P.B.SIDDHARTHA COLLEGE OF ARTS & SCIENCE
DEPARTMENT OF CHEMISTRY
M.Sc – CHEMISTRY (ORGANIC CHEMISTRY)

II SEMESTER
W.E.F 2022-23 (R22 Regulations)

Title of the Paper: MOLECULAR SPECTROSCOPY

Course Code	**22CH2E1**	Course Delivery Method	Class Room / Blended Mode - Both
Credits	**4**	CIA Marks	30
No. of Lecture Hours / Week	**4**	Semester End Exam Marks	70
Total Number of Lecture Hours	**60**	Total Marks	100
Year of Introduction:2017-2018	Year of Offering:	Year of Revision:----	Percentage of Revision: 20 %

S.No	COURSE OUTCOMES	PO`S
	After the completion of the course, Students will be able to	
1	Memorize the basic principles and theory involved in molecular absorption spectroscopy.	2,7
2	Comprehend the advanced concepts of molecular absorption spectroscopy.	1,2,5
3	Apply the knowledge of spectroscopy in calculating the bond length, identifying the functional group present in molecules.	1,5,6
4	Identify the role UV – visible spectroscopy in the determination of absorption maximum and ESR spectroscopy in studying the properties of paramagnetic substances.	1,3,4

Syllabus

Unit	Learning Units	Lecture Hours
I	**Introduction to Molecular Spectroscopy:** Motion of molecules-Degrees of freedom – Energy associated with the degrees of freedom-Type of spectra**.** **Microwave spectroscopy**: Classification of molecules, rigid rotator model, effect of isotopic substitution on the transition frequencies, Intensities non-rigid rotator-Microwave spectra of polyatomic molecules.	12
II	**Infrared spectroscopy:** Harmonic oscillator, vibrational energies of diatomic molecules, zero point energy, force constant and bond strengths, anhormonicity Morse potential energy diagram. Vibration – rotation spectroscopy. PQR braches, Born – oppenheimer approximation, Break down Born – openheimer approximation, normal modes of vibration group frequencies, overtones, hot bands, application of IR spectra to polyatomic molecules.	12
III	**Raman Spectroscopy:** Classical and quantum theories of Raman effects, pure rotational, vibrational and Vibrational- rotational Raman spectra, selection rules, mutual exclusion principle, Resonance Raman spectroscopy, coherent antistrokes Raman Spectroscopy (CARS).	12

IV	**UV- Visible Spectroscopy:** Electronic Spectra of diatomic molecules, vibrational structure of an electronic transition, classification of bands, rotational fine structure of electronic vibrational transition. Electronic Spectra of Polyatomic Molecules.	12
V	**Electron Spin Resonance Spectroscopy:** Basic Principles, zero field splitting and kranners's degeneracy, factors affecting the 'g' value. Istropic and anisotropic hyperfine coupling constants, spin hamiltenia, spin densities measurement techniques - simple applications like methyl radical, ethyl radical etc.,	12

Text books/ Reference books:

1. Introduction to Spectroscopy – D. L. Pavia, G.M. Lampman, G. S. Kriz, 3rd Ed. (Harcourt college publishers).

2. Absorption spectroscopy of organic molecules – V. M. Parikh

3. Nuclear Magnetic Resonance – Basic Principles- Atta-Ur-Rehman, Springer-Verlag (1986).

4. Molecular spectroscopy by Kalidas & B.K.Sharma

5. Vibrational Spectroscopy by D.N.Sathyanarayana New Age Int. Pub.

6. Spectroscopy by Aruldas.

7. Symmetry & Spectroscopy of molecules by K.Veerareddy

M.Sc. DEGREE EXAMINATION
SECOND SEMESTER
Course Code : 22CH2 E1

Elective Paper- :: Molecular Spectroscopy

Time: 3 hours **Maximum Marks: 70**

SECTION – A **(5x4M=20M)**

1 (a). Write a short note on Degrees of Freedom of a rigid body (CO-2, L-2)

(Or)

(b). Explain the effect of Isotopic substitution on the transition frequencies. (CO-2, L-2)

2 (a).Define Zero point Energy and force constant. (CO-1, L-1)

(Or)

(b).Elaborate the importance of Morse Potential in vibration spectroscopy. (CO-1, L-1)

3 (a). State the Mutual Exclusion Principle (CO-2, L-2)

(Or)

(b). Write note on Classical theory of Raman effect. (CO-2, L-2)

4(a). Discuss electronic Spectra of Diatomic molecules. (CO-2, L-2)

(Or)

(b). Explain the classification of bands in Electronic spectroscopy. (CO-2, L-2)

5(a). Give a short account of Krammers degenracy. (CO-2, L-2)

(Or)

(b).Deliberate the spin Hamiltonian in ESR spectroscopy. (CO-2, L-2)

SECTION – B **(5x10M=50M)**

UNIT - I

6.(a) Describe the Non-rigid rotator of rotational spectrum. (CO-2, L-2)

(Or)

(b) Discuss the Microwave spectra of polyatomic molecules . (CO-2, L-2)

UNIT – II

7.(a) Elucidate the importance of Born-oppenheimer approximation in vibrational spectroscopy. (CO-2, L-2)

(Or)

(b) Explain PQR Branches, Overtones and Hot bands in IR spectroscopy. (CO-2, L-2)

UNIT – III

8.(a) Explain the CARS. (CO-2, L-2)

(Or)

(b) Write about Resonance Raman spectroscopy. (CO-3, L-3)

UNIT - IV

9.(a) Discuss in detail Electronic spectra of ployatomic molecules. (CO-3, L-3)

(Or)

(b) Write a note on electronic transtitions and electronic spectra of diatomic molecules.(CO-2, L-2)

UNIT - V

10.(a) Discuss in detail hyper fine splitting in methyl and ethyl radicals . (CO-2, L-2)

(Or)

(b) Describe the factors affecting the ‘g’ value in ESR spectroscopy. (CO-2, L-2)

******