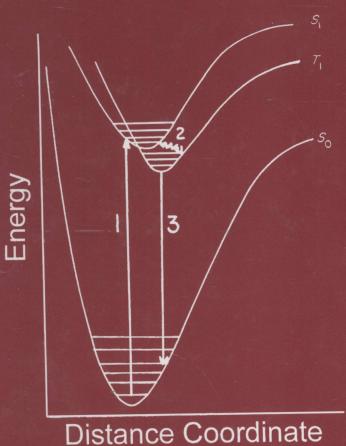
# Spectroscopy of Pharmaceutical Solids



edited by Harry G. Brittain

# Spectroscopy of Pharmaceutical Solids

edited by

Harry G. Brittain

Center for Pharmaceutical Physics Milford, New Jersey, U.S.A.



Published in 2006 by Taylor & Francis Group 270 Madison Avenue New York, NY 10016

© 2006 by Taylor & Francis Group, LLC

No claim to original U.S. Government works Printed in the United States of America on acid-free paper 10 9 8 7 6 5 4 3 2 1

International Standard Book Number-10: 1-57444-893-5 (Hardcover)
International Standard Book Number-13: 978-1-57444-893-1 (Hardcover)

This book contains information obtained from authentic and highly regarded sources. Reprinted material is quoted with permission, and sources are indicated. A wide variety of references are listed. Reasonable efforts have been made to publish reliable data and information, but the author and the publisher cannot assume responsibility for the validity of all materials or for the consequences of their use.

No part of this book may be reprinted, reproduced, transmitted, or utilized in any form by any electronic, mechanical, or other means, now known or hereafter invented, including photocopying, microfilming, and recording, or in any information storage or retrieval system, without written permission from the publishers.

For permission to photocopy or use material electronically from this work, please access www.copyright.com (http://www.copyright.com/) or contact the Copyright Clearance Center, Inc. (CCC) 222 Rosewood Drive, Danvers, MA 01923, 978-750-8400. CCC is a not-for-profit organization that provides licenses and registration for a variety of users. For organizations that have been granted a photocopy license by the CCC, a separate system of payment has been arranged.

**Trademark Notice:** Product or corporate names may be trademarks or registered trademarks, and are used only for identification and explanation without intent to infringe.

Library of Congress Cataloging-in-Publication Data

Catalog record is available from the Library of Congress



Visit the Taylor & Francis Web site at http://www.taylorandfrancis.com

# Spectroscopy of Pharmaceutical Solids

#### DRUGS AND THE PHARMACEUTICAL SCIENCES

A Series of Textbooks and Monographs

# Executive Editor James Swarbrick

PharmaceuTech, Inc. Pinehurst, North Carolina

#### **Advisory Board**

Larry L. Augsburger University of Maryland Baltimore, Maryland

Harry G. Brittain

Center for Pharmaceutical Physics

Milford, New Jersey

Jennifer B. Dressman Johann Wolfgang Goethe University Frankfurt, Germany Anthony J. Hickey University of North Carolina School of Pharmacy Chapel Hill, North Carolina

Jeffrey A. Hughes University of Florida College of Pharmacy Gainesville, Florida

Ajaz Hussain U.S. Food and Drug Administration Frederick, Maryland

Trevor M. Jones The Association of the British Pharmaceutical Industry London, United Kingdom Hans E. Junginger Leiden/Amsterdam Center for Drug Research Leiden, The Netherlands

Vincent H. L. Lee University of Southern California Los Angeles, California

Stephen G. Schulman University of Florida Gainesville, Florida

Jerome P. Skelly Alexandria, Virginia

Elizabeth M. Topp University of Kansas School of Pharmacy Lawrence, Kansas

Geoffrey T. Tucker University of Sheffield Royal Hallamshire Hospital Sheffield, United Kingdom

Peter York University of Bradford School of Pharmacy Bradford, United Kingdom

### **Preface**

Spectroscopic techniques have been widely used in the pharmaceutical sciences to obtain both fundamental and applied information. During the development of any given drug candidate, spectroscopy will be used to establish the structure of the compound and understand its interaction with other constituents. It is also often used as a means for evaluating the analytical characteristics of the bulk drug substance and its formulations. It is no surprise, therefore, that solid-state spectroscopic methods have become extremely important to successful modern drug development.

Many scientists believe themselves to be familiar with the principles that govern the interaction of electromagnetic radiation with matter, and yet their knowledge is often based on partial truths. For instance, most would state that for a molecule to absorb ultraviolet light, an electron must be promoted from one energy level to another. While in some cases there is validity to this belief, the true origin of the transition is a change in the orbital angular momentum of the molecule, and the absorption of a quantum of light causes the transition from one molecular state to another. Genuine knowledge as to the origin of spectroscopic phenomena might not change the routine use of a particular technique, but it would provide a basis that could lead to a more advanced application for that technique.

The reasoning just stated has led to the need for the present volume. However great the use of solid-state spectroscopy might be, a greater degree of fundamental understanding is necessary to obtain maximal use out of each technique. In the present work, the underlying principles of each technique will be sufficiently outlined to provide a thorough and proper understanding of the physics involved, and then applications will be used to illustrate what can be learned through the employment of the method under discussion. Whenever possible, the examples will be drawn from the pharmaceutical literature, but this rule will be violated whenever the author feels that an application from another field might inspire analogous work by a pharmaceutical scientist.

iv Preface

In 1995, I edited a volume entitled "Physical Characterization of Pharmaceutical Solids" in which a fairly extensive overview of methods suitable for work at the molecular, particulate, and bulk levels was provided. Since a substantial portion of this earlier book was concerned with the use of spectroscopy for the characterization of solids having pharmaceutical, the present volume may be viewed as being Volume 1 in the second edition of the older book. In the present volume, the use of spectroscopy for the characterization of pharmaceutical solids has been taken much further, and the range of topics has been greatly extended relative to the coverage of the earlier volume.

Harry G. Brittain

## **Contributors**

**Harry G. Brittain** Center for Pharmaceutical Physics, Milford, New Jersey, U.S.A.

David E. Bugay SSCI, Inc., West Lafayette, Indiana, U.S.A.

**Robert P. Cogdill** School of Pharmacy, Duquesne University, Pittsburgh, Pennsylvania, U.S.A.

**James K. Drennen, III** School of Pharmacy, Duquesne University, Pittsburgh, Pennsylvania, U.S.A.

Ales Medek Pfizer Global R&D, Groton, Connecticut, U.S.A.

- 1. Pharmacokinetics, Milo Gibaldi and Donald Perrier
- 2. Good Manufacturing Practices for Pharmaceuticals: A Plan for Total Quality Control, *Sidney H. Willig, Murray M. Tuckerman, and William S. Hitchings IV*
- 3. Microencapsulation, edited by J. R. Nixon
- 4. Drug Metabolism: Chemical and Biochemical Aspects, *Bernard Testa* and *Peter Jenner*
- 5. New Drugs: Discovery and Development, edited by Alan A. Rubin
- 6. Sustained and Controlled Release Drug Delivery Systems, *edited by Joseph R. Robinson*
- 7. Modern Pharmaceutics, edited by Gilbert S. Banker and Christopher T. Rhodes
- 8. Prescription Drugs in Short Supply: Case Histories, Michael A. Schwartz
- 9. Activated Charcoal: Antidotal and Other Medical Uses, David O. Cooney
- Concepts in Drug Metabolism (in two parts), edited by Peter Jenner and Bernard Testa
- 11. Pharmaceutical Analysis: Modern Methods (in two parts), edited by James W. Munson
- 12. Techniques of Solubilization of Drugs, edited by Samuel H. Yalkowsky
- 13. Orphan Drugs, edited by Fred E. Karch
- 14. Novel Drug Delivery Systems: Fundamentals, Developmental Concepts, Biomedical Assessments, *Yie W. Chien*
- Pharmacokinetics: Second Edition, Revised and Expanded, Milo Gibaldi and Donald Perrier
- Good Manufacturing Practices for Pharmaceuticals: A Plan for Total Quality Control, Second Edition, Revised and Expanded, Sidney H. Willig, Murray M. Tuckerman, and William S. Hitchings IV
- 17. Formulation of Veterinary Dosage Forms, edited by Jack Blodinger
- 18. Dermatological Formulations: Percutaneous Absorption, Brian W. Barry
- 19. The Clinical Research Process in the Pharmaceutical Industry, *edited by Gary M. Matoren*
- 20. Microencapsulation and Related Drug Processes, Patrick B. Deasy
- Drugs and Nutrients: The Interactive Effects, edited by Daphne A. Roe and T. Colin Campbell
- 22. Biotechnology of Industrial Antibiotics, Erick J. Vandamme
- 23. Pharmaceutical Process Validation, edited by Bernard T. Loftus and Robert A. Nash
- 24. Anticancer and Interferon Agents: Synthesis and Properties, edited by Raphael M. Ottenbrite and George B. Butler
- 25. Pharmaceutical Statistics: Practical and Clinical Applications, Sanford Bolton

- 26. Drug Dynamics for Analytical, Clinical, and Biological Chemists, Benjamin J. Gudzinowicz, Burrows T. Younkin, Jr., and Michael J. Gudzinowicz
- 27. Modern Analysis of Antibiotics, edited by Adjoran Aszalos
- 28. Solubility and Related Properties, Kenneth C. James
- Controlled Drug Delivery: Fundamentals and Applications, Second Edition, Revised and Expanded, edited by Joseph R. Robinson and Vincent H. Lee
- 30. New Drug Approval Process: Clinical and Regulatory Management, edited by Richard A. Guarino
- 31. Transdermal Controlled Systemic Medications, edited by Yie W. Chien
- 32. Drug Delivery Devices: Fundamentals and Applications, *edited by Praveen Tyle*
- 33. Pharmacokinetics: Regulatory Industrial Academic Perspectives, edited by Peter G. Welling and Francis L. S. Tse
- 34. Clinical Drug Trials and Tribulations, edited by Allen E. Cato
- 35. Transdermal Drug Delivery: Developmental Issues and Research Initiatives, *edited by Jonathan Hadgraft and Richard H. Guy*
- 36. Aqueous Polymeric Coatings for Pharmaceutical Dosage Forms, edited by James W. McGinity
- 37. Pharmaceutical Pelletization Technology, edited by Isaac Ghebre-Sellassie
- 38. Good Laboratory Practice Regulations, edited by Allen F. Hirsch
- 39. Nasal Systemic Drug Delivery, Yie W. Chien, Kenneth S. E. Su, and Shyi-Feu Chang
- 40. Modern Pharmaceutics: Second Edition, Revised and Expanded, edited by Gilbert S. Banker and Christopher T. Rhodes
- 41. Specialized Drug Delivery Systems: Manufacturing and Production Technology, *edited by Praveen Tyle*
- 42. Topical Drug Delivery Formulations, edited by David W. Osborne and Anton H. Amann
- 43. Drug Stability: Principles and Practices, Jens T. Carstensen
- 44. Pharmaceutical Statistics: Practical and Clinical Applications, Second Edition, Revised and Expanded, *Sanford Bolton*
- 45. Biodegradable Polymers as Drug Delivery Systems, *edited by Mark Chasin and Robert Langer*
- 46. Preclinical Drug Disposition: A Laboratory Handbook, *Francis L. S. Tse and James J. Jaffe*
- 47. HPLC in the Pharmaceutical Industry, edited by Godwin W. Fong and Stanley K. Lam
- 48. Pharmaceutical Bioequivalence, edited by Peter G. Welling, Francis L. S. Tse, and Shrikant V. Dinghe
- 49. Pharmaceutical Dissolution Testing, Umesh V. Banakar

- 50. Novel Drug Delivery Systems: Second Edition, Revised and Expanded, Yie W. Chien
- Managing the Clinical Drug Development Process, David M. Cocchetto and Ronald V. Nardi
- 52. Good Manufacturing Practices for Pharmaceuticals: A Plan for Total Quality Control, Third Edition, *edited by Sidney H. Willig and James R. Stoker*
- 53. Prodrugs: Topical and Ocular Drug Delivery, edited by Kenneth B. Sloan
- 54. Pharmaceutical Inhalation Aerosol Technology, *edited by Anthony J. Hickey*
- 55. Radiopharmaceuticals: Chemistry and Pharmacology, *edited by Adrian D. Nunn*
- 56. New Drug Approval Process: Second Edition, Revised and Expanded, edited by Richard A. Guarino
- 57. Pharmaceutical Process Validation: Second Edition, Revised and Expanded, *edited by Ira R. Berry and Robert A. Nash*
- 58. Ophthalmic Drug Delivery Systems, edited by Ashim K. Mitra
- 59. Pharmaceutical Skin Penetration Enhancement, edited by Kenneth A. Walters and Jonathan Hadgraft
- 60. Colonic Drug Absorption and Metabolism, edited by Peter R. Bieck
- 61. Pharmaceutical Particulate Carriers: Therapeutic Applications, edited by Alain Rolland
- 62. Drug Permeation Enhancement: Theory and Applications, *edited by Dean S. Hsieh*
- 63. Glycopeptide Antibiotics, edited by Ramakrishnan Nagarajan
- 64. Achieving Sterility in Medical and Pharmaceutical Products, Nigel A. Halls
- 65. Multiparticulate Oral Drug Delivery, edited by Isaac Ghebre-Sellassie
- 66. Colloidal Drug Delivery Systems, edited by Jörg Kreuter
- 67. Pharmacokinetics: Regulatory Industrial Academic Perspectives, Second Edition, edited by Peter G. Welling and Francis L. S. Tse
- Drug Stability: Principles and Practices, Second Edition, Revised and Expanded, Jens T. Carstensen
- Good Laboratory Practice Regulations: Second Edition, Revised and Expanded, edited by Sandy Weinberg
- 70. Physical Characterization of Pharmaceutical Solids, *edited by Harry G. Brittain*
- 71. Pharmaceutical Powder Compaction Technology, edited by Göran Alderborn and Christer Nyström
- 72. Modern Pharmaceutics: Third Edition, Revised and Expanded, edited by Gilbert S. Banker and Christopher T. Rhodes
- 73. Microencapsulation: Methods and Industrial Applications, edited by Simon Benita

- 74. Oral Mucosal Drug Delivery, edited by Michael J. Rathbone
- 75. Clinical Research in Pharmaceutical Development, edited by Barry Bleidt and Michael Montagne
- 76. The Drug Development Process: Increasing Efficiency and Cost Effectiveness, edited by Peter G. Welling, Louis Lasagna, and Umesh V. Banakar
- 77. Microparticulate Systems for the Delivery of Proteins and Vaccines, edited by Smadar Cohen and Howard Bernstein
- 78. Good Manufacturing Practices for Pharmaceuticals: A Plan for Total Quality Control, Fourth Edition, Revised and Expanded, Sidney H. Willig and James R. Stoker
- Aqueous Polymeric Coatings for Pharmaceutical Dosage Forms:
   Second Edition, Revised and Expanded, edited by James W. McGinity
- 80. Pharmaceutical Statistics: Practical and Clinical Applications, Third Edition, *Sanford Bolton*
- 81. Handbook of Pharmaceutical Granulation Technology, *edited by Dilip M. Parikh*
- 82. Biotechnology of Antibiotics: Second Edition, Revised and Expanded, edited by William R. Strohl
- 83. Mechanisms of Transdermal Drug Delivery, edited by Russell O. Potts and Richard H. Guy
- 84. Pharmaceutical Enzymes, edited by Albert Lauwers and Simon Scharpé
- 85. Development of Biopharmaceutical Parenteral Dosage Forms, *edited by John A. Bontempo*
- 86. Pharmaceutical Project Management, edited by Tony Kennedy
- 87. Drug Products for Clinical Trials: An International Guide to Formulation
  Production Quality Control, edited by Donald C. Monkhouse and Christopher T. Rhodes
- 88. Development and Formulation of Veterinary Dosage Forms: Second Edition, Revised and Expanded, edited by Gregory E. Hardee and J. Desmond Baggot
- 89. Receptor-Based Drug Design, edited by Paul Leff
- 90. Automation and Validation of Information in Pharmaceutical Processing, edited by Joseph F. deSpautz
- 91. Dermal Absorption and Toxicity Assessment, edited by Michael S. Roberts and Kenneth A. Walters
- 92. Pharmaceutical Experimental Design, Gareth A. Lewis, Didier Mathieu, and Roger Phan-Tan-Luu
- 93. Preparing for FDA Pre-Approval Inspections, edited by Martin D. Hynes III
- 94. Pharmaceutical Excipients: Characterization by IR, Raman, and NMR Spectroscopy, *David E. Bugay and W. Paul Findlay*
- 95. Polymorphism in Pharmaceutical Solids, edited by Harry G. Brittain

- 96. Freeze-Drying/Lyophilization of Pharmaceutical and Biological Products, edited by Louis Rey and Joan C. May
- 97. Percutaneous Absorption: Drugs-Cosmetics-Mechanisms-Methodology, Third Edition, Revised and Expanded, edited by Robert L. Bronaugh and Howard I. Maibach
- 98. Bioadhesive Drug Delivery Systems: Fundamentals, Novel Approaches, and Development, edited by Edith Mathiowitz, Donald E. Chickering III, and Claus-Michael Lehr
- 99. Protein Formulation and Delivery, edited by Eugene J. McNally
- New Drug Approval Process: Third Edition, The Global Challenge, edited by Richard A. Guarino
- 101. Peptide and Protein Drug Analysis, edited by Ronald E. Reid
- 102. Transport Processes in Pharmaceutical Systems, *edited by Gordon L. Amidon, Ping I. Lee, and Elizabeth M. Topp*
- 103. Excipient Toxicity and Safety, edited by Myra L. Weiner and Lois A. Kotkoskie
- 104. The Clinical Audit in Pharmaceutical Development, *edited by Michael B. Hamrell*
- Pharmaceutical Emulsions and Suspensions, edited by Francoise Nielloud and Gilberte Marti-Mestres
- 106. Oral Drug Absorption: Prediction and Assessment, edited by Jennifer B. Dressman and Hans Lennernäs
- Drug Stability: Principles and Practices, Third Edition, Revised and Expanded, edited by Jens T. Carstensen and C. T. Rhodes
- 108. Containment in the Pharmaceutical Industry, edited by James P. Wood
- Good Manufacturing Practices for Pharmaceuticals: A Plan for Total Quality Control from Manufacturer to Consumer, Fifth Edition, Revised and Expanded, Sidney H. Willig
- 110. Advanced Pharmaceutical Solids, Jens T. Carstensen
- Endotoxins: Pyrogens, LAL Testing, and Depyrogenation, Second Edition, Revised and Expanded. Kevin L. Williams
- 112. Pharmaceutical Process Engineering, Anthony J. Hickey and David Ganderton
- 113. Pharmacogenomics, edited by Werner Kalow, Urs A. Meyer and Rachel F. Tyndale
- 114. Handbook of Drug Screening, edited by Ramakrishna Seethala and Prabhavathi B. Fernandes
- 115. Drug Targeting Technology: Physical Chemical Biological Methods, edited by Hans Schreier
- 116. Drug-Drug Interactions, edited by A. David Rodrigues
- 117. Handbook of Pharmaceutical Analysis, edited by Lena Ohannesian and Anthony J. Streeter
- 118. Pharmaceutical Process Scale-Up, edited by Michael Levin

- 119. Dermatological and Transdermal Formulations, *edited by Kenneth A. Walters*
- 120. Clinical Drug Trials and Tribulations: Second Edition, Revised and Expanded, edited by Allen Cato, Lynda Sutton, and Allen Cato III
- 121. Modern Pharmaceutics: Fourth Edition, Revised and Expanded, edited by Gilbert S. Banker and Christopher T. Rhodes
- 122. Surfactants and Polymers in Drug Delivery, Martin Malmsten
- 123. Transdermal Drug Delivery: Second Edition, Revised and Expanded, edited by Richard H. Guy and Jonathan Hadgraft
- 124. Good Laboratory Practice Regulations: Second Edition, Revised and Expanded, *edited by Sandy Weinberg*
- 125. Parenteral Quality Control: Sterility, Pyrogen, Particulate, and Package Integrity Testing: Third Edition, Revised and Expanded, Michael J. Akers, Daniel S. Larrimore, and Dana Morton Guazzo
- 126. Modified-Release Drug Delivery Technology, edited by Michael J. Rathbone, Jonathan Hadgraft, and Michael S. Roberts
- 127. Simulation for Designing Clinical Trials: A Pharmacokinetic-Pharmacodynamic Modeling Perspective, *edited by Hui C. Kimko and Stephen B. Duffull*
- 128. Affinity Capillary Electrophoresis in Pharmaceutics and Biopharmaceutics, edited by Reinhard H. H. Neubert and Hans-Hermann Rüttinger
- 129. Pharmaceutical Process Validation: An International Third Edition, Revised and Expanded, edited by Robert A. Nash and Alfred H. Wachter
- 130. Ophthalmic Drug Delivery Systems: Second Edition, Revised and Expanded, *edited by Ashim K. Mitra*
- 131. Pharmaceutical Gene Delivery Systems, edited by Alain Rolland and Sean M. Sullivan
- 132. Biomarkers in Clinical Drug Development, edited by John C. Bloom and Robert A. Dean
- 133. Pharmaceutical Extrusion Technology, edited by Isaac Ghebre-Sellassie and Charles Martin
- 134. Pharmaceutical Inhalation Aerosol Technology: Second Edition, Revised and Expanded, *edited by Anthony J. Hickey*
- 135. Pharmaceutical Statistics: Practical and Clinical Applications, Fourth Edition, Sanford Bolton and Charles Bon
- 136. Compliance Handbook for Pharmaceuticals, Medical Devices, and Biologics, *edited by Carmen Medina*
- Freeze-Drying/Lyophilization of Pharmaceutical and Biological Products: Second Edition, Revised and Expanded, edited by Louis Rey and Joan C. May
- 138. Supercritical Fluid Technology for Drug Product Development, edited by Peter York, Uday B. Kompella, and Boris Y. Shekunov
- 139. New Drug Approval Process: Fourth Edition, Accelerating Global Registrations, *edited by Richard A. Guarino*

- 140. Microbial Contamination Control in Parenteral Manufacturing, edited by Kevin L. Williams
- 141. New Drug Development: Regulatory Paradigms for Clinical Pharmacology and Biopharmaceutics, *edited by Chandrahas G. Sahajwalla*
- 142. Microbial Contamination Control in the Pharmaceutical Industry, *edited by Luis Jimenez*
- 143. Generic Drug Product Development: Solid Oral Dosage Forms, edited by Leon Shargel and Izzy Kanfer
- 144. Introduction to the Pharmaceutical Regulatory Process, edited by Ira R. Berry
- 145. Drug Delivery to the Oral Cavity: Molecules to Market, *edited by Tapash K. Ghosh and William R. Pfister*
- 146. Good Design Practices for GMP Pharmaceutical Facilities, edited by Andrew Signore and Terry Jacobs
- 147. Drug Products for Clinical Trials, Second Edition, edited by Donald Monkhouse, Charles Carney, and Jim Clark
- 148. Polymeric Drug Delivery Systems, edited by Glen S. Kwon
- Injectable Dispersed Systems: Formulation, Processing, and Performance, edited by Diane J. Burgess
- Laboratory Auditing for Quality and Regulatory Compliance, Donald Singer, Raluca-loana Stefan, and Jacobus van Staden
- 151. Active Pharmaceutical Ingredients: Development, Manufacturing, and Regulation, *edited by Stanley Nusim*
- 152. Preclinical Drug Development, edited by Mark C. Rogge and David R. Taft
- 153. Pharmaceutical Stress Testing: Predicting Drug Degradation, edited by Steven W. Baertschi
- 154. Handbook of Pharmaceutical Granulation Technology: Second Edition, edited by Dilip M. Parikh
- 155. Percutaneous Absorption: Drugs-Cosmetics-Mechanisms-Methodology, Fourth Edition, *edited by Robert L. Bronaugh and Howard I. Maibach*
- 156. Pharmacogenomics: Second Edition, edited by Werner Kalow, Urs A. Meyer and Rachel F. Tyndale
- 157. Pharmaceutical Process Scale-Up, Second Edition, edited by Michael Levin
- 158. Microencapsulation: Methods and Industrial Applications, Second Edition, edited by Simon Benita
- 159. Nanoparticle Technology for Drug Delivery, edited by Ram B. Gupta and Uday B. Kompella
- 160. Spectroscopy of Pharmaceutical Solids, edited by Harry G. Brittain

## **Contents**

Pre	eface	ii
	ntributors	iχ
Pai	rt I. Introduction to Spectroscopy	
1.	Electromagnetic Radiation and Spectroscopy  Harry G. Brittain  Nature of Electromagnetic Radiation 1  Classical Description of Electromagnetic Radiation 3  The Quantum Theory of Electromagnetic Radiation 8  Ionization and Excitation of Atoms 12  Development of the Quantum Theory 17  Overview of Spectroscopy 28  Summary 30  References 31	1
Par	t II. Core Electron Spectroscopy	
2.	Core Electron States and X-Ray Absorption Spectroscopy 3.  Harry G. Brittain  Wave Mechanical Description of the Hydrogen Atom 33  X-Ray Absorption Spectroscopy 53  References 64	3
3.	X-Ray Photoelectron and X-Ray Fluorescence Spectroscopy 67  Harry G. Brittain  X-Ray Emission Spectroscopies 67	7

vi Contents

X-Ray Photoelectron Spectroscopy . . . . 69 X-Ray Fluorescence Spectroscopy . . . . 77

	References 87
Part	III. Valence Electron Spectroscopy
4.	Molecular Orbital Theory and the Electronic Structure of Molecules
5.	UV/VIS Reflectance Spectroscopy
6.	Luminescence Spectroscopy