GAYATRI VIDYA PARISHAD
COLLEGE FOR DEGREE AND PG COURSES (AUTONOMOUS)
Affiliated to Andhra University || Accredited by NAAC and NBA
VISAKHAPATNAM

DEPARTMENT OF ORGANIC CHEMISTRY

M.Sc. (PREVIOUS) CHEMISTRY SYLLABUS
SEMESTER-I
PAPER-I: GENERAL CHEMISTRY-I
(Effective from the admitted batch of 2022-2023)

Credits: 4		Theory: 4 Hours
Max Marks: 100	External: 80	Internal: 20

Course Outcomes (COs)/Course Specific Outcomes (CSOs):
Upon completion of the course the students will be able to:

CO 1: Learn and understand the selection rules and criteria for molecules to exhibit rotational and IR spectroscopy.

CO 2: Understand the Classical and quantum mechanical theories of Raman spectroscopy and basic concepts of electronic spectroscopy.

CO 3: Learn spectroscopic methods based on magnetic resonance principles.

CO 4: Learn basics of group theory and its application in chemistry.

CO 5: Understand the basic concepts of FORTRAN programming and its applications.

Course learning outcome (LOs):
Upon completion of the course the student will be able

LO 1: To apply the spectroscopic methods for structure elucidation of molecules.

LO 2: To apply the spectroscopic methods for structure elucidation of molecules.

LO 3: To acquire knowledge of molecular symmetry and group theory and to solve chemical problems.

LO 4: To determine the group multiplication tables for C2V and C3V point groups.

LO 5: To write FORTRAN programs for simple chemical problems

UNIT – I **[12 Hours]**
Rotational spectra of diatomic molecules-rigid rotor-selection rules-calculation of bond length- isotopic effect, second order stark effect and its applications.
Infrared spectra of diatomic molecules-harmonic and anharmonic oscillators. Selection rules-overtones-combination bands calculation of force constant, anharmonicity constant and zero-point energy, Fermi resonance.
Simultaneous vibration rotation spectra of diatomic molecules.

UNIT-II **[12 Hours]**
Raman effect-classical and quantum mechanical explanations-rotational Raman and vibrational Raman spectra.
Electronic spectra aff diatomic molecules-vibrational coarse structure-intensity of spectral lines-Franck Condon principle-applications, Rotational fine structure-band head and band shading, Charge transfer spectra.

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UNIT-III   **[12 Hours]**

Spin Resonance Spectroscopy: Principle and theory of NMR spectroscopy-Chemical shift and its origin. Spin-Spin interaction. Application of NMR to structural elucidation-Structure of ethanol, dimethylformamide, styrene and acetophenone.

Principle and theory of ESR-g-factor, hyperfine interactions-applications of ESR studies to the structure of free radicals.

UNIT-IV   **[12 Hours]**

Basic concepts of Symmetry and Group theory – Symmetry elements, symmetry operations and point groups – Schoenflies symbols – Classification of molecules into point groups.

Axioms of Group theory – Group multiplication tables for C2V and C3V point groups –Similarity Transformation and classes – Representations – reducible and irreducible representations, Mulliken symbols, Orthogonality theorem and its implications.

UNIT-V [12 Hours]

Microsoft Fortran: constants, variables and operators, arithmetic expressions, assignment and replacement statements, Input and Output statements – Format free and Format directed I/O statements – Iw, Fw.d, Ew.d and Gw.d format specifications, conditional and unconditional statements – Logical IF, Block IF and Go To statements, Do statement – syntax and rules.

Application of Chemical Problems:

Flowcharts and Programs for

1. Statistical Analysis calculation of arithmetic mean, mean deviation, variance and standard deviation of replicate measurements.

2. Calculation of the pH and hydrogen ion concentration of an aqueous solution of a strong acid considering the auto ionization of water.

3. Calculation of the rate constant of a first order reaction.

4. Calculation of molar extinction coefficient using Beer-Lambert's Law by Linear least-squares method.

Text Books:

1. Symmetry and Spectroscopy of Molecules, K Veera Reddy, New Age International Publishers.

2. Physical Chemistry by Peter Atkins and Julio de Paula, Oxford University Press.

3. Chemical Applications of Group Theory, F. A. Cotton Wiley Eastern Limited New Delhi.

4. Group Theory and its Applications to Chemistry, K. V. Raman, Tata McGraw – Hill Publishing Company Ltd., New Delhi.

5. Computer programming in Fortran-IV by V .Rajaraman, Prentice-Hall of India Pvt. Ltd., New Delhi.

6. Molecular Spectroscopy, - Gordon M. barrow

7. Fundamentals of Molecular Spectroscopy – Banwell.

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