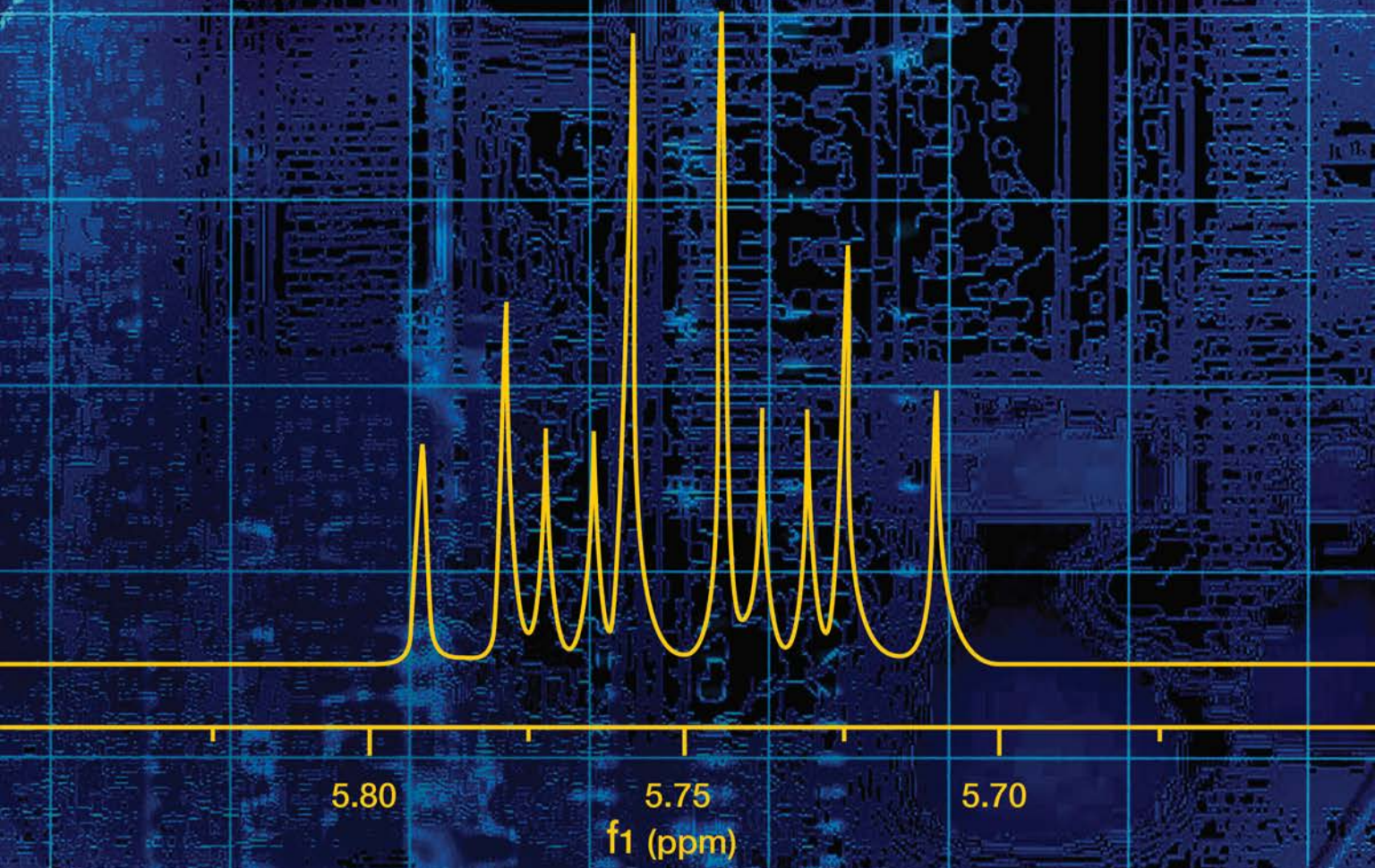
INTRODUCTION TO Spectroscopy

Fifth Edition



PAVIA | LAMPMAN | KRIZ | VYVYAN

FIFTH EDITION

INTRODUCTION TO SPECTROSCOPY

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Cover Designer: Bartay Studio
Cover Image: Expansion of the C-4 methine proton of ethyl 2-methyl-4-pentenoate acquired at 500 MHz. Data acquired and processed by James Vyvyan.
Compositor: MPS Limited

Library of Congress Control Number: 2013950396

ISBN-13: 978-1-285-46012-3

ISBN-10: 1-285-46012-X

Cengage Learning
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Printed in the United States of America
1 2 3 4 5 6 7 17 16 15 14 13

PREFACE

This is the fifth edition of a textbook in spectroscopy intended for students of organic chemistry. Our textbook can serve as a supplement for the typical organic chemistry lecture textbook or as a stand-alone textbook for an advanced undergraduate or first-year graduate course in spectroscopic methods. This book is also a useful tool for students engaged in research. Our aim is not only to teach students to interpret spectra, but also to present basic theoretical concepts. As with the previous editions, we have tried to focus on the important aspects of each spectroscopic technique without dwelling excessively on theory or complex mathematical analyses.

This book is a continuing evolution of materials that we use in our own courses, both as a supplement to our organic chemistry lecture course series and also as the principal textbook in our upper division and graduate courses in spectroscopic methods and advanced NMR techniques. Explanations and examples that we have found to be effective in our courses have been incorporated into this edition.

NEW TO THIS EDITION

This fifth edition of *Introduction to Spectroscopy* contains some important changes. The material on mass spectrometry has been moved closer to the front of the text and divided into two more easily digested chapters. Material on some newer sampling and ionization methods is included, as are additional methods of structural analysis using fragmentation patterns. All of the chapters dealing with nuclear magnetic resonance have been gathered together into sequential chapters. Expanded discussions of diastereotopic systems and heteronuclear coupling are included, as is a revised discussion of solvent effects in NMR.

Additional practice problems have been added to each of the chapters. We have included some additional solved problems, too, so that students can better develop strategies and skills for solving spectroscopy problems. The problems that are marked with an asterisk (*) have solutions included in the Answers to Selected Problems following Chapter 11.

We wish to alert persons who adopt this book that answers to all of the problems are available online from the publisher. Authorization to gain access to the website may be obtained through the local Cengage textbook representative.

ADVICE FOR STUDENTS

Success in working out the solutions to spectroscopy problems comes more easily and is more enjoyable by following some simple suggestions:

1. Carefully study the solved examples that may be found at the end of each chapter. Do not attempt to work on additional problems until you are comfortable with the approach that is being demonstrated with the solved examples.
2. There is great value to be gained in working collaboratively to solve spectroscopy problems. Try standing around a blackboard to exchange ideas. You will find it to be fun, and you will learn more!
3. Don't be afraid to struggle. It is too easy to look up the answer to a difficult problem, and you won't learn much. You need to train your brain to think like a scientist, and there is no substitute for hard work.
4. Work problems concurrently as you study each chapter. That will solidify the concepts in your mind.

Although this book concentrates on organic chemistry examples, be aware that the study of spectroscopy crosses over into many areas, including biochemistry, inorganic chemistry, physical chemistry, materials chemistry, and analytical chemistry. Spectroscopy is an indispensible tool to support all forms of laboratory research.

ACKNOWLEDGMENTS

The authors are very grateful to Mr. Charles Wandler, without whose expert help this project could not have been accomplished. We also acknowledge numerous contributions made by our students, who use the textbook and who provide us careful and thoughtful feedback.

Finally, once again we must thank our wives, Neva-Jean Pavia, Marian Lampman, and Cathy Vyvyan, for their support and patience. They endure a great deal in order to support us as we write, and they deserve to be part of the celebration when the textbook is completed! We honor the memory of Carolyn Kriz; we miss her and the love and encouragement that she provided.

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INTRO TO SPECTROSCOPY FIFTH EDITION SUMMARY OF CHANGES

The order of the chapters was rearranged to better reflect the requests and practices of our users. Mass Spectroscopy was moved to an earlier position, causing the renumbering.

Fourth edition chapter number/title	Fifth edition chapter number/title	Notes
1 Molecular Formulas and What Can Be Learned from Them	1 Molecular Formulas and What Can Be Learned from Them	Section 1.6, A Quick Look Ahead to Simple Uses of Mass Spectra, was deleted. (Mass Spectra were moved earlier into Chapters 3 and 4.) A new Section 1.6 is now titled: "The Nitrogen Rule." References were revised/updated.
2 Infrared Spectroscopy	2 Infrared Spectroscopy	Section 2.6, the solid samples subsection was updated to include ATR techniques. Several figures were revised/updated. Section 2.21, Alkyl and Aryl Halides, was revised. Section 2.23, How to Solve Infrared Spectral Problems, is a new section. The sections that followed were renumbered. Problems were revised. References were revised/updated.
3 Nuclear Magnetic Resonance Spectroscopy Part One: Basic Concepts.	5 Nuclear Magnetic Resonance Spectroscopy Part One: Basic Concepts.	New Section 5.20 References were revised/updated. New online resources were referenced and/or updated.
4 Nuclear Magnetic Resonance Spectroscopy Part Two: Carbon-13 etc.	6 Nuclear Magnetic Resonance Spectroscopy Part Two: Carbon-13 etc.	Section 6.4 introduces a new decoupling notation. New Section 6.12. Sections following 6.12 are renumbered. Several new problems were added. Some spectra replaced/improved. References were revised/updated. New online resources referenced and/or updated.
5 Nuclear Magnetic Resonance Spectroscopy Part Three: Spin-Spin Coupling	7 Nuclear Magnetic Resonance Spectroscopy Part Three: Spin-Spin Coupling	New discussion of splitting in diastereotopic systems. New discussion of heteronuclear splitting between ^{1}H–^{19}F and S–^{31}P Addition of solved example problems. New and revised end-of-chapter problems using coupling constant information and chemical shift calculations. References were revised/updated.
6 Nuclear Magnetic Resonance Spectroscopy Part Four: Other Topics in One-Dimensional NMR	8 Nuclear Magnetic Resonance Spectroscopy Part Four: Other Topics in One-Dimensional NMR	New discussion and examples of solvent effects. Addition of solved example problems. New and revised end-of-chapter problems. References were revised/updated.

(*Continued*)

Fourth edition chapter number/title	Fifth edition chapter number/title	Notes
7 Ultraviolet Spectroscopy	10 Ultraviolet Spectroscopy	Few changes.
8 Mass Spectrometry (first half) Chapter was split.	3 Mass Spectrometry Part One: Basic Theory, Instrumentation, and Sampling Techniques	To highlight the continued development and importance of mass spectrometry (MS) methods, we have moved this material to the early part of the text and split it into two chapters, one on theory and instrumentation (Chapter 3) and the other on detailed structural analysis using characteristic fragmentation patterns of common functional groups (Chapter 4). Expanded and refined discussion of sampling and ionization methods, including atmospheric pressure chemical ionization techniques. Examples of applications for different MS techniques and instrumentation, including pros and cons of different methods.
8 Mass Spectrometry (second half)	4 Mass Spectrometry Part Two: Fragmentation and Structural Analysis	Refined discussion of fragmentations in EI-MS for common functional groups. New examples of use of MS in structure determination. Additional solved example problems. New and revised end-of-chapter problems.
9 Combined Structure Problems	11 Combined Structure Problems	Several new problems were introduced. Two-dimensional spectra were replaced with new, improved ones. References were revised/updated. Online resources were updated.
10 Nuclear Magnetic Resonance Spectroscopy Part Five: Advanced NMR Techniques.	9 Nuclear Magnetic Resonance Spectroscopy Part Five: Advanced NMR Techniques	Sections 9.4 and 9.7 were extensively revised. Many of the two-dimensional spectra were replaced with new, improved ones.
Appendices	Appendices	Old Appendix 11 was removed. Values in some of the tables were updated or revised.