LOYOLA ACADEMY
ALWAL, SECUNDERABAD 500 010 TS
(Autonomous and affiliated to Osmania University)
Re-accredited with 'A' Grade (3.2/4.0 CGPA) by NAAC (III Cycle)
A "College with Potential for Excellence" by UGC
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M.SC ORGANIC CHEMISTRY

PROGRAM OUTCOMES (M.Sc.)

PO1: Scientific Knowledge: Ability to build a strong foundation of knowledge, integrated with the latest developments in science and technology which help students develop critical thinking, reasoning, decision making in process of quality education.

PO2: Problem Analysis: Identify, formulate and analyse the complex scientific problems using the knowledge gained across various streams of science and technology.

PO3: Effective Communication: Ability to articulate ideas, communicate effectively using current tools in the field of ICT along with effective report writing and documentation.

PO4: Development of Skill and Attitude: Enabling the students with the required skill, right attitude, time management and self-discipline for prominent career in industry, research institutes and for further academic study.

PO5: Life Long Learning and Social Responsibility: Recognise the need and ability to engage in lifelong learning and work effectively as an individual and as a member of diverse team. Students get the ability to act with an informed awareness of issues to participate in civic life through volunteering.

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Program Specific Outcomes

PSO1 **Understands, identify and interrelate** with the background of organic reaction mechanisms, complex Stereochemical structures, molecular rearrangements, instrumental method of chemical analysis and separation techniques

PSO2 **Analyses** the importance of various elements in the periodic table, coordination chemistry and structure of molecules, properties of compounds, and structural determination of complexes using theories.

PSO3 **Gathers attention** about the physical aspects of atomic structure, dual behaviour, reaction pathways with respect to time, various energy transformations, molecular assembly in nanolevel, electrochemistry & infer their significance

PSO4 **Learns, constructs and analyses** the potential uses of analytical techniques, medicinal chemistry and green chemistry.

PSO5 **Organise** and carry outexperiments in the area of organic analysis, estimation, separation, derivative process, preparation, conductometric, potentiometric and solve spectral analysis

COMMUNICATIVE COMPETENCE

Credits: 2 **Semester: I**
Subject code: MOC18101 **No. of lecture hours: 30**

Objectives:

- English language course will help students to develop a natural and accurate style of English pronunciation.
- English language course will also improve your ability to express ideas clearly and confidently in English.

Outcome

- Student is able to apply the knowledge of communicative competence to express the ideas clearly

Unit-01:	**6hrs**
• Features of Indian English	1
• Correction of sentences, Structures	1
• Tenses, ambiguity - idiomatic distortions	1
• Informal conversation *Vs* Formal expression	1
• Verbal and non-verbal communication	1
• Barriers to effective communication – kinesics	1
Unit-02:	**6hrs**
• Oral, aural, Writing and reading	1
• Word-Power-Vocabulary- Jargon	1
• Rate of speech, pitch, tone- Clarity of voice	1
• Technical presentations	1
• Types of presentation ,video conferencing	1
• Participation in meetings - chairing sessions	1
Unit-03:	**6hrs**
• Formal and informal interviews	1
• Ambiance and polemics	1
• Interviewing in different settings and for different purposes	1
• e.g., eliciting and giving information	1
• Recruiting, performance appraisal	1
• Group discussions, curriculum vitae	1
Unit-04:	**6hrs**
• Written communication	2
• Differences between spoken and written communication	2
• Features of effective writing such "as clarity, brevity	1
• Appropriate tone clarity, balance etc.	1
Unit-05:	**6hrs**
• Letter-writing business letters	1
• pro forma culture - format - style – effectiveness, promptness	1
• Analysis of sample letters collected from industry –email, fax.	1
• Technical Report writing –Business and Technical Reports	1
• Types of reports - progress reports, routine reports, annual reports - format –	1

- Analysis of sample reports from industry –Synopsis and thesis writing 1

References:

Unit-01-05:

1. Rajendra Pal, J S KorlahaHi, **Essentials of Business Communication**, Sultan Chand & Sons, New Delhi.
2. Andrea J. Rutherford, **Basic Communication Skills for Technology**,Pearson Education Asia, Patparganj, New Delhi-92.
3. V. Prasad,**Advanced Communication Skills**, Atma Ram Publications, New Delhi.
4.Raymond V. Lesikav; John D. Pettit Jr.; **Business Communication; Theory & Application**, All India Traveller Bookseller, New Delhi-51.
5. R. K. Madhukar, **Business Communication**, Vikas Publishing House Pvt. Ltd.

INORGANIC CHEMISTRY-I

Credits: 4 **Semester: I**
Subject Code: MOC19102 **No. of lecture hours: 60**

Objectives

- To impart knowledge of co-ordinate complexes, their reaction mechanisms and their stabilities.
- To acquire the knowledge of symmetry and assigning the same to the molecules.

Course Outcomes

- Understands the concept of bonding in metal complexes
- Interrelates 3-D structures of molecules with their symmetry elements
- Categorises the mechanisms of inorganic complexes
- Analyses the stability of the complexes through equilibria
- Identifies the ligational aspects of diatomic molecules

Unit-01:Bonding in metal complexes-I **12 hrs**

- Crystal Field Theory: Salient features of CFT. Splitting pattern of *d*-orbital in regular Octahedral, tetrahedral, trigonal planar and linear geometries. 6
- John-Tellar Theorem- tetragonally distorted octahedral, square planar 1
- Factors influencing the magnitude of crystal field splitting in octahedral complexes – nature of metal ions, nature of ligands, geometry. 4
- Concept of weak field and strong field–Calculation of crystal field stabilization energies (CFSE's) in six and four coordinate complexes. 1

Unit-02:Symmetry of molecules-I **12 hrs**

- Concept of Symmetry in Chemistry–Symmetry Operations 2
- Symmetry Elements: Rotational Axis of Symmetry and Types of Rotational Axes, Plane of Symmetry and types of Planes, Improper Rotational Axis of Symmetry, Inversion Center and Identity Element. 4
- More about Symmetry Elements-Molecular Point Groups: Definition and Notation of Point Groups 1
- Classification Molecules in to C_1, C_s, C_i, C_n, C_{nv}, C_{nh}, $C_{\alpha v}$, D_n, D_{nh}, D_{nd}, $D_{\alpha h}$, S_n (n=even) 5

Unit-03:Reaction mechanism-I **12 hrs**

- Labile and Inert Complexes. VBT Explanation of Lability and Inertness. Taube's Explanation of Lability and Inertness 2
- Ligand substitution reactions: Energy profile of a reaction – Transition state or Activated Complex 1
- Types of substitution reactions: SE: Electrophilic substitution reaction, S_N1: Substitution, Nucleophilic, Unimolecular Mechanism (Dissociative Mechanism), S_N2: Substitution, Nucleophilic, Bimolecular Mechanism (Associative Mechanism), S_N1CB: Substitution, Nucleophilic, Unimolecular Conjugate Base Mechanism with energy profile diagrams 4
- Ligand substitution reactions in octahedral complexes: Aquation or Acid hydrolysis reactions, Factors effecting Acid Hydrolysis, Base Hydrolysis, Conjugate Base Mechanism, Evidences in favour of S_N1CB Mechanism 4
- Substitution reactions without Breaking Metal-Ligand bond 1

Unit-04:Coordination equilibria **12 hrs**

- Solvation of metal ions- Binary complexes: Formation of binary metal complexes and their stability — 1
- Types of Stability Constants– relation between them- trends in Step-wise Stability Constants (Factors causing decrease and increase in Step-wise Stability) — 1
- Factors influencing the stability constants: (i) Ligand effects: Basicity, Substituent, Steric, Chelate (size and number of chelate rings), Macro cyclic and Cryptate effects; (ii) Metal ion effects: Ionic potential, Effective Nuclear charge and Atomic Number (Irving-William's Order), geometry of metal ion and ligand–chelate effect and its thermodynamic origin — 5
- Jahn-Tellar effect on Stability constants of metal complexes — 1
- Pearson's Theory of Hard and Soft Acids and Bases (HSAB), Applications of HSAB, Electro negativity *vs* Hardness and Softness. Symbiosis — 2
- Methods used for the determination of stability constants (Basic Principles only): pH-metric method and Spectrophotometric method — 2

Unit-05: Ligational aspects of diatomic molecules **12hrs**

- Metal Carbonyls: Carbon monoxide as a ligand, molecular orbital of CO, donor and acceptor molecular orbital of CO; bonding modes of CO: terminal and bridging — 3
- Evidence for multiple bonding from bond lengths and stretching frequencies, 18 valence electron rule and its application — 2
- Metal nitrosyls: NO as a ligand, molecular orbital of NO, donor and acceptor components; bonding modes of NO: terminal (linear, bent) and bridging; structural aspects of $[IrCl(PPh_3)_2(CO)(NO)]^+$ and $[RuCl(PPh_3)_2(NO)_2]^+$ — 3
- Stereochemical control of valance in $[Co(diars)_2(NO)]^{+2}$ and $[Co(diars)_2(NO)(SCN)]^{+1}$ — 2
- Metal dinitrogen complexes: N_2 as aligand – Molecular orbitals of N_2; Bonding modes – Terminal and Bridging; Stretching frequencies; Structures of Ru (II), Mo(II) and Os(II) dinitrogen complexes; Chemical fixation of dinitrogen — 2

References:

Unit-01:

1. J.E.Huheey, K. A. Keiter and R. L. Keiter, 1993, **Inorganic Chemistry** (4th Ed), Harper Cotton's College Publications.
2. G. L. Eichorn, Inorganic Biochemistry, **1982**, Vol 1, Elsevier.
3. R D Madan, G D Tuli and Wahid U Malik. **2011**. **Selected Topics in Inorganic Chemistry** (7th Ed), S Chand & Company Ltd.

Unit-02:

4. Mark Ladd**,** 2000, **Symmetry and Group theory in Chemistry**, Marwood Publishers, London,Mark Ladd.
5. K.Veera Reddy, 1999, **Symmetry and Spectroscopy of Molecules** (1st Ed.), New Age International (P) Limited.

Unit-03:

6. Mark Ladd, 2000, **Symmetry and Group theory in Chemistry,** Marwood Publishers, London.
7. K. Veera Reddy, 1999, **Symmetry and Spectroscopy of Molecules** (1st Ed), New Age International (P) Limited.
8. F.Albert Cotton, 2009, **Chemical Applications of Group Theory** (3rd Ed), Wiley India.

Unit-04& 05:

9. F.A.Cotton, G.Wilkinson, C.A.Murillo and M.Bochmann, 1999, **Advanced Inorganic Chemistry** (6^{th} Edn), Wiley Interscience.
10. M. M. Taqui Khan and A. E Martell, 1974, **Homogeneous Catalysis by Metal complexes** Vol I, Academic Press NewYork.
11. D.F.Shriver, H.D.Kaerz and R.D.Adams, 1990, **The Chemistry of Metal Cluster Complexes.** Oxford University Press, NewYork.

ORGANIC CHEMISTRY-I

Credits: 4 **Semester: I**

Subject Code: MOC19103 **No. of lecture hours: 60**

Objectives

- To impart the knowledge of stereochemistry.
- To understand the mechanisms in organic reactions.
- To apply the knowledge of reactive intermediates and apply the same for various molecular rearrangements.
- To understand the conformational analysis of acyclic system.

Course Outcomes

- Acquires the 3-D aspects of organic molecules
- Understands and compares the organic reaction mechanisms
- Develops the fundamentals of reactive intermediates
- Appreciates the various steps involved in the molecular rearrangements
- Perceives the concept of conformational analysis

Unit-01: Stereochemistry **12 hrs**

- Molecular representation of Fischer, Newman, Sawhorse, Wedge projections and their interconversion — 1
- Molecular symmetry and chirality: Symmetry operations and symmetry elements (C_n&S_n). Criteria for chirality and desymmetrisation — 1
- Axial, planar and helical chirality, configurational nomenclature: Axially chiral allenes, spiranes, alkylidene cycloalkanes, chiral biaryls, and atropoisomerism Planar chiral ansa compounds and *trans*-cyclooctene. Helically chiral compounds. — 3
- Relative and absolute configuration: Determination of absolute configuration. Anomalous X-ray scattering method and chemical correlation methods — 3
- Racemization, racemates and resolution techniques: Resolutions by chiral chromatography and asymmetric transformation — 2
- Determination of configuration in *E, Z*-isomers: Spectral, chemical methods of configuration determination of *E, Z*-isomers — 2

Unit-02: Reaction mechanism-I **12 hrs**

- Effect of structure on reactivity: brief review of inductive effect, electromeric effect, resonance effect, hyper conjugation, steric effect — 2
- Electrophilic addition to carbon carbon double bond: Stereo selective addition to carbon carbon double bond; *anti*-addition: bromination and epoxidation followed by ring opening. *Syn*-addition of OsO_4 and $KMnO_4$, Prevost and Woodward oxidation — 3
- Elimination reactions: E_2, E_1, E_1CB mechanisms. Orientation and stereoselectivity in E_2 eliminations. Pyrolyticsyn elimination and α-elimination, elimination *Vs* substitution — 4
- Determination of reaction mechanism: Energy profiles of addition and elimination reactions, transition states, product isolation and structure of intermediates, use of isotopes, chemical trapping and crossover experiments — 3

Unit-03: Reactive intermediates **12hrs**

Generation, detection, structure, stability and reactions of

- Carbocations (Classical and Non-Classical) carbanions — 4

- Carbenes, nitrenes 4
- Free radicals 2
- Benzyne 2

Unit-04: Molecular rearrangements **12hrs**

- Molecular rearrangements: Definition and classification. Molecular rearrangements involving electron deficient carbon: Wagner-Meerwein, Pinacol-Pinacolone, Allylic and Wolf rearrangement 3
- Electron deficient nitrogen: Hofmann, Lossen, Curtius, Schmidt and Beckmann rearrangements 4
- Electron deficient oxygen: Baeyer-Villiger oxidation 2
- Base catalysed rearrangements: Benzilic acid, Favourski, Transannular, Sommlett-Hauser and Smiles rearrangement, Von-Richter rearrangements 3

Unit-05: Natural Products **12hrs**

- Isolation of natural products by steam distillation, solvent extraction and chemical methods. 2
- Definitions, medical importance, occurrence, detections by various color tests, Classification of alkaloids and terpenoids 1
- Isoprene rule, Special isoprene rule 1
- General methods in structural determination of terpenes 2
- Structure determination and synthesis of α-terpeniol and camphor. Structure determination and synthesis of β- carotene. 3
- General methods of structure determination of alkaloids. Structure determination and synthesis of papaverine 2

References:

Unit-01

1. Ernest L Eliel, Samuel H.Wilen, 2008, **Stereochemistry of Carbon compounds**, John Wiley & Sons INC.
2. D. Nasipuri, 2006, **Stereochemistry of organic compounds- Principles and Applications** (2nd Ed.), New Age International publishers.
3. P S Kalsi, 2010, **Stereochemistry: Conformation & Mechanism** (7th Ed.), New Age International publishers

Unit-02, 03 & 04:

4. Petersykes, **A guidebook of mechanism of organic chemistry** (6th Ed.), Pearson Education, India.
5. Jerry March, 1992, **Advanced Organic Chemistry** (5th Ed.), Wiley-India student edition
6. S. Mukherjee, 2007, **Mechanism and Structure in Organic Chemistry**(3rd Ed.), MacMillan Publishers India Limited

Unit-05:

7. Finar, I.L. 2009. **Textbook of Organic Chemistry**. Vol II. 5th Edition. Pearson Publications.
8. Bhat, S.V. and Nagasampangi, B.A. 2009. **Chemistry of Natural Products**. New Delhi: New Delhi: Narosa Publishing House.
9. Kalsi, P.S. 1983. **Chemistry of Natural Products.** Kalyani Publishers.

PHYSICAL CHEMISTRY-I

Credits: 4 **Semester: I**
Subject Code: MOC19104 **No. of lecture hours: 60**

Objectives

- To understand the thermodynamic properties of reactions.
- To study the nature of electrochemical cells and their applications
- To impart knowledge about the subatomic particles of matter.
- To acquire the knowledge of kinetic mechanism.
- To study the photochemical properties and their applications.

Course Outcomes

- Learns the classical status of thermodynamics
- Recognizes the dynamics of electrode reactions
- Perceives the postulates of quantum chemistry
- Analyses the importance of rates of chemical reactions
- Gains the potential on concepts of photochemical reactions

Unit-01: Thermodynamics-I **12 hrs**

- Brief review of concepts of I and II laws of thermodynamics, concept of entropy, entropy as a state function, calculation of entropy changes in various processes. 2
- Entropy changes in an ideal gas, entropy changes on mixing of ideal gases, entropy as a function of V and T & Entropy as a function of P and T. Entropy change in isolated systems- Clausius inequality, entropy change as criterion for spontaneity and equilibrium. 3
- Third law of thermodynamics: Evaluation of absolute entropies from heat capacity data for solids, liquids and gases, standard entropies and entropy changes of chemical reactions. 1
- Helmholtz and Gibbs free energies (A and G), A and G as a criterion for equilibrium and spontaneity, physical significance of A and G, driving force for chemical reactions- relative signs of ΔH and ΔS. 2
- Thermodynamic relations: Gibbs equations, Maxwell relations, temperature dependence of G. Gibbs- Helmholtz equation. 1
- Chemical potential: Gibbs equations for non-equilibrium systems. Material equilibrium, phase equilibrium, Clapeyron equation and Clausius-Clapeyron equation. 1
- Conditions for equilibrium in a closed system, chemical potential of ideal gases, ideal-gas reaction equilibrium-derivation of equilibrium constant, temperature dependence of equilibrium constant-the van't Hoff equation. 2

Unit-02: Electrochemistry-I **12 hrs**

- Electrochemical Cells: Derivation of Nernst equation–problems, chemical and concentration cells (with and without transference), liquid junction potential (LJP)–derivation, its determination and elimination**.** 3
- Applications of EMF measurements: Solubility product, potentiometric titrations, determination of transport numbers, equilibrium constant measurements. 2
- Decomposition potential and its significance, Electrode polarization: its causes and elimination, concentration over potential. 2

- Types and Classification of Electro analytical Methods. 2
- Conductometry: Definition of terms- Conductivity, specific conductivity, cell constant, mobility of ions. Conductometric titration of weak acid against strong base. 3

Unit -03: Quantum Chemistry- I **12 hrs**

- Black body radiation-Planck's concept of quantization-Planck's equation, average energy of an oscillator (derivation not required). 2
- Wave particle duality and uncertain principle-significance of these for microscopic entities. Emergence of quantum mechanics. Wave mechanics and Schrodinger wave equation. 2
- Operators-operator algebra. Commutation of operators, linear operators. Complex functions. Hermitian operators. Operators ∇ and ∇^2. 2
- Eigen functions and eigenvalues. Degeneracy. Linear combination of eigen functions of an operator. Well behaved functions. Normalized and orthogonal functions. 2
- Postulates of quantum mechanics. Physical interpretation of wave function. Observables and operators. Measurability of operators. Average values of observables. 2
- The time dependent Schrodinger equation. Separation of variables and the time-independent Schrodinger equation. 2

Unit-04: Chemical Kinetics **12 hrs**

- Theories of reaction rates: Collision theory, steric factor, transition state theory, reaction coordinate, activated complex and the transition state, thermodynamic formulation of transition state theory, activation parameters and their significance, the Eyring equation, unimolecular reactions and Lindemann's theory. 4
- Complex reactions: Opposing reactions, parallel reactions and consecutive reactions (all first order type), chain reactions-general characteristics, steady state treatment example: H_2-Br_2 reaction, derivation of rate law. 4
- Effect of structure on reactivity-linear free energy relationships, Hammett and Taft equations-substituent (σ and σ^*) and reaction constant (ρ and ρ^*) with examples, deviations from Hammett correlations, reasons-change of mechanism, resonance interaction, Taft four parameter equation, correlations for nucleophilic reactions. 4

Unit -05: Photochemistry **12 hrs**

- Electronic transitions in molecules, Franck Condon principle, electronically excited molecules- singlet and triplet states, radiative life times of excited states-theoretical treatment, measured lifetimes. 3
- Quantum yield and its determination, Actinomety: Ferrioxalate and Uranyl oxalate actinometers-problems. Derivation of fluorescence and phosphorescence quantum yields, E-type delayed fluorescence- evaluation of triplet energy splitting (ΔE_{ST}). 3
- Photo physical processes, photo physical kinetics of unimolecular reactions, calculation of rate constants of various photo physical processes-problems, state diagrams. 2
- Photochemical primary processes. Types of photochemical reactions- 2

electron transfer, photo dissociation, addition, abstraction, oxidation and isomerization reactions with examples.

- Effect of light intensity on rates of photochemical reactions, photosensitization, quenching, Stern-Volmer equation. 1
- Experimental set up of a photochemical reaction, introduction to fast reactions: Principle of flash photolysis. 1

References:

Unit-01:

1. Peter Atkins and Julio de Paula, **Atkin's Physical Chemistry**, Oxford University press
2. Ira N. Levine, McGraw Hill, **Physical Chemistry**,
3. McQuarrie D. A. and. Simon J. D.**Physical Chemistry-A Molecular approach**, Viva Books Pvt. Ltd
4. McQuarrie D.A. and Simon J.D. **Molecular Thermodynamics**, University Science Books

Unit-02:

5. Glasstone S. **Introduction to Electrochemistry**.
6. Bockris J. O. M. & Reddy A. K. N. Plenum, **Modern Electrochemistry**
7. Samuel Maron H. and Carl Prutton F. **Principles of physical chemistry**, Oxford& IBH

Unit-03:

8. Ira N. Levine, Prentice Hall,**Quantum Chemistry**,
9. Chandra A. K. **Introduction to Quantum Chemistry**, Tata McGraw Hill
10. Prasad R.K. Quantum Chemistry, New Age Publisher, 2010.

Unit-04:

11. Rajaraman and J. Kuriacose, **Kinetics and Mechanism of Chemical Transformations**, J McMillan
12. Laidler K.J. **Chemical Kinetics**, McGraw Hill
13. Espenson J. H. **Chemical Kinetics and Reaction Mechanisms**, McGraw Hill
14. Samuel H. Maron and Carl F. Prutton,**Principles of physical chemistry**, Oxford& IBH
15. Howard Maskill, **The Physical Basis of Organic Chemistry**, Oxford University Press (New York)
16. Isaacs N. S. **Physical Organic Chemistry**, ELBS

Unit-05:

17. Rohtagi-Mukherji K. K. **Fundamentals of Photochemistry**, Wiley-Eastern
18. Turro N. J. **Molecular Photochemistry**, Benjamin
19. Kundall R. P. and Gilbert A. **Photochemistry**, Thomson Nelson
20. Gilbert A. and Baggott J. **Essentials of Molecular Photochemistry**, Blackwell Scientific Publications.
21. Coxon J. M. and Halton B .**Organic Photochemistry**, Cambridge University press.
22. Cox A and Kemp T. J. **Introductory Photochemistry**, McGraw-Hill, London

ANALYTICAL TECHNIQUES AND SPECTROSCOPY-I

Credits: 4 **Semester: I**

Subject Code: MOC19105 **No. of lecture hours: 60**

Objectives

- To acquire knowledge of chromatographic techniques.
- To gain knowledge of various spectroscopic techniques and their applications.

Course Outcomes

- Recognizes the importance of various chromatographic techniques
- Understands the magnetic properties of nuclei
- Analyses the approach of IR and Raman spectra for structural elucidation
- Identifies the electronic transitions in organic molecules
- Gains knowledge about electronic spin spectroscopy

Unit-01: Chromatography Techniques-I **12 hrs**

- Introduction to Chromatography and its classification. Gas Chromatography: Principle, Gas-Solid (GC, Adsorption) and Gas – Liquid (GLC, partition) chromatography — 3
- Performing GC, separations & Instrumentation: Stationary phases, carrier gases, retention indices, detectors (TCD, FID, and NPD). Temperature selection and quantitative measurements. Applications of GC- Analysis of Gasoline, separation of basic drugs, separation of free fatty acids from milk — 4
- High Performance Liquid Chromatography (HPLC): Principles, stationary phases, equipment, normal phase (NPC) and reverse-phase chromatography (RPC), solvents and columns for HPLC. Introduction to fast liquid chromatography. Applications of HPLC-Drug analysis (Antibiotics), Analysis of food products — 4
- Introduction to Ion Exchange Chromatography: Principles, cation and anion exchange resins and applications. — 1

Unit-02: NMR Spectroscopy-I **12 hrs**

- Magnetic properties of nuclei, principles of NMR. Instrumentation, CW and FT NMR — 2
- Equivalent and non-equivalent protons, enantiotopic and diastereotopic protons. Chemical shifts, factors affecting the chemical shifts, electronegativity and anisotropy, shielding and deshielding effects, signal integration — 4
- Spin-spin coupling: vicinal-Karplus equation, geminal, long range and virtual coupling, coupling constants and factors affecting coupling constants — 2
- Applications of ^{1}H NMR spectroscopy: Structure determination, reaction mechanisms (cyclic bromonium ion, electrophilic and nucleophilic substitutions, carbocations and carbanions). *E, Z*-isomers, conformation of cyclohexane and decalins, keto-enol tautomerism, hydrogen bonding, proton exchange process, C-N rotation — 3
- ^{1}H NMR of ethyl benzoate, 2-butanoneand 2-chloropropionic acid — 1

Unit-03: Rotational and Vibrational spectroscopy **12 hrs**

- **Rotational (Microwave) Spectroscopy:** Classification of molecules based on moment of inertia. Diatomic molecule as rigid rotator and its rotational energy — 2

levels. Selection rules (derivation not required)

- Calculation of bond lengths from rotational spectra of diatomic molecules. Isotope effect on rotational spectra. Calculation of atomic mass from rotational spectra. Brief description of microwave spectrometer — 1
- **Vibrational Spectroscopy:** Vibrational energy levels of diatomic molecules, selection rules (derivation not required). Calculation of force constant from vibrational frequency — 1
- Anharmonic nature of vibrations. Fundamental bands, overtones and hot bands, Fermi resonance — 1
- Vibration-rotation spectra diatomic molecules. Vibrations of poly atomic molecules. Normal modes of vibration, concept of group frequencies — 1
- Characteristics of vibrational frequencies of functional groups; Stereochemical effects on the absorption pattern in carbonyl group, cis-trans isomerism and hydrogen bonding — 3
- Applications of IR spectroscopy to the study of metal-ligand bonding modes involving monodentate and bidentate ligands. IR spectra of coordinated NO_3^- and SO_4^{2-} ions — 1
- **Raman Spectroscopy:** Quantum theory of Raman Effect, Vibrational Raman spectra, Stokes and anti- Stokes lines. Complementary nature of IR and Raman spectra — 2

Unit-04: Electronic spectroscopy **12 hrs**

- Overview on terminology and types of transitions — 1
- Electronic spectra: Elementary energy levels of molecules. Selection rules for electronic spectra — 1
- Woodward-Fieser rules for chromophores: Conjugated dienes, trienes, unsaturated carbonyl compounds, benzene, and its derivatives, poly nuclear aromatic hydrocarbons, calculation of λ_{max} — 6
- Solvent and structural influences on absorption maxima, stereo chemical factors. Cis-trans isomers, and cross conjugation — 2
- Quantitative applications of electronic spectroscopy, dissociation constant of a weak acid, Charge transfer spectra — 2

Unit-05: ESR and Photoelectron Spectroscopy **12 hrs**

- Introduction, principle, instrumentation, selection rules — 2
- Hyperfine and super hyperfine Coupling — 1
- Zero field splitting, Kramer's degeneracy and quadrupolar interactions — 2
- Study of free radicals and transition metal complexes — 1
- Study of free radicals and evidence for covalency in complexes, ex: Cu(II) Bis-salcylaldimine, Bis-acetyl acetanatovanadyl(II) — 1
- Introduction, principle and instrumentation, types of Photoelectron Spectroscopy– UPS & XPS Binding Energies, Koopman's Theorem, chemical Shifts — 2
- Vibrational structure of PES bands, potential energy curves — 1
- Interpretation of vibrational spectral data for ionized (M^+) species: photoelectron spectrum of N_2^+ molecule , prediction of nature of molecular orbitals. — 2

References:

Unit-01:

1. Sane and Joshi, 1999, **Electro analytical Chemistry theory and applications,** Quest Publications.
2. Raymond PW Scott, **Techniques and practices of Chromatography,** Marcel Dekker, Inc. New York.
3. WMA Neissen& J V Greef, **Liquid Chromatography- Mass spectrometry Principles & Applications,** Marcel Dekker, Inc. New York.
4. Raymond PW Scott, 1988, **Introduction to analytical Gas Chromatography** (2nd Ed.), Marcel Dekker, Inc. New York

Unit-02, 03 &04:

5. Banwell and Mc Cash, 1966, **Fundamentals of Molecular Spectroscopy,** McGraw-Hill.
6. G.M. Barrow, 1962, **Introduction to Molecular Spectroscopy**, McGraw-Hill.
7. J.R. Dyer, 1965, Absorption **Spectroscopy of Organic Compounds,** Prentice-Hall, Englewood Cliffs, N.J.
8. R.M. Silverstein and F.X. Webster, 1998, **Spectroscopic identification of organic compounds,** (6th Ed), Wiley.
9. William Kemp, 2008, **Organic Spectroscopy** (3rd Ed.), Palgrave.
10. Pavia, 2004, **Introduction to organic spectroscopy** (3rd Ed.), Thomson
11. Jagmohan, 2010, Organic **Spectroscopy, Principles and Applications** (2nd Ed.), Narosa Publication House Pvt. Ltd.

Unit-05:

12. Skoog, Holler and Nieman, Harcourt, 1998, **Principles of Instrumental analysis**, Asia PTE Ltd.
13. Skoog, West, Holler and Crouch, 2000, **Analytical Chemistry-An Introduction,** Saunders College Publishing.
14. Skoog and Leary, **Prinicples of Instrumental Analysis**, Saunders College Publishing.
15. D. Becker and D. Betteridge**,** 1972, **International series of Monographs, Vol. 53, Photoelectron Spectroscopy**

INORGANIC CHEMISTRY PRACTICALS-I

Credits: 2 **Semester: I**

Subject Code: MOC19151 **No. of hours/week: 5**

Objectives

- To synthesize inorganic complexes.
- To understand the techniques involved in the preparation of standard solutions, standardization and estimations of metal ions.

Outcome

- The student will be able to synthesize various inorganic complexes and their estimations.

Calibrations:

- Calibration of weights.

EDTA Back-titrations:

- Estimation of Ni^{2+}.
- Estimation of Al^{3+}

EDTA Substitution titrations:

- Estimation of Ca^{2+}

Preparation of complexes:

- Ammonium tetrathiocyanatodiamminechromate(III)
- Tris(acetylacetanato)manganese
- Tris(ethylenediamine)nickel (II) thiosulphate
- Mercury tetrathiocyanatocobaltate (II)
- Pentaammine(chloro)cobalt (III) chloride
- Potassium dioxalatocuprate(II) dehydrate

Preparation of complexes and calculation of % purity:

- Tetramminecopper(II)sulphate and estimation of NH_3 and calculation of % purity

Redox Titrations

- Estimation of Ferrocyanide and Ferricyanide in a mixture

References:

1. A.I.Vogel, **Text book of Quantitative Inorganic Analysis** (3rd Ed.), ELBS 1969.
2. Jeffery et.al, **Vogel's text book of Quantitative Inorganic analysis** (4th Ed.), ELBS 1988.
3. Jeffery et.al, **Vogel's text book of Quantitative Inorganic analysis** (5th Ed.), ELBS 1989.
4. J. Mendham et.al, **Vogel's text book of Quantitative Inorganic Analysis** (6th Ed.), Pearson education Ltd., 2000.
5. G.Marr and R.W.Rockett, 1972, **Practical Inorganic chemistry**.
6. Mounir A. Malati, 1999, **Experimental Inorganic/Physical Chemistry–An Investigative integrated approach to Practical Project work**.

ORGANIC CHEMISTRY PRACTICALS-I

Credits: 2 **Semester: I**

Subject Code: MOC19152 **No. of hours/week: 5**

Objectives

- To synthesize one-step organic compounds.
- To apply knowledge of Thin Layer Chromatography

Outcome

- The student will develop the skill to carry out the organic synthesis using TLC analysis

Synthesis of the following compounds:

- Tetrahydrocarbazole, 7-hydroxy-4-methyl coumarin, *m*-dinitrobenzene, hippuric acid, anthracene-maleic anhydride adduct, phthalimide, 2,4-dihydroxyacetophenone, 4-chlorotoulene, coumalic acid

Thin layer chromatography:

- Determination of suitable solvent system given 2 mixtures
- Determination of purity of a given 2 samples
- Identification of unknown organic compounds by comparing the R_f values of known standards

Demonstration experiment:

Synthesis of organic compounds by the use of microwave oven (any 2 examples)

References:

1. A.I.Vogel, 1989, **Text book of practical organic chemistry** (5^{th} Ed.).
2. F. G. Mann and B.C. 1990, **Saunders, Text book of practical organic chemistry** (5^{th} Ed.).

PHYSICAL CHEMISTRY PRACTICALS-I

Credits: 2 **Semester: I**

Subject Code: MOC19153 **No. of hours/week: 5**

Objective

- To apply the knowledge of various electro analytical techniques in studying reactions

Outcome

- The student will learn about various electro-analytical techniques.

Physical properties:

- Determination of viscosity of liquids

Colorimetry:

- Verification of Beer's law and calculation of molar absorption coefficient using $CuSO_4$ solution
- Verification of Beer's law and calculation of molar absorption coefficient using $KMnO_4$ solution

Conductometry:

- Titration of strong acid *vs* strong base
- Titration of weak acid *vs* strong base
- Determination of cell constant
- Determination of dissociation constant of a weak acid
- Titration of a mixture of strong and weak acids *vs* strong base
- Mixture of strong acid, weak acid and $CuSO_4$ *vs* strong base
- Determination of the hydrolysis constant of aniline hydrochloride

Polarimetry:

- Determination of specific rotation of sucrose, glucose
- Acid-catalyzed hydrolysis of sucrose (inversion of sucrose)

Chemical kinetics:

- Acid-catalyzed hydrolysis of methyl acetate
- Peroxydisulphate - I^- reaction (overall order)
- Peroxydisulphate - iodide reaction: order w.r.t $[I^-]$ by isolation method
- Peroxydisulphate - iodide reaction: order w.r.t $[S_2O_8^{2-}]$ by initial rate method

Critical Solution Temperature:

- Determination of critical solution temperature of phenol-water system
- Effect of added electrolyte on the CST of phenol-water system

References:

1. B.D. Khosla.**Text book of senior practical physical chemistry**
2. Mounir A.Malati, 1999, **Experimental Inorganic/Physical Chemistry–An Investigative integrated approach to Practical Project work**.
3. J.B. Jadav **Advance Physical Practical Chemistry,** Krishna Publisher
4. A.K. Nad, B. Mahapatra and A. Ghoshal **Advance Course in Practical Chemistry**

HUMAN VALUES & PROFESSIONAL ETHICS

Credits : 2 **Semester: II**
Subject Code : MOC19201 **No. of lecture hours: 30**

Objective

- To emphasize the importance of human values and inculcating them for the betterment of the society.

Outcome

- The student will learn about the human values and professional ethics.

Unit-01: Introduction to Ethics	**6hrs**
• Reasons to have Ethics for Life	1
• Accepted Norms and Counter Values	1
• Happiness as life Goal	2
• Human Context-self and another	2

Unit-02: Towards a new society	**6hrs**
• What is true society	1
• Moral problem of the society	1
• Social desire, social fear, social satence, social indifference	1
• Values revealed and lived in various religions-practicing religious harmony	2
• Eradication of social evil-towards a new society	1

Unit-03: Gender sensitization	**6hrs**
• Why we study it	1
• Socialization-making women and men	1
• Being together as equals-through the lens of gender	1
• Knowledge through the lens of gender	1
• Gender spectrum-beyond the binary	1
• Just relationship-being together as equals	1

Unit-04: Professional ethics		**6hrs**
• Ethics, Professional Ethics, Environmental Ethics		1
• Ethical Situation, Current Ethical Issues	1	
• Values, Policies and Organisation Culture		2
• Moral Situation, Rights and Duties, Codes of Ethics, Their Limitation	2	

Unit-05: Ethics in science		**6hrs**
• Professional Research in Academia and Industry, Scientific fraud		1
• Plagiarism, Conflict of Interest	1	
• Student-Advisor relationship, Intellectual property and Patents	2	
• Accountability and Institutional Practices		2

References:

1. Human Values - Development Programme - AIACHE
2. In Harmony
3. S.S. Dara and D.D. Mishra 2010.**Environmental Chemistry and Pollution Control** New Delhi: S. Chand Publisher.
4. Jeffery Kovac, Ethics in Science, **Accountability in Research** *22*, 312, **2015**.

5. A.Suneetha, B.Uma, D. Vasanta, M. Rama, N. Vasundha, A. Raheed, G**,** Shamala, D. Sreenivas and S. Tharu 201. **Towards a World of Equals: A Bilingual Text on Gender**. Hyderabad: Telugu Akademi

INORGANIC CHEMISTRY-II

Credits: 4 **Semester: II**
Subject Code: MOC19202 **No. of lecture hours: 60**

Objectives

- To impart knowledge of co-ordinate complexes, their reaction mechanisms and metal clusters
- To acquire the knowledge of special symmetry groups and assign the same to the molecules.
- To understand the role of metal ions in biological systems.

Course Outcomes

- **Perceives understanding** about terms, term symbols and icrostates
- **Enlights** the knowledge about higher pointgroups
- **Analyses** the reaction pathways of complex formation
- **Learn** the structural patterns of metal clusters
- **Validate** the role of bioinorganic chemistry in everyday life

Unit-06: Bonding in metal complexes- II **12 hrs**

- Free ion terms and Energy levels: Configurations, Terms, States and Microstates — 3
- Formula for the calculation of Microstates $p^n$and d^nconfigurations: L-S (Russel-Saunders) coupling scheme, j-j coupling scheme — 3
- Determination of terms for various p^n and d^n configurations of metal ins. Hole formalism, Energy ordering of terms (Hund's rules). Inter electron repulsion parameters (Racah parameters), Spin-Orbital coupling parameters — 3
- Effect of weak cubic crystal fields on S, P, D and F terms- Orgel diagrams. Application of electronic spectra of metal complexes-$3d^1$ to $3d^9$ hexaaquo metal complexes — 3

Unit-07: Symmetry of molecules **12 hrs**

- Molecules of special Symmetry: Linear or Infinite groups, Molecules containing multiple higher order axis T, Th, Td, O, O_h, I_h, K_h — 4
- Exercises on point groups, descent in symmetry of molecules with substitution — 2
- Symmetry and stereo isomerism: Symmetry and dipole moment, symmetry criteria for optical activity, symmetry restrictions on dipole moment — 4
- Fullerenes: Structure and symmetry of fullerenes — 2

Unit-08: Reaction Mechanism-II **12 hrs**

- Ligand substitution reactions in square planar complexes: Mechanism of substitution in square planar complexes, trans-effect, Grienberg's polarization theory and π - bonding theory, applications of Trans-effect in synthesis of Pt (II) complexes — 4
- Electron transfer reactions (or Oxidation-Reduction) in Coordination compounds: Mechanism of One-electron transfer reactions: Atom or (group) Transfer or Inner Spheres Mechanism, Direct electron transfer or Outer sphere mechanism. Complementary & non complementary reactions, Cross reactions and Marcus Hush theory — 3
- Nature of bridging ligands. Distinguish between, outer sphere & inner sphere electron transfer reaction mechanism — 3

- Reaction pathways in organometallic complexes. Oxidative addition reductive elimination insertion reactions — 2

Unit-09: Metal clusters — **12 hrs**

- Polyhedral skeletal electron pair theory and total electron count theory, Wade's rules and polyhedral geometries of carbonyl clusters — 2
- Carbonyl clusters: Factors favouring metal-metal bonding — 1
- Classification of clusters: Low nuclearity clusters: M_3 and M_4 clusters. Structural patterns in $M_3(CO)_{12}$ [M=Fe, Ru, Os] and $M_4(CO)_{12}$ [M=Co, Rh, Ir] clusters. Relative stability of bridging and nonbridging structures — 2
- High Nuclearity clusters: M_5, M_6, M_7, M_8 and M_{10} clusters. Capping rule. — 1
- Structural patterns in $[Os_6(CO)_{18}]^{2-}$, $[Rh_6(CO)_{16}]$, $[Os_7(CO)_{21}]$, $[Rh_7(CO)_{16}]^{3-}$, $[Os_8(CO)_{22}]^{2-}$, $[Os_{10}C(CO)_{24}]^{2-}$ and $[Ni_5(CO)_{12}]^{2-}$ — 2
- Metal Halide clusters: Major structural types in Dinuclear Metal-Metal systems: Edge sharing Bioctahedra, Face sharing Bioctahedra, Tetragonal prismatic and Trigonalantiprismatic structures — 2
- Structure and bonding in $[Re_2Cl_8]^{2-}$ and Octahedral halides of $[Mo_6(Cl)_8]^{4+}$ and $[Nb_6(Cl)_{12}]^{2+}$, Trinuclear halides of Re (III) — 2

Unit-10: Bio Coordination Chemistry — **12 hrs**

- Metal ions in biological systems: Brief survey of metal ions in biological systems. Effect of metal ion concentration and its physiological effects — 2
- Oxygen transport and storage: spin-state of iron, Haemoglobin and Myoglobin: Geometric, electronic and magnetic aspects of dioxygen binding, oxygen adsorption isotherms and cooperativity in haemoglobin and its physiological significance. Role of globin chain — 4
- Haemerythrin (Hr) and Haemocyanin (Hc): Introduction-structure of active sites with oxygen and without oxygen. Comparison of Hemerythrin and Hemocyanin with hemoglobin — 3
- Photosynthesis: Structural aspects of chlorophyll. Photo system I and Photo system II — 1
- Vitamin B_6 model systems: Forms of vitamin B6 with structures. Reaction mechanisms of (1) Transamination (2) Decarboxylation and (3) Dealdolation in presence of metal ions — 2

References:

Unit-06:

1. J.E.Huheey, K.A.Keiter and R.L.Keiter, 1993, **Inorganic Chemistry** (4th Ed.), Harper Cottens College Publications.

Unit-07:

2. K.Veera Reddy 2009, **Symmetry and Spectroscopy of Molecules** New Age International Publishers.
3. Mark Ladd, 2000 **Symmetry and Group theory in Chemistry**, Marwood Publishers, London.
4. Robert L.Carter, 1998 **Molecular Symmetry and Group Theory**, John Wiley & Son

Unit-08:

5. K.Veera Reddy, 2005. **Metal ions in Reaction Mechanisms** (1st Ed.), Golgotia Publications (P) Ltd.

6. Richard A Henderson, 1993, **Mechanisms of Reactions in Transition Metal Sites,** Oxford Science Publications, London.
7. F.Basolo and R.G.Pearson, 1967, **Inorganic Reaction Mechanisms** (2nd Ed.), Wiley, New York.

Unit-09:

8. F.A.Cotton, G.Wilkinson, C.A.Murillo and M.Bochmann, 1999, **Advanced Inorganic Chemistry** (6th Edition), Wiley Interscience,New York.
9. G.L.Eichorn, 1982, **Inorganic Biochemistry**(Vol. 1)., Elsevier
10. Keith F.Purcell and John C.Kotz, 1977, **Inorganic Chemistry**, Holt-Saunders International Editions, London.

Unit-10:

11. I.Bertini, H.B.Gray, S.J.Lippard and SJ.Valentine, 1998, **Bioinorganic Chemistry** (1st Ed.), Viva Low- Priced Student Edition, New Delhi.
12. W.Kain and B.Schwederski, 1999, **Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life**, John Wiley and Sons, NY.
13. Keith F.Purcell and John C.Kotz, 1977, **Inorganic Chemistry**, Holt-Saunders International Editions, London.

ORGANIC CHEMISTRY-II

Credits: 4 **Semester: II**

Subject Code: MOC19203 **No. of lecture hours: 60**

Objectives

- To understand the mechanisms in organic reactions involving aromatic systems.
- To acquire knowledge of pericyclic and photochemical reactions.
- To have an understanding of the applications of various reagents in organic reactions.

Course Outcomes

- Develops an understanding about organic reaction mechanisms
- Appreciates the fundamentals of pericyclic reactions
- Apply the theories of pericyclics to molecular reactions
- Understands the importance of photochemistry
- Gains the potential of organic reagents

Unit-06: Conformational Analysis (Acyclic Systems) **12 hrs**

- Introduction to conformational isomerism and concept of dynamic stereochemistry. Klyne-Prelog terminology for conformers and torsion angles — 1
- Conformational analysis of ethane, 1,2-disubstituted ethane derivatives like butane, dihalobutanes, halohydrin, ethylene glycol, butane-2,3-diol, amino alcohols and 1,1,2,2-tetrahalobutanes. Conformations of unsaturated acyclic compounds: propylene, 1-Butene, acetaldehyde, propionaldehyde and butanone — 6
- Conformational diastereoisomers and conformational enantiomers. Factors affecting the conformational stability and conformational equilibrium: Attractive and repulsive interactions. Use of physical and spectral methods in conformational analysis — 3
- Conformational effects on the stability and reactivity of acyclic diastereoisomers, steric and stereo electronic factors with examples — 2

Unit-07: Reaction Mechanism-II **12 hrs**

- Nucleophilic Aromatic substitution: Aromatic Nucleophilic substitution: S_N1 (Ar), S_N2 (Ar), and benzyne mechanisms. Definition and types of ambident nucleophiles — 4
- Neighboring group participation: Criteria for determining the participation of neighboring group. Enhanced reaction rates, retention of configuration, isotopic labeling and cyclic intermediates — 4
- Neighboring group participation involving halogens, oxygen, nitrogen, aryl, cycloalkyl groups, σ and π- bonds, and non-classical carbocations — 4
- Electrophilic substitution at saturated carbon and single electron transfer reactions. Mechanism of aliphatic electrophilic substitution
- SE1, SE2, and SEi. SET mechanism

Unit-08: Pericyclic Reactions-I **12 hrs**

- Introduction, Classification of pericyclic reactions, 4n, 4n+2 systems and examples. — **1**
- Electrocyclic reactions: con rotation and dis rotation. Electrocyclic closure and opening in 4n and 4n+2 systems. — **2**

- Cycloaddition reactions: suprafacial and antara facial additions. 4n and 4n+2 cycloadditions. Stereochemical aspects in supra-supra, supra-antara, antara-supra and antara-antara 4n and 4n+2 cycloadditions, Diels Alder reaction *(endo, exo)*- stereoselectivity **4**
- Sigmatropic reactions [i, j] shifts- suprafacial and antarafacial shifts, Cope, Aza-Cope and Claisen rearrangement reactions **3**
- Molecular orbitals: ethylene, 1, 3-butadiene, 1, 3, 5-hexatriene, allyl cation, allyl radical, pentadienyl cation, pentadienyl radical **2**

Unit-09: Pericyclic Reactions-II **12 hrs**

Theories involved in understanding pericyclic reactions: **4**

- Introduction to Aromatic Transition state Theory: Concept, Woodward-Hoffman se1ection rules for electrocyclic reactions, cycloaddition and sigmatropic reactions based on ATS aromatic transition state (Huckel-Mobius) approach
- Frontier Molecular Orbital Theory: Concept, Woodward- Hoffman selection rules for electrocyclic, cycloaddition, and sigmatropic reactions based on FMO approach **4**
- Conservation of Molecular Orbitals Theory: Construction of correlation diagram for 4n & 4n+2 electrocyclic reactions and cycloaddition (π^2s+π^2s and π^4s+π^2s) systems **4**

Unit-10: Heterocyclic chemistry **12hrs**

- Nomenclature of heterocyclic systems based on ring size, number and nature of hetero atoms 3
- Synthesis and reactivity of indole, benzofuran 4
- Synthesis and reactivity of benzothiophene, quinoline, isoquinoline, coumarin, chromone 5

References:

Unit-06:

1. Ernest L Eliel, Samuel H.Wilen, 2008, **Stereochemistry of Carbon compounds**, John Wiley & Sons INC.
2. D. Nasipuri, 2006, **Stereochemistry of organic compounds- Principles and Applications** (2nd Ed.), New Age International publishers.
3. P S Kalsi, 2010, **Stereochemistry: Conformation & Mechanism** (7th Ed.), New Age International publishers

Unit-07:

4. Jerry March, 1992, **Advanced Organic Chemistry**(5th Ed.), Wiley-India student edition
5. S. Mukerjee,2007, **Mechanism and Structure in Organic Chemistry**(3rd Ed.), MacMillan Publishers India Limited
6. I. L. Finar, 1963, **Organic chemistry** (4th Ed.), Vol. I and II, Longmans
7. D. H. R. Barton and W. D. Ollis, 1978, **Comprehensive organic chemistry**, Vol.5.

Unit-08& 09:

8. Woodward and Hoffmann, 1971, **Conservation of Orbital Symmetry Available** as e-book.
9. Gilchrist and Storr, 1979, **Organic Reactions and Orbital Symmetry**, Cambridge University Press.
10. J.Singh, 2006, **Photochemistry and Pericyclic Reactions** (2nd Ed.), New Age International publishers.

11. Lehr and Merchand, 1972. **Pericyclic Reactions— a problem solving approaches**, Academic Press: New York.

Unit-10:

12. Gilchrist, T. 1987. **Heterocyclic Chemistry.** Pitmann Publishing Ltd.
13. Bansal, R. K. 2005. **Heterocyclic Chemistry**. 4th Edition. New Delhi: New Age International Pvt. Ltd.
14. Joule J.A. and Mills, K. 2004. **Heterocyclic Chemistry**. 4th Edition. Blackwell Publishers.
15. Joule J.A. and Smith. 2010. **Heterocyclic Chemistry**. 5th Edition. ELBS.
16. Acheson. R. M. 1967. **An Introduction to the Chemistry of Heterocyclic Compounds.** 2nd Edition. Wiley & Sons.
17. Gupta R R. Kumar, M. and Gupta V. 2005. Vol-I and Vol-II. **Heterocyclic Chemistry**. 1st Indian Edition Springer publications.

PHYSICAL CHEMISTRY-II

Credits: 4 **Semester: II**

Subject Code: MOC19205 **No. of lecture hours: 60**

Objectives

- To understand the thermodynamic properties of reactions.
- To study the nature of electrochemical cells and their applications
- To impart knowledge about the subatomic particles of matter.
- To acquire the knowledge of kinetic mechanism.
- To understand the concepts of solid state chemistry.

Course Outcomes

- Appreciates the fundamentals of molecular thermodynamics
- Recognizes the various electrochemical reactions
- Applies the wave mechanics for determining atomic structures
- Understands the importance of quantitative mechanics in electronic filling
- Visualizes the macromolecular structures

Unit-06: Thermodynamics-II **12 hrs**

- Solutions: Specifying the Solution composition, partial molar properties-significance, relation between solution volume and partial molar volume. Measurement of partial molar volumes: slope and intercept methods — 3
- The chemical potential, variation of chemical potential with T and P, Gibbs-Duhem equation-derivation and significance — 2
- Ideal solutions: Thermodynamic properties of ideal solutions, mixing quantities, vapour pressure-Raoult's law. Thermodynamic properties of ideally dilute solutionsvapour pressure- Henry's law — 2
- Non ideal systems: Concept of fugacity, fugacity coefficient, determination of fugacity. Non ideal solutions: Activities and activity coefficients, standard-state conventions for non-ideal solutions, determination of activity coefficients from vapour pressure measurements, activity coefficients of nonvolatile solutes using Gibbs-Duhem equation — 4
- Multi component phase equilibrium: Vapour pressure lowering, freezing point depression and boiling point elevation — 1

Unit-07: Electrochemistry-II **12 hrs**

- Potentiometry: Types of electrodes, Hydrogen gas, Calomel, Quinhydrone and glass electrodes. Determination of pH. Potentiometric titration of redox reaction — 2
- Amperometric titrations: Principle, Instrumentation and applications of amperometric titrations, determination of SO_4^{2-}, metal ions viz., Mg^{2+}, Zn^{2+}, Cu^{2+} and other substances — 3
- Cyclic voltammetry: Principle, instrumentation, reversible and irreversible cyclic voltammograms, Application: Cyclic voltammetric study of insecticide parathion — 3
- D.C Polarography: Two and Three electrode assemblies. Dropping mercury electrode, instrumentation — 2
- Types of Currents: Residual, Migration, Limiting. Types of limiting — 2

Currents: Adsorption, Diffusion, Kinetic

Unit-08: Quantum chemistry-II	**12 hrs**
• Theorems of quantum mechanics: Real nature of the Eigen values of a Hermitian operator-significance. Orthogonal nature of the Eigen values of a Hermitian operator-significance of orthogonality. Expansion of function in terms of eigenvalues. Eigen functions of commuting operators-significance. Simultaneous measurement of properties and the uncertainty principle	3
• Particle in a box-one dimensional and three dimensional	2
• Plots of ψ and ψ^2-discussion. Degeneracy of energy levels. Comparison of classical and quantum mechanical particles	1
• Calculations using wave functions of the particle in a box-orthogonality, measurability of energy, position and momentum, average values and probabilities	2
• Application to the spectra of conjugated molecules	1
• Cartesian, Polar and spherical polar coordinates and their interrelations. Schrodinger equation for the hydrogen atom- separation into three equations	3

Unit-09: Quantum chemistry-III	**12 hrs**
• Hydrogen like wave functions. Radial and angular functions. Quantum numbers n, l and m and their importance	2
• The radial distribution functions. Hydrogen like orbitals and their representation. Polar plots, contour pots and boundary diagrams	2
• Many electron systems. Approximate methods. The variation method-variation theorem and its proof. Trial variation function and variation integral	2
• Examples of variational calculations. Particle in a box. Construction of trial functions by the method of linear combinations. Variation parameters. Secular equations and secular determinant	2
• Bonding in molecules. Molecular orbital theory-basic ideas. Construction of MOs by LCAO, H_2^+ ion. The variational integral for H_2^+ ion. Detailed calculation of Wave functions and energies for the bonding and antibonding MOs. Physical picture of bonding and antibonding wave functions. Energy diagram	2
• The MO wave function and the energy of H_2 molecule MO by LCAO method and Valence bond method (detailed calculations not required). The MO wave function and the energy of H_2 molecule MO by LCAO method and Valence bond method (detailed calculations not required)	2

Unit-10: Solid state chemistry	**12 hrs**
• Electrical and Magnetic properties of solids- classification of electrical and magnetic materials, Magnetic susceptibility	2
• Electronic properties of metals, insulators and semiconductors: Electronic structure of solids, Band theory- band structure of metals, insulators and semiconductors	2
• Electrons, holes and excitons, the temperature dependence of conductivity of extrinsic semiconductors, photo conductivity and photovoltaic effect-*p*-*n* junctions	2
• Superconductivity*:* Occurrence of superconductivity, destruction of superconductivity by magnetic fields-Meisner effect, theories of super conductivity- BCS theory	3

- High temperature superconductors*:* Structure of defect pyrovskites. High T_c super conductivity in cuprates, phase diagram of Y-Ba-Cu-O system, crystal structure of $YBa_2Cu_3O_{7-x}$, preparation of 1-2-3 materials, origin of high T_c superconductivity. 3

References:

Unit 06:

1. Peter Atkins and Julio de Paula. **Atkin's Physical Chemistry**, Oxford University press
2. Ira N. Levine. **Physical Chemistry**, McGraw Hill
3. D. A. McQuarrie and J. D. Simon. **Physical Chemistry-A Molecular approach**, Viva Books Pvt. Ltd
4. D. A. McQuarrie and J. D. Simon. **Molecular Thermodynamics**, University Science Books

Unit 07:

5. Heyrovsky, 1966. **Principles of Polarography,** Publishing House of the Czechoslovak Academy of Sciences,
6. Kapoor. R. C. Agarwal B. S. 1991. **Principles of Polarography,**Wiley.
7. Charlot C.1962. **Modern Electro analytical methods,** Elsevier Company.

Unit 08 & 09:

8. Ira N. Levine. **Quantum Chemistry**, Prentice Hall
9. A. K. Chandra. **Introduction to Quantum Chemistry**, Tata McGraw Hill

Unit 10:

10. Leonid V. Azaroff. **Introduction to Solids**, Tata McGraw Hill
11. Chakrabarthy. D. K. **Solid state Chemistry**, New Age International
12. West. A. R. **Solid state Chemistry and its applications**, Plenum.
13. Keer. H. V. **Principles of the Solid State**, New Age International

ANALYTICAL TECHNIQUES AND SPECTROSCOPY-II

Credits: 4 **Semester: II**

Subject Code: MOC19205 **No. of lecture hours: 60**

Objectives

- To acquire knowledge of hyphenated techniques.
- To gain knowledge of various spectroscopic techniques and their applications.

Course Outcomes

- Summarizes the concepts of hyphenated techniques
- Distinguish and identify first and non-first NMR spectra
- Gain knowledge about mass spectrometry
- Analyze the chemical structure using mass fragmentation
- Validates the structure of molecular ions through PES

.

Unit-06: Chromatography Techniques-II	**12 hrs**
• **GC-MS:** Principle, instrumentation; interfaces, jet separators, mass analyzer, mass chromatogram with an example, applications	3
• **GC-FT-IR**: Instrumentation, principles and applications	3
• **LC-MS**: Instrumentation, principles, interfaces and applications	3
• **ICP-MS**: Instrumentation, principles, quantitative analysis and applications	3

Unit-07: NMR spectroscopy-II	**12 hrs**
• First order and non-first order spectra e.g., AX, AX_2, AX_3, A_2X_3, AMX and AB	3
• Simplification of complex spectra: increased field strength, deuterium exchange, Lanthanide shift reagents and double resonance techniques, discrimination of enantiomers by chiral NMR solvents	3
• Nuclear Overhauser enhancement (NOE)	1
• Study of aromaticity and fluxional molecules (eg.$[C_8H_8Ru(CO)_3]$, NMR of paramagnetic compounds: acetylacetone complexes	2
• ^{19}F NMR spectroscopy: ^{19}F chemical shifts, coupling constants. Applications of ^{19}F NMR involving coupling with ^{19}F, ^{1}H and ^{31}P: 2,2,2-trifluoro ethanol, 1,2-dichloro-1,1-difluoro ethane, 5-bromo-1,2,3-trifluoro benzene, BrF_5, SF_4, PF_5, ClF_3, IF_5	2
• Introduction to solid state NMR, Magic angle spinning	1

Unit-08: Mass spectrometry-I	**12 hrs**
• Origin of mass spectrum, principles of EI mass spectrometer	2
• Types of fragments: odd electron and even electron containing neutral and charged species (even electron rule), Nitrogen rule, isotopic peaks, determination of molecular formula and metastable ion peaks	4
• Principle of EI, CI, Fast Atom Bombardment (FAB), Secondary Ion Mass Spectrometry (SIMS), Thermospray (TSI) ionization, and Matrix Assisted Laser Desorption Ionization (MALDI) methods. High resolution mass spectrometry	6

Unit-09: Mass spectrometry-II **12 hrs**

- Fragmentation pattern of organic compounds: cleavage of one, two or more bonds, β-cleavage, McLafferty rearrangement, retro Diels–Alder fragmentation, ortho effect, dehydration, dehydrohalogenation, decarboxylation and elimination of NO. Determination of molecular formula — 8
- Fragmentation of cycloalkanols, cycloalkanones and cyclo alkyl amines — 2
- Application of mass spectrometry to metal carbonyls — 2

Unit-10: Nano chemistry **12 hrs**

- Introduction, definition of a nanosystem, dimensionality and size dependent phenomena, Surface to volume ratio, Fraction of surface atoms, Surface energy — 2
- Preparation of nanoparticles– Bottom-up approach, Top-down approach, chemical vapour deposition method, Thermolysis method, Pulsed laser method — 2
- Carbon-based nano materials (buckyballs, nanotubes, graphene), Core-shell nanoparticles, self- assembled monolayers, magnetic nanoparticles — 4
- Characterisation of Nanomaterials: UV-Visible spectroscopy, SEM, TEM, STM, XRD (principles only) — 3
- Applications of nanomaterials in medicine — 1

References:

Unit-06:

1. Sane and Joshi, 1999, **Electro analytical Chemistry theory and applications,** Quest Publications.
2. Raymond PW Scott, **Techniques and practices of Chromatography,** Marcel Dekker, Inc. New York.
3. WMA Neissen& J V Greef, **Liquid Chromatography- Mass spectrometry Principles & Applications,** Marcel Dekker, Inc. New York.
4. Raymond PW Scott, 1988, **Introduction to analytical Gas Chromatography** (2nd Ed.), Marcel Dekker, Inc. New York

Unit-07:

5. Jag Mohan, 2008, **Organic spectroscopy-Principles applications** (2nd Ed.), Narosa publications.
6. William Kemp, 2008, **Organic Spectroscopy** (3rd Ed.), Palgrave.
7. R.M. Silverstein and F.X. Webster,1998, **Spectroscopic identification of organic compounds,** (6thEd),Wiley.
8. William Kemp,1988, **NMR-A multinuclear introduction**(3rd Ed.), MacMillan.
9. W. Dolbier, 2009, **Guide to Fluorine NMR for organic chemist** (1stEd.),Wiley.

Unit-08 &Unit-09:

10. A. H. Beckett and J.B. Stenlake, 1988, **Practical Pharmaceutical Chemistry**(4th Ed.),WCIR, London
11. Robert Alexander Walker Johnstone, 1996, **Mass Spectrometry for Chemists and Biochemists** (2nd Ed.), Cambridge University Press.
12. Pavia, 2004, **Introduction to organic spectroscopy** (3rd Ed.), Thomson
13. R.M. Silverstein and F.X. Webster, 1998, **Spectroscopic identification of organic compounds,** (6thEd), Wiley.

Unit-10:

12. Pradeep T. 2007, **Nano: the Essentials**. Tata McGraw Hill.
13. Varghes T and Balakrishna K. M. 2012, **Nanotechnology,** Atlantic publishers.
14. Pradeep T.2012. **Textbook of Nano Science and Nanotechnology,** Tata McGraw Hill

CHEMISTRY LAB PRACTICES

Credits: 1 **Semester: II**
Subject Code: MOC19251 **No. of hours/week: 2**
Objectives:

- To learn how to prepare different solutions and reagents.
- To draw and analyse the organic molecules using chemistry software programmes

- **Concept of Concentrations:** Normality, Molarity, ppm, ppb
- Role of an indicator in detecting end point in volumetric analysis- acid base titrations, redox titrations, precipitation titrations and complexometric titrations
- Preparation of indicators and use of indicators: Phenolphthalein, Methyl orange, Methyl-red, Potassium Chromate, Diphenylamine, EBT
- Preparation of buffers – pH 10 ammonical buffer and acetate buffer solutions: Ammonium hydrogen phosphate solution, Bayer's reagent, Benedict's solution, Bromine water, Dimethyl glyoxime reagent, 2,4-Dinitrophenyl hydrazine reagent, Eriochrome black-T reagent
- **Chemistry software programmes:** Chem Draw structures of 2,3-dichloropropene,4-methyl-2-pentanone, methyl-2-furan carboxylate, N-methyl pyridine, ethyl-p-toulenesulphonicacid, papavarine, camphor, abietic acid, morphine, quinine), analysis of IR using ORIGIN data analysis software and NMR using Mestrec or MestreNova NMR processor. EXCEL: Drawing graphs.

References:

1. Vogel's Text Book of Quantitative Chemical Analysis, 5th edition.
2. Vogel's Text Book of macro and semimicro qualitative inorganic analysis. G. Svehla, 5th edition.
3. Chemistry Reagent Manual Prepared by Chemistry Department, SGTB Khalsa College under DBT's Star College Scheme, University of Delhi (Available: online)
4.
5. Silverstein, Bassler and Morrerl, 1998. **Spectrometric Identification of Organic Compounds.** 5th Edition. John Wiley& sons.
6. Field, L.D., Sternhell, S. and Kalman J. R. **Organic Structures from Spectra**. 5th Edition. John Wiley & sons.
7. William Kemp. 2008. **Organic Spectroscopy.** 3rd Edition. Palgrave.
8. Kalsi, P S. 2005. **Spectroscopy of Organic Compounds**. 6th Edition. New Delhi: New Age International publishers.
9. Pavia, 2004. **Introduction to Organic Spectroscopy**. 3rd Edition. Thomson.
10. Jagmohan. 2010. **Organic Spectroscopy, Principles and Applications**. 2nd Edition. New Delhi: Narosa Publication House Pvt. Ltd.

INORGANIC CHEMISTRY PRACTICALS-II

Credits: 2 **Semester: II**

Subject Code: MOC19252 **No. of hours/week: 5**

Objectives

- To analyze the metal ions gravimetrically.
- Separation and analysis of mixture of complexes volumetrically and gravimetrically.

Outcome

- The student will learn to perform gravimetric and volumetric analysis of the inorganic complexes.

One component gravimetric estimations (Use of sintered glass crucible):

- Estimation of Zn^{2+}
- Estimation of Ba^{2+}

Analysis of Two component mixtures:

- Separation of Ni^{2+} and Cu^{2+} in a mixture and estimation of Ni^{2+} (gravimetric) and Cu^{2+} (volumetric)
- Separation of Al^{3+} and Fe^{3+} in a mixture and estimation of Al^{3+} (gravimetric) and Fe^{3+} (volumetric)
- Separation of Ag^{+} and Ca^{2+} in a mixture and estimation of Ag^{+} (gravimetric) and Ca^{2+} (volumetric)

Analysis of three component mixtures:

- Separation of (Ni^{2+} and Cu^{2+}) from Mg^{2+} in the given mixture and estimation of Mg^{2+} (Gravimetric)

Ion exchange methods of analysis:

- Determination of capacity of an ion exchange resin.
  Separation of Zinc and Magnesium on an anion exchange resin and estimation of Mg^{2+} and Zn^{2+}

Applied titrimetric analysis:

- Analysis of iron and calcium in cement
- Determination of calcium in calcium tablets

References:

1. Jeffery et.al, 1988, **Vogel's text book of Quantitative Inorganic analysis** (4^{th} Ed.), ELBS.
2. Jeffery et.al, 1989, **Vogel's text book of Quantitative Inorganic analysis** (5^{th} Ed.), ELBS
3. J. Mendham et.al, 2000, **Vogel's text book of Quantitative Inorganic Analysis** (6^{th} Ed.), Pearson education Ltd.

ORGANIC CHEMISTRY PRACTICALS-II

Credits: 2 **Semester: II**

Subject Code: MOC19253 **No. of hours/week: 5**

Objectives

- To identify the given organic compound and assign its functional group qualitatively.
- To separate an organic mixture and apply systematic functional group analysis.

Outcome

- The student will be able to separate the mixture and analyze the organic functional groups present.

Identification of organic compounds systematic qualitative analysis:

- Physical data BP / MP, Ignition test, solubility classification, Extra elements-N, S & Halogens, (Lassaigne's sodium fusion test)
- Functional groups tests, Preparation of crystalline derivative and determination of their mp's for atleast **3** compounds belonging to strong acid, weak acid, neutral, bases, carbohydrates & hydrocarbons.

Separation of two component mixtures by chemical methods and their identification by chemical reactions

- Separation by using solvent ether, dil. hydrochloric acid, 5 % aqueous sodium bicarbonate and sodium hydroxide solutions.
- Checking the purity of the two components by TLC, identification of the compounds by a systematic study of the physical characteristics (mp/ bp), extra elements (nitrogen, halogens and sulfur), solubility, functional groups, preparation of crystalline derivatives.
- Separation and analysis of a minimum of **5** binary mixtures by these procedures. Following combinations can be given: strong acid **+** neutral including hydrocarbons, strong acid+ weak acid, weak acid+ neutral including hydrocarbon, base+ hydrocarbon, carbohydrate +weak acid, carbohydrate+ strong acid (other than *p*-nitrobenzoic acid)
- Separation of neutral components of binary mixture using column chromatography

Synthesis of the following compounds:

- Benzanilide from benzophenone (Beckmann rearrangement)
- Synthesis of silver nanoparticles

References:

1. A.I.Vogel, 1989, **Text book of practical organic chemistry** (5th Ed.).
2. F. G. Mann and B.C. 1990, **Saunders, Text book of practical organic chemistry** (5th Ed.).

PHYSICAL CHEMISTRY PRACTICALS-II

Credits: 2 **Semester: II**

Subject Code: MOC19254 **No. of hours/week: 5**

Objectives

- To apply the knowledge of various electro analytical techniques in studying reactions

Outcome

- The student will be able to perform various experiments involving different analytical techniques

Potentiometry:

- Titration of strong acid *vs* strong base
- Titration of weak acid *vs* strong base
- Titration of dibasic acid *vs* strong base
- Titration of Fe^{+2} *vs* $Cr_2O_7^{-2}$ (redox titration)
- Titration of Cl^- *vs* Ag^+ (precipitation titration)
- Determination of single electrode potential
- Determination of solubility product

pH metry:

- Calibration of a pH meter and measurement of pH of different solutions
- Preparation of phosphate buffers.
- Monobasic acids *vs* strong base.
- Dibasic acid *vs* strong base

Spectrophotometry:

- Estimation of Cu(II) using EDTA.
- Estimation of Fe(II) using 1,10-phenanthroline

Distribution:

- Distribution of iodine between Cyclohexane and water
- Distribution of I_2 between Cyclohexane and aq.KI solution- calculation of equilibrium constant

Chemical Kinetics:

- Stoichiometry of peroxydisulphate–iodide reaction
- Study of acetone-iodine clock reaction
  - i) Order w.r.t. [iodine]
  - ii) Order w.r.t. [acetone]

Adsorption:

- Adsorption of acetic acid on animal charcoal or silica gel

References:

1. B. D. Khosla, **Text book of senior practical physical chemistry** R. Chand & Co. New Delhi
2. Mounir A.Malati, 1999, **Experimental Inorganic/Physical Chemistry–An Investigative integrated approach to Practical Project work**.
3. J.B. Jadav **Advance Physical Practical Chemistry,** Krishna Publisher
4. A.K. Nad, B. Mahapatra and A. Ghoshal **Advance Course in Practical Chemistry**

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THE DEPARTMENT OF M.Sc. ORGANIC CHEMISTRY

PROGRAM OUTCOMES (M.Sc.)

PO1: Scientific Knowledge: Ability to build a strong foundation of knowledge, integrated with the latest developments in science and technology which help students develop critical thinking, reasoning, decision making in process of quality education.
PO2: Problem Analysis: Identify, formulate and analyse the complex scientific problems using the knowledge gained across various streams of science and technology.
PO3: Effective Communication: Ability to articulate ideas, communicate effectively using current tools in the field of ICT along with effective report writing and documentation.
PO4: Development of Skill and Attitude: Enabling the students with the required skill, right attitude, time management and self-discipline for prominent career in industry, research institutes and for further academic study.
PO5: Life Long Learning and Social Responsibility: Recognise the need and ability to engage in lifelong learning and work effectively as an individual and as a member of diverse team. Students get the ability to act with an informed awareness of issues to participate in civic life through volunteering.

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Program Specific Outcomes

PSO1 **Understands, identify and interrelate** with the background of organic reaction mechanisms, complex Stereochemical structures, molecular rearrangements, instrumental method of chemical analysis and separation techniques

PSO2 **Analyses** the importance of various elements in the periodic table, coordinationchemistry and structure of molecules, properties of compounds, and structural determination of complexes using theories.

PSO3 **Gathers attention** about the physical aspects of atomic structure, dual behaviour, reaction pathways with respect to time, various energy transformations, molecular assembly in nanolevel, electrochemistry &**infer** their significance

PSO4 **Learns, constructs and analyses** the potential uses of analytical techniques, medicinal chemistry and green chemistry.

PSO5 **Organise** and carry outexperiments in the area of organic analysis,estimation,separation,derivative process, preparation,conductometric, potentiometric and solve spectral analysis

COMPUTER APPLICATIONS

Credits: 2 **Semester: III**
Subject code: MOC19301 **No. of lecture hours: 30**

Objective: To study the applications of computer and its techniques in Organic Chemistry.
Outcome: Students will gain knowledge in computer techniques and their application in Chemistry.

Unit-01: Basics in Computers-I	**6 hrs**
• History of computers, generations of computers	1
• Characteristics of computers	1
• Data representation – number system	1
• Binary, octal and hexadecimal	1
• Conversion from one number system to another	1
• Hardware, Software, Translators, Compilers and interpreters	1

Unit-02: Concepts & Commands	**6 hrs**
• System software, application software	1
• Simple operating concepts, flowchart	1
• Algorithms with simple examples	1
• DOS commands – Internal and external commands	2
• File management and directory structure	1

Unit-03: Computer Networks	**6 hrs**
• Network Types : Local Area Network, Metropolitan Network, Wide Area Network	1
• LAN Topologies: Bus Topology, Ring Topology, Star Topology, Communication Protocol	1
• Network Devices**:** Network Interface Card, Repeater, Bridge, Hub, Switch, Router, Gateway	1
• Wireless Networking **:** Bluetooth Technology, Wireless LAN, Wireless WAN	1
• Computer Security**:** Introduction, Security Threat and Security Attack	1
• Malicious Software: Virus, Worms, Torjan Horses	1

Unit-04: Computing Technologies	**6 hrs**
• Cloud computing: IAAS, PAAS, and SAAS, Grid computing	2
• Excel: Creating a new worksheet-select, edit (Copy, move, format, setting column width etc.)	1
• Referencing cells (Addressing methods), Formulae, charts, macros	1
• Functions-logical, mathematical, statistical, date and time	1
• Creating an excel database-sort and filter database. Performing what –if analysis on worksheet data And Analysis data with pivot tables	1

Unit-05: Fundamentals of Database	**6 hrs**
• Introduction	1
• File-Oriented Approach and Database Approach	1
• Characteristics of Database Approach, Data Models, Schema and Instances	1

- Access Basics**:** Database, tables, records, fields, Entering data, Queries 1

References:

Unit-01-05:

1. **Bharihoke, Deepak. 2012. Fundamentals of Information Technology.** Excel Books.
2. Crawford, Sharon and Neil J. Salkind. 1998. **ABCs of Windows.** BPB Publications.
3. Dennis P. Curtin, Kim Foley, Kunal Sen, Cathleen Morin. 2008**. "Information Technology"**, **The Breaking Wake**. Tata Mc.Graw- Hill
4. Anita Goel, 2010. **"Computer Fundamentals"**. Pearson

ORGANIC CHEMISTRY-III

Credits: 4 **Semester: III**
Subject Code: MOC19302 **No. of lecture hours: 60**
Objectives:

- To understand the conformational analysis of cyclic system.
- To enable the student to apply the knowledge of stereochemistry in asymmetric synthesis.
- To impart knowledge to students regarding various synthetic routes for synthesis of compounds.
- To impart knowledge to student regarding the new techniques developed in organic synthesis

Course Outcome:

CO1	**Perceives** the concept of conformational analysis
CO2	**Analyses** the cruciality of stereochemical process
CO3	**Classify** and interrelates types of asymmetric synthesis
CO4	**Understands** and formulates retrosynthesis
CO5	**Learns** new techniques and concepts in organic synthesis

Unit-01: Conformational Analysis (Cyclic Systems) **12 hrs**

• Study of conformations of cyclohexane, mono, di substituted cyclohexane.	4
• Cyclohexene, cyclohexanone (2-alkyl and 3-alkyl ketone effect), and 2-halo cyclohexanones	2
• Stereochemistry of decalins, bicyclo-(3,3,0)-octane and hydrindanes	1
• Conformational structures of piperidine, *N*-methylpiperidine, D-Glucose (Pyranose and Furanose)	1
• Conformational effects on the stability and reactivity of diastereomers in cyclic molecules - steric and stereoelectronic factors – examples	2
• Factors governing the reactivity of axial and equatorial substituents in cyclohexanes	1
• Stereochemistry of addition to the carbonyl group of a rigid cyclohexanone ring	1

Unit-02: Asymmetric Synthesis-I **12 hrs**

• Review on Selectivity in synthesis: Stereospecific reactions (substrate stereoselectivity). Stereoselective reactions (product stereoselectivity): Enantioselectivity and diastereoselectivity	2
• Introduction and terminology: Topocity in molecules Homotopic, stereoheterotopic (enantiotopic and diastereotopic) groups and faces-symmetry, substitution and addition criteria	2
• Prochirality nomenclature: Pro-R, Pro-S, Re and Si	1
• Conditions for stereoselectivity: Symmetry and transition state criteria	1
• % Enantiomer excess, % enantioselectivity, optical purity, % diastereomeric excess and % diastereoselectivity	1
• Techniques for determination of enantioselectivity: Specific rotation, chiral ^{1}H NMR and chiral HPLC	2

- Classification of asymmetric reactions substrate controlled asymmetric synthesis: Nucleophilic additions to chiral carbonyl compounds. 1,2-asymmetric induction, Cram's rule and Felkin-Anh model — 3

Unit-03: Asymmetric Synthesis-II — **12 hrs**

- Chiral auxiliary controlled asymmetric synthesis: α-Alkylation of chiral enolates, evans oxaenolates, azaenolates. Chiral sulfoxides. 1, 4-Asymmetric induction and Prelog's rule. Use of chiral auxiliaries in Diels-Alder reaction — 4
- Asymmetric aldol reaction, Diastereoselective Aldol reaction and its explanation by Zimmerman Traxel model. Auxiliary controlled Aldol reaction. Double diastereoselection-matched and mismatched aldol reactions — 2
- Chiral reagent controlled asymmetric synthesis: Asymmetric reductions using BINAL-H. Asymmetric hydroboration using IPC_2 BH and $IPCBH_2$. Reductions with CBS reagent — 2

Unit-04: New Techniques and Concepts in Organic Synthesis — **12 hrs**

- Solid phase polypeptide synthesis and requirements — 2
- Solid phase oligonucleotide synthesis (Phospharamidite method) — 1
- Strategies in oligosaccharide synthesis (Linear and convergent synthesis) — 1
- Kahne glycosidation — 1
- Tandem synthesis-Electrocyclic Diels- Alder reaction — 1
- Baldwin rules — 2
- Phase transfer catalyst: Crown ethers and quaternary ammonium salts — 2
- Combinatorial synthesis-introduction, definition and types: Haughton's tea bag procedure, Furkas mix and split Method — 2

Unit-05: Photochemistry — **12 hrs**

- Photochemistry of π-π* transitions: Excited states of alkenes, cis-trans isomerisation, and photo stationary state — 2
- Rearrangements: di-π methane, oxa di-π methane rearrangement. Photoisomerisation of benzene — 3
- Photochemistry of n-π* transitions: Excited states of carbonyl compounds. Homolytic cleavage of α-bond Norrish type I reaction in acyclic and cyclic ketones — 2
- Intermolecular abstraction of hydrogen: photoreduction — 1
- Intramolecular abstraction of hydrogen: Norrish type II reaction — 2
- Paterno-Buchi reaction — 1
- Photochemistry of nitrites: Barton reaction — 1

References:

Unit-01:

1. Eliel, E.L. and Wilen, S.H. 2008. **Stereochemistry of Carbon Compounds.** John Wiley & Sons INC.
2. Nasipuri, D. 2006. **Stereochemistry of Organic Compounds, Principles & Applications**. 2nd Edition. New Delhi: New Age International Publishers.
3. Kalsi, P.S. 2010. **Stereochemistry: Conformation & Mechanism.** 7th Edition. New Delhi: New Age International Publishers.
4. Ward, R.S. 1999. **Stereoselectivity in Organic Synthesis**. John Wiley & Sons INC

Unit-02&03:

5. Nogardy, M. 1987. **Asymmetric Synthesis.** VCH Publishers.
6. David Krupadanam, 2013. **Fundamentals of Asymmetric synthesis**. University Press.

Unit-04:

7. Atherton, E. and Sheppard R. A. 1989. **Solid Phase Peptide Synthesis: A Practical Approach.** Oxford University Press.
8. Graham L. Patrick. 2001. **Introduction to Medicinal Chemistry.** 2nd Edition. Oxford University Press.
9. Tse-Lok Ho, 1992. **Tandem Organic Reactions**. John Wiley&Sons
10. Stark, C. M., Liotta C. and M. Halpern, **Phase Transfer Catalysis, Fundamentals, Applications and Industrial perspective**, Academic Press
11. W. P. Weber & G. W. Gokel, 1977. **Phase Transfer Catalysis in Organic synthesis**, Springer

Unit-05:

12. J.Singh, 2006, **Photochemistry and Pericyclic reactions** (2nd Ed.), New Age International publishers.
13. Depuy and Chapman, 1988. **Molecular Reactions and Photo chemistry**, Prentice Hall of India Pvt. Ltd.
14. Nicholas Turro and others, 2009, **Principles of Molecular Photochemistry-An Introduction.** University Science Books.

ORGANIC CHEMISTRY-IV

Credits: 4 **Semester: III**
Subject Code: MOC19303 **No. of lecture hours: 60**

Objectives:

- To acquire knowledge about the organometallic reagents.
- To emphasise the importance of regioselectivity through protection of various functional groups
- To impart knowledge of new synthetic routes developed for organic synthesis
- To gain knowledge about advanced techniques in NMR

Course Outcome:

CO1 **Appreciate** the importance of protecting groups
CO2 **Gains** the potential of organic reagents in synthesis
CO3 **Enlights** the knowledge about new synthetic reactions
CO4 **Determines** the chemical environment of ^{13}C in organic molecules
CO5 **Analyses** the chemical structure using 2D NMR and ORD

Unit-01: Oxidation Reagents **12 hrs**

- Oxidation of active C-H functions: NBS, DDQ and SeO_2 2
- Alcohols to carbonyls: CrVI oxidants-(CrO_3, Jones reagent, Saretts reagent, Collins reagent, PCC, PDC) 3
- Introduction to IBX, DMP, CAN, TEMPO, TPAP 4
- Swern oxidation. Silver Carbonate 1
- Oxidative cleavage of 1,2-diols: Periodic acid and Lead tetra acetate 2

Unit-02: Reduction reagents **12 hrs**

- Catalytic hydrogenation: Homogenous (Wilkinsons's catalytic hydrogenation) and heterogeneous catalytic reduction 2
- Dissolving metal reductions: Birch reduction 2
- Non-metallic reductions: Diimide 1
- Nucleophilic metal hydrides: $LiAlH_4$, $NaBH_4$ and their modifications (alkoxy aluminates, DIBAL-H, sodium cyanoborohydride), K-Selectride 3
- Electrophilic metal hydrides: BH_3, AlH_3 2
- Hydrogenolysis: use of tri-n-butyl tin hydride 1
- Reductive amination: Eschweiler–Clarke reaction 1

Unit-03: Protecting Groups **12 hrs**

- Protection of alcohols by ethers, silyl ether and ester formation 2
- Protection of 1,2-diols by acetals, ketals and carbonate formation 2
- Protection of amines by acetylation, benzoylation, benzyloxycarbonyl, butyloxy carbonyl, fmoc and triphenyl methyl groups 3
- Protection of carbonyl compounds by acetal, ketal and thioacetal formation 2
- Protection of carboxylic acids by ester and ortho ester (OBO) formation 3

Unit-04: Organometallic Reagents and Applications **12 hrs**

- Organo magnesium reagents (Grignard reagents) 2
- Organo lithium reagents 2

- Organo copper reagents 2
- Organo borane reagents 2
- Organo phosphorus reagents: Wittig reagent, modified Wittig reagent, Aza-Wittig reagent 2
- Mannich reaction and Robinson annulation 1
- Stork-enamine reaction and Shapiro reaction 1

Unit-05: Synthetic strategies **12 hrs**

- Brief review on terminology: target, synthon, synthetic equivalent, functional group interconversion, retrosynthetic analysis 2
- Crieteria for selection of target 1
- Linear and convergent synthesis 1
- Synthesis involving chemoselectivity, regioselectivity, reversal of polarity Strategic bond: Criteria for disconnection of strategic bonds 2
- Importance of the order of events in organic synthesis: Salbutamol, Proparacaine. 1
- One group and two group C-X disconnections 1
- One group C-C disconnections. Alcohol and carbonyl compounds 1
- Two group C-C disconnections: Diels-Alder reaction, 1,2-; 1,3- and 1,5-difunctionalised compounds 2
- Synthesis of Salbutamol, Proparacaine, Warfarin by retro synthetic approach 1

References:

Unit-01-04:

1. Michael B Smith. 1994. **Organic Synthesis**. MacGraw Hill International Editions.
2. Jagadamba Singh and Yadav, L.D.S. 2011. **Organic Synthesis.** Pragathi Prakasan Publications.
3. Meckie, R.K., Smith, D. M. and Atken, R. A. 1990. **Guidebook to Organic Synthesis**. 2nd Edition.
4. Carruthers, W. 2004. **Some Modern Methods of Organic Synthesis**. 4th Edition. Cambridge University Press.
5. Willis,C and Willis, M. 1995. **Organic Synthesis.** Oxford University Press
6. Francis, A. Carey. 2008. **Organic Chemistry**. 7th Edition. McGraw Hill International Editions.
7. Jerry March, 1992, **Advanced Organic Chemistry** (5th Ed.), Wiley-India student edition

Unit-05:

1. Jagadamba, Singh and Yadav, L.D.S. 2011. **Organic Synthesis.** New Delhi: Pragathi Prakasan Publications.
2. Warren, S. 2002. **Organic Synthesis-The Disconnection Approach**. John Wiley & Sons.

ORGANIC CHEMISTRY-V

Credits: 4 **Semester: III**
Subject Code: MOC19304 **No. of lecture hours: 60**

Objectives:

- To acquire knowledge about the spectral techniques.
- To emphasise the importance on advanced organic reactions
- To impart knowledge of organic polymer and green methods for organic synthesis

Course Outcome:

CO1 **Appreciate** the importance of ^{13}C and 2D-NMR
CO2 **Gains** the potential of organic polymers
CO3 **Enlights** the knowledge about green chemistry
CO4 **Determines** the chemical environment of ^{13}C in organic molecules
CO5 **Analyses** the chemical structure using 2D NMR and ORD

Unit-01: ^{13}C NMR **12 hrs**

- CW and PFT techniques. 1
- Types of ^{13}C NMR spectra: undecoupled, proton- decoupled, single frequency off-resonance decoupled (SFORD) and selectively decoupled spectra. 4
- ^{13}C chemical shifts, factors affecting the chemical shifts, chemical shifts of organic compounds. 2
- Homonuclear (^{13}C, ^{13}C-J) and Heteronuclear (^{13}C, ^{1}H-J and ^{13}C, ^{2}H-J) coupling. 3
- Applications of ^{13}C NMR spectroscopy: Structure determination, stereochemistry, reaction mechanisms and dynamic processes in organic molecules 1
- ^{13}C NMR spectral editing techniques: principle and applications of APT, INEPT and DEPT methods 1

Unit-02: 2D NMR and ORD **12 hrs**

- Principles of 2D NMR 1
- Classification of 2D-experiments 1
- 2D-J-resolved spectroscopy 1
- Homonuclear and Heteronuclear 2D-J-resolved spectroscopy 1
- Correlation spectroscopy (COSY) Homo COSY (^{1}H-^{1}H COSY) Hetero COSY (^{1}H,^{13}C COSY, HMQC): 2-Pentanone and Ethyl benzoate 2
- NOESY: Sodium 2-methyl acrylate 1

ORD:

- Plain curves and anomalous curves, optical rotation, circular birefringence, circular dichroism and cotton effect 2
- Octant rule, axial halo ketone rule, Application of octant rule to study the absolute configuration and conformations of 3-methyl cyclohexanone, Menthone, Cis-10-methyl-2-decalone 3

Unit-03: New synthetic reactions **12 hrs**

- Baylis-Hillman reaction 1
- Julia-Lythgoe olefination 1
- Peterson's stereoselective olefination 1

- Mukayama aldol reaction 1
- Mitsunobu reaction, McMurrey reaction 1
- Heck reaction 1
- Buchwald-Hartwig coupling, Suziki coupling 1
- Stille coupling, Sonogishira coupling 2
- Eishenmosher-Tanabe fragmentation 1
- Ugi reaction 1
- Click reaction 1

Unit-04: Organic Polymers **12 hrs**

- Introduction to polymers, basic concepts: monomers, repeat units, degree of polymerization. Linear, branched and network polymers 2
- Classification of polymers. Polymerization: condensation, addition, radical chain-ionic and co-polymerization 2
- Molecular weight determination and control of molecular weight 1
- Ziegler-Natta polymerization with mechanism, Stereo regulated polymers, syndiotactic, isotactic and atactic polymers 2
- Resins and plastics: Polystyrene and styrene copolymers, poly(vinyl chloride/vinyl acetate)and related polymers, acrylic polymers, polyesters, phenol-formaldehyde polymers polyurethanes and epoxide polymers with examples 4
- Natural and synthetic rubbers 1

Unit-05: Introduction to Green Chemistry **12 hrs**

- Principles of green chemistry, basic concepts, atom economy, twelve laws of green chemistry, principles of green organic synthesis 4
- Green alternatives of organic synthesis: coenzyme catalyzed reactions 2
- Green alternatives of molecular rearrangements, electrophilic aromatic substitution reactions, oxidation-reduction reactions, clay catalyzed synthesis 4
- Condensation reactions, Green photochemical reactions 2

References:

Unit-01 &02:

1. William Kemp, 2008. **Organic Spectroscopy.** 3rd Edition. Palgrave
2. Atta-ur-Rahman, 2008. Nuclear Magnetic Resonance. **.** 1st Edition. Springer
3. Kalsi, P S. 2005. **Spectroscopy of Organic Compounds**. 6thEdition. New Delhi: New Age International publishers
4. Pavia, 2004. **Introduction to Organic Spectroscopy**. 3rd Edition. Thomson
5. Jagmohan. 2010. **Organic Spectroscopy, Principles and Applications**. 2nd Edition. New Delhi: Narosa Publication House Pvt. Ltd

Unit-03:

6. Jie Jack Li, 2006. **Name Reactions**. (3rd Ed), Springer International Edition.
7. Tse-Lok Ho, 1992. **Tandem Organic Reactions**. John Wiley&Sons

Unit-04:

8. Billmeyer, F. W. Wiley Jr, **Textbook of Polymer Science**.
9. V. R. Gowarikar, N. V. Viswanathan and J. Sreedhar, Wiley-Eastern **Polymer Science**.
10. Takemoto, K. Inaki, Y. and Ottanbrite **Functional Monomers and Polymers**.

Unit-05:

11. Ahuluwalia, V.K. 2006. **Green Chemistry, Environmental Benign Reactions.** New Delhi: Ane Book Publications.

12. Sanghi R. and Srivastava, M.M. 2003. **Green Chemistry, Environment Friendly Alternatives**. New Delhi: Narosa Publications.

ADVANCED HETEROCYCLIC CHEMISTRY

Credits: 4 **Semester: III**
Subject Code: MOC19305A **No. of lecture hours: 60**
Objectives:

- To enable the student to understand and appreciate the importance of heterocyclic compounds
- To understand the mechanism involved in the synthesis and applications of heterocyclic compounds.

Course Outcome:

CO1 **Understands** the background of heterocyclics
CO2 **Compares** the reactivity of aromatic and nonaromatic heterocyclics
CO3 **Differentiate** five and six membered heterocyclics
CO4 **Distinguish** heterocyclics with more than two heteroatoms
CO5 **Recognises** the large ring and other heterocyclics

Unit-01: Non aromatic heterocyclics **12 hrs**

- Different types of strains, interactions and conformational aspects of nonaromatic heterocyclics 3
- Synthesis, reactivity, and importance of the following ring systems of Azirines, Aziridines,Oxiranes, Thiiranes 5
- Synthesis, reactivity, and importance of the following ring systems of Azetidines, Oxetanes, Thietanes 4

Unit-02: Five and six membered heterocyclic with two hetero atoms **12 hrs**

- Synthesis, reactivity, aromatic character and importance of the following heterocycles: Pyrazole, Isoxazole, Isothiazole 3
- Imidazole, Oxazole, Thiazole 3
- Benzimidazole, Benzoxazole and Benzthiazole 3
- Pyridazine, Pyrimidine. Pyrazine 2
- Oxazine, thiazine 1

Unit-03: Heterocyclics with more than two hetero atoms **12 hrs**

- Synthesis, reactivity, aromatic character and importance of the following Heterocycles:
- 1,2,3- Triazoles, 1,2,4-triazoles. Tetrazoles 3
- 1,2,4-Oxadiazole, 1,3,4-oxadiazole 1,2,5- oxadiazole 3
- 1,2,3-Thiadiazoles, 1,3,4- thiadiazoles, 1,2,5- thiadiazoles 3
- 1,2,3-Triazine, 1,2,4- triazine, 1,3,5- triazine, tetrazines 2
- Synthesis and importance of Purines and Pteridines 1

Unit-04: Large ring and other heterocyclics **12 hrs**

- Synthesis, structure, stability and reactivity of following Heterocyclics
- Azepines, Oxepines and Thiepines. 3
- Diazepines rearrangements of 1,2 - diazepines. 1
- Benzoazepines, Benzodiazepines, Benzooxepines, Benzothiepines, Azocines and Azonines. 4
- Selenophenes, Tellerophenes, Phospholes and Boroles. 4

Unit-05: Meso-Ionic heterocycles **12 hrs**

- Introduction, classification of Meso-Ionic Heterocycles 2
- Synthesis, structure and reactivity of Meso-Ionic Heterocycles type A: 1,3-Oxazolium-5-olates (Munchnones), 1,3-diazolium-4-olates, 1,2,3-Oxadiazolium-5-olates (Sydnones) 6
- Synthesis, structure and reactivity of Meso-Ionic Heterocycles type B: 1,2-diazolium-4-aminides, 1,2-dithiolium-4-olates 4

References:

Unit 01-05

1. Gilchrist, T. 1987. **Heterocyclic Chemistry.** Pitmann Publishing Ltd.
2. Bansal, R. K. 2005. **Heterocyclic Chemistry**. 4th Edition. New Delhi: New Age International Pvt. Ltd.
3. Joule, J.A. and Mills, K. 2004. **Heterocyclic Chemistry**. 4th Edition. Blackwell Publishers.
4. Joule, J.A. and Smith. 2010. **Heterocyclic Chemistry**. 5th Edition. ELBS.
5. Acheson. R. M. 1967. **An Introduction to the Chemistry of Heterocyclic Compounds.** 2nd Edition. Wiley & Sons.

GREEN CHEMISTRY

Credits: 4 **Semester: III**
Subject Code: MOC19305B **No. of lecture hours: 60**
Objectives:

- To introduce the concept of Green Chemistry
- To impart knowledge about different methods of Green Synthesis
- To acquire knowledge about ionic–liquids and polymer supported synthesis and multicomponent reactions

Course Outcome:

CO1 **Learns** the basics of green chemistry
CO2 **Understand** the use of ultrasounds and microwave in organic synthesis
CO3 **Appreciates** the importance of solid free synthesis
CO4 **Perceives** the concept of phase transfer catalysis and crown ethers
CO5 **Gains** knowledge about multicomponent reactions

Unit-01: Introduction to Green Chemistry	**12 hrs**
• Principles of green chemistry, basic concepts, atom economy, twelve laws of green chemistry, principles of green organic synthesis	3
• Green alternatives of organic synthesis: coenzyme catalyzed reactions	2
• Green alternatives of molecular rearrangements, electrophilic aromatic substitution reactions, oxidation-reduction reactions, clay catalyzed synthesis	5
• Condensation reactions, Green photochemical reactions	2

Unit-02: Use of Ultrasound and Microwaves in Organic Synthesis	**12 hrs**
• Use of ultrasound**:** Introduction, instrumentation, the phenomenon of cavitation	2
• Sonochemical esterification, substitution, addition, alkylation, oxidation, reduction and coupling reactions	2
• Use of Microwaves: Introduction, concept, reaction vessel/medium, specific effects, atom efficiency (% atom utilization), advantages and limitations	2
• *N*-alkylation and alkylation of active methylene compounds, condensation of active methylene compounds with aldehydes and amines	2
• Diels-Alder reaction. Deprotection of esters and silyl ethers. Oxidation of alcohols and sulphides	2
• Green chemistry in the pharmaceutical industry: Ibuprofen manufacture, biocatalysis	2

Unit-03: Ionic-liquids and Polymer supported reagents in organic synthesis	**12 hrs**
• Introduction, structure, synthesis and applications of some important ionic liquids in organic synthesis	3
• Introduction- properties of polymer support, advantages of polymer supported reagents and choice of polymers	2
• Applications: Substrate covalently bound to the support: Dieckmann cyclisation	2
• Preparation of polymer bound aldehyde and application in aldol and Wittig reactions	2

- Synthesis of polystyryl boronic acid and use in diol protection reaction 1
- Reagent linked to a polymeric material: Preparation of sulfonazide polymer and application in diazotransfer reaction 2
- Synthesis of polymer bound per acid and its applications 1
- Polymer supported catalytic reactions: Preparation of polymer supported $AlCl_3$ and application in etherification and acetal formation reactions 2

Unit-04: Phase transfer catalysis and crown ethers **12 hrs**

- Phase transfer catalysis: Introduction, definition, mechanism of phase transfer catalysis. Types of phase transfer catalysts and reactions and their advantages 3
- Preparation of catalysts and their application in substitution, elimination, addition, alkylation, oxidation and reduction reactions 3
- Crown ethers: Introduction, nomenclature, features, nature of donor site. General synthesis of crown ethers 2
- Synthetic applications: Alkylation, generation of carbenes, aromatic substitution and displacement reactions 2
- Generation and application of superoxide anions. Cation deactivation reactions 2

Unit-05: Multi-component Reactions **12 hrs**

Studies on the mechanistic aspects and use of the following reactions in organic synthesis: 4

- Passerini-Ugi; Hantsch; Biginelli; Doebner-Miller
- Ritter; Jacobson; Betti; Robinson-Schopf 3
- Barbier; Baylis-Hilmann; Ivanov and Suzuki coupling reaction 5

References:

1. Ahuluwalia, V.K. 2006. **Green Chemistry, Environmental Benign Reactions.** New Delhi: Ane Book Publications.
2. Sanghi R. and Srivastava, M.M. 2003. **Green Chemistry, Environment Friendly alternatives**. New Delhi: Narosa Publications.
3. Dehmlov, E.V. and Dehmlov, S.S. 1983. **Phase Transfer Catalysis.** 2nd Edition. Verlagchemie, Wienheim.
4. Mathur, N.K. Narang C. K. and Williams, R. E. 1980. **Polymers as Aids in Organic Synthesis.** New York: Academic Press.

SCIENTIFIC RESEARCH METHODOLOGY AND COMMUNICATIONS

Credits: 1 **Semester: III**

Subject Code: MOC19351 **No. of lab hours: 2 hrs/ week**

Objectives

- To introduce the purpose and importance of research for future development
- Literature search for current awareness and for retrospective survey
- To know the methodology of writing thesis and journal articles
- To present their findings

Outcome:

- The student will acquire knowledge in writing thesis

Unit-1: Meaning of Research **8 hrs**

- The search for knowledge, purpose of research, nature of scientific knowledge, scientific method, role of theory, characteristics of research — 3
- Types of research: fundamental or pure research, applied research, action research, historical research, experimental research — 3
- Assessment and evaluation-purpose and general methodology — 2

Unit-2: The Scientific Writing **8 hrs**

- Scientific writings: research reports, thesis, and journal articles. Requirement of technical communications: eliminating wordiness and repetition of phrases (tautology), redundancy, imprecise words, and superfluous phrases. Lab note book maintenance — 3
- Steps to publish scientific articles in journals: types of publications-communications, articles, reviews; where to publish, specific format required for submission, organization of the material — 3
- Documenting: abstracts-indicative or descriptive abstract, informative abstract, footnotes, end notes, referencing styles, bibliography-journal abbreviations (CASSI), abbreviations used in scientific writing — 2

Unit-3: Seminar-Scientific Communication **14 hrs**

- Recent Advancements in Chemistry: Organic Synthesis, Natural Product Chemistry, Green Chemistry, Material Chemistry, Nano materials

References:

Unit-01, 02 & 03

1. B. E. Cain, ***The Basis of Technical Communicating***, ACS., Washington, D.C., 1988.
2. J. W. Best, ***Research in Education***, 4th ed. Prentice Hall of India, New Delhi, 1981.
3. H. F. Ebel, C. Bliefert and W. E. Russey, ***The Art of Scientific Writing***, VCH, Weinheim, 1988.
4. J. Gibaldi, and W. S. Achtert, ***Handbook for Writers of Research Papers***; 2nd ed.; Wiley Eastern, 1987.
5. J. Joseph, ***Methodology for Research***; Theological Publications, Bangalore, 1986.
6. R. L. Dominoswki, ***Research Methods***, Prentice Hall of India, New Delhi, 1981.
7. H. M. Kanare, ***Writing the Laboratory Notebook***; American Chemical Society: Washington, DC, 1985.
8. J. S. Dodd, Ed., *The ACS Style Guide: **A Manual for Authors and Editors***; American Chemical Society: Washington, DC, 1985.

SYNTHESIS AND ESTIMATION OF DRUGS

Credits: 2 **Semester: III**
Subject Code: MOC19352 **No. of lab hours: 4**

Objectives:

- To enable the student to develop analytical skill in organic quantitative analysis
- To understand the techniques involved in the preparation of standard solutions, standardization and calculations in the estimations of compounds.

Outcome:

The student will learn how to isolate synthesis and estimate drug molecules

Purification of common organic solvents by simple distillation

- Polar and nonpolar combination

Isolation of the following natural products:

- Piperine from pepper (Soxhlet extraction)
- Eucalyptus oil from leaves (steam distillation)

Synthesis of the following drugs:

- Phenacetin
- Phenytoin
- Benzocaine
- 6-Methyl uracil
- 4-Aminobenzene sulfonamide
- FIuorescein
- Antipyrine
- Propronolol

Estimation of the following drugs

- Assay of Ibuprofen /*Isoniazid (Iodometry)*
- Assay of Ascorbic acid
- Chloride in Ringer's lactate (Argentometry)
- Riboflavin (Colorimetry)

References:

1. Mann and Saunders. 2009. **Practical Organic Chemistry.** Pearson education.
2. Vogel. 2000. **A Textbook of Practical Organic Chemistry**. Vol 1 and 2
3. Ahuluwalia, V. K. 2006. **Green Chemistry, Environmental Benign Reactions**. New Delhi: Ane Book Publications.

ORGANIC CHEMISTRY III- PRACTICAL

Credits: 2 **Semester: III**
Course Code: MOC19353 **No. of lab hours: 4**

Objectives:

- To enable the student to develop analytical skill in organic qualitative analysis and to develop preparative skills in organic preparations involving two or three stages.
- To enable to students to understand the mechanism involved in the name reactions and conditions of the reactions involving the preparations

Outcome:

- The student will learn the mechanisms and conditions required for multistep reactions

Synthesis of the following compounds (multi step synthesis)

- p-Bromoaniline from acetanilide
- Vanillyl alcohol from vanillin ($NaBH_4$ reduction)
- Benzilic acid from benzoin (Benzilic acid rearrangement)
- Benzpinacol (photoreduction) and Benzpinacol to Benzpinacolone (Rearrangement)
- 2,4,6-Trimethyl quinolone (Skraup synthesis)
- Allylic alcohols via Baylis-Hillman reaction using DABCO as a catalyst
- Caprolactam (Beckmann rearrangement)

Synthesis and separation of the compounds

- Synthesis of Dihydropyrimidines (MCR, Biginelli reaction)
- Synthesis of 7-Hydroxy-3-methyl flavone (Baker–Venkatraman reaction).
  The products are to be separated by column chromatography or recrystallization and characterized by melting points.
- Synthesis of Ortho and para-nitrophenol from phenol.
  Monitor the progress of the reaction by TLC and separation of isomers by column chromatograph. Characterized by melting points and ^{1}H NMR spectroscopy etc

References:

1. Mann and Saunders. 2009. **Practical Organic Chemistry.** Pearson education.
2. Vogel's **A Textbook of Practical Organic Chemistry**. Vol 1 and 2
3. Ahuluwalia, V. K. 2006. **Green Chemistry, Environmental Benign Reactions**, New Delhi: Ane Book Publications.
4. Kappe, C. O. 1997. **Dihydropyrimidine Synthesis (Beginilli reaction)**. *J. Org. Chem*. 62 (21), 7201–7204.

ORGANIC CHEMISTRY IV- PRACTICAL

Credits: 2 **Semester: III**

Subject Code: MOC19354 **No. of lab hours: 5hrs/week**

Objectives: To learn and apply the principles of spectroscopy for the study and structural elucidation of molecules.

Outcome:
The student will learn interpretation of data and analysis of unknown compounds

- Identification of 30 unknown organic compounds by interpretation of IR, UV, ^{1}H NMR, ^{13}C NMR and mass spectra

References:

1. Silverstein, Bassler and Morrerl, 1998. **Spectrometric Identification of Organic Compounds.** 5th Edition. John Wiley& sons.
2. Field, L.D., Sternhell, S. and Kalman J. R. **Organic Structures from Spectra**. 5th Edition. John Wiley & sons.

ORGANIC CHEMISTRY VI

Credits: 4 **Semester: IV**

Subjected Code: MOC19401 **No. of lecture hours: 60**

Objectives: To impart knowledge to the students regarding drug design and its mechanism of action

Course Outcome:

CO1 **Gains** knowledge about principle of drug design and discovery
CO2 **Appreciates** the role of SAR and QSAR studies
CO3 **Infers** about drugs acting on metabolic processes
CO4 **Identifies** drugs acting on ion channels and receptors
CO5 **Analyses** importance of drugs acting on genetic material

Unit-01: Principles of Drug design and drug discovery	**12 hrs**
• Introduction to drug discovery, pharmacognosy, pharmacokinetics (ADME) pharmacodynamics.	4
• Lead discovery- from natural products, folklore drugs, natural hormones and neurotransmitters, emitting drugs (me too drugs)	2
• Serendipitous discovery of leads e.g.Penicillin and Librium	1
• Definition and principles of design of agonists (Eg: Salbutamol,) and antagonist (Eg: Cimitidin)	3
• Principles of prodrug design	2

Unit-02: SAR and QSAR studies	**12 hrs**
• Binding role of hydroxy group, amino group, aromatic ring, double bond, ketones and amides	1
• Lead modification strategies: Bioisosterism, variation of alkyl substituents, chain homologation and branching, variation of aromatic substituents, extension of structure, ring expansion or contraction, ring variation, variation and position of hetero atoms, ring fusion, simplification of the lead and rigidification of lead. conformational blockers	3
• Structure pruning techniques in lead modification e.g. morphine	1
• Discovery and design of oxaminquine, and captopril	2
• Structure-Activity Relationship studies in benzodiazepines , sulpha drugs	1
• Introduction to Quantitative- Structure Activity Relationship studies. QSAR parameters- pKa, logp, Lipophilicity substituent constant, Hammett substitutent constant, Taft's constant and their relationship with biological activity	2
• Multiparameter QSAR- Hansch analysis, Craig's plot, Topliss method	2

Unit-03: Drugs acting on metabolic processes, cell walls and specific enzymes	**12 hrs**
• Different types of classification of drugs	1
• Introduction to macromolecular targets	1
• Introduction to enzymes and enzyme inhibitors	1
• Folate metabolism in bacteria, Antifolates: Structural formulae of	

sulfaguanidine, dapsone and trimethoprim. Synthesis and mechanism of action of Sulfamethoxazole	2
• Structural formulae β-Lactams antibiotics: penicillin-G, cephalosporin-C, Cefalexin and amoxacillin	2
• Synthesis and mechanism of action of penicillin-G, cephalosporin-C	1
• Inhibitors of ACE, H^+/K^+ ATPase enzymes: Synthesis and mechanism of action of Captopril, Enalapril, Omeprazole	4

Unit-04: Drugs acting on Ionchannels and receptors **12 hrs**

• Introduction to ion channels; Cell membrane	1
• Drugs acting on Ca^{+2}, Na^+ and K^+ channels and their mode of action	1
• Structural formulae of Diltiazem, Tetracaine and 4-aminopyridine Synthesis of Diltiazem	1
• Introduction to nervous system and structure of neurons	1
• Definition and examples of agonists, antagonists, neurotransmitters, receptors	1
• α- Adrenergic receptor agonists and antagonists. Structural formulae of Epinephrine, Nor-epinephrine, Methyldopa and Terazosin. Synthesis of norepinephrine	1
• β- Adrenergic receptor agonists and antagonists. Synthesis of Salbutamol, propronolol	1
• Cholinergic-receptor agonists and antagonists-structural formula of acetyl choline, Succinyl choline, Atropine. Synthesis of succinyl choline	2
• Dopamine receptor agonists and antagonists Synthesis of L-Dopa and Chlorpromazine	2
• Serotonin receptor agonists and antagonists-Structural formulae of Serotonin and Metaclopramide	1
• Histamine receptor agonists and antagonists-Structural formulae of Histamine, Chloropheneramine, Ranitidine and Cimetidine	1

Unit-05: Drugs acting on genetic material and Immune system **12 hrs**

• Introduction to nucleic acid; structure functions	
• DNA-intercalating agents: Structural formulae of Daunomycin, Adriamycin and Amsacrine. Synthesis of Chloroquine	1 2
• DNA-Binding and Nicking agents: Synthesis of Metronidazole, Tinidazole and Dimetridazole	2
• DNA-Polymerase inhibitors: Synthesis of AZT	1
• Inhibitors of transcribing enzymes: Structural formulae of Rifamycins and partial synthesis of Rifampicin	2
• Drugs interfering with translations: Structural formulae of Erythromycin, Chloromycetin, Tetracyclines and Amino glycosides. Synthesis of Chloromycetin	2
• Immunosupressing agent-structural formula and mechanism of action of Cyclosporin. Immunoenhancers-use of vaccines	2

References:

Unit-01 &02:

1. Manfred E. Wolf. 1995. **Burger's Medicinal Chemistry and Drug Discovery.** 5th Edition. John Wiley & Sons.

2. Graham L. Patrick. 2001. **Introduction to Medicinal Chemistry.** 2nd Edition. Oxford University Press.
3. R.B.Silverman. 1992. **Organic Chemistry of Drug Design & Drug Action.** 2nd Edition. Academic Press.
4. Thomas Nogardy. 1988. **Biochemical Approach to Medicinal Chemistry.** 2nd Edition. Oxford University Press.

Unit-03, 04 &05:

5. Kadam 2005. **Principles of Medicinal Chemistry.** 13th Edition. Vol. I &II, Nirali Prakashan Publishers.
6. Gareth Thomas. 2004. **Medicinal Chemistry: An Introduction.** John Wiley & Sons
7. Daniel Ledneiser. 2009. **Strategies for Organic Drug Synthesis and Design**. 2nd Edition. John Wiley & Sons Publishers.
8. Rama Rao N. 2001. **Principles of Organic Medicinal Chemistry**. New Delhi: New Age International Publishers.
9. William Foye. 2013. **Principles of Medicinal Chemistry.** 7th Edition. Lippincott Williams and Wilkins Publishers.
10. Ashutoshkar. 2005. **Medicinal Chemistry.** 3rd Edition. New Delhi: New Age International Publishers.

ADVANCED NATURAL PRODUCTS

Credits: 4 **Semester: IV**
Subject Code: MOC19402A **No. of lecture hours: 60**
Objectives:

- To emphasize the existence and importance of natural products beneficial to mankind.
- To students learn about biosynthetic methods of natural products
- To acquire knowledge about structural elucidation of natural products

Course Outcome:

CO1 **Understands** the importance of natural products
CO2 **Determines** the structure of alkaloids by chemical methods
CO3 **Analyses** the complex structure of steroids and hormones
CO4 **Acquires** the knowledge of prostaglandins
CO5 **Recognises** the Biosynthetic pathways

Unit-01: Alkaloids and terpenoids **12 hrs**

- Isolation, structural elucidation, stereochemistry and synthesis of
- Quinine 2
- Morphine 5
- Abeitic acid 3
- β-Amyrin 2

Unit-02: Steroids and hormones **12 hrs**

- Occurrence, isolation, structure determination, stereochemistry and total synthesis of Cholesterol 6
- Structure determination and synthesis of
- Androsterone 2
- Progesterone 2
- Stereochemical structure and biological activity of Testosterone, Estrone, Estradiol and Aldosterone 2

Unit-03: Prostaglandins **12 hrs**

- Occurrence, classification and physiological activity of prostaglandins 2
- Structure determination and synthesis of
- PGE1α 2
-
- PGE2α 2
- PGE3α 2
- Structure determination and synthesis of rotenone 4

Unit-04: Plant pigments **12 hrs**

- Classification of pigments 1
- Occurrence, Isolation, structural elucidation and synthesis of 3
- Apigenin (Flavone)
- Myricetin (Flavone) 2
- Diadzein (Flavonols) 2
- Classification, isolation and properties of Anthocyanins 1

- Structural elucidation and synthesis of Cyanidin-7-arabinoside 3

Unit-05: Biosynthesis of Natural Products **12 hrs**

- Introduction to biosynthesis and biogenesis 1
- Difference between Laboratory synthesis and biosynthesis 1
- Methods for determination of biosynthetic mechanism. Feeding experiments: use of radioisotopes Measurement of incorporation: absolute incorporation, specific incorporation. Identification of position of labels in labeled natural products by chemical degradation and spectral methods. 2
- Major biosynthetic pathways:
- Mevalonic acid pathway: Biosynthesis of α-terpeniol and camphor 2
- Acetate-Malonate pathway: Biosynthesis of aromatic compounds: Eugenone, pholroglucinol, orsinol and rubrofusarin. 3
- Shikimic acid pathway: Biosynthesis of essential amino acids–phenylalanine, tyrosine, tryptophan and morphine. 3

References:

Unit-01-05:

1. Finar, I.L. 2009. **Textbook of Organic Chemistry**. Vol II. 5th Edition. Pearson Publications.
2. Bhat, S.V. and Nagasampangi, B.A. 2009. **Chemistry of Natural Products**. New Delhi: New Delhi: Narosa Publishing House.
3. Kalsi, P.S. 1983. **Chemistry of Natural Products.** Kalyani Publishers.
4. Rashmi Jain, Alok Sahai, Sandhya Pimplapure, Usha Soni, 2016. **Chemistry of Natural Products**. Pragati Prakashan

BIO ORGANIC CHEMISTRY

Credits: 4 **Semester: IV**
Subject Code: MOC19402B **No. of lecture hours: 60**
Objectives:

- To introduce to biomolecules of importance carbohydrate, proteins, nucleic acids, lipids and enzymes
- To emphasize on the structure reactivity of enzymes and their mechanisms

Course Outcome:

CO1 **Appreciate** the importance of carbohydrates and proteins
CO2 **Visualises** the role of nucleic acids and lipids
CO3 **Categorises** enzymes and their action
CO4 **Identifies** the enzyme models and their transformations
CO5 **Perceives** the concept of coenzymes

Unit-01: Carbohydrates and Proteins	**12 hrs**
• Carbohydrates: Determination of relative and absolute configuration in D (+) Glucose	1
• Occurrence, importance and synthesis of monosaccharide's containing functional groups such as amino, halo and sulphur	2
• Structural elucidation and synthesis of sucrose. Conformational structures of D-(+)-ribose, 2-deoxy-D-ribose, sucrose, lactose, maltose and cellobiose	4
• Structural features of starch and cellulose	2
• Proteins: Acid and enzymatic hydrolysis of proteins	1
• Determination of the amino acid sequence in polypeptides by end group analysis. Chemical synthesis of di and tri peptides. Merrifield's solid phase synthesis	2

Unit-02: Nucleic acids and Lipids	**12 hrs**
Introduction: Structural formulae of bases, nucleosides, nucleotides, and base pairing	2
• Synthesis of nucleoside and nucleotides	2
• Primary, secondary and tertiary structure of DNA. Types of mRNA, tRNA and rRNA	2
• Replication, transcription and translation. Synthesis of nucleosides and nucleotides	2
• Structure and synthesis of acylglycerols, phosphoglycerides and sphingolipids	4

Unit-03: Enzymes and their action	**12 hrs**
• Definition. Classification based on mode of action	1
• Enantiomer discrimination by Three point Contact model. Factors affecting enzyme catalysis. Enzyme inhibition: reversible and irreversible inhibition. Immobilized enzymes	2
• Transition state theory and Acid-Base catalysis	1
• Covalent catalysis: Binding modes of catalysis (i) Proximity effect (ii) Transition state stabilization (iii) Strain and Distortion	4
• Examples of some typical enzyme mechanisms for (i) Triose phosphate	4

isomerase, (ii) α-chymotrypsin and serine protease (iii) Lysozyme (iv) Carboxy peptidase-A (v) Ribonuclease

Unit-04: Enzyme Models and Enzymatic transformations	**12 hrs**
• Introduction: Biomimetic chemical approach to biological systems-Enzyme models Advantage of enzyme models, requirements necessary for the design of enzyme models	3
• Host-guest complexation chemistry. Examples of some host molecules-crown ether cryptanes, cyclodextrins. cyclodextrin based enzyme models-calixarenes, ionophores, micelles and synzymes (synthetic enzymes)-chiral recognition and catalysis	5
• Introduction to industrial enzymes	1
• Enzymatic synthesis of α-amino acids and peptides	1
• Transformations of lipases and esterases	2

Unit-05: Coenzymes	**12 hrs**
• Introduction: Cofactors, cosubstrates, prosthetic groups. Classification: Vitamin derived coenzymes and metabolite coenzymes	2
• Structure and biological functions and mechanism of reactions catalyzed coenzyme A	1
• Thiamine pyrophosphate, pyridoxal phosphate (PLP)	1
• Nicotinamide adenosine dinucleotide/their phosphates	1
• Flavin adenine nucleotide FAD, $FADH_2$ and Flavin mononucleotide (FMN, $FMNH_2$)	2
• Lipoic acid, biotin	1
• Tetrahydrofolate, Ubiquinone	1
• Adenosine triphosphate (ATP) and adenosine diphosphate (ADP)	1
• S-adenosyl methionine (SAM)	1
• Uridine di phospho sugars (UDP-sugars)	1

References:

1. Fersht and Freeman. 1985. **Enzyme Structure and Mechanism.** 2nd Edition. New York: Springer Publication.
2. Hennan Dugas. 1999. **Bio-Organic Chemistry: A Chemical Approach to Enzyme Action.** New York: Springer Publication.
3. D L Nelson and Cox, M.M. 2013. **Lehninger Principles of Biochemistry.** Freeman publications.
4. Conn and Stumpf. 2006. **Outlines of Biochemistry**. 5th Edition. John Wiley & Sons INC.

Interdisciplinary Paper
Chemistry Lab Practices and Awareness

Credits: 4 **Semester: IV**
Subject Code: MOC19403 **No. of lecture hours: 60**
Objectives:

- To train students in understanding laboratory safety rules and to improve the skills in preparation of lab reagents
- To enable the students to understand impact of chemicals towards environment

Course Outcome:

CO1 **Perceives** the concepts the regular practices of chemistry lab
CO2 **Validates** the role of reagents
CO3 **Understands** the importance of awareness of air
CO4 **Analyses** of water pollution
CO5 **Determines** the environment of relevant remedial measures

The student will acquire knowledge of regular practices of chemistry lab, preparation of reagents and awareness of air, water pollution and the.

Unit-01: Safety Rules 12 hrs

- General Rules and regulations for lab safety: minimizing risks of hazards — 2
- Personal Protective Equipment (PPE) - Hair, Dressing for the Laboratory, Eye Protection, Eyewash fountain, Gloves — 3
- Laboratory Protocols, Labeling Chemicals, Careful reading of labels Prevention of Inhaling Harmful Chemicals — 3
- Guide to Chemical Hazards, Chemical Spills etc. Accidents use of fire extinguisher and first aid kit in the laboratory — 3
- Good laboratory practices-maintenance of observation book record — 1

Unit-02: Lab Reagents **12 hrs**

- Concept of Concentrations: Normality, Molarity, ppm, ppb — 2
- Role of an indicator in detecting end point in volumetric analysis-acid base titrations, redox titrations, precipitation titrations and complexometric titrations — 3
- Preparation of indicators and use of indicators: Phenolphthalein, Methyl orange, Methyl-red, Potassium Chromate, Diphenylamine, EBT — 3
- Preparation of buffers: pH 10 ammonical buffer and acetate buffer solutions: Ammonium hydrogen phosphate solution, Bayer's reagent, Benedict's solution, Bromine water, Dimethyl glyoxime reagent, 2,4-Dinitrophenyl hydrazine reagent, Eriochrome black-T reagent — 4

Unit-03: Air Pollution **12 hrs**

- Introduction to environmental pollutions — 2
- Chemistry of Atmosphere: Composition and structure of atmosphere, — 2
- Greenhouse effect, Ozone depletion — 2
- Photochemical smog, Air sampling techniques, Sources, effects — 3

- Monitoring of air pollutants by Instrumental methods, Control of air pollution — 3

Unit-04: Water Pollution — **12 hrs**

- Water quality and common treatments for drinking water system — 2
- Drinking water standards-primary drinking water standards — 2
- Water Pollution, Different types of water pollutants and Sources — 2
- Characteristics and effects of water pollutants — 2
- Monitoring of Water Pollutants (mercury and lead) — 1
- Water Testing : Mineral Analysis, Microbial analysis, Pesticide and other organic chemical test — 3

Unit-05: Remedial Methods for Pollution — **12 hrs**

- Determination of Dissolved oxygen — 2
- Chemical oxygen demand in polluted water through charts, Industrial waste
- Environmental laws in India, Environmental benefits of planting trees. — 2
- Treatment of Municipal Waste Water — 2
- Treatment of Industrial Waste Water — 2

References:

1. Vogel's Text Book of Quantitative Chemical Analysis, 5th edition.
2. Vogel's Text Book of macro and semimicro qualitative inorganic analysis. G. Svehla, 5th edition.
3. Chemistry Reagent Manual Prepared by Chemistry Department, SGTB Khalsa College under DBT's Star College Scheme, University of Delhi (Available: online)

PROJECT

Credits: 6 **Semester: IV**
Subject Code: MOC19452 **Duration: 65 working days**
Objectives:

- To enable the students to have a better understanding in the concepts of organic analysis and apply the same to chemical, industrial and biological streams

Outcome:

- The student will have a hand on experience with the various experimental and analytical techniques.

The final submission of the research project i.e. small thesis, presentation and comprehensive *viva* carries 60% marks.

Note:
1. Student should submit 3 copies of the final research project copy in hard binding format with all declarations and signatures.
2. Journal of Organic Chemistry- ACS journal pattern should be followed