

<<量子化学>>

图书基本信息

书名：<<量子化学>>

13位ISBN编号：9787510029547

10位ISBN编号：7510029546

出版时间：2011-1

出版时间：世界图书出版公司

作者：Iran N. Levine

页数：751

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

a solutions manual for the problems in the book is available.

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.

i have tried to make explanations clear and complete, without glossing over difficult or subtle points. derivations are given with enough detail to make them easy to follow, and i avoid resorting to the frustrating phrase "it can be shown that" wherever possible. the aim is to give students a solid understanding of the physical and mathematical aspects of quantum mechanics and molecular electronic structure. the book is designed to be useful to students in all branches of chemistry, not just future quantum chemists. however, the presentation is such that those who do go on in quantum chemistry will have a good foundation and will not be hampered by misconceptions.

an obstacle faced by many chemistry students in learning quantum mechanics is their unfamiliarity with much of the required mathematics. in this text i have included detailed treatments of operators, differential equations, simultaneous linear equations, and other needed topics. rather than putting all the mathematics in an introductory chapter or a series of appendices, i have integrated the mathematics with the physics and chemistry. immediate application of the mathematics to solving a quantum-mechanical problem will make the mathematics more meaningful to students than would separate study of the mathematics. i have also kept in mind the limited physics background of many chemistry students by reviewing topics in physics.

## 书籍目录

- preface ix
- 1 the schrodinger equation
  - 1.1 quantum chemistry,
  - 1.2 historical background of quantum mechanics,
  - 1.3 the uncertainty principle,
  - 1.4 the time-dependent schrödinger equation,
  - 1.5 the time-independent schrödinger equation,
  - 1.6 probability,
  - 1.7 complex numbers,
  - 1.8 units,
  - 1.9 calculus,
  - 1.10 summary,
- 2 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 summary,
- 3 operators
  - 3.1 operators,
  - 3.2 eigenfunctions and eigenvalues,
  - 3.3 operators and quantum mechanics,
  - 3.4 the three-dimensional, many-particle schrödinger 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 summary,
- 4 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 summary,
- 5 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,

## &lt;&lt;量子化学&gt;&gt;

- 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 summary,
- 8 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 summary,
- 9 perturbation theory
  - 9.1 introduction,
  - 9.2 nondegenerate perturbation theory,
  - 9.3 perturbation treatment of the helium-atom ground state,
  - 9.4 variation treatments of the ground state of helium,
  - 9.5 perturbation theory for a degenerate energy level,
  - 9.6 simplification of the secular equation,
  - 9.7 perturbation treatment of the first excited states of helium,
  - 9.8 comparison of the variation and perturbation methods,
  - 9.9 time-dependent perturbation theory,
  - 9.10 interaction of radiation and matter,

## &lt;&lt;量子化学&gt;&gt;

- 9.11 summary,
- 10 electron spin and the spin-statistics theorem
  - 10.1 electron spin,
  - 10.2 spin and the hydrogen atom,
  - 10.3 the spin-statistics theorem,
  - 10.4 the helium atom,
  - 10.5 the pauli exclusion principle,
  - 10.6 slater determinants,
  - 10.7 perturbation treatment of the lithium ground state,
  - 10.8 variation treatments of the lithium ground state,
  - 10.9 spin magnetic moment,
  - 10.10 ladder operators for electron spin,
  - 10.11 summary,
- 11 many-electron atoms
  - 11.1 the hartree-fock self-consistent-field method,
  - 11.2 orbitals and the periodic table,
  - 11.3 electron correlation,
  - 11.4 addition of angular momenta,
  - 11.5 angular momentum in many-electron atoms,
  - 11.6 spin-orbit interaction,
  - 11.7 the atomic hamiltonian,
  - 11.8 the condon-slater rules,
  - 11.9 summary,
- 12 molecular symmetry
  - 12.1 symmetry elements and operations,
  - 12.2 symmetry point groups,
  - 12.3 summary,
- 13 electronic structure of diatomic molecules
  - 13.1 the born-oppenheimer approximation,
  - 13.2 nuclear motion in diatomic molecules,
  - 13.3 atomic units,
  - 13.4 the hydrogen molecule ion,
  - 13.5 approximate treatments of the  $h_2$  ground electronic state,
  - 13.6 molecular orbitals for  $h_2$  excited states,
  - 13.7 mo configurations of homonuclear diatomic molecules,
  - 13.8 electronic terms of diatomic molecules,
  - 13.9 the hydrogen molecule,
  - 13.10 the valence-bond treatment of  $h_2$ ,
  - 13.11 comparison of the mo and vb theories,
  - 13.12 mo and vb wave functions for homonuclear diatomic molecules,
  - 13.13 excited states of  $h_2$ ,
  - 13.14 scf wave functions for diatomic molecules,
  - 13.15 mo treatment of heteronuclear diatomic molecules,

## &lt;&lt;量子化学&gt;&gt;

- 13.16 vb treatment of heteronuclear diatomic molecules,
- 13.17 the valence-electron approximation,
- 13.18 summary,
- 14 theorems of molecular quantum mechanics
- 14.1 electron probability density,
- 14.2 dipole moments,438
- 14.3 the hartree-fock method for molecules,
- 14.4 the virial theorem,
- 14.5 the virial theorem and chemical bonding,
- 14.6 the hellmann-feynman theorem,
- 14.7 the electrostatic theorem,
- 14.8 summary,
- 15 molecular electronicstructure
- 15.1 ab initio, density-functional, semiempirical, and molecular-mechanics methods,
- 15.2 electronic terms of polyatomic molecules,
- 15.3 the scf mo treatment of polyatomic molecules,
- 15.4 basis functions,
- 15.5 the scf mo treatment of h<sub>2</sub>O,
- 15.6 population analysis and bond orders,
- 15.7 the molecular electrostatic potential, molecular surfaces, and atomic charges,
- 15.8 localized mos,
- 15.9 the scf mo treatment of methane, ethane, and ethylene,
- 15.10 molecular geometry,
- 15.11 conformational searching,
- 15.12 molecular vibrational frequencies,
- 15.13 thermodynamic properties,
- 15.14 ab initio quantum chemistry programs,
- 15.15 performing ab initio calculations,
- 15.16 speeding up hartree-fock calculations,
- 15.17 solvent effects,
- 16 electron-correlation methods
- 16.1 configuration interaction,
- 16.2 m011er-plesset (mp) perturbation theory,
- 16.3 the coupled-cluster method,
- 16.4 density-functional theory,
- 16.5 composite methods for energy calculations,
- 16.6 the diffusion quantum monte carlo method,
- 16.7 relativistic effects,
- 16.8 valence-bond treatment of polyatomic molecules,
- 16.9 the gvb, vbscf, and bovb methods,
- 16.10 chemical reactions,
- 17 semiempirical and molecular-mechanics treatments of molecules

<<量子化学>>

17.1 semiempirical mo treatments of planar conjugated molecules,  
17.2 the hiickel mo method,  
17.3 the pariser-parr-pople method,  
17.4 general semiempirical mo and dft methods,  
17.5 the molecular-mechanics method,  
17.6 empirical and semiempirical treatments of solvent effects,  
17.7 chemical reactions,  
18 comparisons of methods  
18.1 molecular geometry,  
18.2 energy changes,  
18.3 other properties,  
18.4 hydrogen bonding,  
18.5 conclusion,  
18.6 the future of quantum chemistry,  
appendix  
bibliography  
answers to selected problems  
index

## <<量子化学>>

### 编辑推荐

《量子化学(第6版)》共18章，总共750多页，内容非常丰富。书中把量子力学的基本原理，各个不同体系中薛定谔方程及其近似解法，尤其针对化学特有的分子体系的量子力学理论与电子结构计算方法（从头算、密度函数、半经验、分子力学、价键理论）进行了详细介绍，并针对上述方法在计算基态分子性质的性能方面进行了十分详细的对比分析，对实际应用有很好的参考价值。



<<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>