DISCIPLINE SPECIFIC ELECTIVE COURSE CHEM-DSE -6 Quantum Chemistry and Spectroscopy

CREDIT DISTRIBUTION, ELIGIBILITY AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical/ Practice		
Chem-DSE 6: Quantum Chemistry and Spectroscopy	04	02	--	02	Class 12th with Physics, Chemistry, Mathematics	NA

Learning Objectives

The Learning Objectives of this course are as follows:

- To introduce the concepts and methodology of quantum mechanics
- Application of Quantum chemistry to spectroscopy
- To establish the relation between structure determination and spectra.

Learning outcomes

By studying 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.

Syllabus

Unit 1: Quantum Chemistry **(Hours: 16)**

Postulates of quantum mechanics, quantum mechanical operators.

Schrodinger equation and its application to free particle and particle in a 1-D box (complete solution),quantization, normalization of wave functions, concept of zero-point energy.

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.

Unit 2: Spectroscopy (Hours: 14)

Electromagnetic radiation and its interaction with matter. Lambert-Beer's law, Jablonski's diagram. Florescence and Phosphorescence.
Difference between atomic and molecular spectra. Born- Oppenheimer approximation: Separation of molecular energies into translational, rotational, vibrational and electronic components.

Microwave Spectroscopy: 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 fromvibrational spectra. Effect of hydrogen bonding (inter- and intramolecular) and substitution on vibrational frequencies.

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

Practical component Credits:02

(Laboratory periods: 60)

UV/Visible spectroscopy

10. Study the 200-500 nm absorbance spectra of $KMnO_4$ and $K_2Cr_2O_7$ (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).
11. Study the pH-dependence of the UV-Vis spectrum (200-500 nm) of $K_2Cr_2O_7$
12. 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.

Colorimetry

13. Verify Lambert-Beer's law and determine the concentration of $CuSO_4$/ $KMnO_4$/ $K_2Cr_2O_7$/ $CoCl_2$ in a solution of unknown concentration
14. Determine the concentrations of $KMnO_4$ and $K_2Cr_2O_7$ in a mixture.
15. Study the kinetics of iodination of propanone in acidic medium.
16. Determine the amount of iron present in a sample using 1, 10-phenanthroline.
17. Determine the dissociation constant of an indicator (phenolphthalein).
18. Study the kinetics of interaction of crystal violet/ phenolphthalein with sodium hydroxide.

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. McQuarrie, D.A.(2016),**Quantum Chemistry**, Viva Books.
4. Chandra, A. K.(2001),**Introductory Quantum Chemistry**, Tata McGraw-Hill.
5. Dua A and Tyagi P, **Molecular Spectroscopy: Quantum to Spectrum**, (2022) Atlantic Publishers & Distributors Pvt Ltd.
6. Dua A, Singh C, **Quantum Chemistry: Classical to Computational** (2015) ManakinPress.

Practical:

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

Additional Resources:

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

Note: Examination scheme and mode shall be as prescribed by the Examination Branch, University of Delhi, from time to time.