ANALYTICAL CHEMISTRY BY OPEN LEARNING

Microprocessor Applications

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Analytical Chemistry by Open Learning

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Analytical Chemistry by Open Learning

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Analytical Chemistry

This series of texts is a result of an initiative by the Committee of Heads of Polytechnic Chemistry Departments in the United Kingdom. A project team based at Thames Polytechnic using funds available from the Manpower Services Commission 'Open Tech' Project has organised and managed the development of the material suitable for use by 'Distance Learners'. The contents of the various units have been identified, planned and written almost exclusively by groups of polytechnic staff, who are both expert in the subject area and are currently teaching in analytical chemistry.

The texts are for those interested in the basics of analytical chemistry and instrumental techniques who wish to study in a more flexible way than traditional institute attendance or to augment such attendance. A series of these units may be used by those undertaking courses leading to BTEC (levels IV and V), Royal Society of Chemistry (Certificates of Applied Chemistry) or other qualifications. The level is thus that of Senior Technician.

It is emphasised however that whilst the theoretical aspects of analytical chemistry can be studied in this way there is no substitute for the laboratory to learn the associated practical skills. In the U.K there are nominated Polytechnics, Colleges and other Institution who offer tutorial and practical support to achieve the practical objectives identified within each text. It is expected that many institutions worldwide will also provide such support.

The project will continue at Thames Polytechnic to support these 'Open Learning Texts', to continually refresh and update the material and to extend its coverage.

Further information about nominated support centres, the material or open learning techniques may be obtained from the project office at Thames Polytechnic, ACOL, Wellington St., Woolwich, London, SE18 6PF.

How to Use an Open Learning Text

Open learning texts are designed as a convenient and flexible way of studying for people who, for a variety of reasons cannot use conventional education courses. You will learn from this text the principles of one subject in Analytical Chemistry, but only by putting this knowledge into practice, under professional supervision, will you gain a full understanding of the analytical techniques described.

To achieve the full benefit from an open learning text you need to plan your place and time of study.

- Find the most suitable place to study where you can work without disturbance.
- If you have a tutor supervising your study discuss with him, or her, the date by which you should have completed this text.
- Some people study perfectly well in irregular bursts, however most students find that setting aside a certain number of hours each day is the most satisfactory method. It is for you to decide which pattern of study suits you best.
- If you decide to study for several hours at once, take short breaks of five or ten minutes every half hour or so. You will find that this method maintains a higher overall level of concentration.

Before you begin a detailed reading of the text, familiarise yourself with the general layout of the material. Have a look at the course contents list at the front of the book and flip through the pages to get a general impression of the way the subject is dealt with. You will find that there is space on the pages to make comments alongside the ext as you study—your own notes for highlighting points that you eel are particularly important. Indicate in the margin the points you would like to discuss further with a tutor or fellow student. When you come to revise, these personal study notes will be very useful.

When you find a paragraph in the text marked with a symbol such as is shown here, this is where you get involved. At this point you are directed to do things: draw graphs, answer questions, perform calculations, etc. Do make an attempt at these activities. If necessary cover the succeeding response with a piece of paper until you are ready to read on. This is an opportunity for you to learn by participating in the subject and although the text continues by discussing your response, there is no better way to learn than by working things out for yourself.

We have introduced self assessment questions (SAQ) at appropriate places in the text. These SAQs provide for you a way of finding out if you understand what you have just been studying. There is space on the page for your answer and for any comments you want to add after reading the author's response. You will find the author's response to each SAQ at the end of the text. Compare what you have written with the response provided and read the discussion and advice.

At intervals in the text you will find a Summary and List of Objectives. The Summary will emphasise the important points covered by the material you have just read and the Objectives will give you a checklist of tasks you should then be able to achieve.

You can revise the Unit, perhaps for a formal examination, by re-reading the Summary and the Objectives, and by working through some of the SAQs. This should quickly alert you to areas of the text that need further study.

At the end of the book you will find for reference lists of commonly used scientific symbols and values, units of measurement and also a periodic table.

Study Guide

The last decade has seen a rapid growth in the use of computers in the analytical chemical laboratory. Most analytical instruments are now manufactured with an on-board microcomputer system for control purposes or for automatic processing of raw data. Additionally general purpose microcomputers, dedicated to analytical applications by specially written computer programs, are finding increased use. Such systems generally provide the analytical chemist with some flexibility about the way the collected data is to be manipulated. In some cases the software system provided allows a certain amount of programming by the analyst using a specialist language appropriate to the analytical task. Analytical chemists can also use general purpose microcomputers, interfaced to analytical instruments, to develop their own software, although care must be taken not to underestimate the development time required to produce a fully working and well tested system.

Because of the above developments in laboratory computing there is an increasing need for analytical chemists to become computer literate. Even an elementary knowledge of computer programming, computer interfacing, and an appreciation of the scope and limitations of computerisation, would allow the analytical chemist to use computerised equipment more confidently. A more advanced knowledge, although not necessarily appropriate for everyone, would increase the likelihood that existing hardware and software are fully exploited and allow new opportunities in analytical computing to be recognised.

The aim of this Unit is not to attempt to turn analytical chemical technicians into electronic engineers or computer programmers. Our aim is to provide a sufficiently good grounding in both computing and computer interfacing so that the analyst is confident in using computerised equipment and, if necessary, can overcome the 'jargon barrier' to discuss problems or developments with computer specialists and electronic engineers. Those who cope readily with the material of this Unit should find it a useful base for further study of computer applications in analytical chemistry.

Parts 1 to 3 provide an introduction to computing, programming and interfacing for the analytical chemist. Parts 1 and 2 are relatively free standing, but you must understand the contents of both of them before proceeding to Part 3. To satisfactorily complete Part 2 you will need access to a microcomputer with BASIC as a programming language.

Parts 4 to 6 are devoted to applications of the material covered in Parts 1 to 3 to analytical chemistry problems.

Bibliography

For an alternative presentation of much of the contents of Part 1 you may wish to consult the books listed below.

E. Morgan, *Laboratory Computing*, Sigma-Technical Press, Distributed by J. Wiley & Sons, Chichester, 1984.

C. G. Morgan, *The Micro in the Laboratory*, Sigma, Chichester, 1984.

You may also find it useful to refer to the introductory parts of the texts cited in the Overview for Part 3, Microcomputer Interfacing. All of these texts deal with number systems and have some general comments about microcomputers relevant to the content of Part 1.

For an alternative approach to programming (Part 2):

D. M. Monro, *Introduction to Computing with BASIC*, Arnold, 1974.

D. M. Monro, *Basic BASIC*, 2nd. Edn, Wiley, 1985.

C. Prigmore, *30 Hour BASIC*, National Extension College Correspondence Texts, Course M27, 1981.

A good general introduction to computers, computing, data processing and information technology (including some programming) is:

D. R. Sullivan, G. Lewis and C. R. Cook, *Using Computers Today*, Houghton Mifflen, 1986.

As general background reading you are recommended to study the following articles in the literature:

D. Malcolme-Lawes, *Microcomputers in the Chemical Laboratory*, *Chem. Brit.*, **20** (5) 1984, 425.

P. J. Farago, *Peek, Poke and Run*, *Chem. Brit.*, **18** (1), 1982, 40.

A. Hinchliffe, *Microcomputers in Chemistry Teaching*, *Educ. in Chem.* **20**, 1983, 44.

G. S. Owen, *Choosing an Appropriate Computer Language*, *J. Chem. Educ.*, **61** (2), 1984, 440.

R. E. Dessey, *Chemistry and the Microcomputer Revolution*, *J. Chem. Educ.* **59** (4), 1982, 321.

The following books and articles on data processing will be useful reference material in support of Parts 4, 5 and 6.

A. C. Norris, *Computational Chemistry*, Wiley, 1981.

William S. Dorn and Daniel D. McCracken, *Numerical Methods with Fortran IV Case Studies*, Wiley, 1972.

D. Binkley and R. J. Dessy, *J. Chem. Educ.*, **56**, 148, 1979.

A. Savitsky and M. J. E. Golay, *Anal. Chem.*, **36**, 1627, 1964. (Some corrections to the Savitsky and Golay tables are published in Steiner J. *et al*, *Anal. Chem.*, **44**, 1906, 1972.)

Contents

1. Microprocessors and Computing Concepts

Overview

On completing Sections 1.1 and 1.2 of this unit you should be able to relate binary numbers to their decimal and hexadecimal equivalents, and convert numbers from one system to another. You should be able to cope with the material of Section 1 without any previous knowledge of binary numbers.

The content of Section 1.2 requires a knowledge of the material in Section 1.1 to allow you to develop an understanding of the function of the principal components of a microcomputer system. Section 1.2 should introduce you to much of the jargon used with microprocessors. You should also become aware of the variety of microcomputers used in modern analytical laboratories and be able to relate the characteristics of the computer system to the needs of the analysis.

Section 1.3 provides an introduction to the different approaches to computer programming. From this section you should be able to distinguish between machine code, assembler programs and programs written in high-level languages. You should also start to appreciate the scope and limitations of each method of programming.

There are no pre-requisites for Part 1 but it must be studied before Part 3 and later units. Those who wish to study only BASIC programming can skip Part 1 and proceed directly to Part 2.

1.1. COMPUTERS AND NUMBER SYSTEMS

1.1.1. Binary Numbers

Laboratory applications of computers range from small systems dedicated to relatively simple apparatus such as a balance or a pH meter to quite sophisticated systems used with nuclear magnetic resonance spectrometers. Computers may be used to collect and store numeric data from instruments, to undertake calculations and store and retrieve information which may involve text.

All digital computers must reduce the above types of information, as well as the programs which specify what has to be done, to numeric codes expressed in binary. In the familiar decimal system we have ten digits 0, 1 ... 8, 9 but in binary we have only two digits namely 0 and 1. A binary digit is called a bit (Binary digIT). To express a number greater than 9 in decimal requires more than one decimal digit. In the same way to express a number greater than one in binary needs more than one bit. In fact to reach a number as high as 255 we need 8 bits, which is called a byte.

In writing a binary number, as with the decimal system, the least significant digit is written on the right and the most significant one is placed on the left, as shown below for an 8-bit number in which the individual bits have been labelled d0 (least significant bit) to d7.

	most significant bit							least significant bit
	d7	d6	d5	d4	d3	d2	d1	d0
weight of bit	2^7	2^6	2^5	2^4	2^3	2^2	2^1	2^0
	128	64	32	16	8	4	2	1

Thus to write the number 13 using 8 bits we would need to include the bits with weight 1, 4 and 8 as shown below.

0 0 0 0 1 1 0 1

The decimal equivalent of 13 is thus the sum of the weights of the bits set to 1 in the binary representation:

$$\text{decimal } 13 = 1 \times 2^3 + 1 \times 2^2 + 1 \times 2^0$$

SAQ 1.1a

What are the decimal numbers which correspond to each of the following bytes?

(*i*) 01101101

(*ii*) 10000000

(*iii*) 11111111