

<<计算化学>>

图书基本信息

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内容概要

重要的概念（例如，分子力学，从头计算、半经验及密度泛函理论）都辅以其扼要的历史背景和顶尖科。

学家的人物介绍。

计算化学基础理论构架的阐述都配以清晰的计算实例。

2003年第1版以来直到2009年底的学科重要进展，都已纳入本版中。

增加了第1版未涉及的内容，例如，溶剂化效应，如何做CASSCF计算，过渡元素等。

每章章末附有习题，用于测试读者的理解程度。

至于较难的习题，其中有些没有直接明确解的，可到书末寻找答案。

附有大量参考文献，可以帮助读者核查所有关键论点的基础，启发深入思考。

使得《计算化学:分子和量子力学理论及应用导论(原著第2版)》不仅是教科书，还是一部极具参考价值的科学著作。

《计算化学:分子和量子力学理论及应用导论(原著第2版)》特别适合计算化学和理论化学专业的高年级本科生和研究生、科研院所和企业从事计算化学相关领域的专业人员，同时也可用于自学和指导用书。

<<计算化学>>

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书籍目录

1. An Outline of What Computational Chemistry Is All About
 - 1.1 What You Can Do with Computational Chemistry,
 - 1.2 The Tools of Computational Chemistry
 - 1.3 Putting It All Together
 - 1.4 The Philosophy of Computational Chemistry
 - 1.5 Summary
- References
- Easier Questions
- Harder Questions
2. The Concept of the Potential Energy Surface
 - 2.1 Perspective
 - 2.2 Stationary Points
 - 2.3 The Born-Oppenheimer Approximation
 - 2.4 Geometry Optimization
 - 2.5 Stationary Points and Normal-Mode Vibrations - Zero Point Energy
 - 2.6 Symmetry
 - 2.7 Summary
- References
- Easier Questions
- Harder Questions
3. Molecular Mechanics
 - 3.1 Perspective
 - 3.2 The Basic Principles of Molecular Mechanics
 - 3.2.1 Developing a Forcefield
 - 3.2.2 Parameterizing a Forcefield
 - 3.2.3 A Calculation Using Our Forcefield
 - 3.3 Examples of the Use of Molecular Mechanics
 - 3.3.1 To Obtain Reasonable Input Geometries for Lengthier (Ab Initio, Semiempirical or Density Functional) Kinds of Calculations
 - 3.3.2 To Obtain Good Geometries (and Perhaps Energies) for Small- to Medium-Sized Molecules
 - 3.3.3 To Calculate the Geometries and Energies of Very Large Molecules, Usually Polymeric Biomolecules (Proteins and Nucleic Acids)
 - 3.3.4 To Generate the Potential Energy Function Under Which Molecules Move, for Molecular Dynamics or Monte Carlo Calculations
 - 3.3.5 As a (Usually Quick) Guide to the Feasibility of, or Likely Outcome of, Reactions in Organic Synthesis
 - 3.4 Geometries Calculated by MM
 - 3.5 Frequencies and Vibrational Spectra Calculated by MM
 - 3.6 Strengths and Weaknesses of Molecular Mechanics
 - 3.6.1 Strengths
 - 3.6.2 Weaknesses

<<计算化学>>

3.7 Summary

References

Easier Questions

Harder Questions

4 Introduction to Quantum Mechanics in Computational Chemistry

4.1 Perspective

4.2 The Development of Quantum Mechanics The Schrodinger Equation

4.2.1 The Origins of Quantum Theory: Blackbody Radiation and the Photoelectric Effect

4.2.2 Radioactivity

4.2.3 Relativity

4.2.4 The Nuclear Atom

4.2.5 The Bohr Atom

4.2.6 The Wave Mechanical Atom and the Schrodinger Equation

4.3 The Application of the Schrodinger Equation to Chemistry by Huckel

4.3.1 Introduction

4.3.2 Hybridization

4.3.3 Matrices and Determinants

4.3.4 The Simple Huckel Method - Theory

4.3.5 The Simple Huckel Method - Applications

4.3.6 Strengths and Weaknesses of the Simple Huckel Method

4.3.7 The Determinant Method of Calculating the Huckel c's and Energy Levels

4.4 The Extended Huckel Method

4.4.1 Theory

4.4.2 An Illustration of the EHM: the Protonated Helium Molecule

4.4.3 The Extended Huckel Method - Applications

4.4.4 Strengths and Weaknesses of the Extended Huckel Method

4.5. Summary

References

Easier Questions

Harder Questions

5 Ab initio Calculations

5.1 Perspective

5.2 The Basic Principles of the Ab initio Method

5.2.1 Preliminaries

5.2.2 The Hartree SCF Method

5.2.3 The Hartree-Fock Equations

5.3 Basis Sets

5.3.1 Introduction

5.3.2 Gaussian Functions; Basis Set Preliminaries; Direct SCF

5.3.3 Types of Basis Sets and Their Uses

5.4 Post-Hartree-Fock Calculations: Electron Correlation

<<计算化学>>

- 5.4.1 Electron Correlation
- 5.4.2 The Moller-Plesset Approach to Electron Correlation
- 5.4.3 The Configuration Interaction Approach To Electron Correlation - The Coupled Cluster Method
- 5.5 Applications of the Ab initio Method
 - 5.5.1 Geometries
 - 5.5.2 Energies
 - 5.5.3 Frequencies and Vibrational Spectra
 - 5.5.4 Properties Arising from Electron Distribution: Dipole Moments, Charges, Bond Orders, Electrostatic Potentials, Atoms-in-Molecules (AIM)
 - 5.5.5 Miscellaneous Properties - UV and NMR Spectra, Ionization Energies, and Electron Affinities
 - 5.5.6 Visualhation
- 5.6 Strengths and Weaknesses of Ab initio Calculations
 - 5.6.1 Strengths
 - 5.6.2 Weaknesses
- 5.7 Summary
- References N
- Easier Questions
- Harder Questions
-
- 6 Semiempirical Calculations
- 7 Density Functional Calculations
- 8 Some "Special" Topics: Solvation, Singlet Diradicals, A Note on Heavy Atoms and Transition Metals
- 9 Selected Literature Highlights, Books, Websites, Software and Hardware
- Answers
- Index

章节摘录

版权页：插图：Molecular mechanics is based on a model of a molecule as a collection of balls (atoms) held together by springs (bonds) . If we know the normal spring lengths and the angles between them, and how much energy it takes to stretch and bend the springs, we can calculate the energy of a given collection of balls and springs, i.e. of a given molecule; changing the geometry until the lowest energy is found enables us to do a geometry optimization, i.e. to calculate a geometry for the molecule. Molecular mechanics is fast: a fairly large molecule like a steroid (e.g.cholesterol, C₂₇H₄₆O) can be optimized in seconds on a good personal computer.Ab Initio calculations (ab initio, Latin: "from the start", i.e. from first principles) are based on the Schrodinger equation. It is one of the fundamental equations of modern physics and describes, among other things, how the electrons in a molecule behave. The ab initio method solves the Schrodinger equation for a molecule and gives us an energy and wavefunction. The wavefunction is a mathematical function that can be used to calculate the electron distribution (and, in theory at least, anything else about the molecule) . From the electron distribution we can tell things like how polar the molecule is, and which parts of it are likely to be attacked by nucleophiles or by electrophiles.

<<计算化学>>

编辑推荐

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