

Index

A

angular momentum

- [7.1: Introduction to Rotation](#)
- [7.4: Angular Momentum Operators and Eigenvalues](#)

Angular Momentum Eigenvalues

- [7.4: Angular Momentum Operators and Eigenvalues](#)

Angular Momentum Operator

- [7.4: Angular Momentum Operators and Eigenvalues](#)

angular momentum quantum number

- [8.2: The Wavefunctions](#)

antibonding molecular orbital

- [10.4: The Case of \$H_2^+\$](#)

atomic orbitals

- [8.2: The Wavefunctions](#)

atomic term symbols

- [8.8: Coupling of Angular Momentum and Spectroscopic Term Symbols](#)

azimuthal quantum number

- [8.2: The Wavefunctions](#)

B

basis functions

- [9.5: Single-electron Wavefunctions and Basis Functions](#)
- [10.2: The Orbital Approximation and Orbital Configurations](#)
- [10.3: Basis Functions](#)

Bohr magneton

- [8.4: Magnetic Properties and the Zeeman Effect](#)

bonding molecular orbital

- [10.4: The Case of \$H_2^+\$](#)

C

central potential

- [8.1: The Schrödinger Equation](#)

centrifugal stretching

- [7.6: Rotational Spectroscopy of Diatomic Molecules](#)

Compton effect

- [2.4: The Compton Effect](#)

configuration interaction

- [9.8: Configuration Interaction](#)
- [10.9: Correlation Energy and Configuration Interaction](#)

correlation energy

- [10.9: Correlation Energy and Configuration Interaction](#)

Coulomb integral

- [10.4: The Case of \$H_2^+\$](#)
- [10.6: Semi-Empirical Methods- Extended Hückel](#)

cyanine dyes

- [4.2: Cyanine Dyes](#)

cyclic boundary condition

- [7.3: Solving the Rigid Rotor Schrödinger Equation](#)

D

degrees of freedom

- [6.1: Spatial Degrees of Freedom, Normal Coordinates and Normal Modes](#)

E

eigenvalue

- [3.4: Operators, Eigenfunctions, Eigenvalues, and Eigenstates](#)

electron affinity

- [9.9E: Electron Affinity](#)

electron spin

- [8.5: Discovering Electron Spin](#)

electronic spectroscopy

- [8.3: Orbital Energy Levels, Selection Rules, and Spectroscopy](#)

EPR

- [8.5: Discovering Electron Spin](#)

exchange integral

- [10.4: The Case of \$H_2^+\$](#)

expectation value

- [3.8: Expectation Values](#)

Extended Hückel

- [10.6: Semi-Empirical Methods- Extended Hückel](#)

F

fine structure

- [8.8: Coupling of Angular Momentum and Spectroscopic Term Symbols](#)

force constant

- [6.2: Classical Description of the Vibration of a Diatomic Molecule](#)

free particle

- [5.1: The Free Particle](#)

G

Gaussian basis function

- [10.3: Basis Functions](#)

gross population matrix

- [10.7: Mulliken Populations](#)

H

Hamiltonian operator

- [3.4: Operators, Eigenfunctions, Eigenvalues, and Eigenstates](#)

Hermitian operators

- [4.9: Properties of Quantum Mechanical Systems](#)

Hermitian Theorem

- [4.9: Properties of Quantum Mechanical Systems](#)

Hooke's Law

- [6.2: Classical Description of the Vibration of a Diatomic Molecule](#)

hydrogen atom Schrödinger equation

- [8.2: The Wavefunctions](#)

I

ionization energy

- [9.9D: Ionization Potentials](#)

K

Koopmans' Theorem

- [9.9D: Ionization Potentials](#)

L

Laplacian operator

- [3.4: Operators, Eigenfunctions, Eigenvalues, and Eigenstates](#)

Linear Combination of Atomic Orbitals (LCAO)

- [10.4: The Case of \$H_2^+\$](#)

Linear Variational Method

- [9.5: Single-electron Wavefunctions and Basis Functions](#)
- [10.6: Semi-Empirical Methods- Extended Hückel](#)

M

Magnetic Moment

- [8.4: Magnetic Properties and the Zeeman Effect](#)

microwave spectroscopy

- [7.1: Introduction to Rotation](#)
- [7.6: Rotational Spectroscopy of Diatomic Molecules](#)

minimal basis set

- [10.6: Semi-Empirical Methods- Extended Hückel](#)

molecular rotation

- [7.1: Introduction to Rotation](#)

momentum operators

- [3.5: Momentum Operators](#)

Mulliken Populations

- [10.7: Mulliken Populations](#)

N

net population matrix

- [10.7: Mulliken Populations](#)

normal modes

- [6.1: Spatial Degrees of Freedom, Normal Coordinates and Normal Modes](#)

O

orbital approximation

- [10.2: The Orbital Approximation and Orbital Configurations](#)

orbital configurations

- [10.2: The Orbital Approximation and Orbital Configurations](#)

orbital energy eigenvalues

- [8.3: Orbital Energy Levels, Selection Rules, and Spectroscopy](#)

Orthogonality Theorem

- [4.9: Properties of Quantum Mechanical Systems](#)

overlap integral

- [5.3: Linear Combinations of Eigenfunctions](#)

P

particle in a box

- [4.3: The Particle-in-a-Box Model](#)
- [4.4: Spectroscopy of the Particle-in-a-Box Model](#)

photoelectric effect

- [2.3: Photoelectric Effect](#)

primitive Gaussian basis set

- [10.3: Basis Functions](#)

principal quantum number

- [8.2: The Wavefunctions](#)

R

radial probability density

- [8.2: The Wavefunctions](#)

reduced mass

- [6.2: Classical Description of the Vibration of a Diatomic Molecule](#)

resonance integral

- [10.6: Semi-Empirical Methods- Extended Hückel](#)

rigid rotor

- [7.3: Solving the Rigid Rotor Schrödinger Equation](#)
- [7.7: Overview of the Rigid Rotor](#)

rotational Hamiltonian

- [7.2: The Hamiltonian Operator for Rotational Motion](#)

Rotational Spectroscopy of Diatomic Molecules

- [7.6: Rotational Spectroscopy of Diatomic Molecules](#)

S

Schrödinger equation

- [3.3: Invention of the Schrödinger Equation](#)

selection rules

- [4.5: The Transition Dipole Moment and Spectroscopic Selection Rules](#)
- [4.6: Selection Rules for the Particle-in-a-Box](#)

Self Consistent Field (SCF) Method

- [10.8: The Self-Consistent Field and the Hartree-Fock Limit](#)

Separation of Variables

- [3.3: Invention of the Schrödinger Equation](#)

Slater determinant wavefunction

- [9.6: Electron Configurations, The Pauli Exclusion Principle, The Aufbau Principle, and Slater Determinants](#)

Slater Orbitals

- [9.5: Single-electron Wavefunctions and Basis Functions](#)

spontaneous emission

- [7.6: Rotational Spectroscopy of Diatomic Molecules](#)

stimulated emission

- [7.6: Rotational Spectroscopy of Diatomic Molecules](#)

superposition principle

- [5.3: Linear Combinations of Eigenfunctions](#)

T

total angular momentum

- [8.8: Coupling of Angular Momentum and Spectroscopic Term Symbols](#)

transition dipole moment

- [4.5: The Transition Dipole Moment and Spectroscopic Selection Rules](#)

transition moment integral

- [7.6: Rotational Spectroscopy of Diatomic Molecules](#)

triplet state

- [10.10: Electronic States](#)

tunneling

- [6.5: Quantum Mechanical Tunneling](#)

U

uncertainty principle

- [5.2: The Uncertainty Principle](#)

V

Variational Method

- [9.4: The Variational Method](#)

W

wave equations

- [3.2: A Classical Wave Equation](#)

wavefunction

- [3.7: Meaning of the Wavefunction](#)

Z

Zeeman effect

- [8.4: Magnetic Properties and the Zeeman Effect](#)