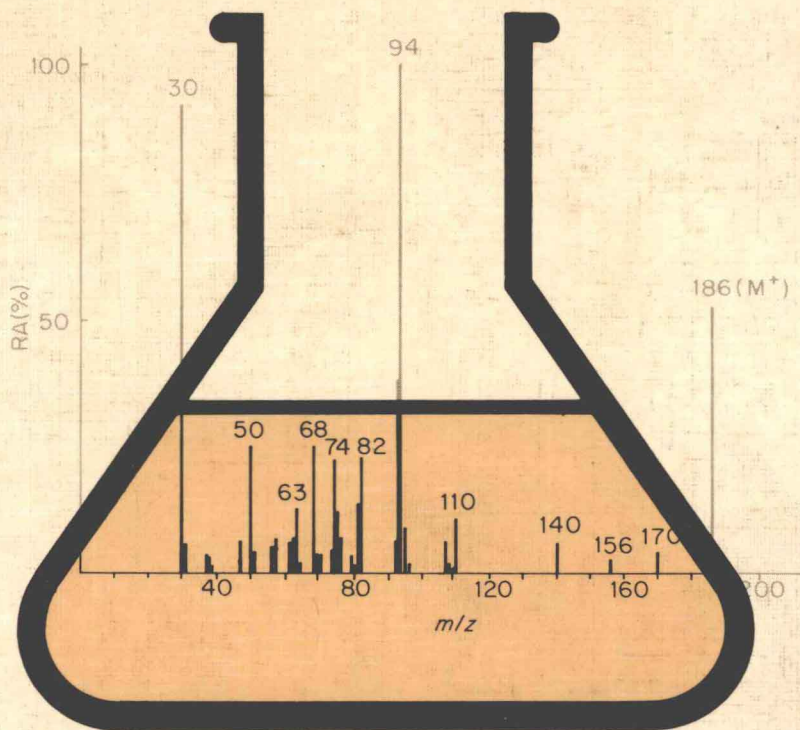


ANALYTICAL CHEMISTRY BY OPEN LEARNING

Mass Spectrometry



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Mass Spectrometry

Analytical Chemistry by Open Learning

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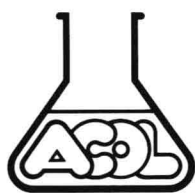
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Analytical Chemistry

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 Institutions 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

text as you study—your own notes for highlighting points that you feel 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.

- II 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

This unit is intended to provide you with a good understanding of mass spectrometry. It covers the basic theory of ion formation and behaviour, the instrumentation and the interpretation of the spectra of organic molecules. There are also sections covering combined gas chromatography – mass spectrometry and liquid chromatography – mass spectrometry, which are two of the most powerful techniques available to the analytical chemist.

Mass spectrometry has undergone a great deal of development as an empirical subject. That is, many useful approaches to the analysis and identification of organic molecules have been developed without a detailed understanding of theory of ion behaviour. This is also the way in which the subject is usually taught and it is the approach adopted here. That does not mean to say that an understanding of ion behaviour is not important – it is, but that understanding is still being developed and we wish to use the technique now.

Understanding the fragmentations of ions formed from organic molecules is greatly aided by an understanding of the basic concepts of organic chemistry which you will have met while studying that subject. Section 9 depends on this knowledge, although some of the most important concepts are highlighted in the text. It is assumed, throughout, that the reader has an understanding of chemistry equivalent to that of a student holding an HNC in Chemistry and a knowledge of physics and mathematics to at least GCE (O-level).

The course is constructed to be used at two levels – by those studying for the LRSC qualification or its equivalent and by those who wish to obtain a very detailed knowledge of mass spectrometry, much

beyond that required for LRSC. Those using the text as preparation for their LRSC examinations are not expected to study the whole unit. They are advised to omit the following sections:

3; 4.3, 4.4; 6.2; 7.4; 8.2; 9.3, 9.4, 9.5.2 to 9.5.7 inclusive, 9.8, 9.9, 9.10; 10.2.

You may find that the coverage given in text-books clarifies some aspects of this text. For this reason a bibliography is provided. We hope you will look at at least one of these books sometime during studying this unit. This will provide balance in the approach to the subject.

Bibliography

1. General Analytical and Spectroscopy books. Most analytical chemistry text books have a chapter on mass spectrometry. These include:

- (a) F. W. Fifield and D. Kealey, *Principles and Practice of Analytical Chemistry*, International Textbook Co Ltd, 2nd Edn 1983.
- (b) H. H. Willard, L. L. Merritt, J. A. Dean and F. A. Settle, *Instrumental Methods of Analysis*, Van Nostrand, 6th Edn, 1981.
- (c) R. L. Pecsok, L. D. Shields, T. Cairns and I. G. McWilliam, *Modern Methods of Chemical Analysis*, J. Wiley and Sons, 2nd Edn 1976.

Spectroscopy books have in some cases just a brief description of mass spectrometry but all have examples for analysis and show how mass spectrometry is used in conjunction with other spectroscopic techniques.

- (d) D. L. Pavia, G. M. Lampman and G. S. Kriz, *Introduction to Spectroscopy*, Saunders, 1979.
- (e) R. Davis and C. H. J. Wells, *Spectral Problems in Organic Chemistry*, International Textbook Co Ltd, 1984.

2. Books specialising in Mass Spectrometry.

- (a) J. H. Beynon and A. G. Brenton, *Introduction to Mass Spectrometry*, Univ Wales Press, 1982.
- (b) I. Howe, D. H. Williams and R. D. Bowen, *Mass Spectrometry, Principles and Applications*, 2nd Ed, McGraw Hill, 1981.

- (c) M. E. Rose and R. A. W. Johnstone, *Mass Spectrometry for Chemists and Biochemists*, Cambridge U.P., 1982.
 - (d) J. R. Majer, *The Mass Spectrometer*, Wykeham, 1977.
 - (e) B. S. Middleditch, *Practical Mass Spectrometry*, Plenum, 1979.
 - (f) G. M. Message, *Practical Aspects of Gas Chromatography – Mass Spectrometry*, Wiley–Interscience, 1984.
 - (g) B. J. Millard, *Quantitative Mass Spectrometry*, Heyden, 1978.
 - (h) J. R. Chapman, *Computers in Mass Spectrometry*, Academic Press, 1978.
 - (i) J. P. Payne, J. A. Bushman and D. W. Hill, *The Medical and Biological Application of Mass Spectrometry*, Academic Press, 1979.
 - (j) H. E. Duckworth, R. C. Barber and V. S. Venkatasubramanian, *Mass Spectroscopy*, 2nd Ed, Cambridge University Press, 1986.
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Figures 9.6f and 9.7d are mass spectra taken from D. L. Pavia, G. M. Lampman and G. C. Kris Jr, *Introduction to Spectroscopy*, Saunders and Co, 1979 with permission from Holt, Rinehart and Winston, Inc.

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