UNIT- III: **[15 Hours]**

Formation and Hydrolysis of Esters: Plurality of mechanism. Mechanism of esterification reactions. Ester hydrolysis-$A_{AC}2$, $B_{AC}2$, $A_{AC}1$ & $A_{AL}1$ mechanism. Transesterification.4 hrs

Addition to Carbon-Carbon Multiple Bonds: Addition reactions involving electrophiles, nucleophiles and free radicals. Cyclic mechanisms. Orientation and stereochemistry. Addition of halogens, hydrogen halides, carboxylic acids and amines. Addition to cyclopropanes, hydroboration, Michael addition. Addition of oxygen across double bonds. 5 hrs

Addition to Carbon-Hetero Multiple Bonds: Electrophilic, nucleophilic and free radical additions to C=O and C=N systems. Addition of Grignard reagents. Reformasky reaction, aldol condensation, Knoevenagel condensation, Perkin reaction and Wittig reactions. 6 hrs

REFERENCES:

1.Organic Reactions and Their Mechanisms- P.S. Kalsi (New Age, New Delhi),1996.

2.Advanced Organic Chemistry 4th Edn- J. March (Wiley, NY) 2000.

3.Organic Reaction Mechanisms- Bansal (Tata McGraw Hill, New Delhi) 1978.

4.Organic Chemistry-Vol.–I & II-Mukherji, Singh and Kapoor(Wiley Eastern, New Delhi) 1985.

5.Mechanism and Theory in Organic Chemistry-Lowry and Richardson Harper and Row, 1987.

6. Reaction Mechanisms in Organic Chemistry-Mukherji, Singh and Kapoor (McMillan) 1978.

7. Organic Chemistry-P.Y. Bruice (Pearson Education, New Delhi) 2002.

8. Organic Reaction Mechanism-R.K. Bansal (Wiley Eastern Limited, New Delhi) 1993.

9. A Guide Book to Mechanism in Organic Chemistry-Petersykes.

10. Advanced Organic Chemistry –Carey and Sundberg, Part A& B, 3rd edition (Plenum Press, New York) 1990.

11. Organic Chemistry-I.L. Finar (ELBS Longmann, Vol. I) 1984.

12. Advanced General Organic Chemistry-S.K. Ghosh (Book and Alleied (P) Ltd) 1998.

CH H 453 : ADVANCED PHYSICAL CHEMISTRY

COURSE OUTCOME:

- It is an advanced level course which helps to understand the concepts of physics and their subsequent applications in the field of chemistry.
- The concepts of chemical thermodynamics helps in the design of processes in chemical industries.
- The concepts of statistical thermodynamics find relevance in understanding the nature of solids and metals in specific.
- It enables to understand chemical bonding, photochemistry and spectroscopy

UNIT I: **[15hours]**

Chemical Thermodynamics:

Entropy: Physical significance, entropy change in an ideal gas. Variation of entropy with Temperature, Pressure and Volume. Entropy change in reversible and irreversible processes. Thermodynamic equations of state.

Free energy, Maxwell's relations and significance. Helmholtz's and Gibbs free energies, Gibbs – Helmholtz equation and its applications.

Nernst heat theorem: Its consequences and applications. Third law of thermodynamics – statements, applications and Comparison with Nernst Heat theorem.
Chemical affinity and thermodynamic functions. Effect of temperature and pressure on chemical equilibrium- van't Hoff reaction isochore and isotherms.
Partial molar properties: Physical significance, determination of partial molar volume and enthalpy. Chemical potential: variation of chemical potential with temperature. Gibbs – Duhem equation.
Thermodynamic functions of mixing, Gibbs – Duhem – Margules equation.
Fugacity: Relationship between fugacity and pressure. Determination of fugacity- graphical method and Lewis Randall rule.
Activity and activity coefficient: Variation of activity and fugacity with temperature and pressure. Determination of activity by vapour pressure method.

UNIT - II: Statistical and Irreversible thermodynamics [15 hours]

Statistical Thermodynamics: Thermodynamic Probability, phase space, micro and macrostates, statistical weight factor, assembly, ensemble-significance, classification and comparison. Distribution laws – Boltzmann law, Maxwell-Boltzmann distribution law. Bose-Einstein and Fermi-Dirac statistics, Limit of applicability of various laws. Relationship between partition function and thermodynamic functions -Average energy, heat capacity, free energy, chemical potential. Introduction to Statistical mechanism of independent, independent and indistinguishable (non-localized) molecules or particles.

Partition function for molecular particles.

Thermodynamic quantities in terms of partition function of particles- Evaluation of Translational, vibrational, rotational, electronic and nuclear derivations of translational, rotational, vibrational and electronic partition functions. Law of equipartition principle. Partition function and equilibrium constant.

Statistical thermodynamic properties of solids (Heat capacity)-Introduction, thermal characteristics of crystalline solid, Einstein model, Debye modification. Nuclear statistics - Introduction, symmetric and nuclear spin, ortho and para nuclear states. Applications of partition function to mono atomic gases, diatomic molecules, equilibrium constant. 9hrs.

Irreversible Thermodynamics – Introduction, Thermodynamics of irreversible processes, Entropy production-rate of entropy production. Phenomenological relations. The principle of microscopic reversibility, Onsager reciprocal relations – validity and applications (Electro kinetic, Thermoelectric phenomena). Irreversible thermodynamics of Non linear regime and biological systems. 6hrs

UNIT III

Postulates of quantum Mechanics. Particle waves, its character and significance. Normalization and orthogonality of wave functions. Operators and their algebra, types and applications, operators for the dynamic variables of a system (position, linear momentum, angular momentum, Kinetic energy, potential energy and total energy) Eigen values and Eigen functions. Quantum numbers and their characteristics. Schrodinger wave equation – significance and derivation. Statistical interpretation of ψ 7 hrs

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