Chemistry

An Introduction for Medical and Health Sciences

Alan Jones

Formerly Head of Chemistry and Physics
Nottingham Trent University

John Wiley & Sons, Ltd

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Other Wiley Editorial Offices

John Wiley & Sons Inc., 111 River Street, Hoboken, NJ 07030, USA

Jossey-Bass, 989 Market Street, San Francisco, CA 94103-1741, USA

Wiley-VCH Verlag GmbH, Boschstr. 12, D-69469 Weinheim, Germany

John Wiley & Sons Australia Ltd, 33 Park Road, Milton, Queensland 4064, Australia

John Wiley & Sons (Asia) Pte Ltd, 2 Clementi Loop #02-01, Jin Xing Distripark, Singapore 129809

John Wiley & Sons Canada Ltd, 22 Worcester Road, Etobicoke, Ontario, Canada M9W 1L1

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Library of Congress Cataloging-in-Publication Data

Jones, Alan, 1941–
Chemistry : an introduction for medical and health sciences / Alan Jones
p. cm.
Includes bibliographical references and index.
ISBN 0-470-09288-2 (cloth) – 0-470-09289-0

1. Biochemistry. 2. Chemistry. 3. Pharmaceutical chemistry. II. Title
QP514.2.J66 2005
612′.015–dc22 2004029124

British Library Cataloguing in Publication Data

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

ISBN 0 470 09288 2 hardback
ISBN 0 470 09289 0 paperback

Typeset in 11/14pt Times by Thomson Press (India) Limited, New Delhi
Printed and bound in Great Britain by Antony Rowe Ltd, Chippenham, Wiltshire
This book is printed on acid-free paper responsibly manufactured from sustainable forestry in which at least two trees are planted for each one used for paper production.

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Preface

Recent years have seen significant changes in the practice, education and training of doctors, medical, nursing and healthcare professionals. Pieces of paper are required to show competency in a wide range of skills. There is also a requirement for continuing professional development in order that people increase their knowledge and skills. The United Kingdom Central Council for Nursing, Midwifery and Health Visiting publication *Fitness for Practice* notes that there will be: 'greater demands upon nurses and midwives for technical competence and scientific rationality'.

The daily use of chemicals in the form of medicines and drugs means that there is a need for a basic understanding of chemistry. Do not be put off by this, as you will not be expected to be a chemical expert, but you will need to have some knowledge of the various chemicals in common medical use. You will not be expected to write complicated formulae or remember the structures of the drugs you administer, but it will be of use to know some of their parameters. Modern healthcare is becoming increasingly scientific, so there is a necessity to have a good introduction to chemical concepts. Scientific and chemical understanding leads to better informed doctors, nurses and healthcare workers.

This book starts each chapter with a self-test to check on chemical understanding, and then proceeds to move through the subject matter, always within the context of current practice. Anyone able to pass well on the self-test can move onto the next chapter. I hope you will find the Glossary a useful reference source for a number of chemical terms.

Finally, I would like to thank Mike Clemmet for his valuable contributions to earlier versions of the book, also Dr Sheelagh Campbell of the University of Portsmouth who reviewed the draft manuscript, and Malcolm Lawson-Paul for drawing the cartoons. Perhaps he has learned a little more about chemistry along the way!

Alan Jones

Introduction

This book is intended to introduce some of the basic chemistry for the medical and healthcare professions. The material is suitable for any such course or as a refresher for people returning to the profession. It is designed to give a basic introduction to chemical terms and concepts and will develop the relevant chemistry of drugs and medicines in common use in later chapters.

It can be used as a self-teaching book since it contains diagnostic questions at the beginning of each chapter together with the answers, at the end of the chapter.

It can also be used to supplement the chemistry done on any suitable course. It is not a compendium or list of current drugs and their contents. It is also suitable for people who have a limited chemical knowledge as it starts with the basic concepts at the start of each chapter.

How to use the book

Read Chapter 1. Just read it through quickly. Do not worry about total understanding at this stage. Use it as an introduction or refresher course for chemical terminology

Take in the 'feeling' of chemistry' – and begin to understand the basic principles. Think, but do not stop to follow up any cross-references yet. Just read it through. That will take about twenty minutes.

When you've read this section through once, and thought about it, read it through again, a few days later, but this time take it more slowly. If you are unclear about the chemical words used in Chapter 1 and the others Chapters, use the Glossary at the end of the book for clarification. After reading the whole of Chapter 1 you will be ready for a more detailed study of the relevant areas of chemistry in later chapters.

At the start of each chapter there are some diagnostic questions. If you get more than 80 % of the questions right (the answers are given at the end of each chapter),

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you probably understand the principles. Be honest with yourself. If you really feel that you do not understand it, talk to someone. Start with a fellow student. Then, if the two of you cannot sort it out, ask your lecturer/tutor – that is what they get paid for! You can always read the chapter again a little later. Sometimes familiarity with the words and concepts from a previous reading helps when you read it a second time. Remember this is a study book for your own professional development not a novel where it does not matter if you cannot remember the characters' names.

It will also be helpful, whenever needed or as an aid to your memory, to check on things by looking up words, concepts and definitions in the Glossary. Keep a notebook handy to jot down useful items to remember later.

Throughout the book, as you would expect, there are formulae and structures of chemical compounds. You need not remember these but they are included to show the principles being covered. You are not expected to work out the names of these compounds or balance equations but after a while some might stick in your memory.

In each of the later chapters there are 'scene setters' for the concepts covered in the chapters. The chapters start up with basic ideas and lead onto more detailed chemistry and applications.

Anyway, here we go! Enjoy it! I did when I wrote it and even later when I re-read it. Excuse my sense of humour; I feel it is needed when studying chemistry.

1 Starting Chemistry

Learning objectives

- To introduce some of the most relevant and commonly used chemical concepts, processes and naming systems.
- To show some of the background upon which medicinal chemistry is based.

Diagnostic test

Try this short test. If you score more than 80 % you can use the chapter as a revision of your knowledge. If you score less than 80 % you probably need to work through the text and test yourself again at the end using the same test. If you still score less than 80 % then come back to the chapter after a few days and read it again.

1. What is the main natural source of drug material for research? (1)
2. What charge has each of the following particles: proton, neutron, electron? (3)
3. Covalent bonding gains its stability by what process? (1)
4. Ionic bonding gains its stability by what process? (1)

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5. From what natural source does aspirin originally come? (1)
6. Who was the first person to come up with the idea of the atom? (1)
7. What is the arrangement called that puts all the elements into a logical pattern? (1)
8. Who discovered penicillin? (1)

Total 10 (80 % = 8)
Answers at the end of the chapter.

1.1 Terminology and processes used in drug manufacture

The terms and nomenclature used in chemistry might seem over-complicated at first, but they have been internationally accepted. In this book we use the scientific names for chemicals, not their trivial or common names, e.g. ethanoic acid is used for acetic acid (a constituent of vinegar).

1.1.1 Separation and preparation of commonly used drugs

Where do drugs come from? Most people knows the story of the discovery of penicillin. In simplified form it tells that Alexander Fleming left a culture of bacteria in a Petri dish open in the laboratory. When he looked at it a few days later, he found a fungus or mould growing on it. There was a ring around each bit of the mould, where the bacteria had died. He decided that the mould must have produced a chemical that killed that bacteria. We might have said, 'Uch, dirty stuff' and thrown it out, but he realized he had discovered something new. He had discovered the first *antibiotic*. This all happened in the late 1920s, although it was not until the 1940s and World War II that it was used to great effect for treating infections.

The following section looks at some of the chemical principles which need to be considered when searching for a cure for a particular disease or condition. SARS in 2003 and the Bird Flu in Asia in 2004 were such examples where immediate new cures were sought to avoid a pandemic. The HIV virus has an uncanny knack of changing its surface proteins to confuse the drugs used in its treatments. Research is being conducted to overcome this problem.

As disease agents, such as MRSA, become more and more resistant to drugs, the search is on for new drugs to combat disease and attack viruses. Where should we look for new sources of combatants against disease? We should look where people have always looked – the natural drugs present in the plant world. There have always been 'witch doctors' and old women who have come up with concoctions which supposedly combat diseases, for example hanging garlic bags around a person's neck to drive away the plague, wearing copper bracelets to counteract arthritis or chewing the leaves of certain plants. Some of these remedies might have real significance.

Some of the most promising places to search for suitable plants are in the tropical rain forests, although even plants in places such as Milton Keynes seem to have medicinal uses, for example willow tree bark. The willow tree was the original source of aspirin-like medicines in Britain. It cured the pains from various complaints.

Herbal concoctions have been the basis of healing and also poisoning for centuries. Curare was used on the tips of poison darts to kill opponents, but in smaller quantities it was used as a muscle relaxant in surgery up to the 1960s.[1] Foxglove (digitalis) extracts, as well as being poisonous, have been found to help reduce blood pressure and aid people with heart problems. 'My mother-in-law used to wrap cabbage leaves around her arthritic knees to give her relief from pain just as her mother before had done'. In 2003 a short note in a British medical journal reported that this 'old wives tale' has been shown to have a scientific reason.[2]

Approximately 80 % of modern drugs came initially from natural sources. There are more different species of plants in the rain forests than in any other area on Earth. Many of these species are yet to be discovered and studied in detail. Every year, thousands of plant samples are collected by drug companies to find out whether they have any anti-disease activity. Many of them do. In the mean time, we continue to destroy the rain forests just to obtain teak furniture or some extra peanuts, but that is another story. This area of research is considered in more detail in Chapter 14.

The principles of how chemicals are isolated from plants will be used as an example. Aspirin has been chosen because it is one of the most widely used drugs in the world and it is also one of the most chemically simple, as well as one of the cheapest.

About 50 000 000 000 aspirin tablets are consumed each year throughout the world. On average, each adult takes the equivalent of 70 aspirin tablets (or tablets containing it) each year in the UK, but where did it all start?

Over 2400 years ago in ancient Greece, Hippocrates recommended the juice of willow leaves for the relief of pain in childbirth. In the first century AD in Greece, willow leaves were widely used for the relief of the pain of colic and gout. Writings from China, Africa and American Indians have all shown that they knew about the curative properties of the willow.

Try this one – it's good for the head after an all night session.

In 1763 the use of willow tree bark was reported in more specific terms by Reverend Edward Stone in a lecture to the Royal Society in London. He used its extracts to treat the fever resulting from malaria (then common in Britain; there are some marshes in the UK where the malarial mosquito still persists). He also found that it helped with 'the agues', probably what is now called arthritis. Other common medicines of the time included opium to relieve pain and Peruvian cinchona bark for fevers (it contained quinine).

In the early part of the 1800s chemists in Europe took willow leaves and boiled them with different solvents to try to extract the active ingredients. In 1825 an Italian chemist filtered such a solution and evaporated away the solvent. He obtained impure crystals of a compound containing some of the active ingredient. Repeated recrystallization and refinement of his experimental technique produced a pure sample of the unknown material (Figure 1.1).

In 1828 Buchner in Germany managed to obtain some pure white crystals of a compound by repeatedly removing impurities from an extract of willow bark. He called it 'salicin' (Figure 1.2). It had a bitter taste and relieved pain and inflammation. This same compound was extracted from a herb called meadowsweet by other chemists. Analysis of salicin showed it to be the active ingredient of willow bark joined to a sugar, glucose.

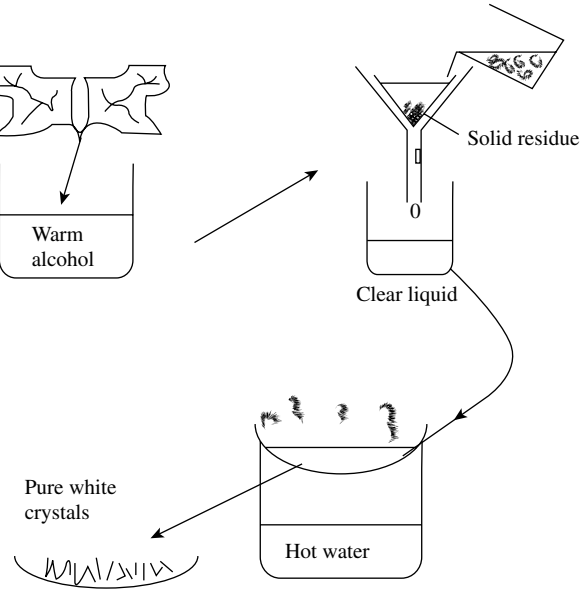


Figure 1.1 Separation of ingredients from willow

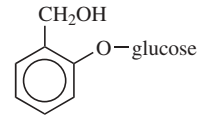


Figure 1.2 Salicin

In the body, salicin is converted into salicylic acid (Figure 1.3) and it was this that was thought to be the active ingredient that relieved pain, but it had such a very bitter taste that it made some people sick. Some patients complained of severe irritation of the mouth, throat and stomach.

The extraction process for making the salicin also proved long and tedious and wasteful of trees: from 1.5 kg of willow bark only 30 g of salicin could be obtained.[3,4] Once the formula was known for salicylic acid, a group of chemists tried to work out how to make it artificially by a less expensive and tedious process.

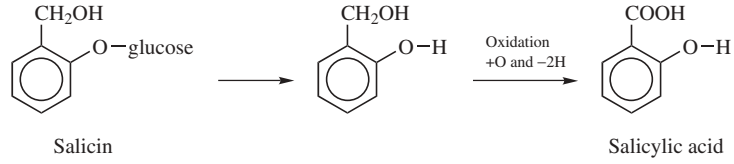
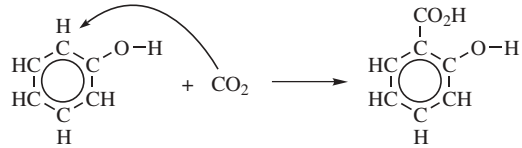


Figure 1.3 Conversion of salicin to salicylic acid



Phenol Salicylic acid

Figure 1.4 Synthesis of salicylic acid

It was not until 1860 that Professor Kolbe found a suitable way of doing this. He heated together phenol, carbon dioxide gas and sodium hydroxide (Figure 1.4; the hexagonal rings in the following figures are an abbreviation of a compound with carbon atoms joined to hydrogen atoms on each point of the hexagon). The phenol was extracted from coal tar and the carbon dioxide, CO_2, was readily made by heating limestone, a carbonate rock, or burning carbon:

$$CaCO_3 \rightarrow CaO + CO_2$$

Because of the ease of its synthesis it was beginning to look as though salicylic acid had a future as a pain-relieving drug, although it still had the drawback of its very bitter taste.

Felix Hoffman worked for the manufacturers Bayer. His father suffered from arthritis and became sick when he took salicylic acid. He challenged his son to find a better alternative. Hoffman did this in 1893 when he made the compound acetyl salicylic acid. This compound went through extensive clinical trials and in 1899 it came on the market as aspirin (Figure 1.5). It proved to be a wonder drug and still is.

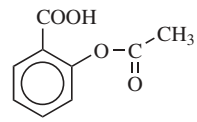


Figure 1.5 Aspirin

It is only in recent years that researchers have found out exactly how it works in our bodies. Previously all they knew was that it worked for a wide range of ailments, thinning the blood, lowering blood pressure and relieving pain for arthritis sufferers.

Aspirin deals with pain that comes from any form of inflammation, but it does cause some stomach bleeding. Therefore, research was undertaken for an alternative that was cheap to manufacture and would not cause stomach bleeding. This search led to the synthesis of paracetamol (Figure 1.6). Paracetamol does not cause stomach bleeding, but large doses damage the liver.

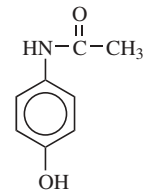


Figure 1.6 Paracetamol

A further series of drugs based on ibuprofen, developed by Boots in the 1980s, looks like being the most successful replacement for aspirin so far. Six hundred different molecules were made and tested before ibuprofen was perfected and clinically trialled. It is now sold over the counter and has few or no side effects (Figure 1.7).

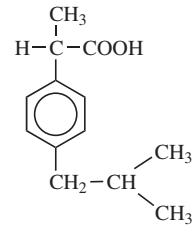


Figure 1.7 Ibuprofen

A similar story to that of aspirin could be told of the discovery and eventual implementation of penicillin and the development of replacements. Mixtures of suitable drugs seem to be a possible answer to combat resistant bacteria – bacteria do not like cocktails!

1.2 Atoms and things

While some Ancient Greek scientists were suggesting medical solutions to common complaints by mixing together natural products, others were 'thinking' and 'wondering' what the composition was of materials in general. Democritus in 400 BCE suggested that all materials were made up of small particles he called atoms. He even invented *symbols* instead of writing the names for elements. In the Western world it was the school teacher and scientist John Dalton, in 1803, who resurrected the idea of the atom. It took until the 1930s for the structure of the atom to be fully

understood. *Atoms* are so small that about 1 000 000 000 atoms of iron would fit onto the point of a pin.

Atoms are composed of a heavy central nucleus containing positively charged protons, and these are accompanied by varying numbers of the same-sized neutral particles called neutrons. Rotating in orbits around the nucleus like planets around the sun are negatively charged, very small particles called electrons. The positive charge on the nucleus keeps the negative electrons in place by mutual attraction. The orbits contain only a fixed number of electrons; the inner shell holds a maximum of two and the outer orbits eight electrons or more.

Each element has its own unique number of *protons* and *electrons*. This is called its *atomic number*. Whenever *elements* react together to form *molecules* they try to arrange their outermost electrons to obtain this complete electron shell (of either two or eight electrons), either by sharing electrons with another atom (called *covalent bonding*) or by donation and accepting electrons (called *ionic bonding*). A more complete explanation of these is given in later chapters.

The naturally occurring hydrogen gas molecules, H_2, shares one electron from each hydrogen atom so that each now has a share of two electrons. This is a covalent bond (Figure 1.8). The other method of bonding to get a complete outer electron

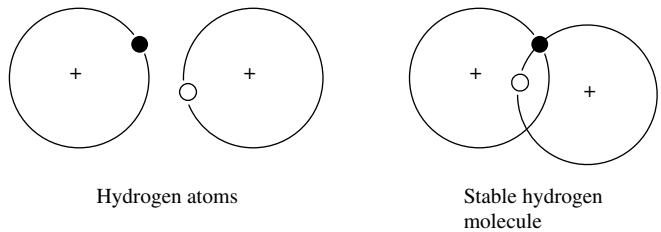


Figure 1.8 Hydrogen atoms and molecule

shell is demonstrated with sodium chloride or common salt. Here the outermost single electron of sodium is completely transferred to the chlorine atom. Sodium loses an electron so it then has a net positive charge, whereas the chlorine gains the electron and so has a net negative charge. These two oppositely charged particles, called ions, attract each other and form a strong ionic bond (Figure 1.9). A more complete explanation of these is given in Chapter 2 and 7.

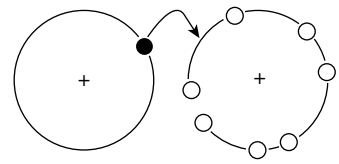


Figure 1.9 Transfer of electrons

As the years progressed, the methods of analysis become more accurate and precise. Scientists were able to detect very small quantities of materials and the structures were worked out. In modern times chemical analysis is done by very accurate and sophisticated techniques. These methods will be discussed in Chapter 11.

1.3 Chemical reactions and the periodic table

Whenever elements and compounds react together to form a stable compound, the atoms always try to rearrange the outer electrons to achieve a complete outer electron shell of two or eight. These complete shells were found to be the structures of the elements in group 8 of the *periodic table*.

The scientists of the nineteenth century discovered new materials that they found to be made up of combinations of simple *elements*. They began to compare the masses of these elements and discovered that this property was a fundamental characteristic of the element – its *atomic mass*.

In 1896 a Russian scientist called Mendeleev found that these numerical values could be put into an ordered pattern which he called the periodic table, which was completed later when more elements were discovered. In about 1932 scientists found that the fundamental property that sequenced the elements in their periodic table order was not their mass but the number of protons in their nucleus. This property is called the *atomic number*, and every element has its own unique atomic number.

In the periodic table according to atomic number all the elements are put in order, each element differing by one unit from its neighbour. It is that simple! (See Appendix 2 for the periodic table.)

The millions of compounds formed by combining these elements together are not so easily systematized. The use of chemical abbreviations and chemical formulae was introduced as some of the molecules were so huge that using names alone for all their contents would lead to impossibly large words. (see *formula* and *symbols for elements* in the Glossary.) There are many millions of compounds made up of approximately 100 different elements. The vast majority of compounds that make up biological tissues are carbon compounds. This branch of chemistry is called *organic chemistry*. There are over a million compounds containing carbon and hydrogen that are arranged into logical groups based upon what is in them and how they react. These groups are called ‘homologous series’. Some of these molecules are very large, and proteins are such a group, containing 2000 or more groups of carbon, hydrogen, nitrogen and oxygen atoms. Similarly sugars (or carbohydrates) and fats (lipids) are vast molecules. Of course there are the famous molecules DNA

(deoxyribosenucleic acid) and RNA (ribosenucleic acid), which are combinations of smaller groups joined together in their thousands. These molecules are in twisted bundles inside cells, and if they were untwined and strung end to end the molecules in our body would stretch to the sun and back 600 times.

When these protein and other molecules inside our cells are working efficiently then we are well, but if they go wrong, something has to be done. Usually our own body mechanisms can correct these faults itself, but sometimes medication and drugs are needed. That is the beginning of our story about the chemistry of cells and drugs.

Understanding of these complex chemicals needs to be built up in small steps by studying the chemistry of their component parts. Drugs and medicines containing hydrocarbon compounds are covered in Chapter 2; compounds containing OH groups are studied in Chapter 3; the precursors of sugars and fats start with a study of carbonyl compounds in Chapter 4; and the starting point for understanding proteins is the study of amino compounds and amino acids in Chapter 5. Some of the processes involved in the chemistry of medicinal compounds require an understanding of what is meant by covalency, acids, oxidation, solubility, the speed of a reaction and the role of metal ions. All these topics are considered in separate chapters. The growth of analytical techniques and radioactivity are covered in Chapters 11 and 12. Recent chemical and biomedical research is summarized in Chapter 14. Chapter 15 was written to put numeracy into a chemical perspective.

Answers to the diagnostic test

1. Plants	(1)
2. Proton, $+1$; neutron, 0; electron, -1	(3)
3. Sharing electrons	(1)
4. Donating and receiving electrons	(1)
5. Willow tree	(1)
6. Democritus	(1)
7. Periodic table	(1)
8. Alexander Fleming	(1)

Further questions

1. What is the difference between an atom and a molecule?
2. What determines the chemistry of an atom, the outer electrons or the nucleus?
3. What is the name given to particles with positive or negative charges?
4. On which side of the periodic table would you find the metals?
5. The huge branch of chemistry devoted to the study of carbon compounds is called what?
6. What is a homologous series?
7. Aspirin has some side effects, what are they? Name a replacement drug that was developed to eliminate these side effects.
8. What is the difference between atomic number and atomic mass?

References

1. A. Dronsfield. A shot of poison to aid surgery. *Education in Chemistry*, May 2003, 75.
2. J. Le Fanu. *The Sunday Telegraph*, Review, 31 August 2003, 4.
3. *Aspirin*. Royal Society of Chemistry, London, 1998.
4. S. Jourdier. A miracle drug. *Chemistry in Britain*, February 1999, 33–35.

2 Covalent Compounds and Organic Molecules

It is assumed that you have fully understood the principles outlined in Chapter 1.

Learning objectives

- To appreciate the significance of covalent bonding for some biological molecules.
- To write, name and understand the structures of some relevant organic compounds.
- To know what is meant by 'isomerism' and appreciate its importance for metabolic processes.
- To appreciate that there are millions of organic molecules.

Diagnostic test

Try this short test. If you score more than 80 % you can use the chapter as a revision of your knowledge. If you score less than 80 % you probably need to work through the text and test yourself again at the end using the same test. If you still score less than 80 % then come back to the chapter after a few days and read it again.

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