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Descrizione fisica	1 online resource (XVIII, 432 p. 27 illus., 21 illus. in color.)
Disciplina	500
Soggetti	Physics Astronomy Physical chemistry Atomic structure Molecular structure Chemistry, Physical and theoretical Quantum physics Chemometrics Physics and Astronomy Physical Chemistry Atomic and Molecular Structure and Properties Theoretical Chemistry Fundamental concepts and interpretations of QM Mathematical Applications in Chemistry
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Nota di contenuto	Chapter1: Concepts and Assumptions of Quantum Mechanics -- Chapter2: Dirac Notation and Principles of Quantum Mechanics -- Chapter3: Harmonic Oscillator and Vibrational Spectroscopy -- Chapter4: Multidimensional Systems and Separation of Variables -- Chapter5: Rotational States and Spectroscopy -- Chapter6: Hydrogen-like Systems and Spin Orbit States of an Electron -- Chapter7: Approximation Methods for Time Independent Schrödinger Equation -- Chapter8: Many Electron Systems and Atomic Spectroscopy -- Chapter9: Polyatomic Molecules and Molecular Spectroscopy --

Chapter10: Quantum Dynamics of Pure and Mixed States -- Chapter11: Theories for Electronic Structure Calculation of Polyatomic Molecules -- Chapter12: Special Topics.

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Sommario/riassunto

This textbook forms the basis for an advanced undergraduate or graduate level quantum chemistry course, and can also serve as a reference for researchers in physical chemistry and chemical physics. In addition to the standard core topics such as principles of quantum mechanics, vibrational and rotational states, hydrogen-like molecules, perturbation theory, variational principles, and molecular orbital theories, this book also covers essential theories of electronic structure calculation, the primary methods for calculating quantum dynamics, and major spectroscopic techniques for quantum measurement. Plus, topics that are overlooked in conventional textbooks such as path integral formulation, open system quantum dynamics methods, and Green's function approaches are addressed. This book helps readers grasp the essential quantum mechanical principles and results that serve as the foundation of modern chemistry and become knowledgeable in major methods of computational chemistry and spectroscopic experiments being conducted by present-day researchers. Dirac notation is used throughout, and right balance between comprehensiveness, rigor, and readability is achieved, ensuring that the book remains accessible while providing all the relevant details. Complete with exercises, this book is ideal for a course on quantum chemistry or as a self-study resource.

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