AnTS *Analytical Techniques in the Sciences*

Barbara H. Stuart

Forensic Analytical Techniques

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FORENSIC ANALYTICAL TECHNIQUES

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WILEY
A John Wiley & Sons, Ltd., Publication

This edition first published 2013

Registered office
John Wiley & Sons Ltd, The Atrium, Southern Gate, Chichester, West Sussex, PO19 8SQ, United Kingdom

Library of Congress Cataloging-in-Publication Data applied for.

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

HB ISBN: 9780470687277
PB ISBN: 9780470687284

Set in 10/12pt Times by Laserwords Private Limited, Chennai,India.
Printed in [Country] by [Printer]

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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 now 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, tables of SI units and important physical constants and, 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

The public profile of forensic science has dramatically increased in recent decades and there has been a corresponding rise in the number of students undertaking forensic science degree courses at a tertiary level with the view to a professional career in this field. During this period the application of modern analytical techniques to the examination of forensic problems has expanded, particularly due to the development of small and portable cost-effective instrumentation. The availability of new techniques has led to a greater choice of tools that can be employed to analyse forensic specimens. An understanding of a broad range of analytical tools is required by today's forensic chemists and is an important aspect of their training.

The aim of this book is to provide an overview of the most commonly used analytical techniques that are of interest to forensic chemists. A clear description of how each technique works and how to prepare specimens for analysis is provided. Some techniques are widely used as standard methods, while others are yet to be established but show great potential. An explanation of how to analyse the data obtained is also provided and, for each technique, the most common forensic applications are described. There are specific issues to consider when examining forensic samples. Apart from the applicability of a technique, the issues of dealing with small quantities of material, whether a technique is non-destructive and the cost and/or portability for fieldwork must be considered.

The reader will note that there is a deliberate focus on forensic chemistry and physical evidence. Topics such as DNA analysis are intentionally not dealt with here, and forensic biology topics are well covered elsewhere. The focus here is on how to analyse samples once collected – the process of evidence collection is, of course, an important aspect of a forensic scientist's training and is an expansive topic in its own right. This book is designed for students who are undertaking a forensic chemistry based programme and require a sound knowledge of analytical techniques. Some basic tertiary mathematical and chemistry knowledge is

assumed. The book will also provide a useful reference for forensic practitioners who may be interested in investigating new forms of evidence or techniques.

I hope that this book helps fill a gap in the world of forensic textbooks. Naturally many forensic science textbooks focus on the collection of evidence, but this book will provide a resource for the teaching of forensic analytical techniques. I would like to acknowledge the valuable conversations with and the data provided by a multitude of hardworking forensic scientists in police forces, law enforcement agencies and universities – not just in Australia, but worldwide. A special thanks to my colleagues and students past and present in the Centre of Forensic Science and the School of Chemistry and Forensic Science at the University of Technology, Sydney.

About the Author

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Barbara Stuart holds the position of Associate Professor at the School of Chemistry and Forensic Science and the Centre for Forensic Science at the University of Technology, Sydney (UTS) in Australia. She received BSc (Hons) and MSc degrees in chemistry from the University of Sydney in Australia and gained her PhD at Imperial College in London in 1993. Barbara held the position of lecturer at the University of Greenwich, London before returning to Australia to take up a position at UTS in 1995. Barbara has contributed to the teaching of a broad range of topics in the chemistry, forensic and materials programmes at UTS. She also has active research interests in the fields of forensic taphonomy and archaeology, as well as in materials conservation and environmental science, and has published many papers on these topics. Barbara is also the author of five other books published by John Wiley & Sons: *Modern Infrared Spectroscopy* and *Biological Applications of Infrared Spectroscopy*, both in the ACOL series of open learning texts, and *Polymer Analysis* and *Infrared Spectroscopy: Fundamentals and Applications* in the current AnTS series of texts, as well as *Analytical Techniques in Materials Conservation*.

Acronyms, Abbreviations and Symbols

AAS	atomic absorption spectrometry
AES	atomic emission spectrometry
AFM	atomic force microscopy
ALS	alternate light source
ANN	artificial neural network
APCI	atmospheric pressure chemical ionization
ATR	attenuated total reflectance
BAC	blood alcohol concentration
BSA	*N*,*O*-bistrimethylsilylic acid
BSE	backscattered electron
BSTFA	*N*,*O*-bistrimethylsilyltrifluoroacetamide
CE	capillary electrophoresis
CI	chemical ionization
CNS	central nervous system
COHb	carboxyhaemoglobin
CZE	capillary zone electrophoresis
Δn	birefringence
DAC	diamond anvil cell
DAD	diode array detector
DART	direct analysis in real time
DC	direct current
DESI	desorption electrospray ionization
DFO	1,8-diazafluoren-9-one
DRIFT	diffuse reflectance infrared by Fourier transform
DSC	differential scanning calorimetry
DTA	differential thermal analysis
DTG	derivative thermogravimetric

ECD	electron capture detector
EDS	energy dispersive X-ray spectroscopy
EDX	energy-dispersive X-ray analysis
EDXRF	energy-dispersive X-ray fluorescence
EELS	electron energy loss spectroscopy
EI	electron ionization
ESEM	environmental scanning electron microscopy
ESI	electrospray ionization
FID	flame ionization detector
GC	gas chromotography
GHB	gamma-hydroxybutyric acid
GFAAS	graphite furnace atomic absorption spectrometry
GRIM	Glass Refractive Index Measurement
GSR	gunshot residue
Hb	haemoglobin
HCA	hierarchical clustering analysis
HDPE	high-density polyethylene
HPLC	high-performance liquid chromatography
IBA	ion beam analysis
IC	ion chromatography
ICDD	International Centre for Diffraction Data
ICP–MS	inductively coupled plasma–mass spectrometry
ILR	ignitable liquid residue
IMS	ion mobility spectrometry
IRMS	isotope ratio mass spectrometry
LC	liquid chromatography
LDA	linear discriminant analysis
LDPE	low-density polyethylene
LIBS	laser-induced breakdown spectroscopy
MDA	methylenedioxyamphetamine
MDMA	methylenedioxymethylamphetamine
MDEA	3,4-methylenedioxyethylamphetamine
MECC	micellar electrokinetic capillary chromatography (*also* MEKC)
MI	medullary index
MS	mass spectrometry
MSP	microspectrophotometry
MSTFA	*N*-methyl-*M*-trimethylsilyltrifluoroacetamide
m/z	mass-to-charge (ratio)
NMR	nuclear magnetic resonance
NOE	Nuclear Overhauser Effect
NRA	nuclear reaction analysis
PC	paper chromatography

PCA	principal component analysis
PD	physical developer
PDMS	polydimethylsiloxane
PE	polyethylene
PET	poly(ethylene terephthalate)
PETN	pentaerythritol tetranitrate
PIXE	particle-induced X-ray emission
PLM	polarizing light microscope
PMMA	poly(methyl methacrylate)
PP	polypropylene
ppb	parts per billion
ppm	parts per million
PS	polystyrene
PSA	prostate-specific antigen (test)
PVC	poly(vinyl chloride)
ρ	density
R^2	coefficient of determination
RBS	Rutherford back scattering spectrometry
RF	radiofrequency
RI	reflective index
RRS	resonance Raman spectroscopy
SAN	styrene–acrylonitrile
SAP	seminal acid phosphatase
SBR	styrene–butadiene rubber
SE	secondary electron
SEM	scanning electron microscopy
SERS	surface-enhanced Raman spectroscopy
SIMS	secondary ion mass spectrometry
SIM	selected ion monitoring
SPE	solid-phase extraction
SPME	solid-phase microextraction
TEA	thermal energy analyser
TEM	transmission electron microscopy
TFAA	trifluoroacetic anhydride
TGA	thermogravimetric analysis
THC	Δ^9-tetrahydrocannabinol
THM	thermally assisted hydrolysis methylation
TLC	thin layer chromatography
TMAH	tetramethylammonium hydroxide
TMB	tetramethylbenzidine
TOF	time-of-flight
TOF-SIMS	time-of-flight secondary ion mass spectrometry