

# TABLE OF CONTENTS

## Licensing

## 1: The Basic Tools of Quantum Mechanics

- 1.1: Operators
- 1.2: Wavefunctions
- 1.3: The Schrödinger Equation
- 1.4: Free-Particle Motion in Two Dimensions
- 1.5: Particles in Boxes
- 1.6: One Electron Moving About a Nucleus
- 1.7: Harmonic Vibrational Motion
- 1.8: Rotational Motion for a Rigid Diatomic Molecule
- 1.9: The Physical Relevance of Wavefunctions, Operators and Eigenvalues

## 2: Approximation Methods

- 2.1: The Variational Method
- 2.2: Perturbation Theory
- 2.E: Approximation Methods (Exercises)

## 3: Nuclear Motion

- 3.1: The Born-Oppenheimer Separation of Electronic and Nuclear Motions
- 3.2: Time Scale Separation
- 3.3: Vibration/Rotation States for Each Electronic Surface
- 3.4: Rotation and Vibration of Diatomic Molecules
- 3.5: Separation of Vibration and Rotation
- 3.6: The Rigid Rotor and Harmonic Oscillator
- 3.7: The Morse Oscillator
- 3.8: Rotation of Polyatomic Molecules
- 3.9: Rotation of Linear Molecules
- 3.E: Exercises
- 3.10: Rotation of Non-Linear Molecules
- 3.11: Chapter Summary

## 4: Atomic Orbitals

- 4.1: Shapes of Atomic Orbitals
- 4.2: Directions of Atomic Orbitals
- 4.3: Sizes and Energies

## 5: Molecular Orbitals

- 5.1: Orbital Interaction Topology
- 5.2: Orbital Symmetry
- 5.3: Linear Molecules
- 5.4: Atoms

## 6: Quantum Mechanics in Reactions

- 6.1: Reduction in Symmetry Along Reaction Paths
- 6.2: Orbital Correlation Diagrams - Origins of the Woodward-Hoffmann Rules

## 7: Further Characterization of Molecular Orbitals

- 7.1: The LCAO-MO Expansion and the Orbital-Level Schrödinger Equation
- 7.2: Determining the Effective Potential
- 7.3: The Hückel Parameterization
- 7.4: The Extended Hückel Method

## 8: Electronic Configurations

- 8.1: Orbitals Do Not Provide the Complete Picture; Their Occupancy By the N Electrons Must Be Specified
- 8.2: Even N-Electron Configurations are Not Mother Nature's True Energy States
- 8.3: Mean-Field Models
- 8.4: Configuration Interaction (CI) Describes the Correct Electronic States
- 8.5: Summary

## 9: Symmetry of Electronic Wavefunctions

- 9.1: Electronic Configurations
- 9.2: Antisymmetric Wavefunctions

## 10: Angular Momentum and Group Symmetries of Electronic Wavefunctions

- 10.1: Angular Momentum Symmetry and Strategies for Angular Momentum Coupling
- 10.2: Electron Spin Angular Momentum
- 10.3: Coupling of Angular Momenta
- 10.4: Atomic Term Symbols and Wavefunctions
- 10.5: Atomic Configuration Wavefunctions
- 10.6: Inversion Symmetry
- 10.7: Review of Atomic Cases

## 11: Evaluating the Matrix Elements of N-electron Wavefunctions

- 11.1: Configuration State Functions can Express the Full N-Electron Wavefunction
- 11.2: The Slater-Condon Rules Give Expressions for the Operator Matrix Elements Among the CSFs
- 11.3: The Slater-Condon Rules
- 11.4: Examples of Applying the Slater-Condon Rules
- 11.S: Evaluating the Matrix Elements of N-electron Wavefunctions (Summary)

## 12: Quantum Mechanical Picture of Bond Making and Breaking Reactions

- 12.1: Concepts of Configuration and State Energies
- 12.2: Mixing of Covalent and Ionic Configurations
- 12.3: Various Types of Configuration Mixing

## 13: Molecular Rotation and Vibration

- 13.1: Rotational Motions of Rigid Molecules
- 13.2: Vibrational Motion Within the Harmonic Approximation
- 13.3: Anharmonicity

## 14: Time-dependent Quantum Dynamics

- 14.1: Time-Dependent Vector Potentials
- 14.2: Time-Dependent Perturbation Theory
- 14.3: Application to Electromagnetic Perturbations
- 14.4: The "Long-Wavelength" Approximation
- 14.5: The Kinetics of Photon Absorption and Emission

## 15: Spectroscopy

- 15.1: Rotational Transitions
- 15.2: Vibration-Rotation Transitions
- 15.3: Electronic-Vibration-Rotation Transitions
- 15.4: Time Correlation Function Expressions for Transition Rates

## 16: Collisions and Scattering

- 16.1: One Dimensional Scattering
- 16.2: Multichannel Problems
- 16.3: Classical Treatment of Nuclear Motion
- 16.4: Wavepackets

## 17: Higher Order Corrections to Electronic Structure

- 17.1: Orbitals, Configurations, and the Mean-Field Potential
- 17.2: Electron Correlation Requires Moving Beyond a Mean-Field Model
- 17.3: Moving from Qualitative to Quantitative Models
- 17.4: Atomic Units

## 18: Multiconfiguration Wavefunctions

- 18.1: Optimization of the Energy for a Multiconfiguration Wavefunction
- 18.2: The Single-Determinant Wavefunction
- 18.3: The Unrestricted Hartree-Fock Spin Impurity Problem
- 18.4: Atomic Orbital Basis Sets
- 18.5: The LCAO-MO Expansion
- 18.6: The Roothaan Matrix SCF Process
- 18.7: Observations on Orbitals and Orbital Energies

## 19: Multi-Determinant Wavefunctions

- 19.1: Introduction to Multi-Determinant Wavefunctions
- 19.2: Different Methods
- 19.3: Strengths and Weaknesses of Various Methods
- 19.4: Further Details on Implementing Multiconfigurational Methods

## 20: Response Theory

- 20.1: Calculations of Properties Other Than the Energy
- 20.2: Ab Initio, Semi-Empirical, and Empirical Force Field Methods

## 21: Problem Sets

## 22: Problems

- 22.1: The Basic Tools of Quantum Mechanics
  - 22.1.1: i. Review Exercises
  - 22.1.2: ii. Exercises
  - 22.1.3: iii. Problems 1-10
  - 22.1.4: iv. Problems 11-18
  - 22.1.5: v. Review Exercise Solutions
  - 22.1.6: vi. Exercise Solutions
- 22.2: Simple Molecular Orbital Theory
  - 22.2.1: i. Review Exercises
  - 22.2.2: ii. Exercises
  - 22.2.3: iii. Problems
  - 22.2.4: iv. Review Exercises Solutions
  - 22.2.5: v. Exercise Solution
  - 22.2.6: vi. Problem Solutions
- 22.3: Electronic Configurations, Term Symbols, and States
  - 22.3.1: i. Review Exercises
  - 22.3.2: ii. Exercises
  - 22.3.3: iii. Problems
  - 22.3.4: iv. Review Exercise Solutions
  - 22.3.5: v. Exercise Solutions
  - 22.3.6: vi. Problem Solutions
- 22.4: Molecular Rotation and Vibration
  - 22.4.1: i. Exercises
  - 22.4.2: ii. Problems
  - 22.4.3: iii. Exercise Solutions
  - 22.4.4: iv. Problem Solutions
- 22.5: Time Dependent Processes
  - 22.5.1: i. Exercises
  - 22.5.2: ii. Problems
  - 22.5.3: iii. Exercise Solutions
  - 22.5.4: iv. Problem Solutions
- 22.6: More Quantitative Aspects of Electronic Structure Calculations
  - 22.6.1: i. Review Exercises
  - 22.6.2: i. Review Exercises-
  - 22.6.3: ii. Exercises
  - 22.6.4: iii. Problems
  - 22.6.5: iv. Review Exercise Solutions
  - 22.6.6: v. Exercise Solutions
  - 22.6.7: vi. Problem Solutions

[Index](#)

[Glossary](#)

[Detailed Licensing](#)