<<量子化学>>

图书基本信息

书名:<<量子化学>>

13位ISBN编号: 9787506272445

10位ISBN编号:750627244X

出版时间:2004-11

出版时间:北京世图

作者: Ira N. Levine

页数:739

版权说明:本站所提供下载的PDF图书仅提供预览和简介,请支持正版图书。

更多资源请访问:http://www.tushu007.com



内容概要

This book is intended for first-year graduate and advanced undergraduate courses in quantum chemistry. The expanding role of quantum chemistry makes it highly desirable for students in all areas of chemistry to understand modern methods of electronic structure calculation, and this book has been written with this goal in mind.



书籍目录

PREFACE1 THE SCHRODINGER EQUATION 1.1 Quantum Chemistry 1.2 Historical Background of Quantum Mechanics 1.3 The Uncertainty Principle 1.4 The Time-Dependent Schr6dinger Equation 1.5 The Time-Independent Schr6dinger Equation 1.6 Probability 1.7 Complex Numbers 1.8 Units 1.9 Summary2 THE PARTICLE IN A BOX 2.1 Differential Equations 2.2 Particle in a One-Dimensional Box 2.3 The Free Particle in One Dimension 2.4 Particle in a Rectangular Well 2.5 Tunneling 2.6 Summary3 OPERATORS 3.1 Operators 3.2 Eigenfunctions and Eigenvalues 3.3 Operators and Quantum Mechanics 3.4 The Three-Dimensional Many-Particle Schrodinger Equation 3.5 The Particle in a Three-Dimensional Box 3.6 Degeneracy 3.7 Average Values 3.8 Requirements for an Acceptable Wave Function 3.9 Summary4 THE HARMONIC OSCILLATOR 4.1 Power-Series Solution of Differential Equations 4.2 The One-Dimensional Harmonic Oscillator 4.3 Vibration of Molecules 4.4 Numerical Solution of the One-Dimensional Time-Independent Schrodinger Equation 4.5 Summary5 ANGULAR MOMENTUM 5.1 Simultaneous Specification of Several Properties, 5.2 Vectors 5.3 Angular Momentum of a One-Particle System 5.4 The Ladder-Operator Method for Angular Momentum 5.5 Summary 6 THE HYDROGEN ATOM 6.1 The One-Particle Central-Force Problem 6.2 Noninteracting Particles and Separation of Variables 6.3 Reduction of the Two-Particle Problem to Two One-Particle Problems, 6.4 The Two-Particle Rigid Rotor 6.5 The Hydrogen Atom 6.6 The Bound-State Hydrogen-Atom Wave Functions 6.7 Hydrogenlike Orbitals 6.8 The Zeeman Effect 6.9 Numerical Solution of the Radial Schrodinger Equation 6.10 Summary 7 THEOREMS OF QUANTUM MECHANICS 7.1 Introduction 7.2 Hermitian Operators 7.3 Expansion in Terms of Eigenfunctions 7.4 Eigenfunctions of Commuting Operators 7.5 Parity 7.6 Measurement and the Superposition of States. 7.7 Position Eigenfunctions 7.8 The Postulates of Quantum Mechanics 7.9 Measurement and the Interpretation of Quantum Mechanics 7.10 Matrices 7.11 Summary8 THE VARIATION METHOD 8.1 The Variation Theorem 8.2 Extension of the Variation Method 8.3 Determinants 8.4 Simultaneous Linear Equations 8.5 Linear Variation Functions 8.6 Matrices, Eigenvalues, and Eigenvectors 8.7 Summary9 PERTURBATION THEORY10 ELECTRON SPIN AND THE PAULI PRINCIPLE11 MANY-ELECTRON ATOMS12 MOLECULAR SYMMETRY13 ELECTRONIC STRUCTURE OF DIATOMIC MOLECULES14 THE VIRIAL THEOREM AND THE HELLMANN-FEYNMAN THEOREM15 AB INITIO AND DENSITY-FUNCTIONAL TREATMENTS OF MOLECULES 16 SEMIEMPIRICAL AND MOLECULAR-MECHANICS TREATMENTS OF MOLECULES 17 COMPARISONS OF METHODSAPPENDIXBIBLIOGRAPHYANSWERS TO SELECTED PROBLEMSINDEX

<<量子化学>>

版权说明

本站所提供下载的PDF图书仅提供预览和简介,请支持正版图书。

更多资源请访问:http://www.tushu007.com