11.1.17. Course Code: DSC17: CHEMISTRY6 (C6)

Course Title: QUANTUM CHEMISTRY AND SPECTROSCOPY

Total Credits: 04 **(Credits: Theory-02, Practical-02)**

(Total Lectures: Theory- 30, Practical-60)

Objectives: The objective of this course is to introduce the students to the concepts and methodology of quantum mechanics, its applications to spectroscopy and establish the relation between structure determination and spectra.

Learning Outcomes:

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

- Understand basic principles of quantum mechanics: operators, eigen values, averages, probability distributions.
- Understand and use basic concepts of microwave, IR and UV-VIS spectroscopy for interpretation of spectra.
- Explain Lambert-Beer's law, quantum efficiency and photochemical processes.

Unit 1: Quantum Chemistry

Postulates of quantum mechanics, quantum mechanical operators.

Free particle. Particle in a 1-D box (complete solution), quantization, normalization of wave functions, concept of zero-point energy.

Schrodinger equation and its application to free particle and particle in a 1D box

Qualitative treatment of H and H like atoms. Setting up of Schrodinger equation for many electron atoms.

Rotational Motion: Schrödinger equation of a rigid rotator and brief discussion of its results (solution not required). Quantization of rotational energy levels.

Vibrational Motion: Schrödinger equation of a linear harmonic oscillator and brief discussion of its results (solution not required). Quantization of vibrational energy levels.

(Lectures: 12)

Unit 2: Spectroscopy

Spectroscopy and its importance in chemistry. Wave-particle duality. Link between spectroscopy and quantum chemistry. Electromagnetic radiation and its interaction with matter.

Types of spectroscopy. Difference between atomic and molecular spectra. Born- Oppenheimer approximation: Separation of molecular energies into translational, rotational, vibrational and electronic components.

Microwave (pure rotational) spectra of diatomic molecules. Selection rules. Structural information derived from rotational spectroscopy.

IR Spectroscopy: Selection rules, IR spectra of diatomic molecules. Structural information derived from vibrational spectra. Vibrations of polyatomic molecules. Group frequencies. Effect of hydrogen bonding (inter- and intramolecular) and substitution on vibrational frequencies.

Electronic Spectroscopy: Electronic excited states. Free electron model and its application to electronic spectra of polyenes. Colour and constitution, chromophores, auxochromes, bathochromic and hypsochromic shifts.

(Lectures: 12)

Unit 3: Photochemistry

Laws of photochemistry. Lambert-Beer's law. Fluorescence and phosphorescence. Quantum efficiency and reasons for high and low quantum yields. Primary and secondary processes in photochemical reactions. Photochemical and thermal reactions. Photoelectric cells.

(Lectures: 6)

PRACTICALS (Credits:02, Laboratory Periods: 60)

1. Study the 200-500 nm absorbance spectra of $KMnO_4$ and K_2Cr2O_7 (in 0.1 M H_2SO_4) and determine the λ_{max} values. Calculate the energies of the two transitions in different units (J molecule^{-1}, kJ mol^{-1}, cm^{-1}, eV).
2. Study the pH-dependence of the UV-Vis spectrum (200-500 nm) of $K_2Cr_2O_7$ (*Use solutions of different pH*)

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. Verify Lambert-Beer's law and determine the concentration of $K_2Cr_2O_7$ in a solution of unknown concentration.
5. Determine the concentrations of $KMnO_4$ and $K_2Cr_2O_7$ in a mixture.
6. Study the kinetics of iodination of propanone in acidic medium.
7. Determine the dissociation constant of an indicator (phenolphthalein).
8. Study the kinetics of interaction of phenolphthalein with sodium hydroxide.
9. Study the kinetics of interaction of crystal violet with sodium hydroxide.

REFERENCES:

Theory

- Banwell, C.N.; McCash, E.M.(2006), Fundamentals of Molecular Spectroscopy, Tata McGraw- Hill.
- Kapoor, K.L.(2015),A Textbook of Physical Chemistry, McGraw Hill Education, ,Vol 4, 5th Edition, McGraw Hill Education.
- McQuarrie, D.A.(2016),Quantum Chemistry, Viva Books.
- Chandra, A. K.(2001),Introductory Quantum Chemistry, Tata McGraw-Hill.

Practical:

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

Additional Resources:

- Castellan, G. W .(2004),Physical Chemistry, Narosa.
- Petrucci, R. H.(1989),General Chemistry: Principles and Applications, Macmillan Publishing

Teaching Learning Process:

- Conventional chalk and board teaching,
- Class interactions and discussions
- Power point presentation on important topics.

Assessment Methods:

- Class Tests at Periodic Intervals.
- Written assignment (s) / Presentation by individual students
- End semester University Theory and Practical Examination

Keywords: Quantisation, Selection rules, Schrodinger equation, Operator, Spectrum, Quantum efficiency.