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FOURTH EDITION

INTRODUCTION TO SPECTROSCOPY

Donald L. Pavia Gary M. Lampman George S. Kriz

James R. Vyvyan

Department of Chemistry Western Washington University Bellingham, Washington



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PREFACE

This is the fourth 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, and it can also be used as a "stand-alone" textbook for an advanced undergraduate course in spectroscopic methods of structure determination or for a first-year graduate course in spectroscopy. 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.

This fourth edition of *Introduction to Spectroscopy* contains some important changes. The discussion of coupling constant analysis in Chapter 5 has been significantly expanded. Long-range couplings are covered in more detail, and multiple strategies for measuring coupling constants are presented. Most notably, the systematic analysis of line spacings allows students (with a little practice) to extract all of the coupling constants from even the most challenging of first-order multiplets. Chapter 5 also includes an expanded treatment of group equivalence and diastereotopic systems.

Discussion of solvent effects in NMR spectroscopy is discussed more explicitly in Chapter 6, and the authors thank one of our graduate students, Ms. Natalia DeKalb, for acquiring the data in Figures 6.19 and 6.20. A new section on determining the relative and absolute stereochemical configuration with NMR has also been added to this chapter.

The mass spectrometry section (Chapter 8) has been completely revised and expanded in this edition, starting with more detailed discussion of a mass spectrometer's components. All of the common ionization methods are covered, including chemical ionization (CI), fast-atom bombardment (FAB), matrix-assisted laser desorption ionization (MALDI), and electrospray techniques. Different types of mass analyzers are described as well. Fragmentation in mass spectrometry is discussed in greater detail, and several additional fragmentation mechanisms for common functional groups are illustrated. Numerous new mass spectra examples are also included.

Problems have been added to each of the chapters. We have included some more solved problems, so that students can develop skill in solving spectroscopy problems.

vi Preface

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.

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

Finally, once again we must thank our wives, Neva-Jean, Marian, Carolyn, and Cathy for their support and their 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!

Donald L. Pavia Gary M. Lampman George S. Kriz James R. Vyvyan

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