the transition that produces the line at 588 nm.



A I→III

 $\mathbf{B} \quad \text{III} \rightarrow \text{I}$ 

 $C \quad II \rightarrow IV$ 

 $\mathbf{D} \quad IV \to II$ 

# Structure 1.3.3, 1.3.4 and 1.3.5 – Electron configuration

Structure 1.3.3 – The main energy level is given an integer number, n, and can hold a maximum of  $2n^2$  electrons.

Deduce the maximum number of electrons that can occupy each energy level.

Structure 3.1 – How does an element's highest main energy level relate to its period number in the periodic table?

Structure 1.3.4 – A more detailed model of the atom describes the division of the main energy level into s, p, d and f sublevels of successively higher energies.

Recognize the shape and orientation of an s atomic orbital and the three p atomic orbitals.

Structure 3.1 – What is the relationship between energy sublevels and the block nature of the periodic table?

Structure 1.3.5 – Each orbital has a defined energy state for a given electron configuration and chemical environment, and can hold two electrons of opposite spin.

Sublevels contain a fixed number of orbitals, regions of space where there is a high probability of finding an electron.

Apply the Aufbau principle, Hund's rule and the Pauli exclusion principle to deduce electron configurations for atoms and ions up to Z = 36.

Full electron configurations and condensed electron configurations using the noble gas core should be covered.

Orbital diagrams, i.e. arrow-in-box diagrams, should be used to represent the filling and relative energy of orbitals.

The electron configurations of Cr and Cu as exceptions should be covered.

# A more sophisticated model is needed for atoms with more than one electron

# Wave and particle models of light and the electron

Although the Bohr model of the atom was able to predict the wavelengths of lines in the emission spectrum of hydrogen with great success, it failed to predict the spectral lines of atoms with more than one electron. The model is a simplification. To develop the model of the atom further, we need to reconsider the nature of light and matter.

We saw earlier that light could either be described by its frequency, f, which is a wave property, or by the energy of individual particles, E (called photons, or quanta, of light), which make up a beam of light. The two properties are related by the Planck equation E = hf. Both wave and particle models have traditionally been used to explain scientific phenomena and you may be tempted to ask which model gives the 'true' description of light. We now realize that neither model gives a complete explanation of light's properties – both models are needed.

- The diffraction, or spreading out, of light that occurs when light passes through a small slit can only be explained by a wave model.
- The scattering of electrons that occurs when light is incident on a metal surface is best explained using a particle model of light.

ток

We have outlined the plum pudding and Bohr models of the atom even though we now know they are incorrect. How can a model be useful even if it is obviously false?

In a similar way, quantum theory suggests that it is sometimes preferable to think of an electron (or indeed any particle) as having wave properties. The diffraction pattern produced when a beam of electrons is passed through a thin sheet of graphite demonstrates the wave properties of electrons. To understand the electron configurations of atoms, it is useful to consider a wave description of the electron.

Demonstration of waveparticle duality. An electron gun is fired at a thin sheet of graphite. The electrons pass through the graphite and hit a luminescent screen, producing the pattern of rings associated with diffraction. Diffraction occurs when a wave passes through an aperture similar in size to its wavelength. Quantum theory shows that electrons have wavelengths inversely proportional to their momentum (momentum is the product of their mass and velocity).



# 8

#### **Nature of Science**

Scientists use models to explain processes that may not be observable. The models can be simple or complex in nature but must match the experimental evidence if they are to be accepted. The power of the wave and particle models is that they are based on our everyday experience, but this is also their limitation. We should not be too surprised if this way of looking at the world breaks down when applied to the atomic scale, as this is beyond our experience. The model we use depends on the phenomena we are trying to explain.

When differences occur between the theoretical predictions and experimental data, the models must be modified or replaced. Bohr's model of the hydrogen atom was very successful in explaining the line spectra of the hydrogen atom but could not explain the spectra of more complex atoms, or the relative intensities of the lines in the hydrogen spectra. It also suffered from a fundamental weakness in that it was based on postulates, which combined ideas from classical and quantum physics in an ad hoc manner, with little experimental justification. Ideally, models should be consistent with the assumptions and premises of other theories. A modification of Bohr's model could only be achieved at the expense of changing our model of the electron as a particle. Dalton's atomic model and quantum theory are both examples of such radical changes of understanding, often called **paradigm shifts**.

What role do paradigm shifts play in the progression of scientific knowledge? Do they play a similar role in other areas of knowledge? ток

# The electron's trajectory cannot be precisely described

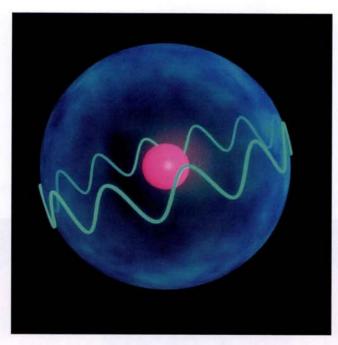
Another fundamental problem with the Bohr model is that it assumes the electron's trajectory can be precisely described. This is now known to be impossible, as any attempt to measure an electron's position will disturb its motion. The act of focusing radiation to locate the electron sends it hurtling off in a random direction.

According to Heisenberg's **Uncertainty Principle** we cannot know where an electron is at any given moment in time – the best we can hope for is a probability picture of where the electron is *likely* to be. The possible positions of an electron are spread out in space in the same way as a wave is spread across a water surface.

# Electrons occupy atomic orbitals

# Schrödinger model of the hydrogen atom

We have seen that the electron can be considered to have wave properties and that only a probability description of its location is possible at a given time. Both of these ideas are encapsulated in the Schrödinger model of the hydrogen atom. Erwin Schrödinger (1887–1961) proposed that a wave equation could be used to describe the behaviour of an electron in the same way that a wave equation could be used to describe the behaviour of light. The equation can be applied to multi-electron systems and its solutions are known as **atomic orbitals**. An atomic orbital is a region around an atomic nucleus in which there is a 90% probability of finding the electron. The shape of the orbitals will depend on the energy of the electron. When an electron is in an orbital of higher energy, it will have a higher probability of being found further from the nucleus.



# Challenge yourself

**2.** State **two** ways in which the Schrödinger model of the hydrogen atom differs from that of the Bohr model.

ток

The Uncertainty Principle states that it is impossible to make an exact and simultaneous measurement of both the position and momentum of any given body. It can be thought of as an extreme example of the observer effect discussed on page 887. The significance of the Uncertainty Principle is that it shows the effect cannot be decreased indefinitely by improving the apparatus. There is an inherent uncertainty in our measurements. What are the implications of this for the limits of human knowledge?

The hydrogen atom shown as a nucleus (a central proton, pink), and an electron orbiting in a wavy path (light blue). It is necessary to consider the wave properties of the electron to understand atomic structure in detail. According to Heisenberg's Uncertainty Principle, the exact position of an electron cannot be defined; atomic orbitals represent regions where there is a high probability of finding an electron.



The progressive nature of scientific knowledge about the atom is illustrated by the Nobel Prizes awarded between 1922 and 1933 to Bohr, Heisenberg and Schrödinger.

Our model of the atom owes a great deal to the work of Niels Bohr and Werner Heisenberg, who worked together in the early years of quantum theory before World War II. But they found themselves on different sides when war broke out. The award-winning play and film Copenhagen is based on their meeting in the city in 1941 and explores their relationship, the uncertainty of the past, and the moral responsibilities of the scientist.

The Pauli exclusion principle states that no more than two electrons can occupy any one orbital, and if two electrons are in the same orbital, they must spin in opposite directions.

a

An electron is uniquely characterized by its atomic orbital and spin. If two electrons occupied the same orbital spinning in the same direction, they would be the same electron – which is impossible!

An orbital shows the volume of space in which the electron is likely to be found.

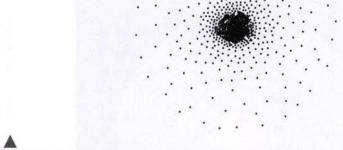


The Schrödinger model of the hydrogen spectrum does not fully explain the fine details of the hydrogen spectrum. The model needs to be further refined: in addition to moving around the nucleus, electrons can also be thought to **spin** on their own axis. They can spin in either a clockwise direction, represented by an upward arrow, or an anti-clockwise direction, represented by a downward arrow. Spin is an important factor in electron—electron interactions. Electrons can occupy the same region of space despite their mutual repulsion if they spin in opposite directions. This leads to the **Pauli exclusion principle**, which states that an orbital can hold only two electrons of opposite spin.

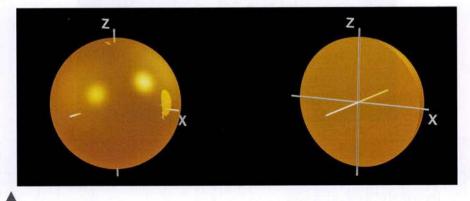
# Atomic orbitals have different shapes and sizes The first energy level has one 1s orbital

We saw that the electron in hydrogen occupies the first energy level in the ground state. This energy level can hold a maximum of two electrons. To highlight the distinction between this wave description of the electron provided by the Schrödinger model and the circular orbits of the Bohr atom, we say the electron occupies a 1s orbital.

The dots in Figure 7 represent locations where the electron is most likely to be found. The denser the arrangement of dots, the higher the probability that the electron occupies this region of space. The electron can be found anywhere within a spherical space surrounding the nucleus.



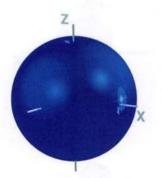
**S1.3 Figure 7** An electron in a 1s atomic orbital. The density of the dots gives a measure of the probability of finding the electron in this region.

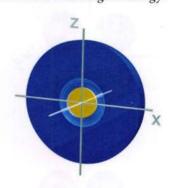


The first energy level consists of a 1s atomic orbital, which is spherical in shape.

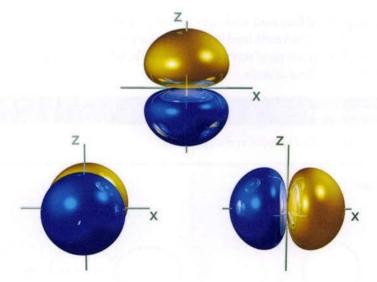
## The second energy level has a 2s and 2p sublevel

The second energy level of the Bohr model is split into two **sublevels** in the Schrödinger model. Further evidence of sublevels comes from a consideration of patterns in first ionization energies, which is discussed on page 74. The 2s sublevel is one 2s orbital and can hold a maximum of two electrons, and the 2p sublevel is three 2p orbitals and can hold six electrons. The 2s orbital has the same symmetry as a 1s orbital but extends over a larger volume. An electron in a 2s orbital is, on average, further from the nucleus than an electron in a 1s orbital and has higher energy.





The three 2p atomic orbitals in the 2p sublevel have equal energy and are said to be **degenerate**. They all have the same dumbbell shape; the only difference is their orientation in space. They are arranged at right angles to each other with the nucleus at the centre.



#### d and f orbitals

We have seen that the first energy level is made up of one sublevel and the second energy level is made up of two sublevels. This pattern can be generalized; the nth energy level of the atom is divided into n sublevels. The third energy level is made up of three sublevels: the 3s, 3p and 3d. The d sublevel is made up of five d atomic orbitals.

The 2s electron orbital. Just as a water wave can have crests and troughs, an orbital can have positive and negative areas. The blue area shows positive values, and the gold area negative. As it is the magnitude of the wave, not the sign, which determines the probability of finding an electron at particular positions, the sign is often not shown.





Investigating orbital shapes with modelling clay. Full details of how to carry out this experiment with a worksheet are available in the eBook.

From left to right, the  $p_{yx}$   $p_{zx}$  and  $p_{xx}$  atomic orbitals, localized along the y, z, and x-axes respectively (the y-axis comes out of the page). As they have the same energy, they are said to be degenerate. They form the 2p sublevel.

The five electron orbitals found in the 3d sublevel. Four of the orbitals are made up of four lobes, centred on the nucleus.

You are expected to know the shapes and names of the s and p atomic orbitals, but not of the d atomic orbitals.

The labels s, p, d and f relate to the nature of the spectral lines the model was attempting to explain. The corresponding spectroscopic terms are sharp, principal, diffuse and fine.

The letters **s**, **p**, **d**, and **f** are used to identify different sublevels and the atomic orbitals that comprise them. The fourth level (n = 4) is similarly made up from four sublevels. The 4f sublevels are made up of seven f atomic orbitals, but you are not required to know the shapes of these orbitals.

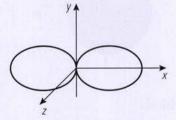
## Worked example

Draw the shapes of a 1s orbital and a 2p<sub>x</sub> orbital.

### Solution



1s orbital

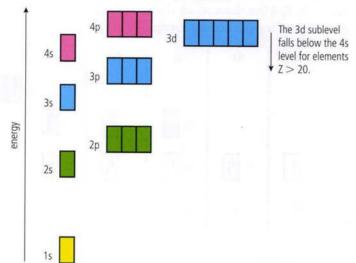


2px orbital

The shapes of a 1s orbital and a 2px orbital. A simple twodimensional drawing is sufficient.

## Each main energy level is divided into sublevels

The atomic orbitals associated with the different energy levels are shown in Figure 8. This diagram is a simplification, as the relative energy of the orbitals depends on the atomic number. The relative energies of the 4s and 3d atomic orbitals are particularly significant and will be discussed in more detail later.



Degenerate orbitals of the same energy form a sublevel; three p orbitals form a p sublevel, five d orbitals form a d sublevel and seven f orbitals form an f sublevel. A single s orbital makes up an s sublevel.

The number of electrons in the sublevels of the first four energy levels are shown in the table.

Level	Sublevel	Maximum number of electrons in sublevel	Maximum number of electrons in level	
n = 1	1s	2	2	
n = 2	2s	2	8	
	2p	6		
n = 3	3s	2	18	
	3p	6		
	3d	10		
n = 4	4s	2	32	
	4p	6		
	4d	10		
	4f	14	13 14	

We can see the following from the table:

- The nth energy level of the atom is divided into n sublevels. For example, the fourth level (n = 4) is made up of four sublevels.
- Each main level can hold a maximum of  $2n^2$  electrons. The 3rd energy level, for example, can hold a maximum of 18 electrons ( $2 \times 3^2 = 18$ ).
- s sublevels can hold a maximum of 2 electrons.
- p sublevels can hold a maximum of 6 electrons.
- d sublevels can hold a maximum of 10 electrons.
- f sublevels can hold a maximum of 14 electrons.

**S1.3 Figure 8** The relative energies of the atomic orbitals up to the 4p sublevel. The 3d sublevel falls below the 4s level for elements 7 > 20



Models are simplifications of complex systems. Details of the historic atomic models of Dalton, Bohr, Schrödinger and Heisenberg will not be assessed.

Aufbau means 'building up' in German.



# The Aufbau principle: constructing arrow-in-box diagrams

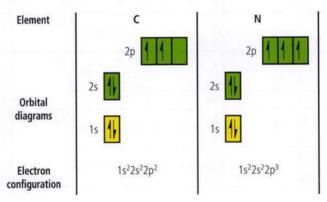
The electron configuration of the ground state of an atom of an element can be determined using the **Aufbau principle**, which states that electrons are placed into orbitals of lowest energy first. Boxes can be used to represent the atomic orbitals, with single-headed arrows to represent the spinning electrons. The **electron configurations** of the first five elements are shown in Figure 9. The number of electrons in each sublevel is given as a superscript.

Element	Н	He	Li	Ве	2p 4
Orbital			2s <b>4</b>	2s <b>4</b>	2s <b>4</b>
diagrams	1s <b>4</b>	1s <b>4</b>	1s <b>4</b>	1s <b>1</b>	1s <mark>{ </mark> }
Electron configuration	1s <sup>1</sup>	1s <sup>2</sup>	1s <sup>2</sup> 2s <sup>1</sup>	1s <sup>2</sup> 2s <sup>2</sup>	1s <sup>2</sup> 2s <sup>2</sup> 2p <sup>1</sup>



\$1.3 Figure 9 The electron configuration of the first five elements.

The next element in the periodic table is carbon. It has two electrons in the 2p sublevel. These could either pair up, and occupy the same p orbital, or occupy separate p orbitals. Following **Hund's third rule**, we place the two electrons in separate orbitals because this configuration minimizes the mutual repulsion between them. As the 2p orbitals are perpendicular to each other and do not overlap, the two 2p electrons are unlikely to approach each other too closely. The electrons in the different 2p orbitals have parallel spins, as this leads to lower energy. The electron configurations of carbon and nitrogen are shown in Figure 10.



Hund's rule: If more than one orbital in a sublevel is available, electrons occupy different orbitals with parallel spins.



\$1.3 Figure 10 Electron configurations of carbon and nitrogen.

The 2p electrons begin to pair up for oxygen  $(1s^22s^22p_x^22p_y^12p_z^1)$  and fluorine  $(1s^22s^22p_x^22p_y^22p_z^2)$ . The 2p sub-shell is completed for neon  $(1s^22s^22p_x^22p_y^22p_z^2)$ .

#### Worked example

Deduce the electron configuration of sulfur.

#### Solution

Sulfur has an atomic number of 16. Therefore it has 16 electrons.

Two electrons occupy the 1s: 1s2

Two electrons occupy the 2s: 2s2

Six electrons occupy the 2p: 2p6

Two electrons occupy the 3s: 3s<sup>2</sup>

Four electrons occupy the 3p: 3p4

So the electron configuration is 1s<sup>2</sup> 2s<sup>2</sup>2p<sup>6</sup> 3s<sup>2</sup> 3p<sup>4</sup>

#### Exercise

- Q5. List the 4d, 4f, 4p, and 4s atomic orbitals in order of increasing energy.
- Q6. State the number of 4d, 4f, 4p, and 4s atomic orbitals.
- **Q7.** Apply the *orbital diagram* method to determine the electron configuration of calcium.
- **Q8.** Deduce the number of unpaired electrons present in a phosphorus atom.
- **Q9.** Deduce the number of orbitals in the n = 4 level and explain your answer.

# Challenge yourself

- **3.** Which of the following provide evidence to support the Bohr model of the hydrogen atom?
  - I. The energy of the lines in the emission spectra of atomic hydrogen.
  - II. The relative intensity of the different spectral lines in the emission spectrum of atomic hydrogen.
    - A I only
- B II only
- C I and II
- D Neither I nor II

75	70	7d	7f	7g	7h	7h
65	бр	δd	6f	6g	6h	
55	5p	5d	<b>5</b> f	5g		
45	4p	4d	45	1		
35	3p	3d	1	1	1	
25	2p	1	1		1	1
15	1				/	1

a

Can you think of a mnemonic for the order of filling orbitals? Figure 11 shows orbitals filled to sublevel 7s. Follow the arrows to see the order in which the sublevels are filled.

**\$1.3 Figure 11** Order of filling sublevels: 1s, 2s, 2p, 3s, 3p, 4s, 3d, 4p, 5s, 4d, 5p, 6s, 4f, 5d, 6p, 7s, 5f, 6d, 7p.

i

TOK

The mathematical nature of the orbital description is illustrated by some simple relationships:

- number of sublevels at nth main energy level = n
- number of orbitals at nth energy level = n<sup>2</sup>
- number of electrons at nth energy level =  $2n^2$
- number of orbitals at Ith sublevel = (2I + 1) where n and I are sometimes known as quantum numbers.

Sublevel	S	p	d	f
1	0	1	2	3

The abstract language of mathematics provides a powerful tool for describing the behaviour of electrons in the atom. The shapes and equations it generates have elegance and symmetry. What do such results tell us about the relationship between the natural sciences, mathematics, and the natural world? Why are many of the laws in the natural sciences stated using the language of mathematics?

When the transition metal atoms form ions they lose electrons from the 4s sublevel before the 3d sublevel.



# The relative energy of the orbitals depends on the atomic number

The energy of an orbital depends on the attraction between the electrons and the nucleus and inter-electron repulsions. As these interactions change with the nuclear charge and the number of electrons – that is, the atomic number – so does the relative energy of the orbitals. All the sublevels in the third energy level (3s, 3p, and 3d), for example, have the same energy for the hydrogen atom and only become separated as extra protons and electrons are added. The situation is particularly complicated when we reach the d block elements. The 3d and 4s levels are very close in energy and their relative separation is very sensitive to inter-electron repulsion. For the elements potassium and calcium, the 4s orbitals are filled before the 3d sublevel. Electrons are, however, first lost from the 4s sublevel when transition metals form their ions, as once the 3d sublevel is occupied the 3d electrons push the 4s electrons to higher energy.

### Worked example

State the full electron configuration of vanadium and deduce the number of unpaired electrons.

#### Solution

The atomic number of vanadium gives the number of electrons: Z = 23.

So the electron configuration is:  $1s^22s^22p^63s^23p^64s^23d^3$ . Note: the 3d sublevel is filled *after* the 4s sub level.

It is useful, however, to write the electron configuration with the 3d sub-shell before the 4s:  $1s^22s^22p^63s^23p^63d^34s^2$  as the 3d sublevel falls below the 4s orbital once the 4s orbital is occupied (i.e. for elements after Ca).

The three 3d orbitals each have an unpaired electron. Number of unpaired electrons = 3.

The worked example asked for the full electron configuration. Sometimes it is convenient to use an abbreviated form, where only the outer electrons are explicitly shown. The inner electrons are represented as a noble gas core. Using this notation, the electron configuration of vanadium is written [Ar]  $3d^34s^2$ , where [Ar] represents the electron configuration of Ar, which is  $1s^22s^22p^63s^23p^6$ .

The electron configurations of the first 30 elements are shown in the table.

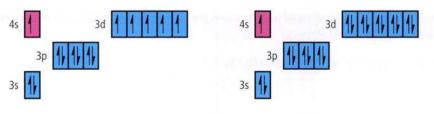
Element	Electron configuration	Element	Electron configuration
1H	1s <sup>1</sup>	16S	1s <sup>2</sup> 2s <sup>2</sup> 2p <sup>6</sup> 3s <sup>2</sup> 3p <sup>4</sup>
<sub>2</sub> He	1s <sup>2</sup>	17Cl	1s <sup>2</sup> 2s <sup>2</sup> 2p <sup>6</sup> 3s <sup>2</sup> 3p <sup>5</sup>
3Li	1s <sup>2</sup> 2s <sup>1</sup>	<sub>18</sub> Ar	1s <sup>2</sup> 2s <sup>2</sup> 2p <sup>6</sup> 3s <sup>2</sup> 3p <sup>6</sup>
<sub>4</sub> Be	1s <sup>2</sup> 2s <sup>2</sup>	19K	1s <sup>2</sup> 2s <sup>2</sup> 2p <sup>6</sup> 3s <sup>2</sup> 3p <sup>6</sup> 4s <sup>1</sup>
<sub>5</sub> B	1s <sup>2</sup> 2s <sup>2</sup> 2p <sup>1</sup>	<sub>20</sub> Ca	1s <sup>2</sup> 2s <sup>2</sup> 2p <sup>6</sup> 3s <sup>2</sup> 3p <sup>6</sup> 4s <sup>2</sup>
<sub>6</sub> C	1s <sup>2</sup> 2s <sup>2</sup> 2p <sup>2</sup>	<sub>21</sub> Sc	[Ar] 3d <sup>1</sup> 4s <sup>2</sup>
<sub>7</sub> N	1s <sup>2</sup> 2s <sup>2</sup> 2p <sup>3</sup>	<sub>22</sub> Ti	[Ar] 3d <sup>2</sup> 4s <sup>2</sup>
8O	1s <sup>2</sup> 2s <sup>2</sup> 2p <sup>4</sup>	23V	[Ar] 3d <sup>3</sup> 4s <sup>2</sup>
<sub>9</sub> F	1s <sup>2</sup> 2s <sup>2</sup> 2p <sup>5</sup>	<sub>24</sub> Cr	[Ar] 3d <sup>5</sup> 4s <sup>1</sup>
<sub>10</sub> Ne	1s <sup>2</sup> 2s <sup>2</sup> 2p <sup>6</sup>	<sub>25</sub> Mn	[Ar] 3d <sup>5</sup> 4s <sup>2</sup>
11Na	1s <sup>2</sup> 2s <sup>2</sup> 2p <sup>6</sup> 3s <sup>1</sup>	<sub>26</sub> Fe	[Ar] 3d <sup>6</sup> 4s <sup>2</sup>
<sub>12</sub> Mg	1s <sup>2</sup> 2s <sup>2</sup> 2p <sup>6</sup> 3s <sup>2</sup>	<sub>27</sub> Co	[Ar] 3d <sup>7</sup> 4s <sup>2</sup>
<sub>13</sub> Al	1s <sup>2</sup> 2s <sup>2</sup> 2p <sup>6</sup> 3s <sup>2</sup> 3p <sup>1</sup>	<sub>28</sub> Ni	[Ar] 3d <sup>8</sup> 4s <sup>2</sup>
14Si	1s <sup>2</sup> 2s <sup>2</sup> 2p <sup>6</sup> 3s <sup>2</sup> 3p <sup>2</sup>	<sub>29</sub> Cu	[Ar] 3d <sup>10</sup> 4s <sup>1</sup>
<sub>15</sub> P	1s <sup>2</sup> 2s <sup>2</sup> 2p <sup>6</sup> 3s <sup>2</sup> 3p <sup>3</sup>	<sub>30</sub> Zn	[Ar] 3d <sup>10</sup> 4s <sup>2</sup>

The electrons in the outer energy level are mainly responsible for compound formation and are called **valence electrons**. Lithium has one valence electron in the outer second energy level  $(2s^1)$ , beryllium has two  $(2s^2)$ , boron has three  $(2s^2p^1)$ , and so on. The number of valence electrons follows a periodic pattern, which is discussed fully in Structure 3.1. Atoms can have many other electron configurations when in an excited state. Unless otherwise instructed, assume that you are being asked about ground-state configurations.

For the d block elements, three points should be noted:

- the 3d sublevel is written with the other *n* = 3 sublevels because it falls below the 4s orbital once the 4s orbital is occupied (i.e. for elements after Ca), as discussed earlier
- chromium has the electron configuration [Ar] 3d<sup>5</sup>4s<sup>1</sup>
- copper has the electron configuration [Ar] 3d104s1.

To understand the electron configurations of copper and chromium, it is helpful to consider the electrons-in-boxes arrangements in Figure 12. As the 4s and 3d orbitals are close in energy, the electron configuration for chromium, with a half-full d sublevel, is relatively stable as it minimizes electrostatic repulsion, with six singly occupied atomic orbitals. This would be the expected configuration using Hund's rule if the 4s and 3d orbitals had exactly the same energy. Half-filled and filled sublevels seem to be particularly stable: the configuration for copper is similarly due to the stability of the full d sublevel.



chromium: [Ar]3d54s1

copper: [Ar]3d104s1



The term 'valence' is derived from the Latin word for 'strength'.

**S1.3 Figure 12** The electron configurations of the 3rd and 4th energy levels for chromium and copper.

**Exercise** Q10. Identify the sublevel that does not exist. 4d A 5d B 3f D<sub>2p</sub> Q11. Which is the correct order of orbital filling according to the Aufbau principle? A 4s 4p 4d 4f 4p 4d 5s 4f C 4s 3d 4p 5s D 4d 4f 5s 5p Q12. State the full ground-state electron configuration of the following elements. (a) V (b) K (c) Se (d) Sr Q13. Determine the total number of electrons in d orbitals in a single iodine atom. 15 A 5 B 10 C D 20 Q14. Identify the excited state (i.e. not a ground state) in the following electron configurations. A [Ne] 3s23p3 [Ne] 3s23p34s1 D [Nel 3s<sup>2</sup>3p<sup>6</sup>3d<sup>1</sup>4s<sup>2</sup> [Ne] 3s<sup>2</sup>3p<sup>6</sup>4s<sup>1</sup> Q15. Deduce the number of unpaired electrons present in the ground state of a titanium atom. C A Q16. Identify the atom that possesses the most unpaired electrons. A 0 B Mg C Ti D Fe

# Electron configuration of ions

As discussed earlier, positive ions are formed by the loss of electrons. These electrons are lost from the outer sublevels. For example, the electron configurations of the different aluminium ions formed when electrons are successively removed are as follows:

- Al+ is 1s<sup>2</sup>2s<sup>2</sup>2p<sup>6</sup>3s<sup>2</sup>
- Al<sup>2+</sup> is 1s<sup>2</sup>2s<sup>2</sup>2p<sup>6</sup>3s<sup>1</sup>
- Al3+ is 1s22s2p6, etc.

When positive ions are formed for transition metals, the outer 4s electrons are removed before the 3d electrons, as discussed earlier.

For example, Cr is [Ar] 3d54s1 and Cr3+ is [Ar] 3d3

The electron configurations of negative ions are determined by adding the electrons into the next available electron orbital:

 $S \ is \ 1s^2 2s^2 2p^6 3s^2 3p^4 \ and \ S^{2-} \ is \ 1s^2 2s^2 2p^6 3s^2 3p^6$ 

### Worked example

Deduce the ground-state electron configuration of the Fe<sup>3+</sup> ion.

#### Solution

First find the electron configuration of the atom. Fe has 26 electrons:  $1s^22s^22p^63s^23p^64s^23d^6$ 

As the 3d sublevel is below the 4s level for elements after calcium, we write this as  $1s^22s^22p^63s^23p^63d^64s^2$ 

Now remove the two electrons from the 4s sublevel and one electron from the 3d sublevel.

Electron configuration of Fe3+ is 1s22s22p63s23p63d5



Note the abbreviated electron configuration using the noble gas core is not acceptable when asked for the *full* electron configuration.

#### **Exercise**

- Q17. State the full ground-state electron configuration of the following ions.
  - (a) O2-
- (b) Cl-
- (c) Ti3+
- (d) Cu2+
- **Q18.** State the electron configuration of the following transition metal ions by filling in the boxes below. Use arrows to represent the electron spin.

(a)	Ion	3d			
	Ti <sup>2+</sup>				
(b)	Fe <sup>2+</sup>				
(b) (c) (d)	Ni <sup>2+</sup>	THE THE PARTY OF T			
(d)	Zn <sup>2+</sup>				

- Q19. (a) State the full electron configuration for neon.
  - **(b)** State the formulas of two oppositely charged ions which have the same electron configuration as neon.
- **Q20.** State the abbreviated electron configuration using the previous noble gas core for:
  - (a) Ni2+
- (b) Pb2+
- (c) S2-
- (d) Si4+

# Electron configuration and the periodic table

We are now in a position to understand the structure of the periodic table (Figure 13):

- elements whose valence electrons occupy an s sublevel make up the s block
- · elements with valence electrons in p orbitals make up the p block
- the d block and the f block are similarly made up of elements with outer electrons in d and f orbitals.

d9/ Ne 2 3 Ar 4 Kr 5 Xe Rn 6 7 d block p block s block f block

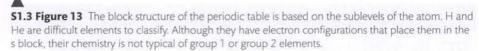
Structure 3.1 - What is the relationship between energy sublevels and the block nature of the periodic table?

The ns and np sublevels are filled for elements in period n. However the (n - 1)d sublevel is filled for elements in period n.

T

Structure 3.1 – How does an element's highest main energy level relate to its period number in the periodic table?

Some versions of the periodic table use the numbering 3-7 for groups 13-17. In this version, group 3 elements have three valence electrons and group 7 elements have seven valence electrons. Although this is simpler, in some respects it can lead to problems. After extensive discussions, the IUPAC concluded that the 1 to 18 numbering provides the clearest and most unambiguous labelling system.



The position of an element in the periodic table is based on the occupied sublevel of highest energy in the ground-state atom. Conversely, the electron configuration of an element can be deduced directly from its position in the periodic table.

Here are some examples.

- Caesium is in group 1 and period 6 and has the electron configuration: [Xe] 6s<sup>1</sup>.
- Iodine is in group 17 and in period 5 and has the configuration: [Kr] 5s<sup>2</sup>4d<sup>10</sup>5p<sup>5</sup>. Placing the 4d sublevel before the 5s gives [Kr] 4d<sup>10</sup>5s<sup>2</sup>5p<sup>5</sup>. Iodine has 7 valence electrons, in agreement with the pattern discussed on page 69.

#### Exercise

- **Q21.** Use the periodic table to find the full ground-state electron configuration of the following elements.
  - (a) Cl
- (b) Nb
- (c) Ge
- (d) Sb
- **Q22.** Identify the elements that have the following ground-state electron configurations.
  - (a) [Ne] 3s<sup>2</sup>3p<sup>2</sup>

(b) [Ar] 3d<sup>5</sup>4s<sup>2</sup>

(c)  $[Kr] 5s^2$ 

- (d) 1s<sup>2</sup>2s<sup>2</sup>2p<sup>6</sup>3s<sup>2</sup>3p<sup>6</sup>3d<sup>1</sup>4s<sup>2</sup>
- Q23. State the total number of p orbitals containing one or more electrons in tin.
- Q24. How many electrons are there in all the d orbitals in an atom of barium?
- Q25. State the electron configuration of the ion Cd<sup>2+</sup>.
- Q26. State the full electron configuration of U<sup>2+</sup>.

### Challenge yourself

- 4. State the electron configuration of thorium.
- **5.** Only a few atoms of element 109, meitnerium, have ever been made. Isolation of an observable quantity of the element has never been achieved and may well never be. This is because meitnerium decays very rapidly.
  - (a) Suggest the electron configuration of the ground-state atom of the element.
  - (b) There is no g block in the periodic table as no elements with outer electrons in g orbitals exist in nature or have been made artificially. Suggest a minimum atomic number for such an element.
- **6.** Consider how the shape of the periodic table is related to the three-dimensional world we live in.
  - (a) How many 3p and 3d orbitals would there be if only the x and y dimensions existed?
  - (b) How many groups in the p and d block would there be in such a twodimensional world?

TOK

Do atomic orbitals exist or are they primarily useful inventions to aid our understanding? What consequences might questions about the reality of scientific entities have for the public perception and understanding of the subject? If they are only inventions, how is it that they can yield such accurate predictions?



#### **Nature of Science**

We have seen how the model of the atom has changed over time. All these theories are still used today. Dalton's model adequately explains many properties of the states of matter, the Bohr model is used to explain chemical bonding, and the structure of the periodic table is explained by the wave description of the electron. In science, we often follow Occam's razor and use the simplest explanation that can account for the phenomena. As Einstein said 'Explanations should be made as simple as possible, but not simpler'.

HL

# Structure 1.3.6 and 1.3.7 - Ionization energies

Structure 1.3.6 – In an emission spectrum, the limit of convergence at higher frequency corresponds to ionization.

Explain the trends and discontinuities in first ionization energy (IE) across a period and down a group.

Calculate the value of the first IE from spectral data that gives the wavelength or frequency of the convergence limit.

The value of the Planck constant h and the equations E = h f and  $c = \lambda f$  are given in the data booklet.

Structure 3.1 – How does the trend in IE values across a period and down a group explain the trends in properties of metals and non-metals?

Nature of Science, Tool 3, Reactivity 3.1 – Why are log scales useful when discussing [H<sup>+</sup>] and ionization energies?

Structure 1.3.7 – Successive ionization energy (IE) data for an element give information about its electron configuration.

Deduce the group of an element from its successive ionization data.

Databases are useful for compiling graphs of trends in IEs.

Structure 3.1 – How do patterns of successive IEs of transition elements help to explain the variable oxidation states of these elements?

# In an emission spectrum, the limit of convergence at higher frequency corresponds to ionization

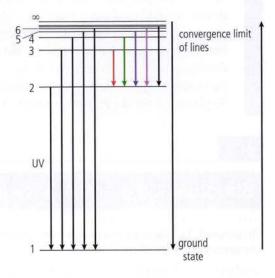
The first ionization energy of an element is the energy needed to remove one mole of electrons from the ground state of one mole of the gaseous atom. For hydrogen it corresponds to the following change, with the electron being removed from the 1s orbital:

$$H(g) \rightarrow H^+(g) + e^-$$

Once removed from the atom, the electron is an infinite distance away from the nucleus and can be considered to be in the  $n = \infty$  energy level.

We saw earlier that the energy levels in hydrogen converge at higher energy. This allows us to calculate the ionization energy from the convergence limit at higher frequency.

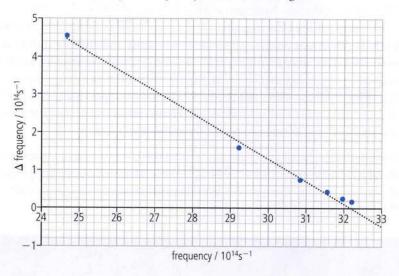
The frequency at which convergence occurs can be obtained graphically. The frequencies of the lines where the transitions involve the electron falling from the excited levels with  $n \ge 1$  to the n = 1 energy level are shown below. The difference between the frequencies in successive lines is given in the third column.



Excited energy level (n)	Frequency, $f/\times 10^{-14}$ s <sup>-1</sup>	$\Delta f/\times 10^{-14} s^{-1}$
2	24.66	4.57
3	29.23	1.60
4	30.83	0.74
5	31.57	0.40
6	31.97	0.24
7	32.21	0.16
8	32.37	

The first ionization energy of an element is the minimum energy needed to remove one mole of electrons from one mole of gaseous atoms in their ground state.

A graph of f against  $\Delta f (f_{n+1} - f_n)$  gives an approximate best-fit straight line with the intercept on the x axis giving the frequency at which convergence occurs.



A graph showing the frequency of the line emitted against the difference in frequency between successive lines in the UV region of the hydrogen atom.

From the graph, convergence occurs when  $\Delta f = 0$  at  $f = 32.3 \times 10^{-14} \text{ s}^{-1}$ 

Using the equation E = h f we have the ionization energy for one atom:

$$E = 32.3 \times 10^{-14}\,\mathrm{s}^{-1} \times 6.63 \times 10^{-34}\mathrm{J}\,\mathrm{s}$$

So for one mole, the ionization energy is given by:

IE = 
$$32.3 \times 10^{-14} \,\text{s}^{-1} \times 6.63 \times 10^{-34} \,\text{J} \,\text{s} \times 6.02 \times 10^{23} \,\text{mol}^{-1}$$
  
=  $1290 \,\text{kJ} \,\text{mol}^{-1}$ 

This is close to the value of 1312kJ mol<sup>-1</sup> given in Section 9 of the data booklet.



#### **Nature of Science**

The best data for making accurate and precise descriptions are often quantitative as you can use this for mathematical analysis. The data can often be presented in a variety of formats that can be analysed. Scientists look for patterns in an attempt to discover relationships.

### Challenge yourself

7. A more accurate value for the convergence limit can also be found by plotting a graph of the frequencies of the lines against  $\frac{1}{n^2}$ . Determine the ionization energy of hydrogen using this method and explain why this method is more accurate.



#### **Nature of Science**

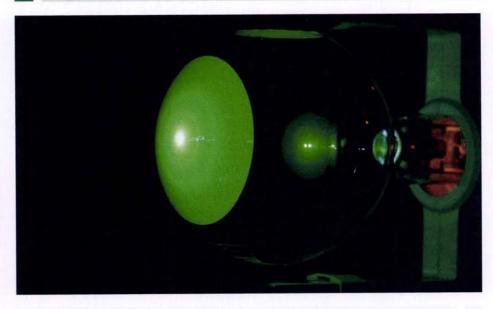
The Bohr model of the hydrogen atom (1913) was able to explain the relationship between the frequency of the lines and the *n* values for the energy levels, but Bohr was unable to provide experimental evidence to support his postulates. They were inconsistent as they came from an unjustified mixture of classical and quantum theory. In general, scientists strive to develop hypotheses and theories that are compatible with accepted principles and that simplify and unify existing ideas. A deeper understanding needed the wave description of the electron suggested by de Broglie (1926).

Many scientific discoveries have come from speculation or simple curiosity about particular phenomena. De Broglie speculated on the wave properties of particles by combining results from Einstein's theory of relativity with Planck's quantum theory.

An electron diffraction tube. The electrons fired at a thin sheet of graphite produce the patterns of rings associated with diffraction. De Broglie (1892–1987) correctly deduced that the electrons would have wavelengths inversely proportional to their momentum ( $\lambda = h/p$ ).

The de Broglie equation  $(\lambda = h/p)$  shows that macroscopic particles have too short a wavelength for their wave properties to be observed. Is it meaningful to talk of properties which can never be observed from sense perception?





Ionization energies can also be used to support this model of the atom.

#### **Exercise**

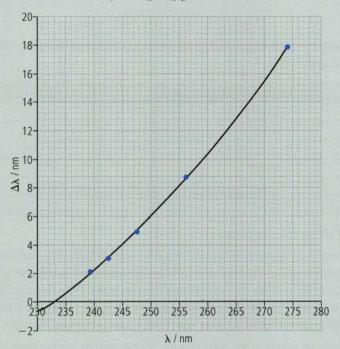
- Q27. Sodium lamps used for street lighting emit a distinctive orange light with a wavelength of 590 nm. Calculate the energy produced by one mole of excited sodium atoms when they give out orange light of this wavelength.
- **Q28.** Some frequencies of the lines in the spectrum of He<sup>+</sup> ion are shown in the table. Determine the convergence limit and ionization energy of the He<sup>+</sup> ion.

Excited energy level (n)	Frequency, $f/\times 10^{-15}$ s <sup>-1</sup>
2	9.87
3	11.72
4	12.36
5	12.66
6	12.82

**Q29.** The convergence limits in the spectra of two single electron ions are shown in the table. Use these values to calculate the ionization energy of the ions.

	Frequency of convergence limit/s-
Li <sup>2+</sup>	$2.97 \times 10^{16}$
Be <sup>3+</sup>	5.27 × 10 <sup>16</sup>

**Q30.** The emission spectrum of lithium includes a number of lines corresponding to the transitions involving the valence electron falling from excited states back to the 2s orbital. The graph shows the wavelength  $\lambda_n$  of a number of these lines in the spectrum, plotted against the difference in wavelength between consecutive lines  $(\Delta \lambda = \lambda_n - \lambda_{n+1})$ .



Determine the wavelength that corresponds to ionization of lithium and calculate the ionization energy.

# Successive ionization energy (IE) data for an element give information about its electron configuration

Additional evidence for the electron configuration of an atom comes from looking at patterns of successive ionization energies. As discussed earlier for aluminium, the first ionization energy corresponds to the following process:

$$Al(g) \rightarrow Al^+(g) + e^-$$

The second ionization energy corresponds to the change:

$$Al^+(g) \rightarrow Al^{2+}(g) + e^-$$

and so on.

The ionization energies for aluminium are shown in Figure 14.

s1.3 Figure 14 Successive ionization energies for aluminium. Note the jumps between the 3rd and 4th and between the 11th and 12th ionization energies as electrons are removed from lower energy levels. As there is a wide range of values, they are best presented on a log scale.

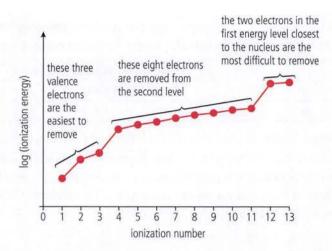
TOK

TOK

How does the method of data presentation influence how the data are interpreted? The use of scale can clarify important relationships but can also be used to manipulate data. How can you as a knower distinguish between the use and abuse of data presentation?

Nature of Science, Tool 3, Reactivity 3.1 - Why are log scales useful when discussing [H\*] and ionization energies?

Which of Dalton's five proposals (page 30) do we now hold to be 'true'? How does scientific knowledge change with time? Are the models and theories of science accurate descriptions of the natural world, or just useful interpretations to help predict and explain the natural world?



The electron configurations of aluminium ions as electrons are successively removed are shown in the table.

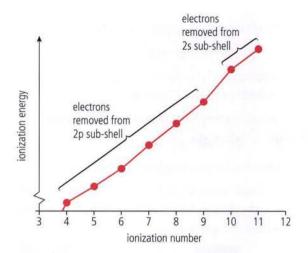
	Electron configuration		Electron configuration
Al	1s <sup>2</sup> 2s <sup>2</sup> 2p <sup>6</sup> 3s <sup>2</sup> 3p <sup>1</sup>	Al6+	1s <sup>2</sup> 2s <sup>2</sup> 2p <sup>3</sup>
Al+	1s <sup>2</sup> 2s <sup>2</sup> 2p <sup>6</sup> 3s <sup>2</sup>	Al <sup>7+</sup>	1s <sup>2</sup> 2s <sup>2</sup> 2p <sup>2</sup>
A 2+	1s <sup>2</sup> 2s <sup>2</sup> 2p <sup>6</sup> 3s <sup>1</sup>	Al8+	1s <sup>2</sup> 2s <sup>2</sup> 2p <sup>1</sup>
Al <sup>3+</sup>	1s <sup>2</sup> 2s <sup>2</sup> 2p <sup>6</sup>	Al9+	1s <sup>2</sup> 2s <sup>2</sup>
Al4+	1s <sup>2</sup> 2s <sup>2</sup> 2p <sup>5</sup>	Al <sup>10+</sup>	1s <sup>2</sup> 2s <sup>1</sup>
Al5+	1s <sup>2</sup> 2s <sup>2</sup> 2p <sup>4</sup>	A 11+	1s <sup>2</sup>

Figure 14 shows two key points.

- There is an increase in successive ionization energies. The first ionization
  energy involves the separation of an electron from a singly charged ion and the
  second IE involves the separation of an electron from a doubly charged ion.
  The process becomes more difficult as there is increasing attraction between the
  higher charged positive ions and the oppositely charged electron.
- There are jumps when electrons are removed from levels closer to the nucleus. The first three ionization energies involve the removal of electrons from the third level. The 3p electron is removed first, followed by the electrons from the 3s orbital. An electron is removed from the second level for the fourth ionization energy. This electron is closer to the nucleus and is more exposed to the positive charge of the nucleus and so needs significantly more energy to be removed. There is similarly a large jump for the 12th ionization energy as it corresponds to an electron being removed from the 1s orbital.

# A closer look at successive ionization energies gives evidence for sublevels in the atom

A closer look at the successive ionization energies shows evidence of the sublevels present with each level. The log graph of all 13 ionization energies showed a 2, 8, 3 pattern in successive ionization energies, which reflects the electron arrangement of the atom, with two electrons in the first level, eight electrons at the second energy level, and three valence electrons in the outer shell. Now we consider the fourth to eleventh ionization energies in more detail. These correspond to the removal of the eight electrons in the second energy level (Figure 15).



The jump between the ninth and tenth ionization energies shows that the eleventh electron is more difficult to remove than we would expect from the pattern of the six previous electrons. This suggests that the second energy level is divided into two sublevels.

This evidence confirms that the **2s sublevel** can hold a maximum of two electrons, and the **2p sublevel** can hold six electrons.

### Worked example

A graph of some successive ionization energies of aluminium is shown in Figure 15.

- (a) Explain why there is a large increase between the ninth and tenth ionization energies.
- **(b)** Explain why the increase between the sixth and seventh values is greater than the increase between the fifth and sixth values.

#### Solution

(a) The ninth ionization energy corresponds to the change:

$$Al^{8+}(g) \rightarrow Al^{9+}(g) + e^{-}$$

Al<sup>8+</sup> has the configuration 1s<sup>2</sup>2s<sup>2</sup>2p<sup>1</sup>. The electron is removed from a 2p orbital.

The tenth ionization energy corresponds to the change:

$$Al^{9+}(g) \rightarrow Al^{10+}(g) + e^{-}$$

Al<sup>9+</sup> has the configuration 1s<sup>2</sup>2s<sup>2</sup>. The electron is removed from a 2s orbital.

Electrons in a 2s orbital are of lower energy than those is 2p orbitals. They are closer to the nucleus and experience a stronger force of electrostatic attraction and so are more difficult to remove.

S1.3 Figure 15 Successive ionization energies for aluminium. The jump between the ninth and tenth ionization energies indicates that the second energy level is divided into sublevels. The smaller jump between the sixth and seventh ionization energies should also be noted and is discussed more fully in the text.





Successive ionization energies database investigation: Full details of how to carry out this activity with a worksheet are available in the eBook.

# **(b)** The sixth ionization energy corresponds to the change:

$$Al^{5+}(g) \rightarrow Al^{6+}(g) + e^{-}$$

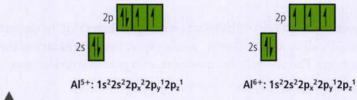
Al<sup>5+</sup> has the configuration  $1s^22s^22p^4$  ( $1s^22s^22p_x^22p_y^22p_y^12p_z^1$ ). The electron is removed from a doubly occupied 2p orbital.

The seventh ionization energy corresponds to the change:

$$Al^{6+}(g) \rightarrow Al^{7+}(g) + e^{-}$$

The electron is removed from a singly occupied 2p orbital.

An electron in a doubly occupied orbital is repelled by its partner, and so is easier to remove than electrons in half-filled orbitals, which do not experience this force of repulsion.



The electron removed from the Al5+ ion is from a doubly occupied 2p orbital. This is easier to remove than an electron in a singly occupied orbital because it is repelled by its partner.

# Successive ionization energies of transition elements

One of the key features of transition metal chemistry is the wide range of oxidation states that the metals display in their compounds. Calcium, for example, only shows the +2 state whereas titanium shows the +4, +3, and +2 states. The difference in behaviour can be related to patterns in successive ionization energies (Figure 16).

Element	Electron configuration
Ca	1s <sup>2</sup> 2s <sup>2</sup> 2p <sup>6</sup> 3s <sup>2</sup> 3p <sup>6</sup> 4s <sup>2</sup>
Ti	1s <sup>2</sup> 2s <sup>2</sup> 2p <sup>6</sup> 3s <sup>2</sup> 3p <sup>6</sup> 3d <sup>2</sup> 4s <sup>2</sup>

12000 10000 onization energy/kJ mol-8000 6000 4000 2000 0 ionization number

**51.3 Figure 16** Successive ionization energies for Ca and Ti.

Structure 3.1 - How do patterns of successive IEs of transition elements help to explain the variable oxidation states of these elements?

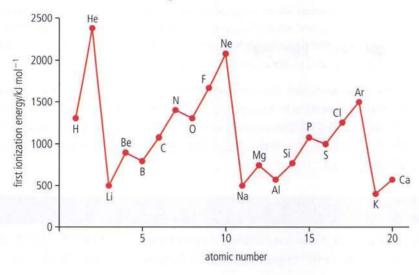


The Ca<sup>3+</sup> ion is energetically unstable because there is a large jump in ionization energy as the third electron is removed from the inner 3p orbital. The increase in successive energies for titanium is more gradual as the 3d and 4s orbitals are close in energy. Titanium shows the +2, +3, and +4 oxidation states. A large jump occurs between the fourth and fifth ionization energies, as the inner 3p electron is removed, so titanium does not form the +5 state.

Further evidence of sub-shells comes from a consideration of patterns in first ionization energies.

# Trends in first ionization energy across periods account for the existence of main energy levels and sublevels in atoms

The periodic arrangement of the elements in the periodic table is also reflected by patterns in the first ionization energies.



The first ionization energies of the first 20 elements.

- Ionization energies generally increase from left to right across a period, as the nuclear charge increases. The electrons are removed from the same main energy level, but there is an increase in the force of electrostatic attraction between the nucleus and outer electrons.
- · Ionization energy decreases down a group as a new energy level, which is further from the nucleus, is occupied. Less energy is required to remove outer electrons that are further from the attractive pull of the nucleus.
- · There are regular discontinuities in the trend across a period, which are explored below. These provide further evidence for the existence of sub-shells.

The metals on the left of the periodic table have low ionization energies and generally form stable positive ions. The non-metals on the right of the periodic table have high ionization energies and do not lose electrons readily. They generally form negative ions. This is explored in more detail in Structure 3.1.

#### Worked example

Further evidence for the existence of sub-shells comes from a study of first ionization energies.

- (a) In period 2, there is a decrease in first ionization energies between Be and B, and in period 3, there is a decrease between Mg and Al. Explain this decrease in ionization energies between group 2 and group 13 elements.
- (b) In period 2, there is a decrease in first ionization energies between N and O, and in period 3, there is a decrease between P and S. Explain the decrease in ionization energies between group 15 and group 16 elements.



Structure 3.1 - How does the trend in IE values across a period and down a group explain the trends in properties of metals and non-metals?

#### Solution

- (a) The group 2 elements have the electron configuration  $ns^2$ . The group 13 elements have the electron configuration  $ns^2np^1$ .
  - The electron removed when the group 13 elements are ionized is a p electron. The electron removed when the group 2 elements are ionized is an s electron. Electrons in p orbitals are of higher energy and further away from the nucleus than s electrons and so are easier to remove.
- **(b)** Group 15 elements have the configuration  $ns^2np_x^1np_y^1np_z^1$ . Group 16 elements have the configuration  $ns^2np_x^2np_y^1np_z^1$ . For group 16 elements, the electron is removed from a doubly occupied p orbital. An electron in a doubly occupied orbital is repelled by its partner and so is easier to remove than an electron in a half-filled orbital.

Databases can be used for compiling graphs of trends in ionization energies.



#### **Exercise**

**Q31.** The first four ionization energies for a particular element are 738, 1450, 7730, and 10550 kJ mol<sup>-1</sup> respectively. Deduce the group number of the element.

A 1

B 2

C

D 4

Q32. Successive ionization energies for an unknown element are given in the table.

First ionization	Second	Third ionization	Fourth
energy /	ionization	energy /	ionization
kJ mol <sup>-1</sup>	energy / kJ mol <sup>-1</sup>	kJ mol <sup>-1</sup>	energy / kJ mol <sup>-1</sup>
590	1145	4912	6491

Identify the element.

A K

B Ca

CS

D Cl

Q33. The successive ionization energies (in kJ mol<sup>-1</sup>) for carbon are shown in the table.

1st	2nd	3rd	4th	5th	6th
1086	2352	4619	6220	37820	47280

- (a) Explain why there is a large increase between the fourth and fifth values.
- (b) Explain why there is an increase between the second and third values.
- **Q34.** Sketch a graph to show the expected pattern for the first seven ionization energies of fluorine.
- **Q35.** The first ionization energies of the period 3 elements Na to Ar are given in Section 9 of the data booklet.
  - (a) Explain the general increase in ionization energy across the period.
  - **(b)** Explain why the first ionization energy of magnesium is greater than that of aluminium.
  - (c) Explain why the first ionization energy of sulfur is less than that of phosphorus.



#### **Nature of Science**

This chapter has highlighted the need for experimental evidence to support our scientific theories.

Scientific ideas often start as speculations which are only later confirmed experimentally. The existence of the Higgs' boson was, for example, first suggested by the physicist Peter Higgs in 1964. It was, however, only detected in 2012 when two separate international teams working at the Large Hadron Collider at CERN independently announced that they had collected evidence to support its existence.

HL end



The discovery of the Higgs boson was greatly facilitated by growth in computing power and sensor technology. Experiments in CERN's Large Hadron Collider regularly produce 23 petabytes of data per second, equivalent to 13.3 years of highdefinition TV content per second. How does computation help people to process data to gain knowledge?



#### **Guiding Question revisited**

How can we model the energy states of electrons in atoms?

In this chapter we have developed models of the energy states of electrons in atoms to explain atomic emission line spectra and patterns in successive ionization energies of an element, and first ionizations.

- Electromagnetic radiation can be described using a wave model or a particle model. The speed of the wave (c) is related to the frequency (f) and wavelength (λ) by the expression: c = f λ
- The existence of lines in an emission spectrum indicates that the electron can only
  exist in discrete energy levels. The lines in the spectra converge at high energies
  because the gaps between energy levels in the atom decrease at higher energies.
- In the Bohr model of the hydrogen atom, the electron travels in orbits of discrete radii around the nucleus. This model correctly predicts the frequencies and wavelengths of the line spectra but does not apply to more complex systems with more than one electron.
- According to the quantum theory, an electron's trajectory can only be described in terms of probabilities and a wave model of the electron is needed.
- Electrons in the atom occupy atomic orbitals, which are regions in which the electron is most likely to be found. Two electrons of opposite spin can occupy one orbital.
- Atomic orbitals have different shapes, sizes and energies. Orbitals of the same energy form sublevels. The first energy level is made up of one sublevel, the second has two sublevels and so on.
- The ground state configuration of an atom is obtained using the Aufbau principle, with electrons occupying the available orbitals of lowest energy.
- The periodic table reflects the periodicity of the electron configuration.
   Elements with valence electrons in s orbitals are in the s block, elements with valence electrons in p orbitals are in the p block, and so on.
- The energy of a photon ( $E_{\text{photon}}$ ) depends on the frequency (f) according to Planck's equation:  $E_{\text{photon}} = hf$ .
- When an excited electron in an atom loses energy, the energy is given out as a photon.  $\Delta E_{\text{atom}} = E_{\text{photon}}$



## **Practice questions**

- 1. What is the electron configuration of the Cr2+ ion?
  - A [Ar] 3d54s1

B [Ar] 3d<sup>3</sup>4s<sup>1</sup>

C [Ar] 3d64s1

D [Ar] 3d44s0

2. Which is correct for the following regions of the electromagnetic spectrum?

	Ultraviolet (UV		Infrared (IR)		
A	high energy	short wavelength	low energy	low frequency	
В	high energy	low frequency	low energy	long wavelength	
C	high frequency	short wavelength	high energy	long wavelength	
D	high frequency	long wavelength	low frequency	low energy	

3. An ion has the electron configuration  $1s^22s^22p^63s^23p^63d^{10}$ . Which ion could it be?

A Ni<sup>2+</sup>

B Cu+

C Cu<sup>2+</sup>

D Co3+

**4.** In the emission spectrum of hydrogen, which electron transition would produce a line in the visible region of the electromagnetic spectrum?

A  $n=2 \rightarrow n=1$ 

 $\mathbf{B} \quad n=3 \to n=2$ 

C  $n=2 \rightarrow n=3$ 

**D**  $n = \infty \rightarrow n = 1$ 

5. The electron configuration of chromium can be expressed as [Ar]4sx3dy.

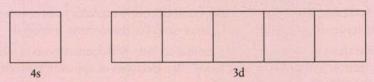
(a) Explain what the square brackets around argon, [Ar], represent.

(1)

**(b)** State the values of *x* and *y*.

(1)

(c) Annotate the diagram below to show the 4s and 3d orbitals for a chromium atom. Use an arrow, and to represent a spinning electron.



(Total 3 marks)

**6. (a)** List the following types of electromagnetic radiation in order of increasing wavelength (shortest first).

I. Yellow light

II. Red light

III. Infrared radiation

IV. Ultraviolet radiation

(1) (1)

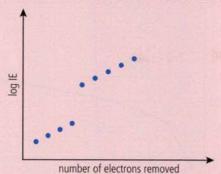
(1)

(b) Distinguish between a continuous spectrum and a line spectrum.

(Total 2 marks)

HL

7. The graph represents the energy needed to remove nine electrons, one at a time, from an atom of an element. Not all of the electrons have been removed.



Which element could this be?

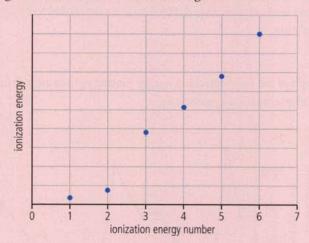
A C

B Si

C P

D S

8. The graph gives the successive ionization energies for an element X.



Deduce the charge of the most stable ion formed by X.

A X+

B X2+

C X3+

D X4+

9. The successive ionization energies of an element, Y, are shown in the table.

	1st	2nd	3rd	4th	5th	6th	7th
Ionization energy / kJ mol <sup>-1</sup>	788	1577	3232	4356	16091	19805	23780

Identify the type of orbital from which the first electron is removed when the first ionization energy is determined.

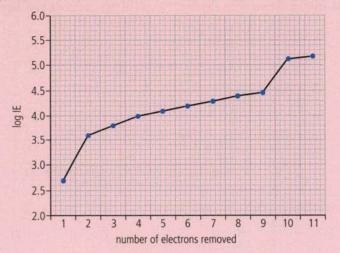
A sorbital

B p orbital

C d orbital

D forbital

10. The graph represents the successive ionization energies of sodium. The vertical axis plots log(ionization energy) instead of ionization energy to allow the data to be represented without using an unreasonably long vertical axis.

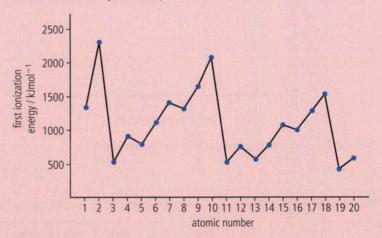


State the full electron configuration of sodium and explain how the successive ionization energy data for sodium are related to its electron configuration.

(Total 4 marks)

(4)

**11.** The graph of the first ionization energy plotted against atomic number for the first 20 elements shows periodicity.



- (a) Explain how information from this graph provides evidence for the existence of main energy levels and sublevels within atoms.
- (b) State what is meant by the term second ionization energy.

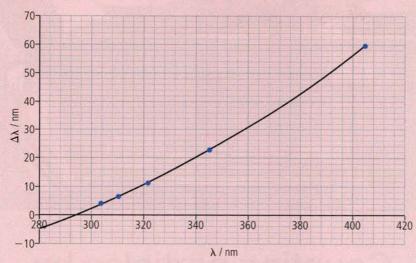
(Total 5 marks)

(4)

(1)

**12.** The emission spectrum of potassium includes a number of lines corresponding to the transitions involving the valence electron falling from excited states back to the 4s orbital. The graph shows the wavelength  $\lambda_n$  of a number of these lines in the spectrum plotted against the difference in wavelength between consecutive lines

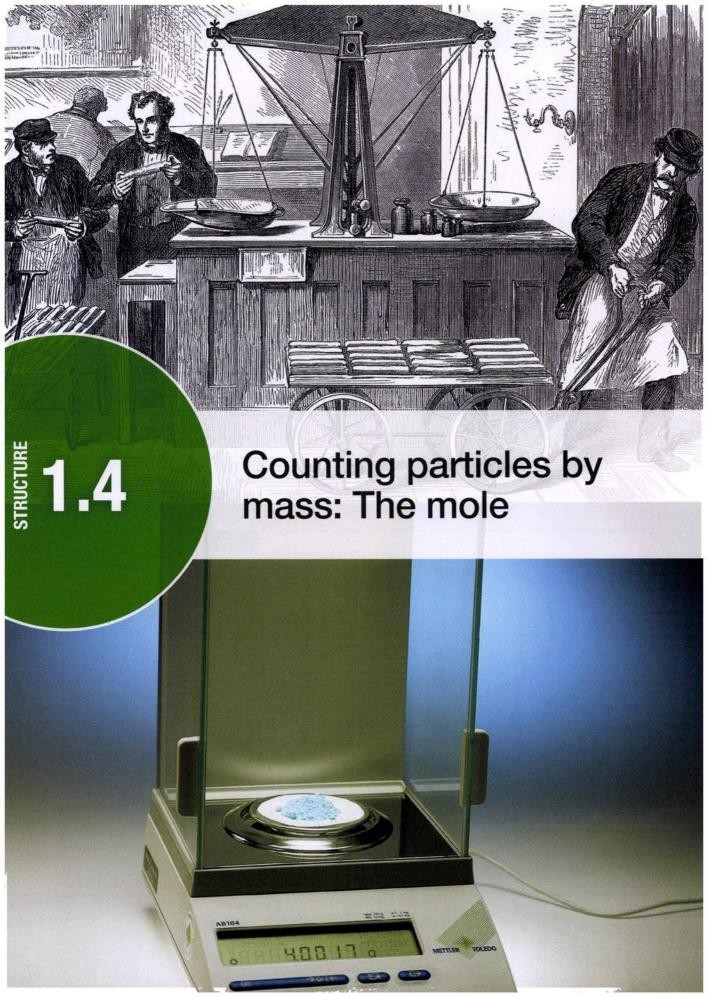
 $(\Delta \lambda = \lambda_n - \lambda_{n+1}).$ 



Determine the wavelength that corresponds to ionization of potassium and calculate the ionization energy in kJ mol<sup>-1</sup>. (2)

(Total 2 marks)

HL end



(Top) Entrance to the Bank of England, London, 1872. Samples of precious metals such as gold and silver are being checked for mass on the balance in the centre. (Bottom) A modern analytical instrument that measures mass to a high degree of precision, accounting for small factors such as dust and airflow.







#### **Nature of Science**

Advances in technology have led to increasingly precise ways of measuring mass, as well as units derived from it, such as concentration. This means that values which were previously too low to be detected can now be reported accurately. This makes possible changes in regulations and laws, such as levels of pollutants in fluids and of illegal drugs in the bloodstream. Authorities and governments often depend on measurements such as these in making judgements and enforcing the law. It is therefore essential that the data collected are reliable and include clearly stated uncertainties.



#### **Guiding Question**

How do we quantify matter on the atomic scale?

Chemical change involves interactions between atoms that have fixed mass. Yet the mass of an individual atom is so small that it is not practical to measure it directly in a laboratory. The upper limit of precision of very high quality analytical balances is generally about  $1\times 10^{-8}\,\mathrm{kg}$ , whereas, for example, a single atom of carbon weighs  $1.99\times 10^{-26}\,\mathrm{kg}$ .

Clearly, we need a way to close the gap between what can be measured and what is happening on the atomic scale. In this chapter we will learn how solving this problem led to the development of the chemical unit of amount, the mole. The mole is a fundamental unit in the SI system and is one of the most widely used tools in chemistry. It allows a form of book-keeping at the atomic level, making that important link between the measurable mass and the number of reacting particles.

# Structure 1.4.1 – The mole as the unit of amount

Structure 1.4.1 – The mole (mol) is the SI unit of amount of substance. One mole contains exactly the number of elementary entities given by the Avogadro constant.

Convert the amount of substance, n, to the number of specified elementary entities.

An elementary entity may be an atom, a molecule, an ion, an electron, any other particle or a specified group of particles.

Avogadro's constant  $(N_A)$  is given in the data booklet. It has the units mol<sup>-1</sup>.

#### The mole. Full details of how to carry out this activity with a worksheet are available in the eBook.





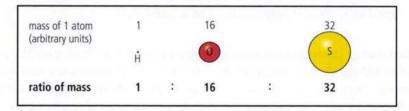
100 atoms of H, O and S have the same mass ratio as one atom of each element. 1:16:32.

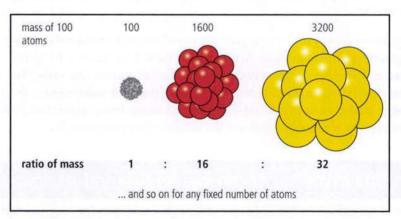
atoms of H, O and S have the same mass ratio as one atom of each element. This number of atoms gives an amount that we can see and measure in grams.

# The Avogadro constant defines the mole as the unit of amount in chemistry

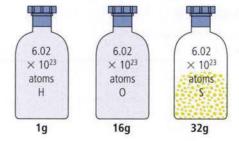
We know that even with the very best experimental apparatus available, we are unable to measure the mass of individual atoms in the laboratory directly. They are simply too small. This is not really a problem because all we need to do is to weigh an appropriately large number of atoms to give a mass that will be a useful quantity in grams. As atoms do not react individually but in very large numbers, this approach makes sense. So how many atoms shall we lump together in our 'appropriately large number'?

Let us first consider that atoms of different elements have different masses because they contain different numbers of particles, mostly **nucleons** in their nucleus, as discussed in Structure 1.2. This means we can compare their masses with each other in relative terms. For example, an atom of oxygen has a mass approximately 16 times greater than an atom of hydrogen, and an atom of sulfur has a mass about twice that of an atom of oxygen. The good news is that these ratios will stay the same when we increase the number of atoms, so long as we ensure we have the same number of each type of atom.





If we could take  $6 \times 10^{23}$  atoms of hydrogen, it would have a mass of 1 g. It follows from the ratios above that the same number of atoms of oxygen would have a mass of 16 g, while the same number of atoms of sulfur would have a mass of 32 g. We now have a quantity of atoms that we can measure in grams (Figure 1).



This number, accurately stated as  $6.02214129 \times 10^{23}$ , is known as the Avogadro number and it is the basis of the unit of **amount** used in chemistry known as the **mole**. In other words, one mole of a substance contains the Avogadro number of particles. Mole, the unit of amount, is one of the base units in the SI system and has the unit symbol **mol**.

The example in Figure 1 is illustrative only, as in reality hydrogen and oxygen do not occur stably as single atoms, but as diatomic molecules,  $H_2$  and  $O_2$ , as explained in Structure 2.2. Other substances exist as particles of different types, so the term **elementary entity** is used to cover the broad range of possible particles. An elementary entity may be an atom, a molecule, an ion, an electron, any other particle or a specified group of particles.

In 2019, the International Union of Pure and Applied Chemistry (IUPAC) published a change to the definition of the mole. The new definition emphasizes that the quantity 'amount of substance' is concerned with counting entities, rather than measuring the mass of a sample.



The SI refers to the metric system of measurement based on seven base units. These are metre (m) for length, kilogram (kg) for mass, second (s) for time, ampere (A) for electric current, kelvin (K) for temperature, candela (cd) for luminous intensity and mole (mol) for amount. All other units are derived from these. The SI system is the world's most widely used system of measurement.



The International Bureau of Weights and Measures (BIPM according to its French initials) is an international standards organization, which aims to ensure uniformity in the application of SI units around the world. The BIPM officially introduced updated definitions to these base units, including the mole, in 2019.

So 'mole' is simply a word that represents a number, just as 'couple' is a word for 2 and 'dozen' is a word for 12. A mole is a very large number, bigger than we can easily imagine or ever count, but it is nonetheless a fixed number. So a mole of any substance contains the Avogadro number,  $6.02 \times 10^{23}$ , of entities. It can refer to atoms, molecules, ions, electrons and so on – it can be applied to any entity because it is just a number. And from this, we can easily calculate the number of particles in any fraction or multiple of a mole of a substance.



i

Amedeo Avogadro (1776-1856) was an Italian scientist who made several experimental discoveries. He clarified the distinction between atoms and molecules, and used this to propose the relationship between gas volume and number of molecules. His ideas were not accepted in his time, largely due to a lack of consistent experimental evidence. After his death, when his theory was confirmed by fellow Italian Cannizzaro, his name was given in tribute to the famous constant that he helped to establish.

a

The mole is the SI unit of amount of substance. One mole contains exactly 6.022 × 10<sup>23</sup> elementary entities. This number is the fixed numerical value of the Avogadro constant, N<sub>A</sub>.

Each sample contains one mole, 6.02 × 10<sup>23</sup> particles, of a specific element. Each has a characteristic mass, known as its molar mass. Clockwise from upper left the elements are: carbon (C), sulfur (S), iron (Fe), copper (Cu) and magnesium (Mg).

addition polymers 276-9 alkenes 325 absolute temperature 21-2, 435, cistrans isomers 370-1 524, 584 addition reactions 277, 787-8, 869 distinguishing from alkanes 839 adsorption 790 absolute zero 21, 22, 128, 129, 521 electrophilic addition reactions of absorbance of light 330-4 air 11 837-40, 854-62 alchemy 882 measuring reaction rates 581, reactions with halogens 838, 600 - 2alcohols 855-6 combustion reactions 489 solutions 112 reactions with hydrogen halides absorption of IR radiation 387-92, general formula 353 oxidation of 779-84 839, 855, 856-7, 860-2 502 physical properties 353-4 reactions with water 837-8, 858 absorption spectra 54, 55 reduction 787-8 abundance (isotopes) 39, 43, 44, primary, secondary and tertiary structural isomers 363-4 compounds 364-5, 779-82 unsymmetrical 860-2 acid-base character 310, 677-9 protons 403 acid-base indicators 559, 683, 699, reaction with carboxylic acid alkyl groups 850 alkynes 364, 787, 788 280-2, 358 719 - 22allotropes 198-203 aldehydes 780-1, 785-7 acid-base theories 672-4, 675, alloys 11, 258, 271-3 alkali metals (group 1) 151-3, 841 - 3acid-base titrations 558-9, 295 - 6alpha particles 32-3 aluminium 77-80, 154, 809 697-701, 715-19, 720-2 electron configuration and ions aluminium chloride 268, 270 155, 258-9 acid deposition 311–13 aluminium ions 70-1 period 3 oxides 310 acid dissociation constant 704-12 aluminium oxide 310, 777-8 acid rain 311-13, 679-80, 696 properties 298, 305 reaction with water 305-6 amide links 282-3, 350 acidic non-metal oxides 310, amines 282-3, 365 reactions with halogens (group 311-13, 679 amino acids 218, 282, 350-1 17) 152-3 acids ammonia 556, 673 reducing agents 756 and buffer solutions 723-7 conjugate bases 159-60 alkaline electrolytes 508-10 Haber process 324, 643-5 ammonium 676 dissociation 689, 690, 691 alkalis 676-7, 723-5 ammonium chloride 673 Lewis acids 186-7, 841-3 alkanes 325, 352-3 alkenes and alkynes reduced to amphiprotic species 677-80 oxidation of metals 759-61 amphoteric oxides 310, 311, 679 pH values 681-4 analytical techniques 379, 405-8 boiling points 208, 362 reactions with bases 673, 674-5, infrared spectroscopy 385-92 carbon content 499-501 693 - 7mass spectrometry 380-4 combustion reactions 489, relative strengths 704-12 nuclear magnetic resonance see also Brønsted-Lowry acids 499-501 and bases; strong acids; weak distinguishing from alkenes 839 (NMR) spectroscopy 393-404 physical properties 353-4 anhydrous salts 101 acids anions (negative ions) 37, 150, reaction with bromine water in activation energy 432, 458, 488, 152, 154, 155-6 UV light 827 586 electrolytic cells 775, 776 reactions with halogens in UV calculated with Arrhenius forming lattice structures 161–3 equation 614-18 light 826-8 anodes 761, 764-8, 776-8, 792, specific energy 500-1 effect of catalysts 592 793 of rate-determining step 598 structural isomers 362-3 substitution reactions 825-8 anodizing 809 activity series 757-8, 760

anti-particles 33-4 base dissociation constant 704-12 bond enthalpies 454-60, 851 approximations 656 bases bond length 184-5, 219-20 aqueous solutions 16, 110 and buffer solutions 723-5, 727 bond polarity 193-6, 455 acidic, neutral or basic 686-7 dissociation 689-90 bond strength 184-5, 205, 219-20 electrolysis 802-8 Lewis bases 841-3 metallic bonds 258-9, 323 endothermic/exothermic pH values 681-4 bond vibrations 387-8, 390 reactions 428-9 reactions with acids 673, 674-5, bonding continuum 168, 195-6, metal and non-metal oxides 693 - 7310 - 13relative strengths 704–12 bonding triangle 265-70 of salts 696 see also Brønsted-Lowry acids Born-Haber cycles 473-8 aromatic compounds 345 and bases; strong bases; weak boron 66, 69 Arrhenius equation 613-18 bases Boyle, Robert 30 Arrhenius factor 614, 616-17 basic metal oxides 310–11, 679 Boyles Law 126-7 Arrhenius plot 615-16 branched-chain isomers 362-3 batteries 763, 768, 770-1 Arrhenius, Svante August 672 benzene 863 bromine 306 arrow-in-box diagrams 66, 69 disubstituted 366-7 addition reactions 855-6 asymmetric synthesis 377 electrophilic substitution displacement reactions 307 atom economy 278, 568-70, 874 reactions 864-8 gas volumes 113-14 atomic models 29-38, 59-67, 73 hybridization 244-5 reaction with alkanes 827 Bohr model 34-5, 56, 59, 60, 76 nitration of 865-6 bromine water 827, 839 Dalton's model 30-2, 60 properties 223-5 Brønsted-Lowry acids and bases energy levels 56-7 ring structure 222-7 671-7, 841-2 Rutherford's nucleus model benzene ring 345 amphiprotic species 677-80 32 - 3beryllium 66, 69, 301 conjugate acid-base pairs 675-6 Schrödinger model of hydrogen bimolecular reactions 849 conjugate acids and bases atom 61-5 biodegradability 275-6 formulas 676-7 subatomic particles 33-4 biofuels 495, 504-8 neutralization reactions 693-7 Thomson's 'plum pudding' biological compounds 495, 496 strong and weak 688-92 model 32 biological reactions 593 buckyballs 202 atomic number 29, 35-6, 37 blood 351, 493 buffer region 716 and orbital energy 68-9 buffers in 727, 729-30 buffer solutions 716, 722-31 atomic radii 298, 321-2 Bohr model of the atom 34–5, 56, buffering capacity 729 atoms 8, 30 59, 60, 61, 76 butane 344, 556 mass of 90-1, 93-5 Bohr, Niels 62 nuclear charge 151-2 boiling 17, 18 caesium 72, 269 Aufbau Principle 66 boiling points 17, 18, 21, 40 caesium fluoride 269 Avogadro, Amedeo 91 alkane isomers 362 calcium Avogadro constant 90-3, 96 covalent compounds 212-13 ionization energies 80 Avogadro's law 113-16, 135, 555 and intermolecular forces 207-9, oxidation states 80 azo-dyes 366 210, 212-13 calibration curves 112, 333-4 ionic compounds 163-4 calorimeters 436-7, 438, 439-40 back-titration 560-1, 565 organic compounds 353-4, 362 carbocation 850, 851, 856 balancing equations 550-3, 554, bond angles 190, 228-30 carbohydrates 490 749-50 bond dipoles 175, 194, 197 carbon 205

chromatography 216-22 catenation 347 allotropes 198–203 chromium 69, 156, 809 cathodes 761, 765-8, 776-8, 792, combustion product (soot) 491–3 cistrans isomers 370-2 covalent bonding 239-42 793 classes of compounds 348-50 electron configuration 66 cations (positive ions) 37, 150, classification systems 8, 11, 289, electron deficient 833 152, 155-6 341, 348–50, 360, 693 charge and radius 258-9 reducing agent 758 electrolytic cells 775, 776 climate change 501-3 relative atomic mass 43-4 clock reactions 582-3 lattice structures 161, 256-7, carbon-12 isotope 258 coal 495-6, 498 comparing masses of atoms cell diagrams 765-6 collision theory 585-8 93 - 5collisions radiocarbon dating 46 Celsius scale 21-2 chain reactions 826-7 energy 586 relative atomic mass 43-4 geometry 587 changes of state 17-21 carbon-14 46 particles 22 charge density 332 carbon chain 344, 355-9 particles and anti-particles 33-4 Charles' law 128-9 branching 362 colorimetry 333-4, 581 chemical environments 398-401 in combustion reactions 488-9, colour change 782 chemical equations 98, 549-53, 782 coloured complexes 324, 329-34 length 353-4 570 - 1combined gas law 134-5 chemical feedstocks 496 carbon content 499-501 chemical formulas 10, 158-9, 160 combustion analysis 99-100, 102, carbon dioxide 105 combustion product 489, 500, chemical properties 304-8 combustion reactions 431, 486-91 cistrans isomers 372 554 alkanes 499-501 enantiomers 376-7 dissolving in water 311, 313 classifying 821 transition metals and compounds equilibrium between dissolved enthalpy changes 436-9 324-6 and gaseous 642-3 incomplete combustion 438-9, chemical reactions 150 greenhouse effect 501-3 491-4 chemical shifts 396-9 neutralization product 695 metals and non-metals 486-8 vibrational modes 388 chemical symbols 9, 31 carbon footprint 498-9, 553 reactants and products 554, 556, chiral carbon atom 372-5 chiral drugs 377-8 carbon monoxide 491-3 standard enthalpy change 464-5, carbon nanotubes 201-2 chiral molecules 372-5, 376-7 chlorine 152-3, 306 carbonates 313, 695-6 466 displacement reactions 307 thermochemical equations 434 carbonic acid 311, 313, 695-6 carbonyl compounds 785-7 isotopes 39-40 combustion theories 552 complete combustion 489, 492-3 carboxylic acids 357 oxidizing agents 755-6 complex ions 186-7, 328-34, photolytic fission 823 reaction with alcohol 280-2, 358 843 - 7reaction with amine 282-3 radicals 823-4 charge on 845-7 reaction with hydrogen 741 reduction 785 colour 329-34, 844 reaction with methane 826-8 catalysts 591-3, 598 ligands 329, 844, 845 relative atomic mass 43 chlorine radicals 824 composite materials 270 chlorine molecules 178 and equilibrium 641-2 chloroalkanes 353-4 compounds 7-8, 10, 31 in methanol fuel cells 510-11 bonding type, bonding triangle transition metals 324-5, 788 chlorofluorocarbons (CFCs) 389, and electronegativity 266-70 594, 823-5 catalytic converters 325, 493

combustion analysis 105 electron configuration 69 covalent network structures empirical formulas 99-103, 104, half-cells 763-7, 791 198-205 105 - 7ions 157 period 3 oxides 309, 310 hydrated 95 redox reactions 740-1 and physical properties 213, molecular formulas 104-7 reducing agent 756-7 214, 215 naming 318-19, 746-7 copper sulfate crystalline solids 163-4 percentage composition by mass electrolysis 806-7 crystallization 13 101 - 3reaction with zinc 440-1, 523. Curie, Marie 36 relative formula mass 94-5 524, 756-7, 762 curly arrows 823, 833, 835, 842, concentration 107-13 Corey, E.J. 891 870 determining 558-61, 750-4 covalent bonding 167, 175-253 cyclic compounds 371 equilibrium 630-1, 638-9, bond formation 176-7, 239-43. cycloalkanes 371 651-7,703280 initial 651-3, 655-6, 703, 706-8 bond length 184-5, 219-20 d block elements 71-2, 157, measuring 579 bond polarity 193-6 292-3, 295-6 and orders of reactions 602-3, bond strength 184-5, 205, atomic radii 322 605 - 7219-20 electron configuration 68, 69, rate of change 575-8 breaking bonds 277, 283-4, 321 - 2and rate of reaction 575-8. 822-5, 834-5 data 912-13, 918 589-90, 600-7 coordination bonds 186-7, 832, databases 904, 906-7 of reactants 589-90 842 primary/secondary 917 condensation 17, 19, 21, 628 formal charge 233-6 simulations 904-5, 907, 917 condensation polymers 280-4 hybridization 239-45 de Broglie equation 76 condensation reactions 280-4, Lewis acid-base reactions 842-3 decomposition reactions 350 - 1Lewis formulas 179-81, 183, balancing equations 551 configurational isomers 370-8 219-20, 233-5 rate equation 600-2 confirmation bias 884 molecular geometry 188-93, thermal decomposition of water conformational isomers 369 197-8, 227-31, 243-4 656 conjugate acid-base pairs 675-6, multiple bonds 182-5, 190, deductive reasoning 889 710 - 11219-22, 238 degenerate orbitals 63, 65 conjugate acids 675–7, 712–14 octet rule and stable arrangement delocalization 219-21 conjugate bases 159-60, 675-7, of atoms 178, 181, 227-30 delocalized electrons 711, 712–14 polyatomic ions 160 covalent bonding 219, 220, 223, conservation of energy 453, 460-1 polymers 274, 277-9, 280 224-5, 245 Contact process 646 pure covalent bonds 195-6 metallic bonding 256-7, 258-9 continuous spectrum 53, 54, 55 sigma and pi bonds 237–8, transition elements 260-1 controlled variables 594 240-2, 245 deposition 17 convergence limit 74-7 VSEPR model 188-93, 230-1, diamond 199-200, 215 coordination bonds 186-7, 329, 243 - 4diastereomers 373-4 832, 835, 842, 844 covalent character 265-70 diffraction 59, 60 coordination number 161, 329, covalent compounds 168 diffusion 16 845 period 3 oxides 309 dihalogeno compounds 838 copper 760 physical properties 212-15 dilutions 111–13 electrodes 806-7 covalent model 175 dimensional analysis 97

dipeptides 350-1 dipole-dipole attraction 208-9 dipole-induced dipole attraction 209 dipole moment 197-8, 387-8, 389, 502 dipoles 207, 208, 209 displacement reactions 307, 756-8 zinc/copper sulfate 523, 524, 756 - 7disproportionation reactions 318, dissociation constants 704-12 distillation 13, 781 double-bonded molecules 370-1, 372 double bonds 182-5, 219-22, 238, 241, 277 effective nuclear charge 151-2, 297, 300 effervescence 695 efficiency of chemical process 566-9 Einstein, Albert 881, 884, 896 electrical conductivity 214-15 ionic compounds 166 measuring rate of reaction 582 silicon 205 transition metals 261 electrochemical cells 761-2 see also electrolytic cells; primary (voltaic) cells; secondary (rechargeable) cells electrode potentials 764-5, 789 electrodes 761, 763-8, 775, 776-8 competing reactions 802-3 copper 806-7 inert 775, 790, 806 electrolysis 774-9 of aqueous copper sulfate 806-7 of aqueous sodium chloride (brine) 805-6 competing reactions in aqueous solutions 802-3

with copper electrodes 806–7 electroplating 808–9 with graphite 'inert' electrodes 806 of molten sodium chloride 775-6of water 804-5 electrolytes 508-9, 770, 775 electrolytic cells 761-2, 774-6, 810 electromagnetic radiation 52-3, 54, 385-6 electromagnetic spectrum 53, 385, electromagnetic waves 54 electromotive force (emf) 789, 795 electron affinities 300-1, 472 electron configuration 68-9, 84 complex ions 329 d block metals 69, 321-2 and ionization energies 81-2 ions 70-1 Lewis formulas 179-81 octet rule 178, 181, 227 and periodic table 71-3, 81-2, 151 - 2and periodicity 295-7 from successive ionization energy 77-80 transition metals 321-2, 326 unreactive/reactive elements 154-5 electron configurations 51, 60, 62 - 70arrow-in-box diagrams 66, 69 from emission spectra 55 ground state 66 electron domain geometry 190-2, 228 - 31electron domains 175, 189-92, 197-8, 227-30 electron-in-boxes 66, 69 electron-pair sharing reactions

831, 868-73

electron pairs 831-2, 833, 835 electron sharing reactions 819 electron spin resonance (ESR) spectroscopy 820 electron transfer reactions 739 see also redox reactions electron transfers 150-4, 158 half-equations 748-50 redox reactions 740-1, 743 electronegativity 235 and bond polarity 193-6 bonding triangle 266–8, 269 and ionic character 167–9 periodic trends/periodicity 302 electrons 29, 32, 33, 35–8 Bohr model of the atom 34–5, energy level transitions 54-5, 56 - 7orbitals 61-70 paired/unpaired 68, 323 and photon emission 54-5 shielded 151-2 spin 62, 66 unpaired 819, 820-1 valence electrons 69, 71, 72, 150-2wave and particle model 59-60 see also covalent bonding; delocalized electrons; lone pairs of electrons electrophiles 831-2, 836, 843, 854-5, 865, 869 electrophilic addition reactions 837-40, 854-62 electrophilic reactants 242 electrophilic substitution reactions 863 - 8electrostatic attraction 81, 149, 152 - 3covalent bond 176-7 metallic bond 257

elementary entity 91

elements 7-9, 30 of hypothetical reactions 453 atomic number 35-6 of ionic compound formation native form 10 472-8 emission spectra 51-8, 74-7 measuring 434-46 empirical formulas 99-103, 104, of neutralization 696 105-7, 118-19, 342, 343 of reaction in solution 428-9, enantiomers 372-6 439-43 endothermic processes 21, 301. and spontaneity of reaction 454-5, 456 533-4 endothermic reactions 428-30 standard enthalpy change 434, energy profiles 432-4 462-3, 464-7 and entropy 524, 525-6 in the system 524 equilibrium 640-1 thermochemical equations 434 spontaneity 432, 533 entropy 517, 518-19, 541-5 energetic stability 430-1 absolute entropy 520-1 energy cycles 453, 461-2, 478-83 of the universe 517, 518-19, 523 Born-Haber cycles 473-8 entropy changes 523-7, 528-34 enthalpy of combustion 467, 470 calculating 521, 525 enthalpy of formation 468, 470 and direction of reaction 523-5 Gibbs cycle 527 predicting 519-20 energy density of fuels 495 and spontaneity of reaction energy level diagrams 460, 462 533-4 energy levels 54-8, 296 of surroundings 523-4 total entropy change 525, 527, complex ions 329 electron configurations 65-73 531 and ionization energies 74-5, enzymes 276, 284, 593 equilibrium 534-9, 627-67 77-80, 81-2 light absorbed/transmitted 330-1 characteristics 629-31 orbitals 62-5 chemical systems 629 energy profiles 432-4, 597-8 closed systems 628 energy transfers 425-6 concentrations 651-7 enthalpy 427 dynamic 627-32 enthalpy changes 427, 447-51, homogeneous equilibria 651 523-34 Le Châtelier's principle 637-47, bond enthalpies 454-60 649,660 calculating from standard physical systems 628 enthalpy changes 466-9 response to change 638-43, calculating from temperature 649 - 50change 435-6 equilibrium constant expression of combustion 436-9, 461-2, 633-4 464-5, 467, 469-70 equilibrium constant (K) 536, as direction of reaction 431-4 538-9, 632-7, 642 of formation 465-7, 468-70 calculating 651-3, 659-60 Hess's law 461-4 calculating equilibrium

concentrations from 654-7 effect of temperature 640-1 extent of reaction and 634-5 magnitude 634-5, 655-6, 660-1 predicting 632-4 reverse reactions 635-6 weak acids and bases 704-12, 720 equilibrium law 633-7, 651-7 equilibrium mixture 535-8, 629, 631 changes in 638-43 quantifying composition of 650 - 7value of equilibrium constant 634 - 5equilibrium position 631, 642, 643, 657-62 equivalence point 698-9, 718, 720-2, 751 equivalent hydrogens 396-7 errors 100, 594-5 ester links 280-2 esterification reaction 659 esters 358 ethane 342-3 ethanoic acid 780 ethanol 381-2, 391 as biofuel 506-7 combustion of 436-8, 489, 490, enthalpy change of formation 466 oxidation 780 synthesis 838 ethene 241-2, 344 addition reactions 855-7, 858 hydration of 838 hydrogenation 521, 788 molecular model 854 production process 547 reaction pathway 350 ethers 359 ethics 892-3

volume 113-16, 555-8 hydrogen bonding 209 ethyne 242 reactivity 153 general formulas 353 evaporation 18, 628 giant covalent structures 198-205 formal charge 233-6 exams and exam preparation period 3 oxides 309, 310 formula units 161 921 - 3and physical properties 213, excitation 239 fossil fuels 494-504, 512 214, 215 exothermic processes 21, 456 fractional distillation 512 giant ionic structures 309, 310 exothermic reactions 428-30, 431 fragmentation patterns 43, 380-4 Gibbs energy 526-7 free radicals 821 energy profiles 432-4, 598 see also radicals calculating 527-30 and entropy 524 and equilibrium 534-9, 657-60 equilibrium 640-1 freeze-drying 19 freezing 17, 21 predicting feasibility of a change neutralization reactions 696 reaction mechanisms 598 freezing points 17 531 - 2and spontaneity 531-2 spontaneity 533 Freon-12 and standard electrode potentials (dichlorodifluoromethane) 824 zinc and aqueous copper sulfate 799-801 frequency (of a wave) 53, 385-6 440 - 1fuel cells 508-12, 772-4 at a temperature 528-9 expanded octets and molecular glassware 109, 113, 559 geometry 227-30 fuels 485, 512-15 alkanes 499-501 gold 760 experimental techniques 909-12 biofuels 495, 504-8 gold foil experiment 32-3 experimental yield 566-7 graphene 200-2 explosives 866-7 carbon content 499-501 graphite 199-202 extended essay 924-31 energy density 495 Green Chemistry 547, 568-70, fossil fuels 494-504 593, 642, 865, 874-7 fullerene 200-2, 215, 600-2 f block elements 71-2, 292-3, 295 greenhouse gases 388-9, 501-3 functional group isomers 366 Faraday constant 93, 800 ground state 54 feasibility of a reaction 526, functional groups 341, 348-52 ground state configurations 66, 71 531-2, 800, 801 and chemical reactivity 350 and classes of compounds group 1 metals see alkali metals fertilizers 102-3 348-50 group 2 elements 81–2, 155, Feynman, Richard 29, 423, 886, 258-9, 301, 320 condensation reactions and 887 group 13 elements 81-2, 155, 320 filtrate 13 amino acids 350-1 group 14 elements 155, 203, 210 condensation reactions and filtration 13 group 15 elements 81-2, 155, 210, polymers 280–3 first ionization energy 74, 78, 320 in general formulas 353 81-2, 152, 299-300, 320-1, group 16 elements 81-2, 154, 155, 472 naming compounds 356–8 oxidation 779-84 210, 320 first-order reactions 602, 604, 606, and physical properties 354 group 17 elements see halogens 607 reduction 785-7 flame tests 52 Haber process 324, 643–5 fluids 16 half-cells 763-9, 789-92, 798 gases 15-16 fluorine half-equations 509-11, 552, changes of state 17, 18, 19, 20-1 electron configuration 66 748-50 measuring change in volume electronegativity and bond 579-80 half-equivalence point 716, 717 polarity 194 halide ions 164, 307, 755, 851 electronegativity and bonding produced in a reaction 579-80 solutions 107 halogenated compounds 857 triangle 269

ê 4		
halogenation 788	hydrated salts 101	hydrogen sulfide 497, 741, 742
halogenoalkanes 839	hydration 837–8	hydrogenation 521, 788
nucleophilic substitution 833-4,	hydrides boiling points 210	hydrogencarbonates 313, 695
848–53	hydrocarbons 184-5	hydrolysis reactions 283-4
primary, secondary and tertiary	combustion 488-9, 491, 493,	
364–5, 612, 848–51	556	ice 17, 20
radical substitution reactions	incomplete combustion 499-500	ideal gas equation 135-40
826–7	molecular formulas 116, 556	ideal gas model 114, 121-4, 138
halogens (group 17) 295-6	solubility 214	ideal gases 121-45
boiling points 208, 210	unsaturated 787-8, 837	gas laws 126-40
displacement reactions 307	see also alkanes; fossil fuels	molar mass 136-7
electron affinities 301	hydrofluorocarbons (HFCs) 389,	molar volume 132-3
electron configuration and ions	825	pressure, temperature and
154, 155	hydrogen	volume 126-33
nucleophilic substitution 833	Bohr model 34–5	incomplete combustion 438-9,
oxidizing agents 755-6	combustion of 98	491–4
properties 306-7	electron configuration 66	indicators 559, 683, 699, 719-22,
reactions with alkali metals	equivalent hydrogens 396-7	751
(group 1) 152–3	gas volumes 113-14	inductive reasoning 888-9
reactions with alkanes in UV	ions formed 155	infrared (IR) active molecules
light 826-8	line emission spectrum 56-7	197–8
reactions with alkenes 838,	loss/gain in redox reactions 741	infrared radiation 53, 56, 387-92
855-6	reaction with chlorine 741	infrared spectroscopy 385-92,
reactivity 153, 306-7, 755-6	relative atomic mass 43	405–8
heat transfers 425-6, 427, 517	released by oxidation of metals	inner electrons 151-2
and entropy 523-4	by acids 759-61	inquiry process 917–19
Heisenberg, Werner 62, 888	Schrödinger model 61-5	inter-particle forces 15, 17, 20, 21
Heisenberg's Uncertainty Principle	hydrogen bonding 209-12, 390	intermediates 596-7, 598
61	hydrogen bromide 856-7, 860-1	intermolecular forces 175, 206-12
helium 66	hydrogen chloride 178, 194, 195,	ideal gas model 122
Hess's law 460-4	673, 826–7	and physical properties 212-15,
heterogeneous mixtures 12	hydrogen economy 805	354
heterogeneous reactions 591	hydrogen fuel cells 508-10, 772-3	real gases 124-5, 140
heterolytic fission 834-5, 848, 857	hydrogen half-cell 789-92	internal assessment (IA) 898-907
hexane combustion 465, 492-3	hydrogen halides	intramolecular forces 209, 211
Higgs' boson 83	acid strength 691	inversely proportional relationships
homeopathy 892	electronegativity and bond	126–7
homogeneous mixtures 11, 12	polarity 195	investigation skills 594-5
homogeneous reactions 634	nucleophilic substitution 834	iodine 306
homologous series 352-5	reactions with alkenes 839, 855,	displacement reactions 307
homolytic fission 822-5, 869	856–7, 860–2	electron configuration 72
Hund's third rule 66, 69	hydrogen ion concentration 680-1,	oxidizing agents 755-6
hybridization 175, 239-45	683–4	redox titrations 751-2
hydrated ions 165	hydrogen molecules 177	starch test 229

The state of the s		
iodine chloride 554 ion hydrolysis 712–14 ionic bonding 149–61 bond strength 162–3 and electronegativity 167–9 ionic bonds 161, 162–3, 167 ionic compounds 101, 157–9, 171–3, 195–6 dissolving in water 164–5 as electrolytes 776–8 formation of 152–3, 472–8 formula 158–9 giant structures 309 ionic character 166–9, 265–70, 309 lattice enthalpies 472–8 lattice structures 149, 161 period 3 oxides 309 physical properties 161–6, 215 ionic equations 760 ionic model 163, 166–7, 170–1 ionic product constant of water 685–7 ionic radii, 163, 164, 298–9	in voltaic cells 765, 768 iron galvanized 809 ions and ionic compounds 157, 158 redox titrations 752–3 relative atomic mass 43 rusting 660 isomers 210 stereoisomers 368–79 structural isomers 361–8 isotopes 39–42, 43–7, 48–9 abundance 39, 43, 44, 45 relative atomic mass 43 IUPAC nomenclature 355–61, 894–5  Kekulé structure 224 Kelvin scale 21–2 ketones 357, 781, 785 Kevlar® 282, 283 kinetic energy (KE) 16, 17 collision theory 585–7 of particles 20–2	Lévi-Strauss, Claude 896 Lewis acid-base reactions 186–7, 842–3, 844 Lewis acids 186–7, 841–3 Lewis bases 186–7, 841–3 Lewis formulas 179–81, 183, 189–92, 233–5 Lewis, Gilbert 179, 841, 842 ligands 186–7, 329, 332, 844–6 light see ultraviolet light; visible light limiting reactant 563–6 line emission spectra 54–5, 56–7 linear relationships 128 liquids 15–16 changes of state 17, 18, 19, 20–1 polar/non-polar 165 solutions 107–8 lithium 66, 69 lithium-ion batteries 770–1 logarithmic scales 680–2 London dispersion forces 207–8, 209, 354 lone pairs of electrons 178, 179,
ionic radii 163, 164, 298–9 ionization extent and acid/base strength 689–90	of particles 20–2 and temperature 20–3, 435, 584–5, 589 kinetic molecular theory 14–18,	lone pairs of electrons 178, 179, 831 in hybridization 243 Lewis acid-base theory 841–3,
of water 685–8 ionization energies 57, 73–82, 85–7, 152, 154	584–5 kinetic stability 826 kinetic theory of gases 121–3, 141	844 and molecular geometry 189–92, 228–31
discontinuities 320–1 first 74, 78, 81–2, 152, 299–300, 320–1, 472 noble gases 155 periodic trends/periodicity 81–2, 152, 299–300, 320–1 successive 77–80 ions 37–8 charge on 153, 154, 155–6 electron configuration 70–1 formation of 150–4 ion pairs 161, 163 Lewis formulas 180–1 oppositely charged 835	Kuhn, Thomas 884  Large Hadron Collider (CERN) 83 lattice enthalpies 162–3, 472–8 lattice structures alloys 271–2 covalent network structures 198–205 ionic compounds 149, 161–3 metallic structure 256–7 Le Châtelier's principle 637–47, 649, 660 lead 157 Lead(II) bromide 776–7	macronutrients 103 magnesium combustion reactions 487 ionization energy 154 mass change on burning 99–100 redox reactions 740–1 magnesium fluoride 163–4 magnesium oxide 99–100, 153, 158, 740–1 dissolving in water 310–11 formation enthalpy changes 475–6

melting point 163–4 oxidation state 315	metal carbonates 695 metal hydroxides 694	molecular geometry 197–8, 227–30
magnetic properties 323-4	metallic bonding 255-63, 271, 323	and hybridization 243-4
magnetic resonance imaging (MRI)	metallic character 265–70	using VSEPR model 188–93,
394–5	metalloids 294, 309	230–1
manganese 156	metals 292–3	molecular orbital theory 240
Markovnikov's rule 860–2	alloys 11, 258, 271-3	molecular orbitals 237–8
mass	combustion 486–8	molecular polarity 175, 196–8,
change in 580	electron transfers 155	232
measuring 89, 580	ionization energies 81–2	and intermolecular forces 207-
of reactants and products 98,	ions 150–2	molecularity 597, 603–4
553–4	oxidation by acids 759–61	molecules 30–1
relative mass of subatomic	oxides 309–11, 694	molten salts 775–9
particles 33	physical properties 257–8	monomers 274, 277, 280, 281,
mass/charge ratio 43, 44	reactions with acids 694	282–3
mass number 35–6, 37, 39	reactivity 756–8	202 3
mass spectra 42–7, 49	reducing agents 756–8	nanotechnology 202
mass spectrometry 380–4, 405–6	methane 241	natural frequency 387
mathematics 617, 914–16	for biogas 507	natural gas 497, 498, 547
Maxwell-Boltzmann energy	combustion 434, 457–8, 553,	natural polymers 274, 281
distribution curve 22, 585,	554	neon 66
586, 589, 592	in natural gas 497	net dipole 232
measurement accuracy 109, 910	reaction with chlorine 826–8	neutralization reactions 693–7
measuring 888, 910	methanol 344, 506, 645	enthalpy changes 442–3, 696
change in concentration 582	methanol fuel cell 510–11	pH curves 697–701
change in transmission of light	methyl orange 720	neutrons 29, 33, 35–8
581–2	microbial fuel cells 511	Bohr model of the atom 34–5
change in volume of gas	microplastics 278	isotopes 39–42
produced 579–80	mixtures 7–8, 11–14	nickel 568, 788
mass 89, 580	alloys 11, 258, 271–3	nickel-cadmium batteries 771–2
pH values 683	separating with chromatography	nitrating mixture 865
standard electrode potentials	216–19	nitration of benzene 865–6
790–2	models 60, 346–7, 890–1	nitric acid 312, 865–6
melting 17	molar concentration 107–13	nitrobenzene 865–6
melting points 17, 21, 40	molar mass 96–8, 117–18, 136–7	nitrogen 66, 209, 301, 489
covalent compounds 212–13	molar volume of a gas 557–8	nitrogen molecules 183
and intermolecular forces 207,	molar volume of an ideal gas	nitrogen oxides 312, 493, 679
208, 212–13	132–3, 134	Nobel, Alfred 867
ionic compounds 163–4, 166,	mole (mol) 89–93, 96–8, 117–18	noble gases (group 18) 295–6
167	and gas volume 113–16, 133	chemical properties 178, 304
metals 259	mole ratios 115–16, 553–62,	ionization energies 155
period 3 chlorides 167, 268	563–5	non-metals 293-4
transition elements 261	molecular formulas 104–7, 116,	combustion 486–8
Mendeleev, Dmitri 291, 292	118–19, 342–3	electron transfers 155
	110 17, 572 5	Steeligh dansiers 133

oxidation of alcohols 780 initial rates method 608-9 ionization energies 81-2 relative strengths 798-9 overall reaction order 602-3, ions 150-2 604, 608-9 oxides 309-10, 311-14, 679 oxygen combustion reactions 486-91 oxidizing agents 755-6 with respect to reactants 602-3, 605 - 7electron configuration 66 reducing agents 758 organic compounds 341, 408-19 hydrogen bonding 209 non-polar liquids 165 hydrogen-oxygen fuel cell non-polar molecules 207-8, 214 analytical techniques 379-408 bond vibrations 387-8 508-10 nuclear charge 151-2 classes 348-50 limited during combustion nuclear magnetic resonance (NMR) combustion 488-94 491 - 2spectroscopy 393-404, 405-8 loss/gain in redox reactions formulas/structural nucleons 29, 33, 90 740 - 1representations 342-7, 353 nucleophiles 785, 831-2, 834, 843, reaction with hydrogen sulfide 869 functional groups 348-52, 353, 356-8, 779-87 741, 742 nucleophilic substitution reactions ozone 219-20 832-4 homologous series 352-5 atmospheric ozone depletion heterolytic fission 834-5 identifying bonds 389-91 389, 594, 823-5 leaving group 833, 834, 849, molecular mass 380 850, 851 naming 355-61 Lewis formula 190-1 ozone layer 458, 459, 594, 823 physical properties 353-4 primary halogenoalkanes 848-9 saturated/unsaturated 350 rate expressions 851-2 skeletal formulas 223 p block elements 71–2, 292–3, reaction profiles 851–2 stereoisomers 368-79 295 - 6secondary halogenoalkanes 851 paper chromatography 13, 216-17  $S_N 1$  and  $S_N 2$  mechanisms 847–53 structural isomers 361-8 paradigm shifts 32, 60, 884-6 oxidation 315 tertiary halogenoalkanes 850-1 particle collisions 22, 33-4 of alcohols 779-84 nucleus 29, 30, 32-3, 40 definitions 740-2 in chemical reactions 585-8 nylon 282-3 in electrochemical cells 761-3. ideal gas model 122-3 real gases 124-5, 139 764 - 5Occam's razor 883-4 particle model 59–60 ocean acidification 313, 723 half equations 749–50 of metals by acids 759-61 particles, term definition 15 octane 493 octet rule 175, 178, 181 relative ease of 755-6 Pauli Exclusion Principle 62 of water 802-3 pentane 489 exceptions to 181, 227 peptide bonds 350-1 see also redox reactions oil (crude) 496-7, 498, 547 percentage by mass 101-3, 753 oxidation numbers 158, 746-7 optical activity 375-6 percentage yield 566-7 oxidation states 80, 156-8, 315-20 optical isomers 372-8 period 3 elements 151 combustion reactions 486-7 orbitals 51, 61-70 ionic character of chlorides 167 limitations 744 and covalent bonding 239-43 properties 298-9 period 3 elements 310 hybridization 240-3 redox reactions 741-5 period 3 oxides 267, 309-11 order of filling 66-7 periodic table 289, 291-2, 293, overlapping 237-8, 240-2 transition metals 326-8 variable 326-8 882 relative energy 65, 68-9 oxides 309-14 and charge on an ion 155-6 order of reaction

oxidizing agents 745-6, 751,

755 - 6

and electron configuration 71-3,

81-2, 151-2

612

determining rate constant units

ionic compounds 166-7	photons 33-4, 54	positrons 33–4
and ionization energies 81-2,	photosynthesis 434, 504-5	ppm (parts per million) 110
152	physical properties 40	precipitate 307-8
metals and non-metals 292-4	alloys 272	pressure
and nuclear charge 151-2	and bonding types 266-70,	changes of state 17, 18, 19
periods and groups 292, 295-6	309–10	at equilibrium 639-40
periodic trends/periodicity 291-2,	cistrans isomers 372	gas laws 113-14, 126-7,
335–9	covalent compounds 212-15	129–32, 134–45
acid-base character 310, 679	enantiomers 375-6	ideal gas model 122-4
boiling points 210	ionic compounds 161-6, 215	and rate of reaction 590
ease of oxidation/reduction	metals 257-8	and states of matter 15
755–8	organic compounds 353-4	units 127
effective nuclear charge 151-2,	transition metals 323	primary carbon atom 364
297, 300	pi bonds 238, 242, 854, 856, 860	primary molecules 364, 365
electron configuration 151-2,	Planck equation 54–5, 59	primary (voltaic) cells 512, 762–9,
295–7	Planck, Max 886	773, 810
electronegativity 194, 302	Planck's constant 54	propane 489, 492, 779-80, 788
group 1 and group 2 258-9	plane-polarized light 375-6	propanone 391
ionization energies 81-2, 152,	plastics 275-6, 277-9	propene 788, 856, 860-1
299–300, 320–1	platinum 790	proportional relationships 129
melting points 259	pOH scale 701-4	proteins 282
metal and non-metal oxides	polar bonds 193–8	proton NMR spectroscopy
309–10	polar compounds 214	393-404, 405-8
metallic bonding 259	polar molecules 164-5, 194,	proton transfer reactions 671, 731-7
period 3 oxides 267	208-9	acid-base reactions 673, 674-5
properties of elements 297-304	polarimetry 375-6	neutralization reactions 442-3,
reactivity 304-8	polyamides 282-3	693-701
PET (positron-emission	polyatomic ions 159-60, 676	protons 29, 33, 35-8
tomography) scanners 34	polyatomic molecules 387-8	Bohr model of the atom 34–5
pH curves 697-701, 715-19	poly(chloroethene) (PVC) 277,	isotopes 39–42
pH scale 680-5, 701-3	279	
pH values	polyester 280-2	quantization 55
acid-base indicators 683, 719-20	poly(ethene) 277, 279	quantum theory 55, 60
and buffer solutions 723, 725,	poly(ethylene furanoate) (PEF)	quarks 33
726–9	282	
calculating 683-5, 708-9	polyethylene terephthalate (PET)	racemic mixture 376, 850
measuring 683	281	radicals 819-22, 828-9
salt solutions 712-15	polymers 273–84	chlorine radicals and ozone
temperature dependent 687-8	polypropene (polypropylene) 277,	depletion 823-5
of water 686, 687	279	formed by homolytic fission
phenylamine 366	polytetrafluoroethene (PTFE) 277,	822–3
phosphorus ions and ionic	279	reaction mechanism 826-7
compounds 154	Popper, Karl 889	substitution reactions of alkanes
photolytic fission 822-4, 826-7	positional structural isomers 363-5	825–8
· 15.	*	

termination reactions 823, 827 radioactive decay 608 radiocarbon dating 46 radioisotopes 40 random errors 594-5 rate constant 602, 603, 612-13 temperature dependence 614-18 rate-determining steps 597-8, 603 - 5,850rate equations 600-11, 612-13 experimental determination of 600 - 3rate-determining steps 603-5 rate of reaction 575, 619-25 collision theory 585-8 defining 575-8 effect of catalysts 591-3 effect of pressure 590 effect of reactant concentration 589-90, 602-3, 605-7 effect of reactant surface area 591 effect of temperature 589 and equilibrium 629–30, 660–1 factors influencing 588-94 investigating 594-5 measuring methods 579-84 and reactant/product concentration change 576-8, 600 - 2reacting ratios 549, 553-4, 555, 699 reaction kinetics graphs 605-7 reaction mechanisms 596-9 elementary steps 596-7 exothermic reaction 598 radical substitution reactions 826 - 8rate-determining steps 597-8 and rate equations 603-5 reaction quotient (Q) 535-6, 648 - 50reactivity 153, 155 and functional groups 350

halogens 755-6 metals 756-8 periodic trends/periodicity 304 - 8reactivity series 760 real gases 124-5, 139-40 redox reactions 739-48, 811-17 change in oxidation state 741-2 electron transfer 740-1 formation of sodium chloride 152 - 3half-equations 748–50 hydrogen fuel cells 508, 772-3 hydrogen loss/gain 741 non-spontaneous 774-6 oxidation states 318, 741-5 oxidizing/reducing agents 745-6 oxygen loss/gain 740-1 reversible 770-2 spontaneity 761-4, 774-5, 797 in voltaic cells 762-72, 790, 791-4, 795-801 see also electrolysis; oxidation; reduction redox titrations 720, 750-4 reducing agents 745-6, 756-8 relative strengths 798-9 reduction of carbonyl compounds 785-7 definitions 740-2 in electrochemical cells 761-2, 764 - 5half equations 749–50 relative ease of 756-8 standard electrode potentials 793 of unsaturated compounds 787-9 see also redox reactions reflux heating 781 relative atomic mass 39, 43, 93-4, 96 from mass spectra 44-5 relative charge 33 relative formula mass 94-5, 96

repeating units 274, 281, 283 residue 13 resolution 376-7 resonance 175, 220, 222 resonance energy 226 resonance hybrid 220, 221, 223 resonance structures 219-23, 233 - 5retardation factor 217, 218-19 reverse reactions 635-6 reversible reactions 629-32, 662-7 direction of reaction 648-50 extent of reaction 634-5 rate of reaction and equilibrium 655, 660-1 see also equilibrium rusting 552, 660, 744 Rutherford, Ernest 32-3 atomic model 32-3 gold foil experiment 32-3 s block elements 71–2, 292–3, 295 - 6oxidation states 326 salt bridge 764, 765-6, 768 salts 693-7, 759-61 electrolysis of molten salts 775-9 solutions pH values 712-15 saturation 350 scanning tunnelling microscope (STM) imaging 30 Schrödinger model of hydrogen atom 61-5 scientific investigation 594-5, 898-907 sea water 166, 313 second-order reactions 606-7 secondary carbon atom 364-5 secondary molecules 364-5 secondary (rechargeable) cells 770-2, 773 selective discharge 802–3

serial dilution 112

shielding effect 151-2 ionic compounds 164-5 determining direction of reaction SI units 91 solute 13, 16, 107-8, 110 spontaneity 797 solutions 119 side chains 357-8 and Gibbs energy changes sigma bonds 237-8, 240-1, 242, absorbance 112 799-801 245 concentration 107-13, 333-4 interpreting 801 significant figures 93 concentration of reactants and measuring 790-2 silicon 203-5, 215 products 558-61 standard enthalpy change 434, electron configuration and ions dilutions 111-13 462 - 3formed 155 enthalpy changes 428-9, 439-43 of combustion 464-5, 466 ionization energy 154 pH values of salt solutions of formation 465-7 silicon dioxide 203-5 712-15 standard entropy change 528-9 silver 157, 760 solvation 13 standard Gibbs energy changes electroplating 809 solvents 13, 16, 107-8, 110 527-8, 535-41, 659-60 half-cells 766-7 ionic 164-5 standard hydrogen electrode silver halide precipitates 307–8 polar/non-polar 214, 215 789-90 simulations 904-5, 907 separating mixtures with 216-19 standard solutions 110, 112 single covalent bonds 184-5, 237, specific energy 495, 500-1 standard temperature and pressure 241 specific heat capacity 435-6 (STP) 133 skeletal formulas 223, 344-6 spectator ions 696, 755, 757 starch test 229 S<sub>N</sub>1 reaction mechanisms 847–8, spectrophotometry 581 stars 55 850 - 3speed of light 53 state symbols 16, 551, 552 S<sub>N</sub>2 reaction mechanisms 598, spin (electrons) 62, 66 states of matter 15, 17-21 847-9, 851-3 spin-spin coupling 402 Staudinger, Hermann 274 sodium 154, 296 splitting patterns 402-3 stereochemical formulas 343-4 sodium atom 151, 152-3 spontaneity 541 stereoisomers 368-79 sodium chloride 10 direction of reaction 797 stereospecific reactions 849 dissolving in water 164-5 and enthalpy changes 533-4 steric hindrance 850 electrolysis 775-6, 805-6 and entropy changes 533-4 stock solution 111 formation of 152-3, 162-3, and Gibbs energy 526, 531-2, stoichiometric coefficients 550 473-4, 693 659 stoichiometry 549, 633 lattice structure 161-2, 474 straight-chain isomers 362-3, 364 redox reactions 761-4, 774-5, properties and bonding types strong acids 689, 690-2 797 268, 270 spontaneous change 517, 518, calculating pH and pOH 703-4 sodium fluoride 163-4 pH curves 699-701, 717 sodium halides 163-4 pH of salts formed 713-14 spontaneous reactions 518, sodium hydroxide 509-10 526 - 7strong bases 689-90, 691 sodium oxide 158 and temperature 533-4 calculating pH and pOH 703-4 pH curves 699-701, 716-17 dissolving in water 310-11 standard cell potentials 795-6 melting point 163-4 standard electrode potentials 793 pH of salts formed 713-14 solids 15, 16 calculating emf 795 structural formulas 343, 345-6 changes of state 17, 19, 20-1 and cell potentials 795-6 structural isomers 361-8 solutions 107-8 comparing oxidizing/reducing sub-shells 80-2 solubility 215 power of half-cells 798 subatomic particles 33–8 covalent compounds 214 deducing electron flow 796 sublevels 63-70, 72

ionization energies 80, 156 and ionization energies 78–9, ideal gas model 123 and ionization of water 687-8 magnetic properties 323-4 81 - 2.300oxidation states 80, 156-7 and kinetic energy (KE) 20-3, sublimation 17, 19 substituent groups 357-8 435, 584-5, 589 successive ionization energies substitution reactions 869 and rate of reaction 589, 614-18 80 and spontaneity of reaction variable oxidation states 326-8 of alkanes 825-8 531 - 4see also complex ions electrophilic 863-8 radical mechanism 826-8 and states of matter 15 transition state 849, 852 triple bonds 182-5, 238 see also nucleophilic substitution units 127, 129 two-step reactions 780 temperature scales 21-2, 129 reactions tertiary carbon atom 365 successive ionization energy tertiary molecules 365 ultraviolet light 56 77-80 theoretical yield 563-7 photolytic fission 822-4, 826-7 sulfur 67, 487 theory of knowledge 878-97 reactions in presence of 826-7, sulfur dioxide assessment 896-7 839 and acid rain 312, 679 formation, enthalpy change knowledge framework 880-93 UV-visible spectroscopy 112 462 - 3optional themes 893-6 uncertainty 109 Lewis formula and formal charge thermochemical equations 434 Uncertainty Principle 61 233 - 4thermodynamics, second law 517, unit cells 161 518-19, 525 units 91, 127, 129 sulfuric acid 312, 318 universal gas constant 135-6 thermolytic fission 822 Contact process 646 unpaired electrons 819, 820-1 thin layer chromatography 217-18 industrial use 547, 646 third-order reactions 603, 604-5 unsaturated compounds 787-9 neutralization reaction 442-3 unsaturated hydrocarbons 787-8, nitration of benzene 865-6 Thomson, J.J. 32, 891 837 sulfurous acid 312, 318 3D models 346-7 uranium isotopes 40 surface area 591, 790 tin 157 urea 101 surroundings 426-7 titanium 80, 156 synthetic polymers 275, 282-3 titrations 113, 558-61 system 426-7 acid-base titrations 558-9, valence bond theory 240 697-701, 715-19, 720-2 valence electrons 69, 71, 72, systematic errors 594-5 back-titration 560-1, 565 150 - 2indicators 559, 699, 720-2, 751 Valence Shell Electron Pair technology 892, 893-4, 912-13 Repulsion (VSEPR) model temperature 557-8 measuring rate of reaction 582 188-93 absolute temperature 21-2, 435, redox titrations 720, 750-4 van der Waals' forces 209 transition elements see transition 524, 584 and activation energy 614, 618 metals vanadium 68 vibrational modes 387-8, 502 transition metal ions 844-5 calculating enthalpy change visible light 52-3, 56 transition metals 70, 80, 260-2, 435 - 6absorbed/transmitted 330-4, changes during reactions in 296 solution 428-9 acting as Lewis acids 844 581 - 2changes of state 17, 18, 19, 20-1 catalysts 592-3 colour 329-34, 581 plane-polarized 375-6 effect on buffer solutions 729 characteristic properties 321-6 reaction rates from change in at equilibrium 640-1 coloured complexes 324, absorbance 600-2 329-34, 844 gas laws 113–14, 128–45, 557

UV-visible spectroscopy 112 wave and particle model 59-60 volatility 215 covalent compounds 213 ionic compounds 164 organic compounds 354 voltage 765, 766-7 voltaic cells 761-2 see also primary (voltaic) cells; secondary (rechargeable) cells volume gas laws 126-9, 130-45 of gaseous reactants and products 555-6, 579-80 molar volume of a gas 132-3, 557-8 reactants and products in solution 558-60 real gases 124-5, 139-40 of a solution 108, 109-10, 111 units 558 volumetric analysis 113, 558-60 volumetric flasks 110, 112

water acting as acid and base 677-8 compound formation 31, 550 electrolysis of 804-5 ionization 685-8 molecule geometry and bond polarity 194 molecule geometry and hydrogen bonding 211 neutralization product 693-6 oxides dissolved in 310-14 oxidizing and reducing agent 746 pH values 686, 687 reactions with alkali metals 305 - 6reactions with alkenes 837-8, 858 solubility of ionic compounds 164 - 5thermal decomposition 656 water of crystallization 101 wave models 59-60

wave-particle duality 60, 891
wavelengths 52–3, 385–6
wavenumbers 385, 389–91
weak acids 655, 689, 690–2
acid-base indicators 719–22
buffer solutions 724, 725, 726–9
dissociation constants 704–10
pH curves 716–18
pH of salts formed 713–14
weak bases 655, 690, 691
buffer solutions 724–5, 726
dissociation constants 704–10
pH curves 717–18
pH of salts formed 713–14

zero-order reactions 605–6, 607 zinc 322, 809 half-cells 763–7, 792 reaction with aqueous copper sulfate 440–1, 523, 524, 756–7, 762 reducing agent 756–7, 760

## Online access to your ActiveBook

Thank you for buying Higher Level Chemistry for the IB Diploma Programme 3<sup>rd</sup> Edition. It comes with four years' access\* to your ActiveBook – an online, digital version of your textbook. You can personalise your ActiveBook with notes, highlights and links to your wider reading. It is perfect for supporting your coursework and revision activities.

\*For new purchases only. If this access code has already been revealed, it may no longer be valid. If you have bought this textbook second hand, the code may already have been used by the first owner of the book.



### How to access your ActiveBook

- Scratch off the panel with a coin to reveal your unique access code. Do not use a knife or other sharp object as this may damage the code.
- Go to www.pearsonactivelearn.com
- If you already have an ActiveLearn or ActiveTeach account, log in and click 'I have a new access code' in the top right of the screen.
  - Type in the code above and select 'Activate'.
  - If you do not have an ActiveLearn or ActiveTeach account, click 'Register'. It is free to do this.
    Type in the code above and select 'Activate'.
    Simply follow the instructions on screen to register.

## Important information

- The access code can only be used once.
- Please activate your access code as soon as possible, as it does have a 'use-by date'. If your code has expired when
  you enter it, please contact our ActiveLearn support site at digital.support@pearson.com
- The ActiveBook will be valid for four years upon activation.

#### Getting help

- To check that you will be able to access an ActiveBook, go to https://pearsonactivelearn.com/check\_requirements.asp
- If you have any questions about accessing your ActiveBook, please contact our ActiveLearn support site at www.pearsonactivelearn.com/support

HIGHER LEVEL

# Chemistry



## for the IB Diploma Programme

3<sup>rd</sup> Edition

Pearson Higher Level Chemistry for the IB Diploma

Programme 3<sup>rd</sup> Edition has been developed in cooperation with the IB and has been fully updated to support the subject guide for first assessments in 2025.

#### The book includes the following features:

- comprehensive coverage of the syllabus written by extremely experienced IB teachers, examiners and curriculum specialists, and reviewed by the IB's subject matter experts
- · emphasis on a flexible conceptual approach
- · labels to clearly identify Higher Level only content
- worked examples, exercises, exam-style practice questions and challenge yourself questions with full answers
- Internal and External Assessment support, including the Extended Essay
- Guiding Questions at the start of each chapter set the context, and are revisited at the end of the chapter as a summary of learning
- Linking Questions to help build a network of knowledge
- Nature of Science and Theory of Knowledge links throughout in addition to a separate TOK chapter
- a global perspective encouraged with international examples in context
- plain language with scientific terms highlighted and explained
- eBook resources including answers, worked solutions, lab skills and activity worksheets, video links and auto-marked quizzes

Catrin Brown taught IB Chemistry and Biology at Pearson College UWC in Canada for over 20 years. She has been involved in the IB world since 1992 with extensive experience as an examiner, senior moderator, site visitor and consultant. Catrin has led teacher training workshops across North America and has played a key role in curriculum development.

Mike Ford teaches at the École Jeannine Manuel in Paris. He has an MA in Chemistry from Oxford University and has been teaching IB Chemistry, Physics and TOK since 1992. He has been an examiner and has led workshops all over the world. Mike has been involved in curriculum development for all the IB sciences.

Oliver Canning teaches IB Chemistry and is the TOK Coordinator at TASIS England. He has taught in the UK, Spain and Singapore. Oliver is the creator of natureofchemistry.com which supports the NOS aspect of the Chemistry course. He was a contributing author to the new Chemistry curriculum.

Andreas Economou is the High School Principal at The Island Private School in Limassol, Cyprus. He has a PhD in Organic Chemistry from the University of Manchester and spent time as a research and development chemist. Since 2016, Andreas has been an IB examiner and Internal Assessment moderator.

Garth Irwin has taught IB Chemistry at Pearson College UWC in Canada since 2002. He has a PhD in Inorganic Photochemistry from the University of Victoria, Canada, and has worked as a research chemist and university lecturer. Garth has co-authored several successful IB Chemistry resources for Pearson.

www.pearson.com/international-scho

Pearson

