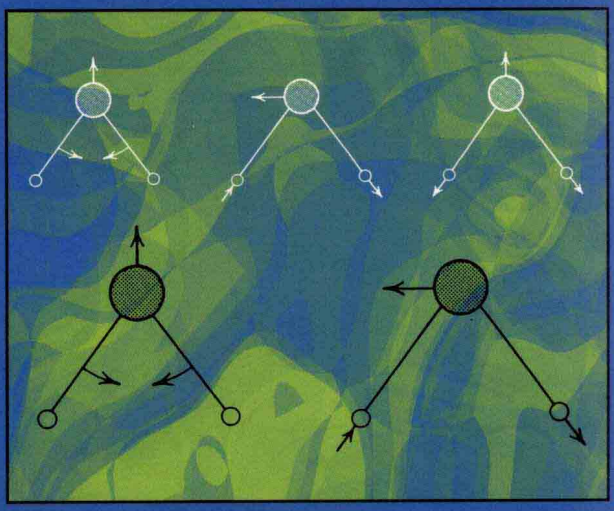
AnTS *Analytical Techniques in the Sciences*

INFRARED SPECTROSCOPY: FUNDAMENTALS AND APPLICATIONS

Barbara Stuart



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Barbara H. Stuart
University of Technology, Sydney, Australia

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INFRARED SPECTROSCOPY: FUNDAMENTALS AND APPLICATIONS

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Series Preface

There has been a rapid expansion in the provision of further education in recent years, which has brought with it the need to provide more flexible methods of teaching in order to satisfy the requirements of an increasingly more diverse type of student. In this respect, the *open learning* approach has proved to be a valuable and effective teaching method, in particular for those students who for a variety of reasons cannot pursue full-time traditional courses. As a result, John Wiley & Sons, Ltd first published the Analytical Chemistry by Open Learning (ACOL) series of textbooks in the late 1980s. This series, which covers all of the major analytical techniques, rapidly established itself as a valuable teaching resource, providing a convenient and flexible means of studying for those people who, on account of their individual circumstances, were not able to take advantage of more conventional methods of education in this particular subject area.

Following upon the success of the ACOL series, which by its very name is predominately concerned with Analytical *Chemistry*, the *Analytical Techniques in the Sciences* (AnTS) series of open learning texts has been introduced with the aim of providing a broader coverage of the many areas of science in which analytical techniques and methods are now increasingly applied. With this in mind, the AnTS series of texts seeks to provide a range of books which will cover not only the actual techniques themselves, but *also* those scientific disciplines which have a necessary requirement for analytical characterization methods.

Analytical instrumentation continues to increase in sophistication, and as a consequence, the range of materials that can now be almost routinely analysed has increased accordingly. Books in this series which are concerned with the *techniques* themselves will reflect such advances in analytical instrumentation, while at the same time providing full and detailed discussions of the fundamental concepts and theories of the particular analytical method being considered. Such books will cover a variety of techniques, including general instrumental analysis,

spectroscopy, chromatography, electrophoresis, tandem techniques, electroanalytical methods, X-ray analysis and other significant topics. In addition, books in the series will include the *application* of analytical techniques in areas such as environmental science, the life sciences, clinical analysis, food science, forensic analysis, pharmaceutical science, conservation and archaeology, polymer science and general solid-state materials science.

Written by experts in their own particular fields, the books are presented in an easy-to-read, user-friendly style, with each chapter including both learning objectives and summaries of the subject matter being covered. The progress of the reader can be assessed by the use of frequent self-assessment questions (SAQs) and discussion questions (DQs), along with their corresponding reinforcing or remedial responses, which appear regularly throughout the texts. The books are thus eminently suitable both for self-study applications and for forming the basis of industrial company in-house training schemes. Each text also contains a large amount of supplementary material, including bibliographies, lists of acronyms and abbreviations, and tables of SI Units and important physical constants, plus, where appropriate, glossaries and references to literature sources.

It is therefore hoped that this present series of textbooks will prove to be a useful and valuable source of teaching material, both for individual students and for teachers of science courses.

Dave Ando
Dartford, UK

Preface

Infrared spectroscopy is one of the most important and widely used analytical techniques available to scientists working in a whole range of fields. There are a number of texts on the subject available, ranging from instrumentation to specific applications. This present book aims to provide an introduction to those needing to use infrared spectroscopy for the first time, by explaining the fundamental aspects of the technique, how to obtain a spectrum and how to analyse infrared data obtained for a wide number of materials.

This text is not intended to be comprehensive, as infrared spectroscopy is extensively used. However, the information provided here may be used as a starting point for more detailed investigations. The book is laid out with introductory chapters covering the background theory of infrared spectroscopy, instrumentation and sampling techniques. Scientists may require qualitative and/or quantitative analysis of infrared data and therefore a chapter is devoted to the approaches commonly used to extract such information.

Infrared spectroscopy is a versatile experimental technique. It can be used to obtain important information about everything from delicate biological samples to tough minerals. In this book, the main areas that are studied using infrared spectroscopy are examined in a series of chapters, namely organic molecules, inorganic molecules, polymers, and biological, industrial and environmental applications. Each chapter provides examples of commonly encountered molecular structures in each field and how to approach the analysis of such structures. Suitable questions and problems are included in each chapter to assist in the analysis of the relevant infrared spectra.

I very much hope that those learning about and utilizing infrared spectroscopy will find this text a useful and valuable introduction to this major analytical technique.

Barbara Stuart
University of Technology, Sydney, Australia

Acronyms, Abbreviations and Symbols

ANN	artificial neural network
ATR	attenuated total reflectance
CLS	classical least-squares
D_2O	deuterium oxide
DAC	diamond anvil cell
DNA	deoxyribonucleic acid
DOP	dioctyl phthalate
DRIFT	diffuse reflectance infrared technique
DTGS	deuterium triglycine sulfate
EGA	evolved gas analysis
en	ethylenediamine
FFT	fast Fourier-transform
FPA	focal plane array
FTIR	Fourier-transform infrared (spectroscopy)
GC–IR	gas chromatography–infrared (spectroscopy)
GC–MS	gas chromatography–mass spectrometry
HDPE	high-density polyethylene
ILS	inverse least-squares
KRS-5	thallium-iodide
LC	liquid chromatography
LDA	linear discriminant analysis
LDPE	low-density polyethylene
MBP	myelin basic protein
MCT	mercury cadmium telluride
MIR	multiple internal reflectance

MMA	methyl methacrylate
NMR	nuclear magnetic resonance (spectroscopy)
PAS	photoacoustic spectroscopy
PCA	principal component analysis
PE	polyethylene
PEO	poly(ethylene oxide)
PET	poly(ethylene terephthalate)
PLS	partial least-squares
PMMA	poly(methyl methacrylate)
PP	polypropylene
PTFE	polytetrafluoroethylene
PU	polyurethane
PVC	poly(vinyl chloride)
PVIE	poly(vinyl isobutylether)
PVPh	poly(vinyl phenol)
RNA	ribonucleic acid
SFC	supercritical fluid chromatography
SNR	signal-to-noise ratio
TFE	trifluoroethanol
TGA	thermogravimetric analysis
TGA–IR	thermogravimetric analysis–infrared (spectroscopy)

A	absorbance
$A_{\parallel}$	absorbance parallel to chain axis
$A_{\perp}$	absorbance perpendicular to chain axis
B	magnetic vector (magnitude)
$B(\bar{\nu})$	spectral power density
c	speed of light; concentration
d_p	penetration depth
D	optical path difference
E	energy; electric vector (magnitude)
h	Planck constant
k	force constant; molar absorption coefficient
I	transmitted light
I_0	incident light
$I(\delta)$	intensity at detector
l	pathlength
L	cell pathlength
n	number of peak-to-peak fringes; refractive index; number of moles
P	pressure
R	reflectance; universal gas constant
T	transmittance; temperature

V	volume
δ	pathlength
ε	molar absorptivity
θ	angle of incident radiation
λ	wavelength
μ	reduced mass
ν	frequency
$\bar{\nu}$	wavenumber

About the Author

Barbara Stuart, B.Sc. (Sydney), M.Sc. (Sydney), Ph.D. (London), D.I.C., MRACI, MRSC, CChem

After graduating with a B.Sc. degree from the University of Sydney in Australia, Barbara Stuart then worked as a tutor at this university. She also carried out research in the field of biophysical chemistry in the Department of Physical Chemistry and graduated with an M.Sc. in 1990. The author then moved to the UK to carry out doctoral studies in polymer engineering within the Department of Chemical Engineering and Chemical Technology at Imperial College (University of London). After obtaining her Ph.D. in 1993, she took up a position as a Lecturer in Physical Chemistry at the University of Greenwich in South East London. Barbara returned to Australia in 1995, joining the staff at the University of Technology, Sydney, where she is currently a Senior Lecturer in the Department of Chemistry, Materials and Forensic Science. She is presently conducting research in the fields of polymer spectroscopy, materials conservation and forensic science. Barbara is the author of three other books published by John Wiley and Sons, Ltd, namely *Modern Infrared Spectroscopy* and *Biological Applications of Infrared Spectroscopy*, both in the ACOL series of open learning texts, and *Polymer Analysis* in this current AnTS series of texts.

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