

# TABLE OF CONTENTS

Licensing

Preface

## 1: Systems and Variables

- 1.1: Thermodynamic Systems
- 1.2: Thermodynamic Variables

## 2: Zeroth Law of Thermodynamics

- 2.1: What is Thermodynamics?
- 2.2: The Zeroth Law of Thermodynamics
- 2.3: Calculation of Heat
- 2.4: Calculation of Work

## 3: First Law of Thermodynamics

- 3.1: Calculation of Internal Energy Changes
- 3.2: The First Law of Thermodynamics
- 3.3: Reversible and Irreversible Processes

## 4: Thermochemistry

- 4.1: Reaction Enthalpies
- 4.2: Standard Enthalpies of Formation
- 4.3: Hess's Law
- 4.4: Calculations of Enthalpies of Reaction at  $T \neq 298\text{ K}$

## 5: Thermodynamic Cycles

- 5.1: Carnot Cycle
- 5.2: Energy, Heat, and Work in the Carnot Cycle
- 5.3: Efficiency of a Carnot Cycle

## 6: Second Law of Thermodynamics

- 6.1: Entropy
- 6.2: Irreversible Cycles
- 6.3: The Second Law of Thermodynamics

## 7: Calculation of Entropy and the Third Law of Thermodynamics

- 7.1: Calculation of  $\Delta S_{\text{sys}}$
- 7.2: Calculation of  $\Delta S_{\text{surr}}$
- 7.3: Clausius Theorem
- 7.4: The Third Law of Thermodynamics

## 8: Thermodynamic Potentials

- 8.1: Fundamental Equation of Thermodynamics
- 8.2: Thermodynamic Potentials

- 8.3: Free Energies
- 8.4: Maxwell Relations

## 9: Gibbs Free Energy

- 9.1: Gibbs Equation
- 9.2: Temperature Dependence of  $\Delta G$
- 9.3: Pressure Dependence of  $\Delta G$
- 9.4: Composition Dependence of  $\Delta G$

## 10: Chemical Equilibrium

- 10.1: Reaction Quotient and Equilibrium Constant
- 10.2: Temperature Dependence of  $K_{eq}$
- 10.3: Pressure and Composition Dependence of  $K_{eq}$

## 11: Ideal and Non-Ideal Gases

- 11.1: The Ideal Gas Equation
- 11.2: Behaviors of Non-Ideal Gases
- 11.3: Critical Phenomena
- 11.4: Fugacity

## 12: Phase Equilibrium

- 12.1: Phase Stability
- 12.2: Gibbs Phase Rule
- 12.3: PT Phase Diagrams
- 12.4: The Clausius-Clapeyron Equation

## 13: Multi-Component Phase Diagrams

- 13.1: Raoult's Law and Phase Diagrams of Ideal Solutions
- 13.2: Phase Diagrams of Non-Ideal Solutions
- 13.3: Phase Diagrams of 2-Components/2-Condensed Phases Systems

## 14: Properties of Solutions

- 14.1: Activity
- 14.2: Colligative Properties

## 15: Chemical Kinetics

- 15.1: Differential and integrated rate laws
- 15.2: Complex Rate Laws
- 15.3: Experimental Methods for Determination of Reaction Orders
- 15.4: Temperature Dependence of the Rate Coefficients

## 16: The Motivation for Quantum Mechanics

- 16.1: Introduction
- 16.2: Quantum Mechanics is Bizarre
- 16.3: The Ultraviolet Catastrophe
- 16.4: The Photoelectric Effect
- 16.5: Wave-Particle Duality

## 17: Classical Mechanics

- 17.1: Newtonian Formulation
- 17.2: Lagrangian Formulation
- 17.3: Hamiltonian Mechanics

## 18: The Schrödinger Equation

- 18.1: The Time-Independent Schrödinger Equation
- 18.2: The Time-Dependent Schrödinger Equation

## 19: Analytically Soluble Models

- 19.1: The Free Particles
- 19.2: The Particle in a Box
- 19.3: The Harmonic Oscillator
- 19.4: The Rigid Rotor

## 20: The Hydrogen Atom

## 21: Operators and Mathematical Background

- 21.1: Operators in Quantum Mechanics
- 21.2: Eigenfunctions and Eigenvalues
- 21.3: Common Operators in Quantum Mechanics

## 22: Spin

- 22.1: Stern-Gerlach Experiment
- 22.2: Sequential Stern-Gerlach Experiments
- 22.3: Spin Operators

## 23: Postulates of Quantum Mechanics

- 23.1: Postulate 1- The Wave Function Postulate
- 23.2: Postulate 2- Experimental Observables
- 23.3: Postulate 3- Individual Measurements
- 23.4: Postulate 4- Expectation Values and Collapse of the Wavefunction
- 23.5: Postulate 5- Time Evolution
- 23.6: Postulate 6- Pauli Exclusion Principle

## 24: Quantum Weirdness

- 24.1: The Double-slit Experiment
- 24.2: Heisenberg's Uncertainty Principle
- 24.3: Tunneling

## 25: Many-Electron Atoms

- 25.1: Many-Electron Wave Functions
- 25.2: Approximated Hamiltonians

## 26: Introduction to Molecules

- 26.1: The Molecular Hamiltonian
- 26.2: The Born-Oppenheimer Approximation

- [26.3: Solving the Electronic Eigenvalue Problem](#)

## [27: The Chemical Bond in Diatomic Molecules](#)

- [27.1: The Chemical Bond in the Hydrogen Molecular Cation](#)
- [27.2: The Chemical Bond in the Hydrogen Molecule](#)

## [28: The Chemical Bond in Polyatomic Molecules](#)

- [28.1: The Chemical Bond in the Water Molecule Using a Minimal Basis](#)
- [28.2: Hartree-Fock Calculation for Water](#)
- [28.3: Shapes and Energies of Molecular Orbitals](#)

## [29: Spectroscopy](#)

- [29.1: Rotational Spectroscopy](#)
- [29.2: Vibrational Spectroscopy](#)
- [29.3: Electronic Spectroscopy](#)

## [30: Appendix](#)

- [30.1: Thermodynamic Data of Inorganic Substances at 298 K](#)
- [30.2: Thermodynamic Data of Organic Substances at 298 K](#)

[Index](#)

[Glossary](#)

[Detailed Licensing](#)