

Keywords:

Amino acids, peptides, proteins, solid phase peptide synthesis, Killiani-Fischer synthesis, Amadori rearrangement, Lobry de Bruyn van Ekenstein rearrangement, Krebs cycle, Glycolysis, Enzymes, Inhibitors.

Course Code: CHEMISTRY - CXII: PHYSICAL CHEMISTRY-V

Course Title: Quantum Chemistry & Spectroscopy

Total Credits: 06

(Credits: Theory-04, Practical-02)

(Total Lectures: Theory- 60, Practical-60)

Objectives:

The aim of this course is to make students understand the limitations of classical mechanics and the need of quantum chemistry, familiarize them with postulates of quantum chemistry and apply the same to derive equations for various models and hydrogen atoms. Understand the basis of molecular spectroscopy and its applications.

Learning Outcomes:

By the end of this course, students will be able to:

- Learn about limitations of classical mechanics and solution in terms of quantum mechanics for atomic/molecular systems.
- Develop an understanding of quantum mechanical operators, quantization, probability distribution, uncertainty principle and application of quantization to spectroscopy.
- Interpret various types of spectra and know about their application in structure elucidation

Unit 1:

Quantum Chemistry: Postulates of quantum mechanics, quantum mechanical operators and commutation rules, Schrödinger equation and its application to free particle and particle in a box (rigorous treatment), quantization of energy levels, zero-point energy and Heisenberg Uncertainty principle; wave functions, probability distribution functions, nodal properties, Extension to two and three dimensional boxes, separation of variables, degeneracy.

Qualitative treatment of simple harmonic oscillator model of vibrational motion: Setting up of Schrödinger equation and discussion of solution and wave functions. Vibrational energy of diatomic molecules and zero-point energy.

Angular momentum. Rigid rotator model of rotation of diatomic molecule. Schrödinger equation in Cartesian and spherical polar coordinates (derivation not required). Separation of variables. Spherical harmonics. Discussion of solution (Qualitative).

(Lectures: 22)

Unit 2:

Qualitative treatment of hydrogen atom and hydrogen-like ions: setting up of Schrödinger equation in spherical polar coordinates, radial part and quantization of energy (only final energy expression). Average and most probable distances of electron from nucleus. Setting up of Schrödinger equation for many-electron atoms (He, Li). Need for approximation methods. Statement of variation theorem and application to simple systems (particle-in-a-box, harmonic oscillator, hydrogen atom).

(Lectures: 8)

Unit 3:

Molecular Spectroscopy: Interaction of electromagnetic radiation with molecules and various types of spectra; Born Oppenheimer approximation.

Rotation spectroscopy: Selection rules, intensities of spectral lines, determination of bond lengths of diatomic and linear triatomic molecules, isotopic substitution.

Vibrational spectroscopy: Classical equation of vibration, computation of force constant, amplitude of diatomic molecular vibrations, anharmonicity, Morse potential, dissociation energies, fundamental frequencies, overtones, hot bands, degrees of freedom for polyatomic molecules, modes of vibration, concept of group frequencies.

Vibration-rotation spectroscopy: diatomic vibrating rotator, P, Q, R branches.

Raman spectroscopy: Qualitative treatment of Rotational Raman effect; Vibrational Raman spectra, Stokes and anti-Stokes lines; their intensity difference, rule of mutual exclusion.

Electronic spectroscopy: Franck-Condon principle, electronic transitions, singlet and triplet states, fluorescence and phosphorescence, dissociation and predissociation, calculation of electronic transitions of polyenes using free electron model.

Nuclear Magnetic Resonance (NMR) spectroscopy: Principles of NMR spectroscopy, Larmor precession, chemical shift and low resolution spectra, different scales (δ and τ), spin-spin coupling and high resolution spectra, interpretation of PMR spectra of simple organic molecules like methanol, ethanol, acetaldehyde, acetic acid and aromatic proton.

(Lectures:30)

Practical:

(Credits: 2, Laboratory periods: 60)

Colorimetry:

1. Verify Lambert-Beer's law and determine the concentration of $\text{CuSO}_4/\text{KMnO}_4/\text{K}_2\text{Cr}_2\text{O}_7$ in a solution of unknown concentration.
2. Determine the concentrations of KMnO_4 and $\text{K}_2\text{Cr}_2\text{O}_7$ in a mixture.
3. Study the kinetics of iodination of propanone in acidic medium.

4. Determine the amount of iron present in a sample using 1, 10-phenanthroline.
5. Determine the dissociation constant of an indicator (phenolphthalein).
6. Study the kinetics of interaction of crystal violet/ phenolphthalein with sodium hydroxide.

Spectrophotometry:

1. Study the 200-500 nm absorbance spectra of KMnO_4 and $\text{K}_2\text{Cr}_2\text{O}_7$ (in 0.1 M H_2SO_4) and determine the λ_{max} values. Calculate the energies of the two transitions in different units (kJ molecule^{-1} , kJ mol^{-1} , cm^{-1} , eV).
2. Study the pH-dependence of the UV-Vis spectrum (200-500 nm) of $\text{K}_2\text{Cr}_2\text{O}_7$.
3. Record the 200-350 nm UV spectra of the given compounds (acetone, acetaldehyde, 2-propanol, acetic acid) in water. Comment on the effect of structure on the UV spectra of organic compounds.
4. Analysis of the given vibration-rotation spectrum of HCl (g)

References:

Theory:

1. Banwell, C.N.; McCash, E.M.(2006), **Fundamentals of Molecular Spectroscopy**, Tata McGraw-Hill.
2. Kapoor, K.L.(2015), **A Textbook of Physical Chemistry**, McGraw Hill Education, ,Vol 4, 5th Edition, McGraw Hill Education.
3. House, J.E.(2004), **Fundamentals of Quantum Chemistry**, 2nd Edition, Elsevier.
4. McQuarrie, D.A.(2016), **Quantum Chemistry**, Viva Books.
5. Chandra, A. K.(2001), **Introductory Quantum Chemistry**, Tata McGraw-Hill.
6. Kakkar, R. (2015), **Atomic & Molecular Spectroscopy**, Cambridge University Press.

Practical:

1. Khosla, B.D.; Garg, V.C.; Gulati, A. (2015), **Senior Practical Physical Chemistry**, R. Chand & Co, New Delhi.
2. Kapoor, K.L. (2019), **A Textbook of Physical Chemistry**, Vol.7, 1st Edition, McGraw Hill Education.
3. Garland, C. W.; Nibler, J. W.; Shoemaker, D. P.(2003), **Experiments in Physical Chemistry**, 8th Edition, McGraw-Hill, New York.

Additional Resources:

1. Engel, T.; Reid, P.(2013), **Quantum Chemistry and Spectroscopy**, Pearson.
2. Atkins, P.W.; Friedman, R. (2010), **Molecular Quantum Mechanics**, 5th Edition, Oxford University Press.

Teaching Learning Process:

- Teaching Learning Process for the course is visualized as largely student-focused.
- Transaction through an intelligent mix of conventional and modern methods.

- Engaging students in cooperative learning.
- Learning through quiz design.
- Problem solving to enhance comprehension.

Assessment Methods:

Students' evaluation will be done on the basis of regular class test, presentations and assignments as a part of internal assessment during the course as per the curriculum. End semester university examination will be held for both theory and practical. In practical, assessment will be done based on continuous evaluation, performance in the experiment on the date of examination and viva voce.

Keywords:

Quantum mechanics, Operators, Schrodinger equation, Hydrogen like atoms, Approximation methods, Spectroscopy, Franck-Codon principle, Raman effect.

SEMESTER VI

Course Code: CHEMISTRY - CXIII: INORGANIC CHEMISTRY - IV

Course Title: Organometallic Chemistry & Bio-inorganic Chemistry

Total Credits: 06

(Credits: Theory-04, Practical-02)

(Total Lectures: Theory- 60, Practical-60)

Objectives:

The course introduces some important topics of Inorganic Chemistry in a compact way. Unit 1 of the course introduces students to the basic principles of qualitative inorganic analysis. The influence of solubility products and the common ion effect on the separation of cations is made clear. Interfering anions are identified and their removal is studied. Unit 2, an introduction to the very important area of organometallic chemistry including classification of organometallic compounds, the concept of hapticity and the 18-electron rule governing the stability of a wide variety of organometallic species. Specific organometallic compounds are studied in detail to further understand the basic concepts: metal carbonyls, metal alkyls, Zeise's salt and ferrocene. Unit 4 takes this a step further by covering catalysis, an important application of organometallic compounds. Under Unit 3, bioinorganic chemistry, the student learns the importance of inorganic chemical species, especially metals, in biological systems, through discussions on metal-containing enzymes, the sodium-potassium pump and the applications of iron in physiology, including iron transport and storage system.

Learning Outcomes:

By the end of the course, the students will be able to:

- Understand and explain the basic principles of qualitative inorganic analysis