Jyoti Nivas College Autonomous

Department of Chemistry

Objectives of Chemistry Course (PG): M.Sc. Chemistry (Organic)

Semester I

Sl. No.	Code No.	Title	Theory / practical hrs / Week	Duration of Examination Hours	Max. Marks for ESE	CIA	Total Marks	Total No. of credits
1.	JOC 101	Inorganic Chemistry - I	4	3	70	30	100	4
2.	JOC 102	Organic Chemistry – I	4	3	70	30	100	4
3.	JOC 103	Physical Chemistry - I	4	3	70	30	100	4
4.	JOC 104	Principles of Chemical Analysis	4	3	70	30	100	4
5.	JOC 105	Mathematics for Chemists (Softcore)	3	3	70	30	100	3
6.	JOC 106	Inorganic Chemistry Practicals - I	4	4	35	15	50	2
7.	JOC 107	Inorganic Chemistry Practicals - II	4	4	35	15	50	2
8.	JOC 108	Physical Chemistry Practicals - I	4	4	35	15	50	2
9.	JOC 109	Physical Chemistry Practicals - II	4	4	35	15	50	2
					490	**210**	**700**	**27**

Scheme for Internal Assessment

- **Theory (each paper)**

Maximum Marks (Examination): **70**
Marks for Internal Assessment: **30** *(Continuous evaluation)*
Attendance: 05 Marks
Seminar: 05 Marks
Test: 20 Marks
Total: 30 Marks

* Seminars to be conducted every semester.

- **Practical (each paper)**

Maximum Marks (Examination):	**35**
Marks for Internal Assessment:	**15** *(Continuous evaluation)*
Attendance:	03 Marks
Record book:	02 Marks
Prefinal:	10 Marks
Total:	**15 Marks**

Record book for the Practical has to be assessed as internal assessment. There should be no marks for record book during Practical Examination.

JOC 101: Inorganic Chemistry -I

Objectives:

This course aims to impart to the student, knowledge of:

- Advanced principles of bonding in inorganic compounds.
- The chemistry of coordination compound with Pi acceptor ligands
- The structure of important silicon containing compounds and the correlation between their structure and applications.
- The chemistry of non-metal containing compounds such as boranes, borazines, sulphur-nitrogen compounds and phosphorus-nitrogen compounds.
- The structure and applications of isopoly and heteropoly anions of vanadium, molybdenum and tungsten and metal carbonyl clusters.
- The various principles and applications of solvent system, hard-soft acid base (HSAB), theories of acids and bases and concept of super acids.

Learning Outcomes:

On completion of the course, students should be able to:

- Appreciate the different theories of chemical bonding and be able to apply these theories to solve structures
- Be able to apply IR spectroscopy to discuss structures of pi acceptor containing complexes
- Choose an appropriate solvent for carrying out any chemical reaction based on the principles of acids and bases.
- Correctly write the structures of heteropoly, isopoly anions and metal carbonyl clusters and relate the structure to chemical reactivity.
- Understand the three dimensional structure of silicates and catalytically important molecules such as aluminosilicates (zeolites) and apply their knowledge towards selectivity based on structure.

- Write the structure of non metallic compounds and classify boranes based on STYX.

Syllabus:

Unit I

1. Chemical Bonding 1: **15 hrs**

Ionic bond: Lattice energy, Born-Lande equation, Kapustinskii equation, Born-Haber cycle and its applications, Fajan's rules, Slater's rules, radius-ratio rules, structures of crystal lattices (NaCl, CsCl and ZnS).

Hybridisation, VSEPR model, shapes of molecules – XeF_2, ClF_3, XeF_4, ICl_4^-,XeF_6, $TeCl_6^{2-}$, IF_7, NO_2, NO_2^+, NO_2^-, CO_3^{2-}, SO_4^{2-}

Energetics of hybridization and Bent's rules and, Electronegativity and partial ionic character, Covalent bonding: M.O. Theory: σ, π and δ molecular orbitals, MOs of diatomic molecules: homo - N_2 and O_2 and heteronuclear – CO, NO, HF, ICl, Walsh diagrams of BeH_2 and H_2O.Co-ordinate and quadruple bonds. Hydrogen bonds-types and detection, Agostic bond.

Unit II

2. Chemical Bonding 2: **11 hrs**

Synergic bonding: simple metal carbonyls, nitrosyl, and tertiary phosphine complexes. Structure and bonding in hydride, dihydrogen, dinitrogen, isocyanide. Stereochemical non-rigidity: (TBP, CO scrambling), Stereoisomerism-chirality, optical activity. Absolute configurations, CD, ORD, Cotton effect and magnetic circular dichroism

Unit III

3. Compounds of non-metals: **07 hrs**

Structure and bonding in boranes, carboranes, metallo-carboranes, styx code explanation with examples (B_2H_6, B_4H_{10}, B_5H_9, B_6H_{10}, B_5H_{11} and $B_{10}H_{14}$), Wade's rules,preparation, properties, structure and bonding of borazine, phosphazenes – tri and tetra, sulphur-nitrogen compounds – S_2N_2, S_4N_4, $(SN)_x$.

4. Silicates: **06 hrs**

Principles of structure of silicates, Classification and structures of silicates, isomorphous replacement, pyroxenes, amphiboles, layered (double and triple, distinction between structure of talc and muscovite) and vitreous silicates, zeolites – synthesis of sodalite and ZSM-5, application as molecular sieves, ion-exchange and catalyst.

Unit IV

5. Concepts of Solvent systems and Acids-Bases: **06 hrs**

Solvent systems; Bronsted and Lewis acids and bases, pH and pKa, Hard and Soft acids and bases (HSAB) - concept, application and limitations, levelling effect, super acids, acid-base concept in non-aqueous media, reactions in liquid BrF_3 and liquid N_2O_4.

6. Isopoly and heteropoly acids of W, Mo and V: 04 hrs

Preparation and structure of: Isopoly vanadates – VO_4^{3-}, $V_2O_7^{4-}$, $(VO_3)_n^{n-}$, $[V_{10}O_{28}]^{6-}$; Isopoly molybdates – di, para ($Mo_7O_{24}^{6-}$), tri, tetra (meta), octa ($Mo_8O_{26}^{4-}$); Isopoly tungstates – normal, para, meta ($W_{12}O_{42}^{12-}$, $H_2W_{12}O_{40}^{6-}$); Heteropoly acids of Mo and W – 12 molybdoheteropoly acids, 12 tungstoheteropoly acids; General applications of isopoly and heteropoly acids.

7. Metal clusters: 03 hrs

M-M bond and metal atom clusters, bonding in $Re_2Cl_8^{2-}$; Metal carbonyl clusters – LNCC's and HNCC's. Electron counting in carbonyl clusters: Wades-Mingos and Lauher rules

References

1. Basic Inorganic Chemistry, F.A. Cotton, G. Wilkinson and P.L. Gaus, John Wiley and Sons (1995)
2. Advanced Inorganic Chemistry 3rd, 5th and 6th Editions, F. A. Cotton and G. Wilkinson
3. Inorganic Chemistry, 4th Edition, J.E. Huheey, E.A. Keiter and R.L. Keiter, Addison - Wesley (1993)
4. Inorganic Chemistry, 2nd Edition, D.F. Shriver, P.W. Atkins and C.H. Langford, ELBS (Oxford Univ. Press) (1994)
5. Concise Inorganic Chemistry, 5th Edition, J.D. Lee (1996).
6. Chemistry of the Elementals, N.N. Greenwood and A.E. Earnshaw, Butterworth Heinemann (1997)
7. Essential trends in Inorganic Chemistry, D.M.P. Mingos, Oxford Univ. Press (1998)
8. Materials Science, J.C. Anderson, K.D. Lever, J.M. Alexander and R.D. Rawlings, ELBS, (2000).
9. Structural Inorganic Chemistry, A.F. Wells, Oxford: Clarendon Press, 1984.
10. Inorganic Chemistry, James E. House, Latest ELBS edition.
11. Basics of Inorganic Chemistry by William Jolly, Latest edition

JOC 102: Organic Chemistry - I

Objectives:

This course aims to impart to the student, knowledge of:

- Basic concepts of bonding, structures, resonance, aromaticity, hyperconjugation and tautomerism in organic molecules.
- Generation, structure, stability and reactivity of reactive intermediates.

- Classification of reactions with mechanism, determining reaction mechanism using suitable methods.
- Stereochemistry of organic compounds, isomerism, different projection formulae with nomenclature and prochirality.
- Conformation and stability of substituted cyclic systems, nomenclature and conformations of fused rings and bridged ring systems.
- Use of various oxidizing and reducing agents and their applications in the synthesis of industrially and pharmaceutically important compounds.
- Synthetic molecular receptors, their significance and functions.

Learning Outcomes:

On completion of the course, the student should be able to:

- Apply the concepts of bonding, resonance, aromaticity, hyperconjugation and tautomerism to higher organic compounds.
- Predict the products, identify reaction intermediates and propose suitable mechanism for organic reactions.
- Identify stereogenic centres, recognize enantiomers, diastereomers, meso compounds, draw stereochemical structures, and provide R/S designations of stereocenters.
- Draw stable conformations for substituted cyclic compounds, fused and bridged rings.
- Use of various oxidizing and reducing reagents for application in organic transformations of industrially and pharmaceutically important organic compounds.
- Understand the host-guest interactions in molecular receptors.

Syllabus:

Unit I

1. Nature of Bonding in Organic Molecules **06 hrs**

Delocalized chemical bonding: Conjugation, cross conjugation, resonance.

Aromaticity. Huckel's rule of aromaticity. Craig's rule. Aromatic systems with electron numbers other than six (including azulene, tropone, tropolone and annulenes). Antiaromaticity. Aromaticity in benzenoids, meso-ionic compounds. Homo-aromaticity. Alternant and nonalternant hydrocarbons, Energy levels in odd and even-alternant hydrocarbons, energy levels for the benzyl cation, benzyl free-radical and benzyl carbanion. Hyperconjugation. Tautomerism

2. Reaction Mechanisms - I **10 hrs**

Generation, structure, stability and reactivity of carbocations, carbanions, carbon free radicals, carbenes and nitrenes

Classification of reactions and mechanisms: Thermodynamic and kinetic requirements, kinetic and thermodynamic control, Hammond postulate, Curtin-Hammett principle. Potential energy diagrams, transition states and intermediates

Methods of determining mechanisms: Based on the structure of products, determination of the presence of intermediates, isotopic labeling, isotope effects, from stereochemical evidence
Acids and bases: Hard and soft acids and bases. Effect of structure on the strengths of acids and bases
Effect of structure on reactivity: Resonance and field effects; steric effects. The Hammett equation and linear free energy relationship, substituent and reaction constants, Taft equation

3. Reaction Mechanisms - II **04 hrs**

Nucleophilic substitution reaction at saturated carbon: S_N1, S_N2, S_Ni and SET mechanism, Effect of substrate structure, attacking nucleophile, leaving group, Ambident nucleophiles and substrates

Unit II

4. Stereochemistry **10 hrs**

Fischer, Newman, Sawhorse and flying wedge projections and their interconversions Optical isomerism: Elements of symmetry and chirality, D-L conventions, CIP rules, R-S and M-P conventions, Chirality in compounds with a stereogenic centre, in allenes, alkylidene, cycloalkanes and spiranes (with a stereogenic axis), Cram's and Prelog's rules
Conformational analysis: Conformational analysis of cycloalkanes: cyclobutane, cyclopentane, cychexanes (monosubstituted e.g., methyl, *iso*-propyl, *tert*-butyl and di-substituted cyclohexanes e.g., dialkyl, dihalo, diols) and cycloheptane
Nomenclature and conformations of fused rings and bridged ring systems.
Prochirality: Enantiotopic and diastereotopic atoms, groups and faces.

Unit III

5. Oxidations **09 hrs**

CrO_3, $K_2Cr_2O_7$, $KMnO_4$, OsO_4, SeO_2, $Pb(OAc)_4$, HIO_4, Oxygen (singlet & triplet), ozone, peroxides (H_2O_2, t-BuOOH, dibenzoylperoxide) and peracids (CF_3COOOH, m-CPBA, Dakin-West reaction) as oxidizing agents. Synthesis and application of Jones reagent, Chromyl chloride, Dess Martin reagent, Chloramine-T. Opppenaur oxidation.

6. Reductions **09 hrs**

Complex metal hydrides ($LiAlH_4$, $NaBH_4$), dissolving metal reductions (Na/liq.NH_3, Birch, Clemmensen reductions), Baker's Yeast, diimide reduction, catalytic hydrogenation (homogenous and heterogeneous), organoboranes, NaH, LiH, hydrazine as reducing agents; Wolf-Kishner reduction, Meerwein-Ponndorf-Verley reduction.

Unit IV

7. Synthetic Molecular Receptors **04 hrs**

Definition and significance, Structure and function of receptors with molecular clefts, molecular tweezers, receptors with multiple hydrogen bonding sites, cryptates, cyclodextrins, cyclophanes and calixarenes.

References

1. Advanced Organic Chemistry – Reactions, Mechanism and Structure, Jerry March, John Wiley (2008).
2. Advanced Organic Chemistry, F A Carey and R J Sundberg Plenum, (1990).
3. A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, Longman, (2000).
4. Structure and mechanism of Organic Chemistry, C K Ingold, Cornell University Press (1999).
5. Organic Chemistry, R T Morrison and R N Boyd, Prentice-Hall, (1998).
6. Principles of Organic Synthesis, R O C Norman and J M Coxon, Blackie Academic and Professional, (1996).
7. Stereochemistry of Organic Compounds, D Nasipuri, New-Age International, (1999).
8. Stereochemistry of Carbon Compounds, E L Eliel, S H Wilen and L N Mander, John Wiley, (1994).
9. Organic Synthesis, Jagadamba Singh and L. D. S. Yadav, Seventh Edition, 2011.
10. Organic Reaction Mechanisms, V. K. Alhuwalia and Rakesh Kumar Parashar, 4th Edition, 2012.
11. Some modern methods of Organic Synthesis, W. Carruthers, Cambridge Uni. Press London, 2nd Edn., 1998.
12. Understanding organic reaction mechanisms, A. Jacob, Cambridge, University Press, 1997.
13. Introduction to organic chemistry, A. Streitweiser, Jr. and C. H. Heathcock, Macmillan, 1985.
14. Organic Chemistry, Volumes I and II, I L Finar, Longman, (1999).

<u>JOC 103: Physical Chemistry - I</u>

Objectives:

This course aims to impart to the student, knowledge of:

- Mathematical framework for thermodynamics of open system.
- Concepts in classical laws of thermodynamics and their application, postulates of statistical mechanics, statistical interpretation of thermodynamics, ensembles.
- Statistical mechanics are used to develop the statistics for Bose-Einstein, Fermi-Dirac and photon gases.
- How probability theory can be used to derive relations between the microscopic and macroscopic properties of matter.

- The collision model of chemical reactions and how various factors such as temperature and catalyst can affect reaction rate and mechanism of thermal and photochemical hydrogen-halogen reactions.
- Different theories of unimolecular reactions; Perrin theory, Lindemann-Christiansen Hypothesis, Hinshelwood treatment, RRK treatment and RRKM treatment.
- Surface and colloid chemistry from a physical-chemical perspective.

Learning Outcomes:

On completion of the course, students should be able to:

- Account for the physical interpretation of partition functions and be able to calculate thermodynamic properties of model systems with using Boltzmann -, Fermi-Dirac and Bose-Einstein statistics.
- Account for the physical interpretation of distribution functions and discuss and show how these can be used in calculations of basic thermodynamic properties.
- Use kinetic data to check the viability of a mechanism.
- Recall and explain why certain factors such as concentration, temperature, medium and the presence of a catalyst will affect the speed of a chemical reaction.
- Understand the concept of activation energy and its calculation from kinetic data
- Define and explain surface and interfacial phenomenon.

Syllabus:

Unit I: Classical Thermodynamics

1.1 Systems of variable composition **04 hrs**

Partial molar properties – introduction, Partial molar free energy (chemical potential), partial molar volume and their significance. Gibbs-Duhem equation. Variation of chemical potential with temperature and pressure. Simultaneous determination of partial molar volumes of two components of a binary liquid mixture by intercept (reciprocal density) method. Determination of PMV of a solute in a solution by apparent molar volume method. Problems.

1.2 Gases and Solutions **07 hrs**

The concept of fugacity and fugacity coefficient. Determination of fugacity of a gas by graphical and compressibility factor methods. Problems. Raoult's law. Types of deviations of non-ideal solutions from the ideal behaviour. Gibbs-Duhem-Margules equation and its application: Derivation of Rault's Law, Henry's Law, Phase rule and Nernst Distribution law based on Chemical Potential. Thermodynamic functions of mixing of non-ideal/ideal solutions. Excess thermodynamic functions G^E, S^E, HE and V^E. Activity and activity coefficient. Determination of mean-ion activity coefficient of an electrolyte (HCl) by EMF method and a sparingly soluble salt by solubility method.

Unit II: Statistical Thermodynamics

2.1 Introductory Aspects and Distribution Laws **05 hrs**

Scope. Concepts of distribution, probability of a distribution (apriori probability and thermodynamic probability) and most probable distribution. The concept of an ensemble. Types of ensembles. Stirling's approximation.Maxwell-Boltzmann, Bose-Einstein and Fermi-Dirac statistics. Derivation of the respective distribution laws using the Lagranges method of undetermined multipliers. Comparison of M.B., B.E. and F.D. statistics.

2.2 Partition function **04 hrs**

Definition and physical significance. Derivation of expressions for translational, rotational, vibrational and electronic partition functions. Expression of the thermodynamic functions like internal energy, enthalpy, entropy, free energy and heat capacity in terms of partition function. Sackur-Tetrode equation and its significance. Relation between equilibrium constant of a reaction and partition function.

2.3 Applications of statistical thermodynamics **02 hrs**

A brief account of the theory of heat capacity of solids: Einstein and Debye Theories. Application of Fermi-Dirac statistics: Evaluation of the electronic contribution to heat capacity of metals.

Unit III

3.0 Non-Equilibrium Thermodynamics **05 hrs**

Thermodynamic criteria for non-equilibrium states. Entropy production and entropy flow. Transformations of the generalized fluxes and forces. Phenomenological laws and Onsager's reciprocity relations. Coupled and non-coupled reactions. Electrokinetic phenomena. Principle of detailed balance (microscopic reversibility) as the basis of Onsager's Reciprocity Relations.

Unit IV: Chemical Kinetics

4.1 Introduction to Chemical Kinetics **05 hrs**

Macroscopic and Microscopic Kinetics. Review of theories of reaction rate – Arrhenius equation – characteristics, significance of energy of activation, temperature coefficient and its evaluation Collision Theory and Transition State Theory. Comparison of collision theory with transition state theory. Thermodynamic formulation of reaction rates (Wyne-Jones and Eyring treatment). Reaction between ions in solution – influence of ionic strength on reaction rates (primary and secondary salt effects).

4.2 Steady State Kinetics **04 hrs**

Chain reactions – general characteristics, chain length and chain inhibition. Comparison of photochemical and thermal reactions. Mechanisms of thermal reactions (hydrogen-bromine, hydrogen-chlorine, pyrolysis of acetaldehyde, decomposition of ethane) and photochemical reactions (hydrogen- bromine and hydrogen-chlorine). Comparative study of thermal and photochemical hydrogen-halogen reactions.

4.3 Techniques for Fast reactions **03 hrs**

Introduction – need for special techniques. Stopped flow method. Relaxation method (Principle of temperature jump for unimolecular reaction, bimolecular reaction, derivation not required), flash photolysis and shock tube methods.

4.4 Unimolecular Reactions **04 hrs**

Introduction - Perrin theory, Lindemann-Christiansen Hypothesis, Hinshelwood treatment, RRK treatment (Qualitative treatment only), RRKM treatment (Qualitative treatment only).

4.5 Kinetics of homogeneous Catalysis **06 hrs**

General catalytic mechanisms – Equilibrium treatment: Arrhenius intermediates, Steady state treatment: vant Hoff intermediates, activation energies for catalysed reactions, application to acid base catalysis.

Enyme catalysis: Comparison of enzymes with chemical catalysts. Mechanism (lock and key) and kinetics of enzyme catalysed reactions – Henri-Michaelis-Menten mechanism, significance of Michaelis-Menten constant, Lineweaver-Burke plot. Effect of enzyme concentration, pH, temperature, activators on enzyme activity. Inhibition of enyzymes (Competitve, Non-competitve and uncompetitive, identification based on L.B plots).

Unit V

5.0 Colloids and Surface Chemistry **03 hrs**

Stability and properties of colloids. Types of adsorption isotherms. BET adsorption isotherm and its use in the determination of surface area of a solid. Gibbs adsorption isotherm and its significance.

References

1. Glasstone S., Thermodynamics for Chemists, Affiliated East-West Press Pvt. Ltd., (1960).
2. Mc. Quarrie D.A., Simon J.D., Molecular Thermodynamics, University Science Books, (1999).
3. Gupta M.C. Statistical Thermodynamics, Wiley Eastern Ltd., (1993).
4. Laidler K.J., Chemical Kinetics 3rd Edition, Pearson Publ., (2013).
5. House J.E., Principles of Chemical Kinetics, Wm C Brown Publisher, Boston (1997).
6. Glasstone S., Text Book of Physical Chemistry, 2nd Edition, Macmillan India Ltd., (1991).
7. Atkins P.W., de Paula J., Physical Chemistry, 7th Edition, Oxford Publ., (2002).
8. Puri B.R, Sharma L.R, Pathannia M.S., Principles of Physical Chemistry, 47th Edition., Shoban Lal Nagin Chand Co., (2017).

<u>JOC 104: Principles of Chemical Analysis</u>

Objectives:

This course aims to impart to the student, knowledge of:

- Errors, statistical treatment of analytical data and use of various computational tools on interpreting experimental data
- Principles, terminologies, types and applications of chromatography.
- Optical and thermal methods of chemical analysis; principle, instrumentation and applications.
- Various concepts of volumetric analysis - equivalence point, theory of indicators, use of chemical equations and equilibrium constants to illustrate the chemical changes that occur during the titration.

Learning Outcomes:

On completion of the course, students should be able to:

- Organize, analyze and interpret data using the tools learned in an ethically responsible approach and present it systematically.
- Describe and adopt suitable separation techniques.
- Interpret data obtained from optical and thermal methods of chemical analysis.
- Write balanced chemical equations, plot titration curves and calculate concentrations of analyte from neutralization, redox, complexometric, precipitation and gravimetric titrations.

Syllabus:

Unit I

1. Introduction to Data Analysis: **08 hrs**

Review: Errors in chemical analysis, accuracy and precision, types of errors- absolute, relative, systematic, random, constant and proportional.

Detection of systematic errors. Nature of random errors, sources, distribution of experimental results. Statistical treatment: samples and population, mean and median. Properties of Gaussian curves – Population mean and sample mean, population standard deviation, area under the curve, sample standard deviation, standard error of the mean. Variance, relative standard deviation (RSD), Coefficient of variation (CV). Confidence intervals. Bivariate data, Correlation coefficients, Regression Analysis: regression lines. Testing of hypothesis: t-test. Determination of Outlier: Q-test.

2. Separation Techniques: **10 hrs**

Solvent extraction: Types- Batch, Continuous, efficiency, selectivity, distribution coefficient, Nernst Distribution law, derivation, applications and numerical problems.

Chromatography: Types, Terminology, principles and functioning of Paper, Thin layer, Column, Gas Chromatography, High Performance Liquid Chromatography, Reversed Phase Liquid Chromatography, Super Critical Fluid (SCF) Chromatography, 2D- Thin Layer Chromatography.

Unit II

3. Optical Methods of Chemical Analysis: 06 hrs

Interaction of electromagnetic radiation with matter, deviations from Beer Lambert Law, choice of solvent for UV- Visible spectrophotometry, Sandel sensitivity, Ringbom's plot, Photometric titrations, single and Double beam UV-Visible spectrophotometer, Application of quantitative and qualitative analysis, Principles and Applications of Fluorimetry, Turbidimetry and Nephelometry. Numerical problems on all these techniques.

4. Thermal methods of analysis: 02 hrs

Introduction, general principles and applications of thermogravimetric analysis (TGA), differential thermal analysis (DTA) and differential scanning calorimetry (DSC).

Unit III

4. Neutralization Titrations: 05 hrs

Solutions and indicators for acid base titrations- standard solutions, Acid-base indicators, Titration curves: Strong acid vs. strong base, weak acids vs. strong base, and weak base vs. strong acid, pH calculations, polyfunctional acids and bases - phosphoric acid system, composition of polyprotic acid as a function of pH- phosphoric acid, titration curve, titration of amphiprotic species - acid-base behavior of amino acid system.

5. Redox Titrations: 06 hrs

Introduction: Nernst equation, Standard & Formal potentials. Constructing Redox Titration curves - electrode potential during redox titrations, equivalence point potential. Detection of end point: Oxidation reduction indicators: General Redox Indicators, iron (II) complexes of orthophenanthrolines, starch/iodine solutions. Applications: Iron (II) solutions, iodometric titration (involving sodium thiosulfate) Oxidants such as Permanganate, dichromate, Ce (IV), Bromate. Determining water with Karl Fisher reagent.

6. Complexometric Titrations: 05 hrs

Introduction: Formation of complexes, complexation equilibria, suitability of polydentate ligand as titrants, expressions for the different forms of EDTA in solution as a function of pH, conditional formation constants, Effect of pH and titration curve, Selectivity by pH control, masking and demasking reagents, Theory of metal ion indicators, types of EDTA titrations: direct and back titrations.

7. Precipitation titrations: 04 hrs

Introduction: Argentometric titration, shape of titration curves, Solubility product, Theoretical principles of precipitation: Titration curves, Detection of end point, Mohr, Volhard and Fajan's indicators. Applications: Estimation of F^-, K^+, CO_3^{2-}, $C_2O_4^{2-}$ and mixture of halides.

Unit IV

8. Gravimetric analysis: 06 hrs

Precipitation Gravimetry: properties of precipitates and precipitating agents, factors affecting particle size, mechanism of precipitate formation, experimental control of particle size, conditions for quantitative precipitations, Formation and treatment of precipitates, co-precipitation, precipitation from homogeneous solution, drying and ignition of precipitates, calculation of results from gravimetric data, important precipitating agents such as dimethylglyoxime (DMG) in the estimation of nickel, 8-hydroxyquinoline (oxine) in estimation of aluminium and their significance in inorganic analysis.

References

1. Skoog and West's Fundamentals of Analytical Chemistry, 9th Ed., Holler and Crouch; Cengage Learning, (2014).
2. Analytical Chemistry, G.D. Christian, 5th edition, John-Wiley and Sons Inc.,(1946).
3. Instrumental Analysis, Skoog, Holler & Crouch, Cengage Learning, (2007).
4. Instrumental methods of Chemical Analysis, H.H. Willard, L.L. Merrit, J.A. Dean and F.A. Set, CBS Publishers (1996).
5. Quantitative Chemical Analysis, Daniel C. Harris, 8th Ed., W H Freeman & Co. (2010).
6. Unified Separation Science, J. Calvin Giddings, Wiley-Blackwell, (1991).
7. Instrumental methods of Chemical Analysis, G.W. Ewing, 5th Ed., McGraw-Hill, New York, (1988).
8. Vogel's text book of quantitative chemical analysis, 6th Ed., Jaffrey et.al ELBS/Longman, (1989).
9. Modern Methods of Chemical Analysis- Pecsok, Shields, Cairns and Mc Williams, 2nd Ed., John Wiley and sons (1976).
10. Vogel's Textbook of Quantitative Inorganic Analysis, Bassett, Denney, Jeffery and Mendham, 4th Ed., ELBS (1989).
11. Treaties on analytical Chemistry- Kolthoff, Elving and Krivan 2nd Ed., John-Wiley and Sons (1986).
12. Commercial Methods of analysis- Snell and Biffen, McGraw-Hill, (1944).
13. Hand Book of Instrumental Techniques for Analytical chemistry, Frank Settle, Prentice Hall PTR (1997).

JOC 105: Mathematics for Chemists (Soft Core)

Objectives:

This course aims to impart to the student, knowledge of:

- Mathematical concepts like vectors, matrices, calculus (differentiation, integration and differential equations), Fourier transform and probability.

- Use of these concepts in physical chemistry, spectroscopy, crystallography, analytical chemistry, nature of bonding etc.

Learning Outcomes:

On completion of the course, students should be able to:

- Apply the concepts of calculus in understanding the derivations of thermodynamics and quantum mechanics.
- Discuss the applications of matrices in HMO concept and group theory.
- Understand the advantages in image resolution of infrared spectra using Fourier transform.
- Understand the complex motion of electrons and electronic wave functions which are based on probability.
- Apply matrix and vector methods in understanding diffraction patterns from crystal structures

Syllabus:

Unit I

1. Vectors: **04 hrs**

Vectors, dot and cross products; scalar and vector triple products and their applications.

2. Matrix Algebra: **08 hrs**

Review of different types of matrices (including Hermetian and skew Hermetian); matrix addition and multiplication; determinant of a square matrix, transpose, adjoint and inverse of a square matrix. Solution to system of linear equation (a) by matrix method and (b) by Cramer's Rule. Characteristic equation of a square matrix, eigenvalues and eigen vectors.

Unit II

3. Calculus: **12 hrs**

Rule for differentiation; Chain rule (for f(x)=Un, sin u, log u etc). Implicit differentiation and parametric differentiation and successive differentiation of order 2 (for explicit functions only). Applications of differentiation: Derivative as a slope of the tangent, derivative as a rate measure-velocity and acceleration. Increasing and decreasing functions-Maxima and minima-second derivative test-point of inflections-problems restricted to polynomial.

Unit III

4. Integrations: **03 hrs**

Basic rules-simple substitution-Method of partial fractions-Integration by parts, Define integral and application to areas of plane curves. Functions of several variables: partial derivatives; co-ordinate transformation from cartesian coordinates to spherical and cylindrical coordinates and vice-versa.

5. Elementary differential equation: **03 hrs**

Variable separable, exact first order equations, linear and homogeneous equation, Second order homogeneous differential equation with constant coefficients f(D), y=0. Solution of differential equation by power series method

6. Fourier series: **03 hrs**

Simple problems.

7. Probability: **03 hrs**

Review of permutations and combinations. Probability and addition theorem for mutually exclusive events and multiplication theorem for independent events, Curve fitting-Method of least squares

References

1. Mathematical Preparation for physical chemistry, F. Daniells, M. Graw Hill Inc., US, 1959.
2. Mathematics for chemists, D. M. Hirst, Chemical Publishing Company Incorporated, New York, 1979.
3. Mathematics for chemists, P. G. Francis, Springer, 2011.
4. Basic Mathematics for chemists, P. Tebutt, Wiley-Blackwell, 1994.
5. Calculus and analytic geometry, 9th edition, G. B. Thomas, R.L. Finney, Addison-Wesley Publishing Company, Inc. 1996.
6. Short Course in differential equations, Rainvilles and Bedient, IBH publishers, 1968.
7. Mathematics for chemistry, G. Doggett and B. T. Sutcliffe Longmann Publishers, 1995.

<u>JOC 106: Inorganic Chemistry Practicals - I</u>

Objectives:

This course aims to impart to the student mastery over

- Preparation of solutions required for an experiment.
- The various techniques involved in the preparation of coordination compounds.

Learning Outcomes:

On completion of the course, students should be able to:

- Design a scheme for synthesis of coordination compound and execute it based on the principles learned.
- Solve problems encountered during a synthesis.
- Communicate the results of the experiment in a written and oral form.

Syllabus:

Synthesis of complexes:

Preparation and determination of yield of inorganic complexes:

1. Ferrous oxalate
2. Potassiumtris-oxalatoferrate(III) trihydrate
3. Hexamminecobalt(III) chloride
4. Cis -potassium dioxalatodiaquochromium (III)
5. Mercurytetrathiocyanatocobaltate(II)
6. Chloropentaamminecobalt(III) chloride

References

1. Vogel's Text Book of Quantitative Chemical Analysis, J. Bassett, G.H. Jeffery, J. Mendham and R.C. Demmy, 5th Edition, Longman Scientific and Technical (1999).
2. Practical Inorganic Chemistry by G. Marr and B. W. Rockett, London; New York: Van Nostrand Reinhold, (1972).

JOC 107: Inorganic Chemistry Practicals - II

Objectives:

This course aims to impart to the student, knowledge of:

- Reagents required for qualitative analysis inorganic salts and how to prepare them.
- The principles of qualitative analysis of a mixture of inorganic salts containing rare elements and the skills required for the analysis

Learning Outcomes:

On completion of the course, students should be able to:

- Prepare reagents required for analysis
- Carry out qualitative tests and identify inorganic radicals in a salt mixture.

Syllabus:

Qualitative analysis of inorganic salt mixture

Semi-micro qualitative analysis of mixtures containing two each of common cations and anions and one of the following less familiar elements: W, Mo, Ce, Th, Zr, V, U and Li.

References

1. Inorganic Semi – micro Qualitative Analysis, Dr. V V Ramanujam, 3rd Edition, The National Publishing Company (2008).
2. Vogel's Text Book of Qualitative Chemical Analysis, J. Bassett, G.H. Jeffery and J. Mendham, ELBS (1986).

JOC 108: Physical Chemistry Practicals - I

Objectives:

This course aims to impart to the student knowledge and skills for the

- Preparation and standardization of solutions
- Kinetic studies of a reaction
- Construction of a phase diagram of a two/three component system

Learning Outcomes:

On completion of the course, students should be able to:

- Devise and carry out an experiment to study the kinetics of a reaction.
- Interpret the experimental data in terms of a rate equation
- Plot data in two dimensions
- Learn to work in teams
- To plot phase diagram of two/three component systems and interpret them.
- Communicate the results of the experiment in a written and oral form.

Syllabus:

A. Chemical Kinetics

1. Determination of the velocity constant, catalytic coefficient, temperature coefficient, $t_{½}$ and energy of activation for the acid hydrolysis of methyl acetate
2. Evaluation of Arrhenius parameters for the reaction between potassium persulphate and potassium iodide (1st order).
3. Velocity constant for the saponification of ethyl acetate.
4. Determination of the order of reaction between hydrogen peroxide and potassium iodide (Clock reaction).

B. Phase Diagram

5. Construction of phase diagram of a two-component system and determination of eutectic temperature and eutectic composition.
6. Construction of phase diagram of a three-component system.

C. Adsorption

7. Adsorption of oxalic acid on charcoal. Verification of Langmuir adsorption isotherm.

References

1. Advanced Practical Chemistry by J.B. Yadav, Goel Publication House, Merrut (1989).
2. Experiments in Physical Chemistry by Shoemaker and Garland, McGraw Hill International Ed. (1996).
3. Experimental Physical Chemistry, V.D. Athawale and Parul Mathur, New Age International, New Delhi (2001).

JOC 109: Physical Chemistry Practicals - II

Objectives:

This course aims to impart to the student skills and knowledge required for

- Preparation and standardization of solutions required for an experiment.
- Use of a colorimeter in the study of the kinetics of a reaction.
- Use of a colorimeter for titrations.
- Use of a colorimeter in the estimation of mixtures.
- Determination of partial molal volume of solutions

Learning Outcomes:

On completion of the course, students should be able to:

- Identify wavelength of maximum absorbance
- Collect data using a colorimeter/spectrophotometer.
- Use colorimeter/spectrophotometer for colorimetric estimations, titrations and kinetic studies.
- Calculate the molal volume of a system at STP using experimental data.
- Learn to work in teams and present experimental results in both oral and written form

Syllabus:

A. Colorimetry

1. Test for validity for Beer-Lambert's law and determination of the unknown concentration of solution. Calculation of molar extinction coefficient.
2. Titration of ferrous ammonium sulphate with potassium permanganate colorimetrically.
3. Simultaneous estimation of Mn and Cr in a solution of $KMnO_4$ and $K_2Cr_2O_7$.
4. Kinetics of reaction between $K_2S_2O_8$-KI colorometrically.
5. Determination of concentration of Fe by spectrophotometric titration using EDTA.

C. Cryoscopy

6. Determination of molecular weight of a solute by cryoscopy.
7. Determination of degree of dissociation of an electrolyte and association of benzoic acid in benzene.

D. Partial Molar Volume

8. Determination of partial molar volume of ethanol by reciprocal density method.

9. Determination of PMV by apparent molar volume method, NaCl-H_2O system.

References

1. Advanced Practical Chemistry by J.B. Yadav, Goel Publication House, Merrut (1989).
2. Experiments in Physical Chemistry by Shoemaker and Garland, McGraw Hill International Ed. (1996).
3. Experimental Physical Chemistry, V.D. Athawale and Parul Mathur, New Age International, New Delhi (2001).

Semester II

Sl. No.	Code No.	Title	Theory / practical hrs / Week	Duration of Examination Hours	Max. Marks for ESE	CIA	Total Marks	Total No. of credits
1.	JOC 201	Inorganic Chemistry – II	4	3	70	30	100	4
2.	JOC 202	Organic Chemistry – II	4	3	70	30	100	4
3.	JOC 203	Physical Chemistry - II	4	3	70	30	100	4
4.	JOC 204	Spectroscopy-I	4	3	70	30	100	4
5.	JOC 205	Biomolecular Chemistry (Softcore)	3	3	70	30	100	3
6.	JOC 206	Inorganic Chemistry Practicals – III	4	4	35	15	50	2
7.	JOC 207	Inorganic Chemistry Practicals - IV	4	4	35	15	50	2
8.	JOC 208	Physical Chemistry Practicals – III	4	4	35	15	50	2
9.	JOC 209	Physical Chemistry Practicals - IV	4	4	35	15	50	2
					490	**210**	**700**	**27**

Scheme for Internal Assessment

- **Theory (each paper)**

Maximum Marks (Examination): **70**
Marks for Internal Assessment: **30** *(Continuous evaluation)*
Attendance: 05 Marks

Seminar:	05 Marks
Test:	20 Marks
Total:	**30 Marks**

* Seminars to be conducted every semester.

- **Practical (each paper)**

Maximum Marks (Examination):	**35**
Marks for Internal Assessment:	**15** *(Continuous evaluation)*
Attendance:	03 Marks
Record book:	02 Marks
Prefinal:	10 Marks
Total:	**15 Marks**

Record book for the Practical has to be assessed as internal assessment. There should be no marks for record book during Practical Examination.

JOC 201: Inorganic Chemistry - II

Objectives:

This course aims to impart to the student, knowledge of:

- Kinetic and thermodynamic parameters as a measure of stability of coordination compounds.
- Advanced theories of bonding in complexes along with their stereochemistry.
- Mechanisms of inorganic redox reactions involving coordination compounds.
- Electronic spectroscopy and magnetic properties of coordination compounds.

Learning Outcomes:

On completion of the course, the student should be able to:

- Understand and apply the principles of stability of complexes in synthesis of new molecules.
- Relate the structure of complexes to their properties.
- Use electronic spectroscopy as an analytical tool in the structural elucidation of complexes.
- Interpret the magnetic properties of transition metal complexes based on magnetic measurements

Syllabus:

Unit I

1. Metal - Ligand Equilibria in Solution **13 hrs**

Step-wise and overall formation constant and their relationship, trends in step-wise constant, kinetic and thermodynamic stability of metal complexes, factors affecting the stability of metal

complexes with reference to the nature of the metal ion and ligand, chelate and macrocyclic effects and their thermodynamic origin , determination of binary formation constants by pH-metry, spectrophotometry, polarography and by ion exchange methods.
Mechanism of redox reaction - outer and inner sphere electron transfer. Marcus equation (only mention to be made).

Unit II

2. Metal – Ligand Bonding **13 hrs**

Stereochemistry - coordination numbers 3 to 8. Crystal field theory, salient features, spectrochemical series, splitting of d-orbitals in octahedral, tetrahedral, tetragonal, square planar, trigonal bipyramidal and square-pyramidal geometry, applications of CFT- colours of transition metal complexes, magnetic properties of octahedral complex, distortion of octahedral complex, CFSE and their uses, factors affecting CFSE, limitations of CFT, experimental evidence for metal-ligand covalent bonding in complexes, nephelauxetic effect, Ligand Field Theory, MO theory: tetrahedral and octahedral complexes (including π-bonding)

Unit III

3. Electronic Spectra of Transition Metal Complexes **13 hrs**

Spectroscopic ground states, selection rules, term symbols for d^n ions, Racah parameters, Orgel correlation and Tanabe-Sugano diagrams (d^2), spectra of 3d metal aqua complexes of trivalent V,Cr, divalent Mn, Co and Ni, $[CoCl_4]^{2-}$, calculation of Dq, B and β parameters, charge transfer spectra. Spectral properties of Lanthanide and Actinide metal complexes.

Unit IV

4. Magnetic Properties of Metal Complexes **06 hrs**

Magnetic susceptibility and its determination: Gouy, Faraday, VSM method. Types of magnetic behaviour, diamagnetic corrections, orbital contribution, spin-orbit coupling, Ferro and antiferromagnetic coupling,spin crossover. Magnetic properties of Lanthanide and Actinide metal complexes.

5. Photochemical reactions of transition metal complexes **07 hrs**

Basic photochemical processes, Kasha's rule, Jablonski diagram, quantum yield, photosubstitution reactions, photo-redox reactions, ligand photoreactions, photoreactions and solar energy conversion.

References

1. Basic Inorganic Chemistry, F. A. Cotton, G. Wilkinson and P. L. Gaus, John wiley & sons Inc, 6th Edition (1999)
2. Inorganic Chemistry,4th Edition, J. E. Huheey, E. A. Keiter and R. L. Keiter, Addition - Wesley (1993)

3. Inorganic Chemistry, 2nd Edition, D. F. Shriver, P. W. Atkins and C. H. Langford, ELBS (Oxford Uni. Press) (1994)
4. Inorganic Chemistry – A Unified Approach by W. W. Porterfiled, Elsevier 2005, 2nd Edition.
5. Inorganic Electronic Spectroscopy, A. B. P. Lever, Elsevier.
6. Essential trends in inorganic chemistry, D. M. P. Mingos, Oxford Univ. Press (1998) Magneto Chemistry, R. L. Carlin, Springer Verlag.
7. Electronic Absorption Spectroscopy and Related techniques, D. N. Sathyanarayana, Universities Press (2001).
8. Textbook of Inorganic Chemistry by G. S. Sodhi, Viva books Pvt. Ltd. (2011).
9. Inorganic Chemistry, Miessler and Tarr, Pearson Prentice Hall, 4th Edition.

JOC 202: Organic Chemistry - II

Objectives:
This course aims to impart to the student, knowledge of:

- Mechanisms and evidences for aromatic electrophilic and nuleophilic substitutions, addition reactions, elimination reactions and rearrangements.
- Effect of substrate structure, leaving group and attacking species in the above reactions.
- The orientation and stereochemistry of the product formed.
- Synthesis and applications of selected reagents used for various organic transformations.
- Widely used name reactions and rearrangements for the synthesis of industrially and pharmaceutically important compounds.

Learning Outcomes:
On completion of the course, the student should be able to:

- Explain the mechanistic pathway for aromatic substitutions, addition reactions, elimination reactions and rearrangements.
- Predict the stereochemistry of the products formed.
- Design reactions with the help of name reactions and rearrangements and use of suitable reagents.

Syllabus:

Unit I

1. Aromatic Substitution Reactions **13 hrs**

Electrophilic Substitution Reactions: The arenium ion mechanism. Orientation and reactivity, Energy profile diagrams. The *ortho*/*para* ratio, *ipso* attack, orientation in other ring systems; Quantitative treatment of reactivity in substrates and electrophiles; Effect of leaving group; Amination, sulfonylation reactions, Diazonium coupling, Vilsmeier-Haack reaction, Gatterman reaction, Gatterman-Koch reaction and Hoesch reaction

Nucleophilic substitution reactions: The S_NAr, S_N1, benzyne and $S_{RN}1$ mechanisms. Reactivity: effect of substrate structure, leaving group and attacking nucleophile. Goldberg reaction, Bucherer reaction, Schiemann reaction, von Richter reaction, Sommelet-Hauser and Smiles rearrangements

Unit II

2. Addition Reactions **09 hrs**

Addition to carbon-carbon multiple bonds: mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals. Regio, stereo and chemoselectivities. Orientation and reactivity. Addition to cyclopropane ring. Hydrogenation of double and triple bonds, hydrogenation of aromatic rings. Addition of alkenes and/or alkynes to alkenes and/or alkynes; Ene synthesis, Michael reaction

Addition to carbon-heteroatom multiple bonds: Addition of Grignard reagents and organolithium reagents to carbonyl compounds and unsaturated carbonyl compounds. Conversion of aldehydes to nitriles. Hydrolysis of nitriles and addition of amines to isocyanates. Formation of xanthates. Wittig, Mannich and Stobbe reactions.

Unit III

3. Elimination Reactions **05 hrs**

The E_2, E_1 and E_1cB mechanisms and their spectrum.E_{2C} and E_{2H} mechanisms. Orientation of the double bond, Reactivity-effects of substrate structure, attacking base, the leaving group and the medium, Mechanism and orientation in pyrolytic elimination reactions (including Chugaev reaction)

4. Rearrangements **11 hrs**

Wagner-Meerwein, Pinacol-Pinacolone, Fries, Beckmann, Hofmann, Curtius, Lossen and Schmidt rearrangements, Benzil-benzilic acid rearrangement, Arndt-Eistert reaction (Wolff), Tiffeneau-Demjanov reaction, Firtsch-Buttenberg-Wiechell rearrangement, Stevens, Wittig and Favorskii rearrangements, Dienone-phenol, Baker-Venkatraman rearrangement, Baeyer-Villiger oxidation, Neber rearrangement, Benzidine rearrangement and Nametkin rearrangement

Unit IV

5. C-C and C-N bond forming reactions **07 hrs**

Chichibabin reaction, Darzen's reaction, uses of acetylides in C-C bond formation reactions. Acid catalysed self condensation of olefins, Skraup synthesis, Prins reaction, Shapiro reaction, Reformatsky reaction, Robinson annelation, Hofmann-Loffler-Freytag reaction, Stork-enamine synthesis, Meyer synthesis, Hell-Volhard-Zelenskii reaction.

Unit V

6. Reagents in Organic Synthesis **07 hrs**

Use of the following in Organic synthesis and functional group transformations:

LDA, DCC, DDQ, Me_3SiCl, 1.3-Dithiane (reactivity and umpolung), Woodward and Prevost hydroxylation, Diazomethane, Fenton's reagent, Silver carbonate, NBS, Corey-Chaykovsky reagent, Yamaguchi reagent.

References

1. Advanced Organic Chemistry – Reactions, Mechanism and Structure, Jerry March, John Wiley (1999).
2. Advanced Organic Chemistry, F.A. Carey and R. J. Sundberg, Plenum (1990).
3. A Guide Book to Mechanism of Organic Chemistry, Peter Sykes, Longman (2000).
4. Structure and Mechanism of Organic Chemistry, C.K. Ingold, Cornell University Press.
5. Principles of Organic Synthesis, R.O.C Norman and J.M. Coxon, Blackie Academic and Professional.
6. Stereochemistry of Organic Compounds, D. Nasipuri, New-Age International (1999).
7. Organic Synthesis, Jagadamba Singh and L. D. S. Yadav, Seventh Edition, 2011.
8. Organic Reaction Mechanisms, V. K. Alhuwalia and Rakesh Kumar Parashar, 4th Edition, 2012.
9. Some modern methods of Organic Synthesis, W. Carruthers, Cambridge Uni. Press London, 2nd Edn., 1998.
10. Introduction to organic chemistry, A. Streitweiser, Jr. and C. H. Heathcock, Macmillan, 1985.
11. Stereochemistry: Conformation and mechanism, P. S. Kalsi, 7th Edition (2008).

JOC 203: Physical Chemistry - II

Objectives:

This course aims to impart to the student, knowledge of:

- Time dependent and time independent Schrödinger equations with solutions in simple systems.
- Matrix representation of quantum mechanics is discussed together with approximate methods.
- Spin and angular momentum representations.
- The advanced theories explaining the behavior of electrolytes such as Debye-Huckel theory and Bjerrum theory of ion association.
- Structural models of electrified interface.
- The kinetics and thermodynamics of electrochemical recations

Learning Outcomes:

On completion of the course, students should be able to:

- Show an understanding of wave mechanics in three dimensions.
- Describe the structure of the hydrogen atom and show an understanding of quantisation of angular momentum.
- Apply variational method, time independent perturbation theory and time dependent perturbation theory to solve simple problems.
- Describe the difference between kinetically and mass transport controlled electrochemical processes.
- Explain fundamental aspects of electrochemical reaction in terms of thermodynamics, kinetics and mass transport.
- Explain the structure of electric double layer at the interface and its role on electrode reactions.

Syllabus:

Unit I: Quantum Chemistry (28 Hrs)

1. **Introduction to Quantum Mechanics:** **03 Hrs**

Review: The need for Quantum Mechanics, Blackbody radiation – Planck's Law of radiation, Photoelectric Effect, Electron waves, De Broglie Equation, Heisenberg Uncertainty Principle, Classical wave equation,

Eigenfunctions and Eigenvalues. Schrödinger wave equation and its relation to the classical wave equation. Wave function and its physical meaning, Conditions for Acceptable Wave Function – Normalisation and Orthogonality. Postulates of Quantum Mechanics (with detailed explanation).

2. Quantum Mechanical Formalism: **04 Hrs**

Operator Algebra: Addition and Subtraction, Multiplication; Commutative property – Commutator Operator, Linear Operator, Laplacian Operator, Hamiltonian operator, Hermitian Condition and Hermitian Operators.

3. Application of Quantum Mechanics to Simple Systems: **07 Hrs**

Free particle system, Particle in a box – One dimensional box and the utility of the model, Three dimensional box, Physical representation of the wave function (detailed explanation for finite potential barriers). Vibrational Motion of a particle (Harmonic Oscillator) – Hermite's differential equation and Hermite's Polynomials. Wave functions and physical interpretation. Rotational Motion of a Particle – Particle on a ring, Particle on a Sphere: Legandre and Associated Legandre functions and polynomials. Wave functions and spherical harmonics. Rigid Rotor model. Hydrogen atom: Spherical coordinates, Solutions to the ϕ, θ, and R equation, Lagurre and associated Lagurre polynomials, Radial and Angular Plots. Significance of Quantum

Numbers n, l and M_l. Zeeman Effect and Magnetic Quantum number. Quantum Mechanical Tunneling (No derivation).

4. Approximate Methods: 03 Hrs

The need for approximate methods, Variation Method with proof, Perturbation Method (qualitative treatment, no derivation). Application of Variation and Perturbation to Multielectron Atoms – Helium atom.

5. Angular momentum and Electron Spin 06 Hrs

Classical and Quantum mechanical concept, Angular momentum operators and Physical significance. Ladder operator for angular momentum. Eigenfunctions and eigenvalues of angular momentum. Angular momentum in Many-Electron atoms – Atomic states, Atomic terms and term symbols. Stern-Gerlach experiment. Orbital and spin momenta, antisymmetry and Pauli Exclusion Principle, Slater determinants. Coupling of angular momenta – Russel saunders and JJ coupling. Spin-orbital interaction and explanation of term multiplicities – Na-D doublet.

6. Chemical Bonding: 05 Hrs

HMO Theory – Introduction, Assumptions (qualitative). Application to simple systems: Ethylene, Allyl system, Butadiene and Benzene.

Unit II: Electrochemistry (24 Hrs)

7. Electrochemistry - I: 10 hrs

Electrochemistry of Solutions: Ionic atmosphere, physical significance of κ (kaapa), Debye-Huckel theory to the problem of activity coefficient. Debye-Huckel limiting law. Debye-Huckel equation for appreaciable concentration. The huckel and Brønsted equation. Qualitative verification of Debye-Huckel equation. Debye-Huckel-Onsagar conductance equation. Bjerrum theory of ion association – triples. Ion conductance minima. Thermodynamics of electrified interface derivation of Lipmann’s Equation, Surface excess – thermodynamic aspects. Method of determination and measurement of interfacial tension as a function of applied potential difference across the interface.

8. Electrical Double Layer: 04 hrs

Structure of Electrified Interface – Helmholtz-Perrin model, Guoy – Chapman and Stern Models. Semiconductor-Solution interface – Garrett-Brattain space charge inside an intrinsic semiconductor.

9. Electrochemistry - II: 10 hrs

Overpotential: Types. Electrolytic polarization. Dissolution and deposition potential. Determination of anode and cathode overpotential. Concentration polarization - variation of current with cell potential. Metal deposition overpotential. Thickness of diffusion layer. Derivation of Butler – Volmer Equation. Tafel plots. Exchange current density, factors affecting exchange current density. Influence of current density, pH, temperature, rate of growth on overpotential. Electrocatalysis – Mechanism of electrocatalysis, Volcano plots.

References

1. Prasad R.K., Quantum Chemistry, 4th Edition, 2010, New Age International Publishers.
2. McQuarrie D.A. and Simon J.B., Physical Chemistry: A Molecular Approach, 1st Edition, 2011, Viva Books Private Limited.
3. Anderson J.M., Mathematics for Quantum Chemistry, 1st Edition, 2005, Dover Publications.
4. Atkins P.W, Molecular Quantum Mechanics, 5th Edition, 2010, Oxford University Press.
5. Chandra A.K., Introductory Quantum Chemistry, 4th Edition, 2010, Tata McGraw Hill Publications.
6. Levine I.N., Quantum Chemistry, 6th Edition, 2009, Prentice hall of India Private Limited.
7. Glasstone S.L., Introduction to Electrochemistry, 1st Edition, 2006, Affiliated East West Press Private Limited.
8. Bockris J.O'M. and Reddy A.K.N., Modern Electrochemistry Volume 1: Ionics, 2nd Edition, Springer.
9. Bockris J.O'M., Reddy A.K.N. and Gamboa-Adelco S., Modern Electrochemistry Volume 2A: Introduction to Electrodics, 2nd Edition, Springer.
10. Potter E.C., Electrochemistry: Principles and Applications. 1st edition, 1961, Cleaver Hume Press.
11. Crow D.R., Principles and Applications of Electrochemistry, 3rd Edition, 1988, Chapman Hall.
12. Glasstone S.L., Text Book of Physical Chemistry, 2nd Edition, 1991, Mac Millan India Limited.

JOC 204: Spectroscopy - I

Objectives:

This course aims to impart to the student, knowledge of:

- Basic concepts of group theory and its applications.
- Fundamental aspects of classifying molecules based on various symmetry elements, point groups and constructing character table.
- Principles and instrumentation of different molecular spectroscopic methods.
- Qualitatively predict which signals are to be observed in the rotational, vibrational or electronic spectrum of various materials ranging from single atoms (atomic spectroscopy) to molecules (IR, Raman, UV- Vis Spectroscopy).

Learning Outcomes:

On completion of the course, students should be able to:

- Recognize symmetry elements, identify point groups of molecules, construct and explain character table for simple molecules.
- Categorize molecules based on their symmetry properties and predict their molecular properties.
- Combine, evaluate and interpret information from the various spectroscopic techniques in determination of molecular structures.

Syllabus:

Unit I

1. Symmetry and Group Theory in Chemistry 07 hrs

Principles of Group Theory– Symmetry elements, symmetry operations, Properties of group, Abelian, non-Abelian and cyclic group and subgroups, Multiplication Tables, Classes, Molecular point groups, Schoenflies symbols, Matrices for symmetry operations, Reducible and irreducible representations, Great Orthogonality theorem and its corollaries, Construction of character tables, C_{2v}, C_{2h}, C_{3v}-Explanation of a Character Table.

2. Applications of Group Theory 08 hrs

Standard reduction formula relating reducible and irreducible representations-Hybridization schemes for atoms in molecules of different geometry, AB_4 tetrahedral, AB_3 triangular planar, AB Linear molecules. Symmetries of vibrational modes in non-linear molecules (H_2O, NH_3 and BF_3), Symmetries of vibrational modes in linear molecules (HCN, CO_2, C_2H_2), Transition probability integral, Selection rules, symmetry and spin forbidden transitions.

Unit II

3. Microwave Spectroscopy 06 hrs

Rotations of molecules, rigid diatomic molecule, rotational energy expression, energy level diagram, rotational wave functions and their symmetry, selection rules, expression for the energies of spectral lines, computation of intensities, effect of isotopic substitution, centrifugal distortion and spectrum of a non-rigid rotor. Rotational spectra of poly atomic molecule-linear, symmetric top and asymmetric top molecules; Stark effect, techniques and instrumentation

Unit III

4. Infrared Spectroscopy 12 hrs

Vibrations of molecules, harmonic and anharmonic oscillators-vibrational energy, selection rules, expression of energies of spectral lines, computation of diatomic vibrating rotor, Born-Oppenheimer approximation, vibrational rotational spectra of diatomic molecules, P, Q and R branches, breakdown of the Born-Oppenheimer approximation.

Vibrations of poly atomic molecules: Normal coordinates translations, vibrations and rotations, vibrational energy levels and wave functions, fundamentals, overtones and combinations.

Vibration-rotation spectra of poly atomic molecules, parallel and perpendicular vibrations of linear and symmetric top molecules,
Techniques and instrumentation, FTIR

5. Raman Spectroscopy **07 hrs**

Classical theory of the Raman effect, polarizability as a tensor, polarizability ellipsoids, quantum theory of the Raman effect, Pure rotational Raman Spectra of Linear and asymmetric top molecules, vibrational Raman Spectra, Raman activity of vibrations, rule of mutual exclusions, rotational fine structure, O and S branches, Polarization of Raman scattered photons. Structure determination from Raman and IR spectroscopy-AB_2 and AB_3 molecules, Techniques and instrumentation

Unit IV

6. Electronic Spectroscopy **12 hrs**

Vibrational coarse structure, intensities by Franck-Condon principle, Dissociation energy, rotational fine structure, Fortrat diagram, pre-dissociation
Electronic structure of diatomic molecules- basic results of MO theory, classification of states by electronic angular momentum-σ, π, δ and ϕ molecular orbitals, selection rules, spectrum of singlet and triplet molecular hydrogen
Electronic spectra of polyatomic molecules- localized MOs, spectrum of HCHO, change of shape on excitation
Decay of excited states- radiative (fluorescence and phosphorescence) and non-radiative decay, internal conversion

References

1. Chemical Applications of Group theory, F. A. Cotton, Wiley Eastern (1976).
2. Symmetry and Spectroscopy of molecules, K. Veera Reddy, 2 Ed., New Age Science Ltd (2009).
3. Group Theory in chemistry, M.S. Gopinathan and V. Ramakrishnan, Vishal Publishing Co., (1988).
4. Molecular Symmetry, D. S. Schonland, Van Nostrand (1965)
5. Introduction to Molecular Spectroscopy, C. N. Banwell, TMH Edition (1994)
6. Introduction to Molecular Spectroscopy, G. M. Barrow, McGraw Hill, Int. Studens Edition (1988)
7. Molecular Spectroscopy, J. D. Graybeal, McGraw Hill, Int. Studens Edition (1990)
8. Basic principles of spectroscopy, R. Chang, New Jersy, Englewood Cliffs (1978)
9. Spectroscopy vol. 1,2,3 B. P. Straughan and S. Walter, New York and London (1976)
10. Vibrational Spectroscopy, D.N. Satnarayana, New Age Publishers, Latest edition

<u>JOC 205: Biomolecular Chemistry (Soft Core)</u>

Objectives:
This course aims to impart to the student, knowledge of:

- The structure, nomenclature, reactivity, synthesis and reactions of heterocyclic compounds.
- Heterocyclic structures in biologically active compounds.
- Synthesis and design of biologically active compounds derived from heterocyclic compounds.
- Biologically important molecules and their monomers.
- Various aspects of the principles of organic chemistry in the structure, classification, nature of bonding and functions of bio-molecules.
- Structural elucidation of bio-molecules and steps involved in their chemical synthesis and reactions.

Learning Outcomes:
On completion of the course, the student should be able to:

- Classify heterocyclic compounds based on the characteristics of the heteroatom and explain their reactivity and properties.
- Correlate how the structure of bio-molecules determines their chemical properties and reactivity.
- Design new methods for synthesis of bio-molecules using principles and reagents learned.

Syllabus:

Unit I

1. Heterocyclic compounds – I **06 hrs**

Nomenclature of heterocyclic compounds, Structure, reactivity, synthesis and reactions of pyrazole, imidazole, oxazole, isoxazole, thiazole, isothiazole, pyrimidine and purine; Preparation and reactions (Nucleophilic and Electropholic) of quinoline, isoquinoline, indole and coumarins.

2. Heterocyclic compounds – II **02hrs**

Anthocyanins: Basic structural features of chromones, flavones and isoflavones. Synthesis of quercetin and wedelolactone.

Unit II

3. Carbohydrates **06 hrs**

Determination of configuration of the monosaccharides; General reactions of monosaccharides (glucose and fructose); Conformational analysis of glucose and galactose. Synthesis of aldonic, uronic, aldaric acids and alditols.
Polysaccharides: Determination of molecular weights, Structural elucidation of sucrose and maltose; Structures of starch and cellulose; Photosynthesis of carbohydrates.

4. Vitamins **06 hrs**

Biological importance and synthesis of vitamins A, B_1 (thiamine), B_6 and its interconversion (pyridoxine), C, E(α-tocopherol), H(biotin), K_1, K_2, folic acid, pantothenic acid and riboflavin.

Unit III

5. Amino acids and Peptides **08 hrs**

Synthesis and reactions of amino acids, Classification and nomenclature of peptides, Sanger and Edman methods of sequencing, Cleavage of peptide bond by chemical and enzymatic methods. Peptide synthesis: Protection of amino group (Boc-, Z- and Fmoc-) and carboxyl group as alkyl and aryl esters. Use of EEDQ, HOBt and active esters, acid halides, anhydrides in peptide bond formation reactions. Deprotection and racemization in peptide synthesis. Solution and solid phase techniques, Structure of oxytocin, gramicidin, enkephalins, LH-RH, Introduction to peptidomimetics

6. Nucleic Acids **04 hrs**

Introduction, components of nucleic acids, nucleosides, nucleotides. Base pairing in DNA (C-G, A-T). Methods of protection for hydroxy group in sugar and phosphate functions. Methods of formation of internucleotide bonds: phosphodiester approach, phosphotriester approach, phosphite triester and phosphoramidite methods. Solid phase synthesis of dinucleotides.

Unit IV

7. Metabolism of lipids **04 hrs**

Ketone Bodies: Ketogenesis, utilization of ketone bodies, Biosynthesis of fatty acids, Lipoproteins: structure and classification.

References

1. Organic Chemistry, Volumes I and II, I L Finar, Longman, (1999).
2. Peptides Chemistry: A practical text book, M. Bodansky, Springer-Verlag NY, 1988.
3. Heterocyclic Chemistry, Vols. 1-3, R. R. Gupta, M. Kumar and V. Gupta, Springer Verlag.
4. Heterocyclic Chemistry, J. A. Joule, K. Mills and G. F. Smith, Chapman and Hill.
5. Heterocyclic Chemistry, T. L. Gilchrist, Longman Scientific Tech.
6. Comprehensive Heterocyclic Chemistry, A. R. Katritzky and C. W. Rees, Eds. Pergamon Press.
7. Heterocyclic Chemistry, Raj K. Bansal, 5^{th} Edition, (2010).
8. Biochemistry, U. Satyanarayana and U. Chakrapani, Fourth Edition, 2014.
9. Textbook of Medical Biochemistry, M. N. Chatterjea and Rana Shinde, 8^{th} Edition, 2012.
10. Organic Chemistry, Paula Y. Bruce, 7^{th} Edition, 2014.
11. Natural Products Chemistry, jagadamba singh, S. M. Ali, jaya Singh, 1^{st} Edition, (2010).
12. Organic Chemistry, Natural Products, Vol I & II, O. P. Agarwal, 36^{th} Edition (2009).

<u>JOC 206: Inorganic Chemistry Practicals - III</u>

Objectives:

This course aims to impart to the student, knowledge of:

- Basic and advanced techniques required for the separation of metal ions of a binary mixture.
- Techniques of gravimetric estimation of ions.

Learning Outcomes:

On completion of the course, students should be able to:

- Outline a protocol and carry out separation of metal ions in a mixture
- Carry out the gravimetric estimation of a metal ion.
- Solve problems encountered during an analysis.
- Report the results of the experiment.

Syllabus:

Quantitative gravimetric analysis

a) Gravimetric determination of Fe in an iron ore as Fe_2O_3.
b) Gravimetric determination of Ni in a mixture of Cu and Ni solution.
c) Gravimetric estimation of Cu in a mixture of Cu and Fe solution.
d) Gravimetric estimation of Cu in a mixture of Cu and Zn solution.
e) Gravimetric estimation of Ni in a mixture of Ni and Zn solution.
f) Gravimetric estimation of Cu in German silver.
g) Gravimetric estimation of Ni in Steel.
h) Gravimetric estimation of Sn in Solder.

References

1. Vogel's Text Book of Qualitative Chemical Analysis, J. Bassett, G.H. Jeffery and J. Mendham, ELBS (1986).
2. Vogel's Text Book of Quantitative Chemical Analysis, J. Bassett, G.H. Jeffery, J. Mendham and R.C. Demmy, 5th Edition, Longman Scientific and Technical (1999).

JOC 207: Inorganic Chemistry Practicals - IV

Objectives:

This course aims to impart to the student, knowledge of:

- Basic and advanced techniques required for the separation of metal ions of a binary mixture
- Volumetric techniques of quantitative analysis of metal ions

Learning Outcomes:

On completion of the course, students should be able to:

- Outline a protocol and carry out separation of metal ions in a mixture
- Carry out the volumetric estimation of a metal ion
- Solve problems encountered during an analysis
- Report the results of the experiment in written and verbal form

Syllabus:

Quantitative volumetric analysis

a) Volumetric estimation of Cu in a mixture of Cu and Ni solution.
b) Volumetric estimation of Fe in a mixture of Cu and Fe solution.
c) Volumetric estimation of Zn in a mixture of Cu and Zn solution.
d) Volumetric estimation of Zn in a mixture of Ni and Zn solution.
e) Volumetric estimation of Zn in German silver.
f) Volumetric estimation of Fe and Cr in Steel.
g) Volumetric estimation of Pb in Solder.

References

1. Vogel's Text Book of Qualitative Chemical Analysis, J. Bassett, G.H. Jeffery and J. Mendham, ELBS (1986).
2. Vogel's Text Book of Quantitative Chemical Analysis, J. Bassett, G.H. Jeffery, J. Mendham and R.C. Demmy, 5th Edition, Longman Scientific and Technical (1999).

JOC 208: Physical Chemistry Practicals - III

Objectives:

This course aims to impart to the student mastery over

- The use of a conductivity meter for determination of specific conductance and solubility of electrolytes
- The use of conductivity meter for titrations (acid base, redox, precipitation).
- Plotting of data in two dimensions and identifying the end point of the titration

Learning Outcomes:

On completion of the course, students should be able to:

- Use the conductivity meter as a tool for quantitative analysis
- Use conductivity measurements to distinguish between electrolytes (strong and weak)
- Identify problems where conductivity measurements can be used and devise protocols for the experiment.
- Carry out an experiment based on the protocol and find solutions to problems encountered during the experiment

- Report the results of the experiment in written and verbal form

Syllabus:
Conductometry

1. Determination of solubility of sparingly soluble salt.
2. Titration of mixture of strong and weak acids against strong base.
3. Titration of mixture of strong acid, weak acid and salt (copper sulphate) against strong base
4. Titration of weak acid against weak base.
5. Precipitation titration: lithium sulphate against barium chloride.
6. Dissociation constant of weak electrolyte (weak base-NH_4OH; weak acid-CH_3COOH).
7. Verification of Onsagar's equation – determination of λ_0 of an electrolyte.

References

1. Advanced Practical Chemistry by J.B. Yadav, Goel Publication House, Merrut (1989).
2. Experiments in Physical Chemistry by Shoemaker and Garland, McGraw Hill International edn. (1996).
3. Experimental Physical Chemistry, V.D. Athawale and Parul Mathur, New Age International, New Delhi (2001).

<u>JOC 209: Physical Chemistry Practicals - IV</u>

Objectives:
This course aims to impart to the student mastery over the

- The working, calibration and use of a potentiometer.
- The use of different reference and working electrodes.
- Methodology of a potentiometric titration for different classes of reactions: acid base, redox, precipitation.

Learning Outcomes:
On completion of the course, students should be able to:

- Use the potentiometer as a tool for quantitative analysis
- Identify problems where potentiometry measurements can be used and devise protocols for the experiment.
- Carry out the experiment based on the protocol and solve problems encountered during the experiment
- Report the results of the experiment in written and verbal form

Syllabus:
Potentiometry

1. Determination of single electrode potential of Cu^{2+}/Cu and Zn^{2+}/Zn and testing the validity of Nernst equation.
2. Determination of pH of buffers by using quinhydrone electrode and comparison of the pH values obtained with glass electrode.
3. Potentiometric titration of ferrous ammonium sulphate against potassium dichromate - calculation of formal redox potential of Fe^{3+}/Fe^{2+}.
4. Potentiometric titration of potassium iodide against potassium permanganate.
5. Titration of silver nitrate against potassium chloride.
6. Determination of EMF of a concentration cell and calculation of solubility product of AgCl.
7. Titration of weak acid against strong base using quinhydrone electrode and calculation of pKa value of the weak acid.
8. Titration of a mixture of HCl and CH_3COOH potentiometrically and determination of the composition of the mixture.

References

1. Advanced Practical Chemistry by J.B. Yadav, Goel Publication House, Merrut (1989).
2. Experiments in Physical Chemistry by Shoemaker and Garland, McGraw Hill International Ed. (1996).
3. Experimental Physical Chemistry, V.D. Athawale and Parul Mathur, New Age International, New Delhi (2001).

III Semester

Sl. No.	Code No.	Title	Theory / practical hours / Week	Duration of Examination Hours	Maximum Marks for ESE	CIA	Total Marks	Total No. of credits
1.	JOC 301	Organic Reaction Mechanisms	4	3	70	30	100	4
2.	JOC 302	Organic Spectroscopy	4	3	70	30	100	4
3.	JOC 303	Chemistry of Natural Products	4	3	70	30	100	4
4.	JOC 304	Open Elective*	4	3	70	30	100	4
5.	JOC 305	Organic Chemistry Practical – I	4	4	35	15	50	2
6.	JOC 306	Organic Chemistry Practical – II	4	4	35	15	50	2

7.	JOC 307	Organic Chemistry Practical – III	4	4	35	15	50	2
8.	JOC 308	Organic Chemistry Practical – IV	4	4	35	15	50	2
					420	**180**	**600**	**24**

*Non-chemistry paper

- **Theory (each paper)**

Maximum Marks (Examination): **70**
Marks for Internal Assessment: **30** *(Continuous evaluation)*

Scheme for Internal Assessment

Attendance: 05 Marks
Seminar: 05 Marks
Test: 20 Marks
Total: 30 Marks

* Seminars to be conducted every semester.

- **Practical (each paper)**

Maximum Marks (Examination): **35**
Marks for Internal Assessment: **15** *(Continuous evaluation)*

Scheme for Internal Assessment

Attendance: 03 Marks
Record book: 02 Marks
Prefinal: 10 Marks
Total: 15 Marks

Record book for the Practical has to be assessed as internal assessment. There should be no marks for record book during Practical Examination.

JOC 301: Organic Reaction Mechanisms

Objectives:

This course aims to impart to the student, knowledge of:

- Evidences for the mechanisms of substitution reactions.
- Factors affecting rate of substitution reaction.
- Formation, structure, stability, reactivity and reactions of free radicals.
- Principles and terminologies in photochemistry and photochemical reactions
- Molecular orbital diagram and conservation of orbital symmetry.
- Pericyclic reactions, rules governing them and their applications.

Learning Outcomes:

On completion of the course, the student should be able to:

- Explain the mechanistic pathway for aliphatic substitutions and free radical reactions with stereochemistry.
- Describe and explain photochemical and photophysical processes with mechanisms, and apply established experimental methods for the investigation of these processes.
- Predict and rationalise the outcomes of pericyclic reactions with stereochemistry.

Syllabus:

UNIT I

1. Aliphatic Nucleophilic and Electrophilic Substitution Reactions 11 hrs

Aliphatic Nucleophilic substitution reactions: Substitution at allylic, vinylic and trigonal carbon atoms; Hydrolysis of esters- mechanisms; Neighbouring group participation; selected reactions: Von Braun reaction, Dieckmann condensation and Williamson reaction

Aliphatic electrophilic substitution reactions: S_E1, S_E2 and S_Ei mechanisms - Effect of structure, leaving group, attacking nucleophile and solvent, selected reactions; Migration of double bonds; Halogenation of aldehydes, ketones and acids; Aliphatic diazonium coupling, nitrosation at carbon and nitrogen, diazo transfer reactions, carbene and nitrene insertion, decarboxylation of aliphatic acids, haloform reactions, Haller-Bauer reaction

2. Free Radical Chemistry 03 hrs

Generation of free-radicals: Thermal homolysis of peroxides, peresters and azo compounds, photochemical methods.

Hydrogen abstraction, chain process - stability - steric, resonance and hyperconjugative effects and stereochemistry of free radicals

UNIT II

3. Free Radical Reactions 05 hrs

Addition, Substitution, elimination, rearrangement and electron transfer reactions; Neighbouring group assistance in free radical reactions; Reactivity for aliphatic substrates, reactivity at a bridgehead, reactivity in aromatic substrates; Use of free radicals in organic synthesis

Orton reaction, Gomberg-Bachmann reaction, Meerwein arylation, Sandmeyer reaction, Kolbe reaction and Hunsdiecker reaction

4. Photochemistry 12 hrs

General consideration: Activation in thermal and photochemical reactions; Light absorption and excitation, Singlet and triplet states; Morse curve, Frank – Condon principle

Deexcitation: Physical process, Jablonski diagram (basic and modified), Photosensitization (donor acceptor concept); Chemical process, quantum efficiency - quantum and chemical yields

Photochemistry of functional groups:

i) Olefins: Cis-trans isomerism, [2+2] Cycloaddition, rearrangements. Reactions of conjugated olefins, di-π methane rearrangement
ii) Ketones: Excited state of C=O. Norrish type-I and type- II cleavages. Paterno-Buchi reaction; α,β unsaturated ketones. [2+2] addition, cis-trans isomerisation, rearrangements of cyclohexadienones
iii) Aromatic compounds: Photo rearrangement of benzene and its derivatives and cycloaddition of benzene
iv) Photochemical oxidations and reductions: Cycloaddition of singlet molecular oxygen; Oxidative coupling of aromatic compounds and photoreduction by hydrogen absorptions.

UNIT III

5. Pericyclic reactions **11 hrs**

Molecular orbital symmetry, frontier orbitals of ethylene, 1-3 butadiene, 1,3,5-hexatriene and allyl system; Classification of pericyclic reactions; Woodward-Hoffmann correlation diagrams; FMO and PMO approach

Electrocyclic reactions: conrotatory and disrotatory motions. 4n, [4n+2] and allyl systems

Cycloadditions: antarafacial and suprafacial additions [$_{\pi}m_s$+$_{\pi}n_a$] and [$_{\pi}m_s$+$_{\pi}n_s$] cycloadditions; [$_{\omega}2_a$ + $_{\pi}2_s$] and [$_{\pi}4_s$ + $_{\omega}2_s$] cheletropic reactions; regio, enantio and endo selectivities in Diels-Alder reactions; Hetero Diels-Alder reaction

Sigmatropic rearrangements: suprafacial and antarafacial shifts of H, sigmatropic shifts involving carbon moieties. [*i, j*]- sigmatropic rearrangements (including Walk, Claisen, Cope, oxy and aza-Cope rearrangements).

UNIT IV

6. Biochemical mechanisms **10 hrs**

Introduction: The mechanistic role of the following in living systems:

i) Thiamine pyrophosphate (TPP) in decarboxylation of α-ketoacids and in the formation of α-ketols
ii) Pyridoxal phosphate (PLP) in transamination, decarboxylation, dealdolisation and elimination reactions of amino acids
iii) Lipoic acid in the transfer of acyl group reactions
iv) Coenzyme A (CoASH) in the transfer of acyl group
v) Biotin in the carboxylation reactions
vi) Tetrahydrofolic acid in one- carbon transfer reactions
vii) Vitamin B_{12} coenzymes in molecular rearrangement reactions and in the synthesis of methionine and methane
viii) Nicotinamide in biological redox reactions
ix) Flavin coenzymes in biological redox reactions
x) Vitamin KH_2 coenzyme in carboxylation reactions

References

1. Introduction to Organic Chemistry, A. Streitweiser.Jr. and C.H. Heathcock, Macmillan 1998.
2. Physical and Mechanistic Organic Chemistry, R.A.Y. Jones, 1st Ed. Cambridge Univ. Press, 1979.
3. P.J. Garratt in Comprehensive Organic Chemistry, D. Barton and W.D. Ollis 1st Edition, Pergamon Press, Oxford, 1979.
4. Mechanisms of Molecular Migrations, Vol I and II, B.S. Thiagarajan, 1st Edition, Pergamon Press, Oxford, 1979.
5. Radicals in Organic Synthesis, B. Giese, Pergamon Press, 1986.
6. Stereoelectronic effects in Organic Chemistry, P. Deslongchamps, 1st Edition, Pergamon Press, 1983.
7. Frontier Orbitals and Organic Chemical Reactions, Ian Fleming, Oxford University Press, 1980.
8. Molecular Orbital Theory for Organic Chemistry, A. Streitweiser, 1st Edition, Wiley & sons, NY 1969.
9. Organic photochemistry, J.M. Coxon and B. Halton, 1st Edition, Cambridge Univ. Press, London 1974.
10. Orbital symmetry, R.E. Lehr and A.P. Marchand, Academic Press, 1972.
11. Molecular reactions and photochemistry, C.H. Deputy and D.S. Chapman, 1st Edition, Prentice-Hall India, New Delhi, 1972.
12. Advanced Organic Chemistry, Jerry, March 4th Ed, John Wiley and sons, 1999.
13. Bio chemistry, G. Zubey, Macmillan, NY, 1998.
14. Bio chemistry, D. Voet and J.G. Voet, John Wiley and sons, 1998.
15. Principles of Biochemistry, A.L. Lehninger, D.L. Nelson and M. M. Cox, 2nd Edition, Worth Publishers, NY 1999.

JOC 302: Organic Spectroscopy

Objectives:

This course aims to impart to the student, knowledge of:

- Spectroscopic techniques including the basic principles for recording of NMR, IR, UV, and MS spectra.
- Applications of UV-Vis spectroscopy.
- Identification and characteristics of functional groups using IR spectroscopy.
- Principles of nuclear magnetic resonance spectroscopy of ^{1}H, ^{13}C (1D and 2D) and other nuclei (^{15}N, ^{19}F, ^{29}Si and ^{31}P).
- Fragmentation pattern, effect of isotopes in Mass spectroscopy.

Learning Outcomes:

On completion of the course, the student should be able to:

- Combine information from experimental NMR, IR, UV, and MS spectra and elucidate the structure of unknown organic compounds.
- Argue for a suggested molecular structure from analysis of the spectral data.
- Predict the NMR, IR, UV-Vis and MS spectra from a given molecular structure.

Syllabus:

UNIT I

1. Ultraviolet and visible spectroscopy **03 hrs**

Classification of electronic transitions, terminology, substituent and solvent effects, UV spectral study of alkenes, polyenes, enones and aromatic compounds; Empirical rules for calculating λ_{max} in conjugated dienes, aromatic hydrocarbons and α,β-unsaturated carbonyl compounds

2. Vibrational Spectroscopy **09 hrs**

Sampling techniques, Group frequencies, factors affecting group frequencies, Bond order, Mass effect, Conjugation, Inductive, resonance, steric effects and Intramolecular interactions. Application of IR in the study of H-bonding, stereoisomerism and tautomerism. Complimentarity of IR and Raman spectroscopy.

Identification of the following organic functional groups by IR: Alkanes, Alkenes, Alkynes, Aromatic compounds, Aldehydes, Ketones, Alcohols, Acids, Acid chlorides, Amides, Amines, Esters, Halides, Nitro compounds. Problems using UV and IR.

UNIT II

3. Nuclear magnetic resonance spectroscopy **15 hrs**

Introduction, Magnetic properties of nuclei-Resonance condition, basic NMR equation. Nuclear spin, population of nuclear spin levels and NMR isotopes, Relaxation methods. Instrumentation and sample handling, FT-NMR

Chemical shift- Mechanism of shielding and deshielding in Alkanes, Alkyl halides, Alkenes, Aromatic compounds, Carbonyl compounds and Annulenes; Diamagnetic and paramagnetic effects and magnetic anisotropy; Equivalence of protons-chemical and magnetic equivalence; Spin-systems: First order and higher order coupling. First order splitting rules, Pascal's triangle-low and high resolution, spectrum of ethanol. Simplifications of complex spectra; Problems.

Spin-spin interactions- AX, AX_2, AX_3, AMX, AB types; Vicinal, geminal and long range coupling-Spin decoupling. Chemical shift reagents and deuterium exchange. Stereochemistry and hindered rotations; Karplus Curve, Temperature effects.

CIDNP, Nuclear Overhauser Effect (NOE). Factors influencing coupling constants and Relative intensities. Protons attached to elements other than carbon.

UNIT III

4. ^{13}C NMR and Correlation Spectroscopy **10 hrs**

^{13}C NMR Spectroscopy- Types of CMR spectra-undecoupled, broad band decoupled, Off-resonance decoupled. Selectivity decoupled and gated decoupled spectra. ^{13}C chemicals shifts of Alkanes, Alkyl halides, Alkenes, Alcohols, Ethers, Carbonyl compounds and aromatic compounds. Factors affecting the chemical shifts. Applications of ^{13}C NMR Spectroscopy in confirmation of structure; Introduction to 2D-NMR Pulse sequences. FT-Methods. Classification of 2D Experiments. 2D-J-resolved spectroscopy. HOMO and HETERO-2D-J-Resolved spectra. Correlation Spectroscopy (^{1}H-^{1}H). (^{13}C-^{13}CJ)-INADEQUATE, and heteronuclear (^{13}C-^{1}H) couplings. DEPT. Applications in structure elucidation of simple organic molecules.
Dynamic NMR, NMR spectroscopy of other nuclei with spin I = ½. Introduction to **^{15}N, ^{19}F,^{29}Si** and**^{31}P** NMR spectroscopies; Chemical shift values for **^{15}N, ^{19}F, ^{29}Si** and**^{31}P** containing compounds.

UNIT IV

5. Mass spectrometry **08 hrs**

Basic principles-instrumentation – ion production-ion analysis-magnetic sector instruments-Quadrapole mass spectrometers; Time of flight mass spectrometers; ion cyclotron resonance spectrometers- Mass spectrum-molecular ion-types of ions in mass spectra and effects of isotopes on mass spectra. Methods of ionization, EI, FAB mass and MALDI methods; Fragmentation of: Alkanes, Alkenes, alkyl halides, alcohols, aldehydes, ketones, acids, esters, ethers, amines, nitro and halo compounds Nitrogen rule, Factors affecting cleavage patterns
McLafferty and McLafferty+1 rearrangment. Determination of molecular formula. Composite problems. Use of HRMS to determine exact molecular formulae of compounds

6. Problems based on Spectral Data **07 hrs**

Application of NMR and MS methods and chemical reactions in structure elucidation of organic compounds.

References

1. Applications of Absorption Spectroscopy to Organic compounds, J.R. Dyer, Prentice- Hal, New Delhi, 1969.
2. Organic Spectroscopy, P. Laszlo and P. Stang, Harper &Row, New York, 1971.
3. Organic Spectroscopy, W. Kemp, ELBS London, 2000.
4. Spectrometric Identification of Organic Compounds, R.M. Silverstein and W.P. Weber, 2005.
5. Introduction to Spectroscopy, 3rd Edition, D.L. Pavia, G.M. Laupman and G.S. Kriz, Harcourt College Publishers, 2001.
6. Organic Mass Spectroscopy, K.R. Dass & E.P. James, IBH New Delhi, 1976.
7. Interpretation of Organic Mass Spectra, F.W. McLafferty, W.A. Benjamin, London, 1973.
8. Practical Organic Spectroscopy, 2nd Ed. J.R. Chapman, John Wiley, NY, 1993.

9. The IR Spectra of Complex Molecules, Vol. I & II, L.J. Bellamy, Chapman and Hall, London 1975.
10. Spectroscopic Techniques for Organic Chemists, J.W. Cooper, John Wiley, NY, 1980.
11. Biomolecular NMR Spectroscopy, JNS Evans, Oxford Univ., 1995.
12. Mass Spectrometry-a foundation course, K. Downard, RSC, Cambridge, 2004
13. Mass Spectrometry of Organic Compounds, H. Budzkiewicz, Djerassic and D.H. Williams, Holden Day, NY, 1975.
14. Modern NMR Techniques and Their Applications, Ed. A.I. Popou, Marcel Dekker, 1991.
15. Modern Structural Theory of Organic Compounds, L.N. Ferguson, Prentice-Hall, New Delhi, 1973.
16. Fundamentals of Molecular Spectroscopy, 4^{th} Edn., C.N. Banwell and E.M. McCash, Tata McGraw – Hill, New Delhi, 1999.
17. Instrumental Methods of Analysis, H.H. Williard, L.L. Merrit, I.A. Dean and F.A. Settle, CBS Publishers and Distributors, 1986.

JOC 303: Chemistry of Natural Products

Objectives:
This course aims to impart to the student, knowledge of:
- Classification, nomenclature, structure, biosynthesis, occurrence, analysis and pharmaceutical perspectives of natural products.
- Structural elucidation of these natural products by elemental analysis and characterization by different spectroscopic techniques.
- Industrial synthesis of these natural products with stereochemistry and separation techniques.
- Classification, synthesis and use of insect pheromones used in pest control.

Learning Outcomes:
On completion of the course, the student should be able to:
- Understand extraction and purification methods of natural compounds from available sources.
- Design efficient total synthesis of complex molecules by recognizing substructures amenable to known transformations.
- Familiarize with various types of natural products from different sources and their applications.

Syllabus:

UNIT I

1. Terpenoids and Carotenoids **11 hrs**

Classification, nomenclature, occurrence and isolation; Isoprene rules; Stereochemistry of citral, farnesol, limonene, 1,8-cineole, menthols and borneols; Correlation of configuration of terpenoids. Structural elucidation of α-pinene, camphene, β-caryophyllene, α-santonin and gibberrillic acid

Synthesis and biosynthesis of: Linalool, α-terpeneol, fenchone, eudesmol and abietic acid. Commercial synthesis of camphor, Biosynthesis of squalene and cyclisation of squalene into α-lanosterol

Carotenoids: methods of isolation, structural relationship of α-, β- and γ-carotenes. Structural elucidation and synthesis of β-carotene

UNIT II

2. Steroids **12 hrs**

Occurrence, nomenclature, basic skeleton, Diels hydrocarbon and stereochemistry, isolation, structure and structural elucidation of sterols and bile acids, sex hormones, cortico-steroids; synthesis of cholestrol, estrone, progesterone, epiandrosterone, testosterone; Photo products of ergosterol - Vitamin D; Barton reaction for the synthesis of aldosterone; Marker degradation; Brief discussion of (dl) norgestrel and ethinyl oestradiol; Manufactures as applicable

UNIT III

3. Alkaloids **10 hrs**

Definition, Nomenclature, Occurrence, isolation, classification, general methods of structural elucidation

Synthesis and biosynthesis of: Ephedrin, hygrine, coniine, cocaine, cinchonine and morphine, Structural elucidation of papaverine, reserpine and ergotamine

Photochemical synthesis of Nuciferine and tylophorine

4. Insect Pheromones: **05 hrs**

Introduction, Classification, Pheromones in pest control

Synthesis of (One synthesis should be stereoselective):

- i) Grandisol (component of boll weevil pheromone)
- ii) Farenal (trail pheromone of pharaoh's ants)
- iii) Brevicomin (pheromone from Dendroitis brevicomis)
- iv) (+) – Disparlure (gypsy moth sex pheromone)
- v) 3,11-dimethyl-1,2-nonacosanone (pheromone of German Cockroaches)
- vi) Bombykol (sex pheromone of silkworm moth)
- vii) Multistriatin (Elm bark beetle sex pheromone)

UNIT IV

5. Porphyrins and Vitamin B_{12} **07 hrs**

Structural elucidation and synthesis of haemin and chlorophyll - a, Vitamin B_{12} (synthesis from cobyric acid only)

6. Prostaglandins, Prostacyclins and thromboxanes 07 hrs

Introduction, Nomenclature, classification and biological role of prostaglandins, prostacyclins and thromboxanes; Structural elucidation and stereochemistry of PGE_1 PGE_2 and PGE_3; Synthesis of PGE_1 and PGE_2 by Corey's and Stork's approaches, PGE_3 by Upjohn's approach; synthesis of prostacyclin I_2 and thromboxane B_2

References

1. Natural Products: Their Chemistry and Biological Significance- J. Mann, R.S. Davidson, J.B. Hobbs, D.V. Banthorpe & J.B. Harbone, Longman, UK, 1994.
2. Terpenes, J. Verghese, Tata McGraw- Hill, New Delhi, 1982.
3. Chemistry of Terpenes and Terpenoids, A. Newman, Academic Press, London, 1975.
4. Handbook of Naturally Occurring Compounds Vol II: Terpenes, T.K. Davon, A.I. Scott, Academic Press NY, 1972.
5. Natural Products Chemistry Vol I Vol II, K. Nakanishi, T. Goso, S. Ito, S. Natori & S. Nozoe, Academic Press, NY, 1974.
6. Total Synthesis of Natural Products Vol I & VI, Apsimon, John Wiley, NY, 1973-1981.
7. Organic Chemistry Vol II, I.L. Finar, 6^{th} Ed. Longman,1992
8. Chemistry of Natural Products Vol I & II, O.P. Aggarwal, Goel Publishing house, 6^{th} edn. 1982.
9. Total Synthesis of Steroids, Akhaun & Titov, Jerusalem, 1969.
10. Medicinal Natural products: A biosynthetic approach, P.M. Dewick, John Wiley, Chichester, 1997.
11. The Colours of Life, An introduction to the chemistry of porphyrins and related, L.R. Milgrom, Wiley Chichester, 1995.
12. Interpretation of the UV Spectra of Natural Products, A.I. Scott, Pergamon Press, Oxford, 1964.
13. Spectral Data of Natural Products, Vol.I, K. Yamaguchi, Elsevier publishing Co., London, 1970.
14. Chemistry of Natural Products: A Unified Approach, N.R. Krishnaswamy, University Press, India, 1999.
15. Organic Chemistry Vol I & II, I.L. Finar Longman, 1999.

JOC 304: Chemistry in Daily Life (Open Elective for Non-Chemistry students)

Objectives:

This course aims to impart to the student, knowledge of:

- Basis of thermal energy technologies those are common for combustion and fuels.

- Different types of corrosion and principles and applications of primary and secondary batteries and fuel cell.
- Air pollution, its adverse effects and preventive measures to control and reduce it.
- Hydrological cycle, and tests and parameters for water analysis.
- The composition and analysis of dairy products and beverages, importance of food additives, preservatives, artificial food sweeteners, flavors and colorants.
- Methods of applying dyes to the fabric, types of paints and distempers, nanomaterials and their applications in energy storage devices, sensors and medicines.

Learning Outcomes:

On completion of the course, the student should be able to:

- Identify problems of plastic waste management and how to address this issue.
- Recognise the ongoing role of combustion, both of fossil and bio-fuels, in providing a more sustainable energy source for society, and the environmental challenges to be met to achieve this.
- Have a better understanding of air and water pollution and be aware of effective methods of mitigation.
- Be aware of the different standards of water quality and have a basic understanding of the tests to determine the same.
- Advantages & disadvantages of beverages, food additives, preservatives, artificial food ingredients, applications of dyes, paints and nanomaterials in various fields.

Syllabus:

UNIT I

1. Dairy Products **02 hrs**

Composition and properties of milk. Milk processing, milk products (skimmed milk, cream, butter, cheese, ghee). Analysis of fat content, minerals and micro-organisms in milk. Estimation of added water in milk.

2. Beverages, food additives and preservatives **03 hrs**

Composition and types of coffee and tea. Analysis of caffeine in coffee and tea, composition of soft drinks, Alcoholic beverages- Wine, Beer.

Introduction and importance of food additives and preservatives, Uses of sodium benzoate, sorbates. Adulterants and contaminants in spices.

3. Artificial sweeteners, flavours and food colourants **02 hrs**

Introduction and importance of sweeteners, flavours and colourants in food. Permitted colorants. Use of Aspartame, saccharin, Vanillin and monosodium glutamate, Erythrosine and sunset yellow FCF.

4. Dyes & Paints **03 hrs**

Classification of dyes. Methods of applying dyes to the fabrics using azo dyes, Mordant brown, Congo red and methyl orange. Paints and distempers: Requirement of a good paint. Solvents and thinners for paints. Emulsions, latex; luminescent paints. Fire retardant paints and enamels.

5. Nanomaterials **03 hrs**

Introduction and definition of nanoparticles, Properties of nanomaterials depending upon their size and shape; applications of nanomaterials in energy storage devices, sensors and medicines.

UNIT II

6. Air Pollution **03 hrs**

Air pollutants, prevention and control, Green house gases and acid rain. Ozone hole and CFC's. Photochemical smog and PAN. Catalytic converters for mobile sources. Bhopal gas tragedy.

7. Hydrological cycle **04 hrs**

Sources, criteria and standards of water quality - safe drinking water. Public health significance and measurement of water quality parameters - (Colour, turbidity, total solids, acidity, alkalinity, hardness, sulphate, flouride, phosphate, nitrite, nitrate, BOD and COD). Water purification for drinking and industrial purposes.

8. Toxic chemicals **03 hrs**

Toxic chemicals in the environment. Detergents- pollution aspects, eutrophication. Pesticides and insecticides-pollution aspects. Heavy metal pollution. Solid pollutants- treatment and disposal. Treatment of industrial liquid wastes. Sewage and industrial effluent treatment.

9. Composition of soil and fertilizers **03 hrs**

Inorganic and organic components in soil-micro and macronutrients. Classification of Fertilizers-Straight Fertilizers, Compound/Complex Fertilizers, Fertilizer Mixtures. Manufacture and general prosperities of Fertilizer products- Urea and DAP.

UNIT III

10. Carbohydrates **02 hrs**

Classification; sources and functions of glucose, fructose, galactose, maltose, lactose, sucrose, starch, cellulose

11. Proteins **02 hrs**

Introduction and composition of proteins, classification of amino acids, peptide bond, properties and structure of proteins, denaturation of proteins, nutritional importance.

12. Nucleic Acids **01 hr**

Introduction, components of nucleic acids, nucleosides, nucleotides, base pairing, DNA and RNA.

13. Vitamins **02 hrs**

Classification; Sources, functions and deficiency diseases of Vitamin A, Vitamin B, Vitamin C, Vitamin D, Vitamin E & Vitamin K.

14. Drugs **02 hrs**

Introduction and classification of drugs; Functions, mode of action and side effects of: antibiotics (pencillin V), analgesics (aspirin), anti-inflammatory agents (ibuprofen), cardiovascular drugs (amyl nitrite), antimalarials (chloroquine), antifertility drug (norethindrone)

15. Oils and fats **02 hrs**

Composition of edible oils, detection of purity, rancidity of fats and oil; Tests for adulterants: aregemone oil in mustard oil and mineral oil in edible oil.

16. Soaps & Detergents **02 hrs**

Types, cleansing property of soaps, difference between soaps and detergents

UNIT IV

17. Fuels **03 hrs**

Introduction, characteristics and classification of fuels; Chemical processing of petroleum; Cracking-thermal cracking fluidized catalytic cracking; Knocking of petrol and diesel and its prevention; Alternatives to petrol and diesel- power alcohol, biodiesel, biogas.

18. Principles of Reactivity **03 hrs**

Basis kinetic concepts, rates of simple and complex chemical reactions, empirical rate equations. Temperature dependence of rates and activation parameters. Le-Chatelier principle, Enzyme catalysed reactions.

19. Corrosion **02 hrs**

Types and prevention, corrosion failure and analysis

20. Chemical energy system **02 hrs**

Chemical energy system and limitations, principles and applications of primary& secondary batteries and fuel cell; Basics of solar energy; future energy store.

21. Polymers **03 hrs**

Types and classification of polymers. Source and general characteristics of natural and synthetic polymers. Typical examples of polymers used as plastics, in textiles, in electronic and automobile components, in the medical and aerospace materials. Problems of plastic waste management. Strategies for the development of environment friendly polymers.

References

1. B. K. Sharma, Introduction to Industrial Chemistry, Goel Publishing, Meerut (1998)
2. Medicinal Chemistry by Ashutosh Kar.
3. Drugs and Pharmaceutical Sciences Series, Marcel Dekker, Vol. II, INC, New York.
4. Chemical Analysis of Foods – H. E. Cox and Pearson.
5. Foods: Facts and Principles, N. Shakuntala Manay and S. Swamy, 4th Ed. New Age International (1998)
6. Nano: The Essentials- T. Pradeep, Tata McGraw Hill Education Private Limited, 2013.
7. Biochemistry- U. Satyanarayana, U. Chakrapani, 4th Ed. Elsevier, 2013.
8. Physical Chemistry - Peter Atkins and Julio de Paula – 7th Ed. 2002, Oxford University Press.
9. Handbook on Fertilizer Technology by Swaminathan and Goswamy, 6th ed. 2001, FAI.
10. Organic Chemistry by I.L. Finar, Vol. 1 & 2.
11. Polymer Science and Technology, J. R. Fired (Prentice Hall).

JOC 305: Organic Chemistry Practicals - I

Objectives:

This course aims to impart to the student, knowledge of:

- The principles of separation and qualitative analysis of binary mixture of mono- and bi-functional organic compounds.

Learning Outcomes:

On completion of the course, students should be able to:

- Carryout effective separation (pilot and bulk) of mixture of organic compounds.
- Determine the functional group of the unknown compounds by systematic analysis in a semi-micro scale.

Syllabus:

Qualitative analysis of binary mixtures:

Separation of a binary mixture of organic compounds and identification of the separated components by systematic qualitative organic analysis.

References

1. Semi-Micro Qualitative Organic Analysis, Cheronis, Entrikin and Hoanett

2. Laboratory Manual of Organic Chemistry- B.B. Dey, M.V. Sitaraman and T.R. Govindachari, Allied Publishers, New Delhi, (1996).
3. Practical Organic Chemistry-Mann and Saunders, (1980).
4. Text Book of Practical Organic Chemistry- A.I. Vogel, (1996).
5. A Handbook of Organic Analysis-Clarke and Hayes, (1964).
6. Comprehensive Practical Organic Chemistry: Qualitative analysis, V.K. Ahluwalia, S. Dhingra, Universities Press (India), 2000.
7. Advanced Practical Organic Chemistry, J. Mohan, Vol. I and II, Himalaya Publishing House, 1992.
8. Practical Organic Chemistry(Quantitative analysis), B.B. Dey, M V. Sitaraman and T.R. Govindachari , Allied Publishers, New Delhi, 1992.
9. Laboratory Techniques in Organic Chemistry, V.K. Ahluwalia, Pooja Bhagat and Renu Aggarwal, I.K. International Publishing House, New Delhi, 2005.
10. Intermediates for Organic Synthesis, V.K. Ahluwalia, Pooja Bhagat, Ramesh Chandra and Renu Aggarwal, I.K. International Publishing House, New Delhi, 2005.
11. Spot Tests in Organic Analysis, F. Feigl, 7th Ed. Elsevier, 2005.

JOC 306: Organic Chemistry Practicals - II

Objectives:

This course aims to impart to the student, knowledge of:

- Laboratory set up, safe handling of chemicals, workup procedures and effective disposal of organic waste.
- Various methods of preparing organic compounds in a single step.

Learning Outcomes:

On completion of the course, students should be able to:

- Design and carry out experiments, accurately record and analyze the results of such experiments.

Syllabus:

Single Step Preparations:

1. Cannizarro reaction: benzaldehyde.
2. Claisen-Schmidt reaction: acetone and benzaldehyde.
3. Sandmeyer reaction: p- chlorotoluene from p-toluidine.
4. Pechmann reaction: resorcinol and ethylacetoacetate.
5. Oxidation of cyclohexanol.
6. Preparation of S-benzylisothiuronium chloride.
7. Synthesis of acetanilide.
8. Synthesis of trans-stilbene.

9. Synthesis of 2,4-dichlorophenoxyacetic acid.
10. Synthesis of 1-bromo-2-naphthol from 2-naphthol.

References

1. Laboratory Manual of Organic Chemistry-B.B. Dey, M.V. Sitaraman and T.R. Govindachari, Allied Publishers, New Delhi, (1996).
2. Practical Organic Chemistry-Mann and Saunders, (1980).
3. Text Book of Practical Organic Chemistry- A.I. Vogel, (1996).
4. Test Book of Quantitative Organic Analysis-A.I. Vogel, (1996).
5. Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis, V.K. Ahluwalia, Renu Aggarwal, Universities Press (India), 2000.
6. An Advanced Course in Practical Chemistry, A. Ghoshal, B. Mahapatra and A.Kr. Nad, New central book agency, Calcutta, 2000.
7. Intermediates for Organic Synthesis, V.K. Ahluwalia, Pooja Bhagat, Ramesh Chandra and Renu Aggarwal, I.K. International Publishing House, New Delhi, 2005.

JOC 307: Organic Chemistry Practicals - III

Objectives:

This course aims to impart to the student, knowledge of:

- Quantitative estimation of organic compounds using various methods.

Learning Outcomes:

On completion of the course, students should be able to:

- Carry out quantitative analysis of organic compounds systematically.

Syllabus:

Quantitative analysis:

1. Determination of equivalent weight of dicarboxylic acids.
2. Estimation of glucose (Bertrand's method).
3. Estimation of carbonyl group.
4. Estimation of aromatic amines by acylation method.
5. Estimation of phenols by acylation method.
6. Estimation of nitro group by reduction method using $SnCl_2$.
7. Saponification value of oil.
8. Iodine value of oil (chloramine-T method).
9. Colorimetric estimation of cholesterol.

References

1. Test Book of Quantitative Organic Analysis-A.I. Vogel, (1996).

2. Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis, V.K. Ahluwalia, R. Aggarwal, Universities Press (India), 2000.
3. An Advanced Course in Practical Chemistry, A. Ghoshal, B. Mahapatra and A.Kr. Nad, New central book agency, Calcutta, 2000.
4. Advanced Practical Organic Chemistry, J. Mohan, Vol. I and II, Himalaya Publishing House, 1992.
5. Practical Organic Chemistry (Quantitative analysis), B.B. Dey, M V. Sitaraman and T.R. Govindachari , Allied Publishers, New Delhi, 1992.
6. Laboratory Techniques in Organic Chemistry, V.K. Ahluwalia, Pooja Bhagat and Renu Aggarwal, I.K. International Publishing House, New Delhi, 2005.

JOC 308: Organic Chemistry Practicals - IV

Objectives:
This course aims to impart to the student, knowledge of:

- Laboratory set up, safe handling of chemicals, workup procedures and effective disposal of organic waste.
- Preparation of organic compounds in multiple steps.

Learning Outcomes:
On completion of the course, students should be able to:

- Design and carry out experiments, accurately record and analyze the results, calculate overall yield of the final product.

Syllabus:
Multistep Preparations:

1. p-nitroaniline from acetanilide.
2. p-bromoaniline from acetanilide.
3. m-nitrobenzoic acid from methyl benzoate.
4. Anthranilic acid from phthalic acid.
5. 2,4-dinitrophenylhydrazine from chloronitrobenzene.
6. Benzanilide from benzophenone.
7. Benzilic acid from benzoin.
8. Synthesis of acridone.
9. Synthesis of hydantoin.

References

1. Laboratory Manual of Organic Chemistry-B.B. Dey, M.V. Sitaraman and T.R. Govindachari, Allied Publishers, New Delhi, (1996).
2. Practical Organic Chemistry-Mann and Saunders, (1980).

3. Text Book of Practical Organic Chemistry- A.I. Vogel, (1996).
4. Test Book of Quantitative Organic Analysis-A.I. Vogel, (1996).
5. Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis, V.K. Ahluwalia, R. Aggarwal, Universities Press (India), 2000.
6. An Advanced Course in Practical Chemistry, A. Ghoshal, B. Mahapatra and A.K. Nad, New central book agency, Calcutta, 2000.
7. Intermediates for Organic Synthesis, V.K. Ahluwalia, Pooja Bhagat, Ramesh Chandra and Renu Aggarwal, I.K. International Publishing House, New Delhi, 2005.

Semester IV

Sl. No.	Code No.	Title	Theory / practical hours / Week	Duration of Examination Hours	Maximum Marks for ESE	CIA	Total Marks	Total No. of credits
1.	JOC 401	Stereochemistry and Retrosynthetic Analysis	4	3	70	30	100	4
2.	JOC 402	Organic Synthesis	4	3	70	30	100	4
3.	JOC 403	Organometallic and Heterocyclic Chemistry	4	3	70	30	100	4
4.	JOC 404	Medicinal Organic Chemistry	4	3	70	30	100	4
5.	JOC 405	Organic Chemistry Practical – V	4	4	35	15	50	2
6.	JOC 406	Organic Chemistry Practical – VI	4	4	35	15	50	2
7.	JOC 407	Project Review	8	4	100	-	100	4
					450	**150**	**600**	**24**

- **Theory (each paper)**

Maximum Marks (Examination): **70**
Marks for Internal Assessment: **30** *(Continuous evaluation)*

Scheme for Internal Assessment

Attendance: 05 Marks
Seminar: 05 Marks
Test: 20 Marks
Total: 30 Marks

∗ Seminars to be conducted every semester.

- **Practical (each paper)**

Maximum Marks (Examination):	**35**
Marks for Internal Assessment:	**15** *(Continuous evaluation)*
Scheme for Internal Assessment	
Attendance:	03 Marks
Record book:	02 Marks
Prefinal:	10 Marks
Total:	**15 Marks**

Record book for the Practical has to be assessed as internal assessment. There should be no marks for record book during Practical Examination.

JOC 401: Stereochemistry and Retrosynthetic Analysis

Objectives:

This course aims to impart to the student, knowledge of:

- Stereochemistry of organic compounds exhibiting atropisomerism and chirality due to the presence of heteroatoms.
- Methods used in determining absolute configuration by various techniques.
- Disconnection approach to organic synthesis.
- Protecting and deprotecting of functional groups in organic synthesis.
- Strategies needed to devise routes for the synthesis of simple to complex target compounds.

Learning Outcomes:

On completion of the course, students should be able to:

- Identify stereogenic centres and provide R/S designations for atropisomers and compounds with heteroatoms.
- Determine absolute configuration of organic by various rules and techniques.
- Analyse target compounds by retrosynthetic strategy and devise suitable anionic, cationic and radical synthons.
- Apply the knowledge and understanding of essential facts, concepts, principles and theories relating to retrosynthetic analysis for the synthesis of organic target molecules.

Syllabus:

UNIT I

1. Stereochemistry - I **10 hrs**

Optical activity in the absence of chiral atoms

Chirality in biphenyls, adamentanes, ansa compounds, cyclophanes, *trans*-cyclooctene, catenanes, rotaxanes and helicenes. Assignment of R, S- configuration to these classes of compounds.

Optical activity due to the presence hetero atoms

Chirality of organic compounds due to the presence of silicon, nitrogen, phosphorous, arsenic and sulphur atoms; Determination of R, S-configuration of these compounds using CIP rules.

UNIT II

2. Stereochemistry - II **12 hrs**

Methods of determining absolute configuration

i) Chemical correlation: a) Without affecting bonds attached to a stereo centre and b) affecting bonds attached to a stereo centre in a predictable manner.
ii) Optical rotatory dispersion: α-axial haloketone rule and octant rule, application of these rule in the determination of absolute configuration of cyclohexanones, decalones and cholestanones.
iii) Study of quasi-racemates.
iv) Anomalous X- ray scattering technique.

Transannular reactions

Conformational analysis of medium rings; Trasnannular reactions: Hydrolysis of medium ring epoxides and bromination of C_8–C_{10} cyclic dienes.

UNIT III

3. Retrosynthetic Analysis - I **20 hrs**

Disconnection approach

Introduction to synthons, and synthetic equivalents, disconnection approach; Basic principles and terminologies used in disconnection approach; One group C-X and two group C-X disconnections; Chemoselectivity, reversal of polarity, cyclisation reactions

Protecting groups

Principle of protection of alcohols, amines, acids and carbonyl groups

C-C one group and C-C two group disconnections

Alcohols, carbonyl compounds, alkenes; Use of acetylides and aliphatic nitro compounds in organic synthesis; Diels-Alder reaction, 1,3-difunctionalised compounds, α,β-unsaturated compounds, carbonyl compounds condensations, 1,5-difunctionalised compounds; Michael addition and Robinson annelation.

UNIT IV

4. Retrosynthetic Analysis - II **10 hrs**

Ring Synthesis: Saturated heterocycles, synthesis of 3-, 4-, 5- and 6-membered rings

Synthesis of some complex molecules: Application of the above in the synthesis of following compounds: Camphor, longifolene, cortisone, reserpine, vitamin-D and aphidicolin.

References

1. Stereochemistry of carbon compounds, E.L. Eliel, S.H. Wilen and L.N. Mander, John Wiley & Sons, 1994.

2. Stereochemistry, Potapov, MIR, Moscow, 1984.
3. Stereochemistry, D. Nasipuri, New Age, 1999.
4. Advanced Organic Chemistry, J. March, 4th Ed. John Wiley, 2008.
5. Organic Chemistry, R.E. Ireland Prentice-Hall India, New Delhi, 1975.
6. Some modern methods of Organic Synthesis, W. Caruthers, Cambridge Uni. Press London, 2nd Ed., 1998.
7. Stereochemistry of Organic Compounds- Principle and applications, D. Nasipuri, 2nd Ed., New Age International Publishers, 2001.
8. Organic synthesis: The synthon approach, S. Warren, John Wiley & Sons, New York, 1st. Ed. 1983.
9. Designing Organic Synthesis: A disconnection approach, S. Warren, John Wiley & Sons, New York, 2nd Ed. 1987.
10. Organic Synthesis, C. Willis and M. Wills, Oxford University Press, 1995.
11. Organic Synthesis: Concepts, methods and starting materials, J. Furhfop and G. Penzillin, Verlag VCH.
12. Principles of Organic Synthesis, R. Norman and J.M. Coxon, Blackie Academic & Professional.
13. Advanced Organic Chemistry Part B, F.A. Carrey and J. Sundberg, Plenum Press, 1999.
14. Organic chemistry Vol. 2, 6th Ed., I.L. Finar, Longman, 1992.

<u>JOC 402: Organic Synthesis</u>

Objectives:

This course aims to impart to the student, knowledge of:

- Principles and terminologies in asymmetric synthesis and the importance of chirality in organic synthesis.
- Stereoselective, diastereoselective and enantioselective strategies and the use of chiral auxiliary components for asymmetric synthesis.
- Ultrasound, microwave, ionic liquids, phase transfer catalysts, polymer supports in organic synthesis.
- Multi-component reactions as a tool for efficient atom economical reactions.

Learning Outcomes:

On completion of the course, the student should be able to:

- Understand the importance of asymmetric synthesis and propose syntheses of molecules with control of the stereochemistry.
- Design chemical processes and products that eliminate the use or generation of hazardous substances.
- Use ultrasound, microwave, ionic liquids, phase transfer catalysts, polymer supports and multi-component reactions for various organic transformations.

Syllabus:

UNIT I

1. Asymmetric Synthesis **15 hrs**

'*ee*' and methods of determination of '*ee*'.

Stereoselectivity: classification, terminology and principle; Asymmetric synthesis and asymmetric induction; Double diastereoselection and double asymmetric induction

Acyclic stereoselection: Addition of nucleophiles to carbonyl compounds (1,2- 1,3- and 1,4- asymmetric induction), Felkin-Ahn model. Asymmetric aldol condensation, addition of allyl metal and allyl boranes to carbonyl group

Diastereoselection in cyclic systems: Nucleophilic addition to cyclic ketones (formation of axial and equatorial alcohols, catalytic hydrogenation, alkylation, diastereoselective oxidations and stereoselective cyclization of poylenes)

Enantioselective synthesis: Reduction with chiral hydride donors like (S)-PBMgCl,(-)-$^{i}BOAlCl_2$, alpine-borane, (S)-BINAL-H, (R,R)-DIOP and (S,S)-CHIRAPHOS); Enantioselective alkylation of ketones via hydrazones; Enantioselective alkylation with chiral PTC; Enantioselective Michael addition, intramolecular aldol condensation; Use of (+)- and (–)- DET in asymmetric epoxidation

Polymer-bound chiral catalysts in asymmetric induction; Asymmetric amplification

UNIT II

2. Use of ultrasound and Microwaves in Organic Synthesis **08 hrs**

Use of ultrasound: Introduction, instrumentation, the phenomenon of cavitation, Sonochemical esterification, substitution, addition, oxidation, reduction and coupling reactions

Use of Microwaves: Introduction, concept, reaction vessel/medium, specific effects, atom efficiency (% atom utilization), advantages and limitations. N-alkylation and alkylation of active methylene compounds, condensation of active methylene compounds with aldehydes and amines. Diels - Alder reaction, Deprotection of esters and silyl ethers, Oxidation of alcohols and sulfides

3. Ionic liquids **03 hrs**

Introduction, structure, synthesis of some important ionic liquids and their applications in alkylation, hydroformylation, epoxidation, alkene metathesis, alkoxy carbonylation, Knoevenagel condensation, Heck reaction, Rosenmund-von-Braun reaction, C-O bond formation, Michael addition, oxidation, reduction.

UNIT III

4. Polymer supported reagents in organic synthesis **07 hrs**

Introduction - properties of polymer support, advantages of polymer supported reagents and choice of polymers. Applications: i) Substrate covalently bound to the support: Synthesis of oligosachcharides, Preparation of polymer bound aldehyde and application in aldol reaction. Synthesis of polystyryl boronic acid and use in diol protection reaction; ii) Reagent linked to a polymeric material: Preparation of sulfonazide polymer and application in diazotransfer reaction. Synthesis of polymer bound per acid and Baeyer Villiger Oxidation; iii) Polymer supported catalytic reactions: Preparation of polymer supported $AlCl_3$ and application in acetal formation reactions.

5. Phase transfer catalysis and Crown ethers **07 hrs**

Phase transfer catalysis: Introduction, definition, mechanism of phase transfer catalysis. Types of phase transfer catalysts, general preparation, their application in substitution, elimination, addition, oxidation and reduction reactions and their Advantages

Crown ethers: Introduction, nomenclature, features, nature of donor site. General synthesis of crown ethers and their applications in generation of carbenes, aromatic substitution and displacement reactions. Generation and application of superoxide anions, Cation deactivation reactions

UNIT IV

6. Industrially important Multi - component Reactions **12 hrs**

Studies on the mechanistic aspects and use of the following reactions in organic synthesis: Passerini - Ugi; Hantsch; Biginelli; Doebner - Miller; Ritter; Jacobson; Betti; Robinson - Schopf; Barbier; Baylis - Hilmann; Ivanov reaction, PADAM, Mitsinobu, Chan-Lam coupling, Corey-Bakshi-Shibata reduction.

References

1. Stereochemistry of carbon compounds, E.L. Eliel, S.H. Wilen and L.N. Mander, John Wiley & Sons, 1994.
2. Stereochemistry, Potapov, MIR, Moscow, 1984.
3. Stereochemistry, D. Nasipuri, New Age, 2001.
4. Principles and applications of asymmetric synthesis, G.D. Lin, Y.M. Li and A.S.C. Chan, Wiley Interscience, 2001.
5. Organic Chemistry, R. E. Ireland Prentice-Hall India, New Delhi, 1975.
6. Some modern methods of Organic Synthesis, W. Caruthers, Cambridge Uni. Press London, 2nd Edn., 1998.
7. Understanding organic reaction mechanisms, A. Jacob, Cambridge, University Press, 1997.
8. Introduction to organic chemistry, A. Streitweiser, Jr. and C.H. Heathcock, Macmillan, 1985.
9. Modern synthetic reactions H.O. House and W.A. Benzamin California, 2nd edition, 1972.
10. Comprehensive Organic Chemistry, D. Barton and W.D. Wallis, Pergamon Press Oxford, 1983.
11. Organic reaction mechanisms, 3rd edition V.K. Ahluwalia and R.K. Parashar, Narosa, New Delhi, 2005.

JOC 403: Organometallic and Heterocyclic Chemistry

Objectives:

This course aims to impart to the student, knowledge of:

- σ-bonded and π-bonded ligands, metal-carbon bonding, 18- and 16-electron rules, Green rules for nucleophilc addiditon, complexation and decomplexation of organometallic compounds.
- Transition metal complexes as protecting and stabilizing groups, electrophiles and nucleophiles in organic transformations, as catalysts in isomerization, oxidation, reduction, carbonylation and coupling reactions.
- Application of various organometallic compounds in organic synthesis.
- Synthesis, properties and reactions of 3-, 4-, 5-, 6-, 7- and 8-membered heterocyclic compounds.
- Classification, synthesis and applications of mesoionic compounds.

Learning Outcomes:

On completion of the course, students should be able to:

- Understand the scope, diversity and applications of organometallic compounds.
- Predict the stability, reactivity of metal complexes and stereochemistry of products formed.
- Rationalize the synthesis, structure and applications of organometallic compounds for organic transformations.
- Design the synthesis of industrially important compounds.

Syllabus:

UNIT I

1. Organometallic Compounds in Organic Synthesis I **17 hrs**

Chemistry of Organotransition metal complexes: General introduction. 18- and 16-Electron rules; Green rules, back bonding in π-bonded systems.

Complexation and De-complexation Reactions: σ-Bonded systems η^1 ligands. π-bonded systems involving dihapto to octahapto ligands such as olefins, acetylenes, allyl, butadiene, cyclobutadiene, cyclopentadienyl, arenes, cycloheptadienyl and cyclooctatetraene moieties.

Use of organotransition metal complexes as protecting and stabilizing groups: Protection of olefins, acetylenes and dienes. Stabilization of cyclobutadines and norbornadienones

Organometallics as electrophiles and nucleophiles: Nucleophilic addition to η^2, η^5 and η^6 complexes. Electrophilic addition to η^4, η^6 and carbene complexes

Organometallics in coupling and cyclization reactions: Coupling reactions- Heck reaction, Suzuki coupling, Stille coupling, Sonogashira coupling, Hiyama coupling, Negishi coupling and Felkin's reaction.

Organometallics in isomerization, oxidation and reduction reaction*s*: Isomerization of olefins, allylic alcohols and allylic ethers. Oxidation of olefins (including Wacker's process and epoxidation) and reduction of olefins and α,β-unsaturated compounds (including Wilkinson's reaction).

Carbonylation reactions: Use of zirconium complexes in the synthesis of esters, acids, aldehydes or acyl halides from alkyl halides and in the hydroformylation of olefins and dienes; Use of iron complexes for the insertion of CO group into organic molecules such as dienes, alkyl halides, and vinyl epoxides; Use of cobalt complexes in the synthesis of ketones from epoxides, lactones from allylic alcohols and in the hydroformylation of olefins; Use of palladium complexes for the carbonylation of alkyl halides, dienes and allenes

UNIT II

2. Organometallic Compounds in Organic Synthesis II **13 hrs**

Application of the following organometallics in Organic Synthesis:

Organozinc reagents: Preparation, reaction with compounds containing acidic protons, reaction with C-C multiple bonds, trans-metallation, addition reactions of zinc reagents with carbonyl compounds. Simmons Smith, and Reformatsky reaction.

Organolithium reagents: Preparation. Deprotonation reactions, nucleophilic addition reactions, reactions with imines, nitriles and isonitriles.

Organocopper reagents: (Gilman reagents-lithium dialkyl cuprates): Preparation, reactions with alkyl, allyl, vinyl, benzyl and aryl halides, aldehydes, ketones (including a,b-unsaturated carbonyl compounds) and epoxides, Ullmann reaction.

Organoselenium reagents: preparation. Use of organoseleniums in the synthesis of alkenes fromalkyl halides, α,β-unsaturated carbonyl compounds from carbonyl compounds.

Organotellurium reagents*:* Debromination of vic-dibromides, deoxygenation of epoxides, oxidation of hydroquinone and synthesis of biaryls.

Organoalanes: Preparation, hydroalumination and carboalumination of alkenes. Nucleophillic addition reactions with carbonyl compounds and Hydrocyanation. Preparation of alkenyldialkylalanes and their reactions

Organosilicon reagents: Introduction, preparation and general reactions of trialkylsilyl halides. Peterson olefination.

Organotin reagents: Preparation and reactions of tri-n-butyltin hydride, Barton decarboxylation and Barton-McCombie reaction.

Organocerates: Preparation and reactions of organocerates.

Organomercurials: Preparation, Electrophilic substitution reactions, Solvomercuration, de-mercuration and cyclopropanation of alkenes.

UNIT III

3. Heterocyclic Chemistry I **11 hrs**

Small ring heterocycles: Properties and reactions of 3- and 4- membered heterocycles: oxiranes, thiranes, aziridines, azetidines, oxetanes and thietanes.

Benzo-fused heterocycles: Synthesis and reactions of benzofurans, benzothiophenes, benzoxazoles, benzothiazoles and benzimidazoles.

Six-membered heterocycles with two or more heteroatoms: Synthesis of Diazines, triazines, tetrazines and thiazines.

UNIT IV

4. Heterocyclic Chemistry II **11 hrs**

Seven and large membered heterocycles: Synthesis and reactions of azepines, oxepines, thiepines, diazepines, thiazepines, azocines, diazocines, dioxocines and dithiocines

Heterocycles containing P, As, Sb and B: Synthesis of 5- and 6- membered heterocycles with P, As, Sb and B containing one and two hetero atoms.

Mesoionic compounds: General classification, chemistry of some important meso-ionic heterocycles of type-A and type-B and their applications

References

1. Organometallic Chemistry-A Unified Approach, R. C. Mehrotra and A. Singh, 2nd Ed. Wiley, Eastern, 1991.
2. The Organometallic Chemistry of the transition metals, R.H. Crabtree, 6th Ed., 1988.
3. Principles and application of the organotransition metal chemistry, J.P. Collman, L.S. Hegedus, University Science books, 1980.
4. An introduction to Organometallic Chemistry, A.W. Parkins and R.C. Poller, Macmillan, 1986.
5. Modern Synthetic Reactions, H.O. House, W.A. Benjamin, California, 2nd Ed. 1972.
6. Organometallics, Vol. 1 & 2, M. Bochmann, Oxford Chemistry primers, Oxford University Press, 1994.
7. Advanced Organic Chemistry, J. March, 4th Ed. John Wiley, 2008.
8. Organotransition metal chemistry, S.G. Davies, Pergamon Press, Oxford, 1982.
9. Heterocyclic Chemistry, Vols. 1-3, R.R. Gupta, M. Kumar and V. Gupta, Springer Verlag.
10. The Chemistry of Heterocycles, T. Eicher and S. Hauptimann, Thieme.
11. Heterocyclic Chemistry, J.A. Joule, K. Mills and G.F. Smith, Chapman and Hill.
12. Heterocyclic Chemistry, T.L. Gilchrist, Longman Scientific Tech.
13. Contemporary Heterocyclic Chemistry, G.R. Newkome, and W. W. Paudler, Wiley-Inter Science.

14. An introduction to Heterocyclic Compounds, R. M. Acheson, John Wiley.
15. Comprehensive Heterocyclic Chemistry, A. R. Katritzky and C. W. Rees, Eds. Pergamon Press.

JOC 404: Medicinal Organic Chemistry

Objectives:
This course aims to impart to the student, knowledge of:

- Basic biological and pharmacological interactions of drugs with their targets.
- Process of drug discovery.
- The relation of structure and physical properties of drugs to their pharmacological activity.
- Synthesis and mode of action of the different classes of drugs.
- Development of nanomedicine.

Learning Outcomes:
On completion of the course, students should be able to:

- Use of the knowledge gained for the development of biologically and clinically active drugs.
- Describe the current challenges and opportunities in medicinal chemistry in light of contemporary developments in the field of drug discovery.

Syllabus:

UNIT I

1. Introduction **13 hrs**

Chemotherapy, pharmacokinetics, pharmacodynamics, metabolites and antimetabolites; Prodrugs and soft drugs, agonists and antagonists; Concept of drug receptors; Elementary treatment of drug receptor interactions; Quantitative structure activity relationship (QSAR); Theories of drug activity: Occupancy theory, rate theory and induced fit theory; Computer-aided drug design and molecular modeling; General principles of dosage form design and drug administration.

Brief discussion of the recent developments in chemotherapy; Lead compounds and their isolation from natural and synthetic sources; Generics and analogues; Biosimilars, biopharmaceuticals (immunoglobins, herceptins).

Nanomedicines- Introduction, approach to developing nanomedicines, Kinds of nanosystems (nanoshells, nanopores). Nanodrug administration (oral, nasal, ocular). Materials used in diagnostic and therapeutic applications (gold nanoparticles, magnetic nanoparticles and quantum dots).

UNIT II

Introduction, classification, synthesis and mode of action of the following classes of drugs:

2. Antipyretics, analgesics and Anti-inflammatory Drugs **03 hrs**

Aspirin, paracetamol, phenacetin, novalgin, Phenylbutazone, ibuprofen, naproxen

3. Antibiotics **07 hrs**

Penicillins V & G, semi-synthetic pencillins - Methicillin, ampicillin. chloramphenicol, cephalosporin-C, tetracyclins - aureomycin and terramycin, streptomycin.

4. Antidiabetics **03 hrs**

Classification of oral hypoglycemic agents and mode of action of different classes, structure of insulin and factors that affect release of insulin (IIDM and NIIDM). Structure of sulphonyl urea drugs (Tolbutamide), glibenclamide, metformin and pioglitazone.

UNIT III

5. Antihistamines **02 hrs**

Methapyrilene, chlorpheniramine, ranitidine.

6. Antineoplastic agents **04 hrs**

Introduction, alkylating agents and antimetabolites in treatment of cancer. Synthesis and mode of action of mechlorethamine, melphalan, uracil mustards and 6-mercaptopurine, cyclophosphamide, 6-Fluoro uracil. Mention of carcinolytic antibiotics and mitotic inhibitors, immunotherapy and hormonal therapy (general only).

7. Antivirals **02 hrs**

Introduction and classification. Synthesis and mode of action of acyclovir, amantidine, rimantidine and zidovudine.

8. Cardiovascular drugs **04 hrs**

Introduction, synthesis and mode of action of amyl nitrite, sorbitrate, diltiazem, quinidine, verapamil, methyldopa.

UNIT IV

9. Local anti-infective drugs **07 hrs**

Introduction, Sulphonamides-synthesis of sulphadiazine, sulfanilamide, sulphanillic acid and general mode of action. Synthesis of furazolidone, nalidixic acid, ciprofloxacin, dapsone, aminosalicylic acid, isoniazid, ethionamide, ethambutal, griseofulvin and chloroquin.

10. Psychoactive drugs **07 hrs**

Introduction, Structure-activity relationship of barbiturates and their general mode of action. Classification of anticonvulsants. Synthesis and mode of action of Phenobarbital, pethidine, methadone, chlordiazepoxide, diazepam, meprobamate, chloropromazine, phenytoin, ethosuximide, trimethadione, thiopental sodium, glutethimide and caffeine.

References

1. Introduction to Medicinal Chemistry, A. Gringuage, Wiley-VCH.
2. Wilson and Gisvold's Text book of Organic Medicinal and Pharmaceutical Chemistry, Ed Robert F. Dorge.
3. An Introduction to Drug Design, S.S. Pandey and J.R. Dimmock, New Age International Burger's Medicinal Chemistry and Drug Discovery, Vol-1 Ed. M. E. Wolff, John Wiley
4. Goodman and Gilman's Pharmacological Basis of Therapeutics, McGraw-Hill.
5. The Organic Chemistry of Drug Design and Drug Action, R.B. Silverman, Academic Press
6. Strategies for Organic Drug Synthesis and Design, D. Lednicer, John Wiley.
7. Medicinal Chemistry, A. Kar, Wiley, 2000.
8. Synthetic Drugs, G.R. Chatwal, Himalaya, New Delhi, 1995.
9. Comprehensive Organic Chemistry, Vol.5 (Antibiotics), D.H.R. Barton, W.D. Ollis, Pergamon Press, NY, 1979.
10. Instant Notes on Medicinal Chemistry, P. Graham, Viva, New Delhi, 2002.

JOC 405: Organic Chemistry Practicals-V

Objectives:

This course aims to impart to the student, knowledge of:

- Preparation of organic compounds by various methods.

Learning Outcomes:

On completion of the course, students should be able to:

- Design and carry out experiments employing suitable techniques, accurately record and analyze the results, calculate overall yield of the final product.

Syllabus:

1. Preparations:

1. Preparations of NBS from succinic acid
2. Application of NBS in benzylic bromination reaction.
3. Preparation of benzpinacolone from benzophenone.
4. Preparation of 2-phenylindole from phenylhydrazine.
5. Synthesis of anthrone from anthracene.

6. Synthesis of methyl red.
7. Preparation of 2,4,5-triphenyloxazole from benzoin.
8. Biosynthesis of ethanol from sucrose.
9. Synthesis of hippuric acid.
10. Synthesis of 2-methoxynaphthalene from 2-naphthol.

References

1. Preparation of Organic Intermediates, D.A. Hirley, John Wiley
2. Text book of Practical Organic Chemistry, A.I. Vogel, Pearson, 5th Ed. Delhi, 2004
3. Organic Synthesis, Collective Vols. I to X, 1956-1999
4. Organic Experiments, L.F. Fieser, 2nd Edition, D.C. Heath & Co.USA, 1974-2000
5. Practical Organic Chemistry F.G. Mann and B.C. Saunders, 4th Edition, Longman, 2002
6. Comprehensive Practical Organic Chemistry: Preparation and quantitative analysis, V.K. Ahluwalia, R. Aggarwal, Universities Press (India), 2000
7. An Advanced Course in Practical Chemistry, A. Ghosal, B. Mahapatra and A.K. Nad, New central book agency, Calcutta, 2000
8. Advanced Practical Organic Chemistry, J. Mohan, Vol. I and II, Himalaya Publishing House, 1992
9. Laboratory Techniques in Organic Chemistry, V.K. Ahluwalia, Pooja Bhagat and Renu Aggarwal, I.K. International Publishing House, New Delhi, 2005
10. Intermediates for Organic Synthesis, V.K. Ahluwalia, Pooja Bhagat, Ramesh Chandra and Renu Aggarwal, I. K. International Publishing House, New Delhi, 2005

JOC 406: Organic Chemistry Practicals-VI

Objectives:

This course aims to impart to the student, knowledge of:

- Recording of spectral data using various spectroscopic techniques.
- Methods employed for extraction/isolation of important natural products.
- Chromatographic separation of mixtures.

Learning Outcomes:

On completion of the course, students should be able to:

- Carry out spectral analysis and confirmation of structure of organic compounds.
- Design extraction, isolation and purification (using chromatographic techniques) of natural products.

Syllabus:

1. Instrumental methods in organic analysis:

Recording of spectra using UV, IR, NMR and GC-MS techniques for the compounds prepared in JOC 306 (Organic Practical-II), JOC 308 (Organic Practical-III), JOC-405(Organic Practical-III).

2. Extraction:

1. Extraction of piperine from pepper.
2. Extraction of caffeine from tea leaves.
3. Isolation of Lactose from milk.
4. Isolation of (+) limonene from citrus rinds.

3. Separations:

1. Separation of p-rosaniline and methyl red by column chromatography.
2. Separation of amino acids by paper chromatography.
3. Separation of carbohydrates by thin layer chromatography.

References

1. Text book of Practical Organic Chemistry, A.I. Vogel, Pearson, 5th Ed. Delhi, 2004
2. Natural Products, Laboratory Manual, Ikan, 2000
3. Organic Experiments, L.F. Fieser, 2nd Edition, D.C. Heath & Co.USA, 1974-2000
4. Practical Organic Chemistry F.G. Mann and B.C. Saunders, 4th Edition, Longman, 2002
5. An Advanced Course in Practical Chemistry, A. Ghosal, B. Mahapatra and A.K. Nad, New central book agency, Calcutta, 2000
6. Laboratory Techniques in Organic Chemistry, V.K. Ahluwalia, Pooja Bhagat and Renu Aggarwal, I.K. International Publishing House, New Delhi, 2005
7. Spectrometric Identification of Organic Compounds, R.M. Silverstein and W.P. Weber, 2005.
8. Introduction to Spectroscopy, 3rd Edition, D.L. Pavia, G.M. Laupman and G.S. Kriz, Harcourt College Publishers, 2001.
9. Fundamentals of Molecular Spectroscopy, 4th Ed., C.N. Banwell and E.M. McCash, Tata McGraw – Hill, New Delhi, 1999.
10. Organic Spectroscopy, W. Kemp, ELBS London, 2000.

JOC 407: Project and Review

Objectives:

This course aims to impart to the student, knowledge of:

- The working protocols and systematic methodology followed in research.
- Demands, skill sets, work ethics in industries.

Learning Outcomes:

On completion of the course, the student should be able to:

- Apply skills and knowledge acquired through the course in a real-life environment.

- Identify skills and capabilities that intersect effectively with the needs of industry enhancing employ ability.
- Communicate research findings efficiently in written (report) and verbal (viva-voce) forms.

Syllabus:

The students have to carry out an internship/project work in industries or in-house projects for a period of 45 days (1.5 months) and submit the report on the same.

****