中国科学院研究生教学丛书

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分子光谱

MOLECULAR SPECTROSCOPY

Jeanne L. McHale

科学出版社

影印版

中国科学院研究生教学丛书

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MOLECULAR SPECTROSCOPY

(影印版)

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内 容 简 介

本书为中国科学院研究生教学丛书之一。

本书为化学工作者提供了最新的分子光谱理论与应用信息，内容覆盖了原子光谱、转动光谱、振动光谱及电子光谱，并特别讨论了凝聚相分子光谱。本书从简要说明量子力学原理入手，系统介绍了光的性质、物质的电磁性质及电动力学等知识，结构安排合理，便于读者理解和掌握。

本书可供从事化学，特别是物理化学研究工作的大学高年级本科生、研究生、教师及广大的科研工作者参考。

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《中国科学院研究生教学丛书》序

在21世纪曙光初露，中国科技、教育面临重大改革和蓬勃发展之际，《中国科学院研究生教学丛书》——这套凝聚了中国科学院新老科学家、研究生导师们多年心血的研究生教材面世了。相信这套丛书的出版，会在一定程度上缓解研究生教材不足的困难，对提高研究生教育质量起着积极的推动作用。

21世纪将是科学技术日新月异，迅猛发展的新世纪，科学技术将成为经济发展的最重要的资源和不竭的动力，成为经济和社会发展的首要推动力量。世界各国之间综合国力的竞争，实质上是科技实力的竞争。而一个国家科技实力的决定因素是它所拥有的科技人才的数量和质量。我国要想在21世纪顺利地实施“科教兴国”和“可持续发展”战略，实现邓小平同志规划的第三步战略目标——把我国建设成中等发达国家，关键在于培养造就一支数量宏大、素质优良、结构合理、有能力参与国际竞争与合作的科技大军。这是摆在我国高等教育面前的一项十分繁重而光荣的战略任务。

中国科学院作为我国自然科学与高新技术的综合研究与发展中心，在建院之初就明确了出成果出人才并举的办院宗旨，长期坚持走科研与教育相结合的道路，发挥了高级科技专家多、科研条件好、科研水平高的优势，结合科研工作，积极培养研究生；在出成果的同时，为国家培养了数以万计的研究生。当前，中国科学院正在按照江泽民同志关于中国科学院要努力建设好“三个基地”的指示，在建设具有国际先进水平的科学研究基地和促进高新技术产

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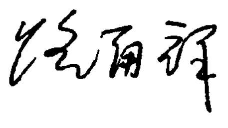
业发展基地的同时，加强研究生教育，努力建设好高级人才培养基地，在肩负起发展我国科学技术及促进高新技术产业发展重任的同时，为国家源源不断地培养输送大批高级科技人才。

质量是研究生教育的生命，全面提高研究生培养质量是当前我国研究生教育的首要任务。研究生教材建设是提高研究生培养质量的一项重要的基础性工作。由于各种原因，目前我国研究生教材的建设滞后于研究生教育的发展。为了改变这种情况，中国科学院组织了一批在科学前沿工作，同时又具有相当教学经验的科学家撰写研究生教材，并以专项资金资助优秀的研究生教材的出版。希望通过数年努力，出版一套面向21世纪科技发展、体现中国科学院特色的高水平的研究生教学丛书。本丛书内容力求具有科学性、系统性和基础性，同时也兼顾前沿性，使阅读者不仅能获得相关学科的比较系统的科学基础知识，也能被引导进入当代科学研究的前沿。这套研究生教学丛书，不仅适合于在校研究生学习使用，也可以作为高校教师和专业研究人员工作和学习的参考书。

“桃李不言，下自成蹊。”我相信，通过中国科学院一批科学家的辛勤耕耘，《中国科学院研究生教学丛书》将成为我国研究生教育园地的一丛鲜花，也将似润物春雨，滋养莘莘学子的心田，把他们引向科学的殿堂，不仅为科学院，也为全国研究生教育的发展作出重要贡献。



PREFACE

This book is the crystallization of the lecture notes I have been compiling since 1981, the year I first taught a graduate course in spectroscopy. At the time, I was disappointed to learn that Ira N. Levine's *Molecular Spectroscopy* (John Wiley and Sons, New York, 1975) was out of print. Since then, I have made use of several excellent texts, but I felt that the time had come to mainstream the topics of condensed phase spectroscopy and time-dependent theory into the conventional introductory spectroscopy course. I wanted to write a book that would bridge tradition and innovation, that would present the necessary theoretical foundations and help students acquire the intuition needed to solve practical problems in the spectroscopy laboratory. I wanted the book to be rigorous, but not at the expense of clarity. I didn't want to follow the typical style of a foreign-language textbook, where students learn all the fine details of gender and verb conjugation, only to later visit a country where the language is spoken and find that they can't get around, having failed to learn words like "upstairs" and "outside." I wanted to write a book that would enable students to "get around" in the field.

Spectroscopy is very much the study of applied quantum mechanics. This book assumes that the reader has previously taken a one-term course in quantum mechanics, at the level of Levine's *Quantum Chemistry* (Prentice-Hall, Upper Saddle River, N.J., 1999) or P. W. Atkins' *Molecular Quantum Mechanics, 2nd ed.* (Oxford University Press, New York, 1983). Some previous exposure to statistical mechanics, as in an undergraduate physical chemistry class, will also be helpful. Chapter 1 summarizes the necessary background in these two subject areas. Even for the student with a very strong background, I recommend Chapter 1 as it will help establish some notation and recurring themes that appear throughout the book. Chapter 2 discusses both the classical and quantum mechanical theory of electromagnetic radiation, and Chapter 3 describes the electric and magnetic properties of matter on which the light-matter interaction depends. Time-dependent perturbation theory, the foundation of spectroscopic theory, is developed in Chapter 4, and in Chapter 5 I discuss the use of time-correlation functions in rotational and vibrational spectroscopy. Applications of the time-correlation function formalism are further described in Chapters 8 and 12. Chapter 6 describes the connection between theoretical quantities, such as the electric dipole transition moment, and experimental observables, such as the intensity of absorption, emission and scattering. Chapters 7 through 12 take up specific types of spectra and applications: Chapter 7 develops atomic spectroscopy in order to introduce electronic transitions, Chapter 8 covers rotations and internal rotations, vibrational spectra are considered in Chapters 9 and 10, and molecular electronic spectroscopy is covered in Chapter 11. Chapter 12 unifies the topics of Raman and resonance Raman spectroscopy, and provides a brief introduction to nonlinear techniques. Group theory is used extensively in Chapters 10, 11, and 12, and is reviewed in Appendix C. While it is assumed that the reader has had some exposure to group theory, particularly molecular symmetry, the basic tools required for working problems are presented in Appendix C. Appendix A covers some necessary math skills and Appendix B presents some details of doing calculations in electrostatics, particularly relevant to Chapter 3. For a general review of helpful math skills, I recommend *Applied Mathematics for Physical Chemistry, 2nd ed.* (Prentice-Hall, Upper Saddle River, N. J., 1998) by James R. Barrante. I have made a strong effort to use consistent notation throughout the book, and I place great emphasis on the power as well as the limitations of approximations. A Solutions Manual for this text is available to adopting instructors (ISBN 0-13-920083-5).

In addition to the many students who helped to shape my early lecture notes and rough drafts of this book, there are many people to thank for critical reading of all or part of the manuscript. At the University of Idaho, my colleagues Phil Deutchman, Dan Edwards, Dave Marshall and Pam Shapiro reviewed chapters and contributed many suggestions. Special thanks are due to Luke Emery and Doug Daniel for critical reading of the entire book, and countless helpful comments and criticisms. The following UI graduate students used the manuscript as the text for the course and made helpful corrections and suggestions: Xuan Cao, Connor Flynn, Brian Keller, Scott Larkin, Ron Mallery, John Streiff, Robert Tolbert, Husheng Yang, Bai Yin, and Mike Wojcik. I am also indebted to my good colleagues, Frank Baglin of the University of Nevada and Nina Veas of Michelin, for careful reading and thoughtful comments on several chapters. I am very grateful to the following reviewers for their helpful suggestions: Robert R. Birge, Syracuse University; David Farrelly, Utah State University; H. Bruce Friedrich, University of Iowa; Daniel P. Gerrity, Reed College; Darla K. Graff, Los Alamos National Labs; Bruce S. Hudson, Syracuse University; Fred Northrup, Northwestern University, Thomas B. Rauchfuss, University of Illinois - Urbana/Champaign; David J. Simkin, McGill University; and Michael Trenary, University of Illinois at Chicago. I owe much to my teachers Jack Simons and Bill Guillory at the University of Utah for their inspiration. I would also like to acknowledge my editors Deirdre Cavanaugh and John Challice at Prentice-Hall for their guidance. Of course, it is customary to thank someone for doing an excellent job of typing. I only wish I could do so! Instead, I express my deepest gratitude to Robert Tolbert and John Jegla for patiently helping me in my struggle to learn LaTeX. This book would not have been possible without their advice. Finally, my biggest debt is to my husband, Fritz Knorr, not only for

his constant encouragement and support during the writing of this book, but more importantly for creating all the drawings. I literally could not have produced this book without him.

I continue to welcome comments and suggestions from readers. Throughout the chapters that follow, you will notice that I chose to use the first person plural. Who are "we?" We are the author and the reader together. It is my strong hope that the reader will follow along with me when *we* consider a topic, and when *we* show that something is true. As an active participant in uncovering the working formulas of spectroscopy, readers will surely discover a few new tricks of their own. In this way, *we* make contributions to future developments in spectroscopy.

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