Solution of SWE for simple systems-particle in a box (1D & 3D), particle in a ring, simple harmonic oscillator, rigid rotor, the H atom (solution of r,θ,Φ equations). Chemical Bonding in diatomics: Covalent bond-Valence bond and molecular orbital approaches with comparison.

Molecular orbital theory applied to homonuclear and heteronuclear diatomic molecules. Introduction to Huckel molecular orbital theory of conjugated systems and its applications.

8hrs

REFERENCES:

1.Thermodynamics for Chemists- S Glasstone(East West press)
2.Physical Chemistry-P W Atkins.
3.Chemical Themodynamics, Rajaram and Kuriokose (East-West)Pearson, Chennai, 2013.
4. Thermodynamics, 3rd Ed., R.C. Srivastava and Subit K Saha (Prentice-Hall of India, Delhi), 2007.
5. Statistical Thermodynamics, M. C. Gupta (New ge International, Delhi)2007.
6.Principles of Physical chemistry; B.R.Puri, L.R.Sharma and M.S.Pathania, Vishal Publishers(2014)
7.Atomic Structure and Chemical Bond , Manasa Chanda, Tata McGraw Hill Publishers(1991).
8.Quantum Chemistry, R.K.Prasad, New Age International (1991)
9.Advanced Physical Chemistry- Gurdeep R Chatwal (Goel Publishes, Meerut), 1992.
10.Introductory Quantum Chemistry – A.K.Chandra (Tata McGraw Hill) 1994.
11.Quantum Chemistry, A.B.Sannigrahi (Book and Allied Pvt.Ltd., Kolkatt), 2013.
12.Quantum Chemistry, Donald A.P (Viva Books, Delhi), 2013.

CH S 454: ORGANIC SPECTROSCOPIC TECHNIQUES

COURSE OUTCOME:

- Enable the students to understand the principle, theory, instrumentation and applications of UV-Visible, Electronic, NMR (^{1}H, ^{13}C, ^{19}F, ^{31}P) and Mass spectroscopy.
- To solve the composite problems involving the applications of UV-Visible, IR, NMR (^{1}H &^{13}C) and Mass spectroscopic techniques.
- To develop the ability to analyse the spectrum and arrive at the correct structure of compound.
- Overall students can get confidence in solving spectroscopic problems.

UNIT–I: **[12 hours]**

UV/Electronic Spectroscopy: Basic principles, Chromophores, auxochromes, Instrumentation and application. Factors affecting the positions of UV bands. Electronic transitions and empirical correlations of predicting λ_{max} of organic compounds. Woodward–Fieser rules. UV absorption of
aromatic compounds - effect of substituents and solvent effects. Emperical rules to calculate $\lambda_{max.}$ Application of UV spectroscopy in the structural study of organic molecules.5 hrs

IR Spectroscopy: Basic principles, Application of infrared spectroscopy in the structural study-identity by finger printing and identification of functional groups. Characteristic vibrational frequencies of common functional groups (alkanes, alkenes, alkynes, aromatic compounds, alcohols, ethers, phenols and amines). Study of vibrational frequencies of carbonyl

compounds (ketones, aldehydes, esters, amides, anhydrides and acids). Factors affecting band positions and intensities such as effect of hydrogen bonding, phase and solvent on vibrational frequencies, overtones, combination bands and Fermi resonance. 7 hr

UNIT-II: Nuclear Magnetic Resonance Spectroscopy **[12 hours]**

Theory and principle, NMR spectrometer, FT NMR and its advantages. Solvents used, chemical shift and its measurements, factors affecting chemical shift. Integration of NMR signals, spin-spin coupling, coupling constant. Shielding and deshielding. Chemical shift assignment of major functional groups, Classification (ABX, AMX, ABC, A_2B_2), spin decoupling, effects of chemical exchange, fluxional molecules, Hindered rotation through NMR spectrum, Karplus relationships (Karplus curve–variation of coupling constant with dihedral angle), double resonance techniques, NMR shift reagents, solvent effects and Nulear Overhauser Effect. High resolution ^{1}H NMR. Applications of NMR spectroscopy in structure elucidation of simple organic and inorganic molecules. Pulse techniques in NMR, two dimensional and solid state NMR. Use of NMR in Medical diagnostics. 10 hrs

NMR of nuclei other than proton: ^{13}C chemical shift & factors affecting it. Decoupling-Noise decoupling & broad band decoupling. Off-resonance proton decoupling-some representative examples. Introduction to 19F &31P NMR. 2 hrs

UNIT-III: Mass Spectrometry **[12 hours]**

Basic principles, Instrumentation, interpretation of mass spectra, resolution, exact masses of nucleides, molecular ions, meta-stable ions and isotope ions. Fragmentation processes-representation of fragmentation, basic fragmentation types and rules. Factors influencing fragmentations and reaction pathways. McLafferty rearrangement. Fragmentations associated with functional groups- alkanes, alkenes, cycloalkanes, aromatic hydrocarbons, halides, alcohols, phenols, ethers, acetals, ketals, aldehydes, ketones, quinines, carboxylic acids, esters, amides, acid chlorides, nitro compounds and amines. Ion analysis, ion abundance, retro Diels-Alder fragmentation. Nitrogen rule. High resolution mass spectroscopy. 9 hrs

Composite problems involving the applications of UV, IR, ^{1}H and ^{13}C NMR and mass spectroscopic techniques. Structural elucidation of organic molecules. 3 hrs

REFERENCES:

1. Spectrometric Identification of Organic Compounds - Silverstein, Bassler & Monnill (Wiley)1981.

2. Applications of Absorption Spectroscopy of Organic Compounds-Dyer(Prentice Hall,NY) 1965.

3. Spectroscopy of Organic Compounds-3rd Ed.-P.S.Kalsi (New Age, New Delhi) 2000.

4. Analytical Chemistry-Open Learning : Mass spectrometry.

5. Spectroscopic Methods in Organic Chemistry - Williams and Fleming, TMH.

6. Spectroscopy, Donald L.Pavia (Cengage learning India Pvt.Ltd., Delhi), 2007.

7. Organic Spectroscopy-3rd ed.-W.Kemp (Pagrave Publishers, New York), 1991.