

Physical Chemistry

SC CHEM 3010.40 – Winter Term

OUTLINE

Four “Units”

1. QUANTUM THEORY
2. ATOMIC AND MOLECULAR SPECTRA AND STRUCTURE
3. ROTATIONAL, VIBRATIONAL, ELECTRONIC SPECTRA
4. STATISTICAL THERMODYNAMICS

Text

Physical Chemistry, P.W. Atkins, 6th (or 7th) Edition,
Publisher, W.H. Freeman.

Unit One

QUANTUM MECHANICS

- The failures of classical physics
- Wave particle duality
- The Schrödinger Equations
- Born interpretation of ψ
- The information in the wave function
- The uncertainty principle
- ψ for translational motion in 1 & 2D

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- Particle tunnelling
- ψ for rotation in 2D and 3D
- Spin

Atkins, Chapters 11, 12

Unit 2

(a) Atomic Structure and Spectra

- Structure of hydrogenic atoms
- Atomic orbitals and their energies
- Spectroscopic transitions
- Structure of many-electron atoms
- Self consistent field orbitals
- Singlet & triplet states
- Spin-orbit coupling
- Term symbols and selection rules

(b) Molecular structure

- Born-Oppenheimer approximation
- Valence bond theory
- Molecular orbital theory

Atkins, Chapters 13, 14

Unit 3 (a)

Molecular spectroscopy

- Pure rotational spectra
- Rotational energy levels
- Rotational transitions
- Rotation Raman spectra
- Vibrations of diatomics
- Selection rules
- Anharmonicity
- Vibration – rotation spectra and Raman spectra
- (Polyatomics?)

Unit 3 (b)

Electronically excited states

- Fluorescence & phosphorescence
- Dissociation & predissociation

Lasers

- General principles
- Practical lasers
- Applications in Chemistry

Photoelectrons spectroscopy

- UV – PES
- Xray – PES

Atkins, Chapters 16, 17 and additional material

Unit 4 (a)

Statistical Thermodynamics

Concepts:

Distribution of molecular states

- Configurations and weights
- The Molecular Partition Function

The internal energy and the Entropy

- Internal energy
- Statistical entropy

The Canonical Partition Function

- Canonical ensemble
- Thermodynamic information in the part function
- Independent molecules

Atkins, Chapter 19

Unit 4 (b)

Using statistical thermodynamics

- The thermodynamic functions
- Evaluating Q from spectroscopic data

Mean energies

Heat capacities

Equations of state

Residual entropies

Equilibrium constants

Atkins, Chapter 20