



# YOGI VEMANA UNIVERSITY

Vemanapuram, KADAPA-516003, Andhra Pradesh, INDIA

<http://www.yogivemanauniversity.ac.in>

## DEPARTMENT OF CHEMISTRY

### CURRICULUM (CBCS) – MSc (ORGANIC CHEMISTRY)

(With effect from the academic year 2018-19, for the M. Sc. Previous)

#### M. Sc. Previous

Sl. No.	Paper Code	Title of the paper	Allotted per Week (Hours)		Uni. Exam Duration (Hours)		Distribution of Marks						No of Credits
I-SEMESTER			L	P	T	P	IE	TE	PE	R	V	TOTAL	
1	15031	Inorganic Chemistry	4	-	3	-	25	75	-	-	-	100	4
2	15032	Organic Chemistry	4	-	3	-	25	75	-	-	-	100	4
3	15033	Physical Chemistry	4	-	3	-	25	75	-	-	-	100	4
4	15034	General Chemistry	4	-	3	-	25	75	-	-	-	100	4
5	15031P	Inorganic Chemistry Practical	-	9	-	3	-	-	75	10	15	100	4
6	15032P	Organic Chemistry Practical	-	9	-	3	-	-	75	10	15	100	4
7		Seminar	2	-	-	-	-	-	-	-	-	-	-
		Total Hours/Week	18	18	-	-	Total Marks/credits					600	24

Sl. No.	Paper Code	Title of the paper	Allotted per Week (Hours)		Uni. Exam Duration (Hours)		Distribution of Marks						No of Credits
II-SEMESTER			L	P	T	P	IE	TE	PE	R	V	TOTAL	
1	25031	Inorganic Chemistry	4	-	3	-	25	75	-	-	-	100	4
2	25032	Organic Chemistry	4	-	3	-	25	75	-	-	-	100	4
3	25033	Physical Chemistry	4	-	3	-	25	75	-	-	-	100	4
4	25034	Spectroscopy	4	-	3	-	25	75	-	-	-	100	4
5	25031P	Organic chemistry Practical	-	7	-	3	-	-	75	10	15	100	4
6	25032P	Physical chemistry Practical	-	7	-	3	-	-	75	10	15	100	4
7	25035 NC	Basics of Chemistry		4	3	-	25	75				100*	-
8		Seminar	2										
		Total Hours/Week	18	18	-	-	Total Marks/credits					600	24

\*Students need to pass the Non-Core paper but marks will not be added to grade points

NC: non-Core

L: Lecture

P: Practical

T: Theory

IE: Internal Examination

TE: Theory Examination

PE: Practical Examination

R: Record

V: Viva-Voce

**M. Sc. Final**

Sl. No.	Paper Code	Title of the paper	Allotted per Week (Hours)		Uni. Exam Duration (Hours)		Distribution of Marks						No of Credits
III-SEMESTER			L	P	T	P	IE	TE	PE	R	V	TOTAL	
1	35031	Inorganic Chemistry	4	-	3	-	25	75	-	-	-	100	4
2	35032	Organic Chemistry	4	-	3	-	25	75	-	-	-	100	4
3	35033	Physical Chemistry	4	-	3	-	25	75	-	-	-	100	4
4	35034	Chromatography & Medicinal Chemistry	4	-	3	-	25	75	-	-	-	100	4
5	35031P	Multistep Synthesis of Organic Compounds	-	7	-	3	-	-	75	10	15	100	4
6	35032P	Spectral Identification of Organic Compounds	-	7	-	3	-	-	75	10	15	100	4
7	35035 NC	Drug Discovery, Design and Development		4	3	-	25	75				100*	-
8		Seminar	2										
		Total Hours/Week	18	18	-	-	Total Marks/credits					600	24

\*Students need to pass the Non-Core paper but marks will not be added to grade points

Sl. No.	Paper Code	Title of the paper	Allotted per Week (Hours)		Uni. Exam Duration (Hours)		Distribution of Marks					No of Credits
IV-SEMESTER			L	P	T	P	IE	TE	D	V	TOTAL	
1	45031	Reagents in Organic Synthesis	4	-	3	-	25	75	-	-	100	4
2	45032	Designing and Modern Topics of Organic Synthesis	4	-	3	-	25	75	-	-	100	4
3	45033	Chemistry of Heterocyclic Compounds	4	-	3	-	25	75	-	-	100	4
4	45034	Chemistry of Natural Products	4	-	3	-	25	75	-	-	100	4
5	45031P	Project Work	-	18	-	6	-	-	150	50	200	8
7		Seminar	2	-	-	-	-	-	-	-	-	
		Total Hours/Week	18	18	-	-	Total Marks/credits				600	24

NC: non-Core

L: Lecture

P: Practical

T: Theory

IE: Internal Examination

TE: Theory Examination

PE: Practical Examination

R: Record

V: Viva-Voce

D: Dissertation

**FIRST SEMESTER**  
**15031: INORGANIC CHEMISTRY**

**UNIT – I: Metal-ligand Bonding Theories**

**UNIT – II: Metal-ligand Equilibria in Solution and Theory of HSAB**

**UNIT – III: Reaction Mechanisms of Complexes**

**UNIT – IV: Carbonyl and Nitrosyl Complexes, and Metal Atom Clusters**

**UNIT – I: Metal-ligand Bonding Theories**

**15 Hrs**

Crystal Field Theory (CFT) for bonding in transition metal complexes, crystal field splitting of 'd'-orbitals in octahedral, tetrahedral, tetragonal and square planar fields. Crystal Field Stabilization Energy (CFSE) and its calculation in six and four coordinated complexes, Spectrochemical series with reference to ligands and metal ions. Factors affecting the magnitude of  $\Delta_o$  in octahedral complexes, Jahn-Teller effect and its consequences. Shortcomings of CFT; Covalency: Evidence for covalency, Nephelauxetic effect; Molecular orbital theory: Concept of Ligand Groups Orbitals (LGOs), MO diagrams for octahedral, tetrahedral and square planar complexes, MO treatment of  $\pi$ -bonds.

**UNIT – II: Metal-ligand Equilibria in Solution and Theory of HSAB**

**15 Hrs**

**(A) Metal-ligand Equilibria in Solution**

Stepwise and overall formation constants and their interrelationship, Trends in stepwise formation constants, Factors affecting the stability of metal complexes, Chelate effect, Determination of binary formation constants by  $p^H$ -metry and spectrophotometric methods.

**(B) Theory of HSAB**

Hard and soft acids and bases, Classification, Acid-base strength and hardness, Symbiosis, Electronegativity and hardness, Application of HSAB: Biological functions and toxicology of metals, and medicinal applications.

**UNIT – III: Reaction Mechanisms of Complexes**

**15 Hrs**

Reactivity of metal complexes, Inert and labile complexes, Kinetics and mechanisms of substitution reactions, Kinetics of substitution reactions in octahedral complexes, Acid hydrolysis, Factors affecting acid hydrolysis, Base hydrolysis, Conjugate base mechanism, Anation reactions, Substitution reactions in square planar complexes, Trans effect, Mechanism of trans effect, Electron transfer reactions, Inner sphere and outer sphere mechanisms, Marcus theory.

**UNIT – IV: Carbonyl and Nitrosyl Complexes, and Metal Atom Clusters**

**15 Hrs**

**(A) Metal Carbonyl and Nitrosyl Complexes**

Metal carbonyls: Preparation of metal carbonyls of Mn, Fe, Co and Ni, Bonding in carbonyls, EAN and 18-electron rule in carbonyls,  $\pi$ -Bonding in carbonyls, Terminal and bridging carbonyls, Measurement of  $\pi$ -bond strength in carbonyls, Structures of mononuclear, binuclear, trinuclear and tetranuclear carbonyls; Metal nitrosyls: Chemistry of linear and bent nitrosyls, Nitrosyls as  $NO^+$  and  $NO^-$  donors, Analytical uses of nitrosyl complexes.

**(B) Metal Atom Clusters**

Cage structures, Higher boranes, Carboranes, Metal-metal bonds in carbonyl cluster, LNCCs and HNCCs, Isoelectronic and isolobal relationships, Hetero atom in metal atom clusters, Electron counting schemes for HNCCs,

HNCCs of Fe, Co, Ni, Ru, Rh, Pd, Os, Ir and Pt, Lower halide and chalcogenide clusters, Triangular clusters, Solid state extended arrays.

**Books suggested:**

1. Advanced Inorganic Chemistry, F. A. Cotton, G. Wilkinson, M. Bochmann and R. N. Grimes, 5<sup>th</sup> Ed. (John Wiley & Sons Inc.).
2. Inorganic Chemistry: Principles of Structure and Reactivity, J. E. Huheey, E. A. Keiter and R. L. Keiter, 4<sup>th</sup> Ed. (Prentice Hall).
3. Inorganic Chemistry: G. Wulfsberg (University Science Books).
4. Introduction to Ligand Fields, B. N. Figgis (Krieger Pub Co.).
5. Concise Inorganic Chemistry, J. D. Lee, 5<sup>th</sup> Ed. (Wiley-Blackwell).
6. Modern Inorganic Chemistry, W. L. Jolly, 2<sup>nd</sup> Ed. (McGraw-Hill).
7. Coordination Compounds, S. F. Kettle (Springer).

## **15032: ORGANIC CHEMISTRY**

### **UNIT – I: Electronic Effects and Criteria of Aromaticity**

### **UNIT – II: Reaction Mechanism and Reactive Intermediates**

### **UNIT – III: Substitution Reactions**

### **UNIT – IV: Stereo Chemistry**

### **UNIT – I: Electronic Effects and Criteria of Aromaticity**

**15Hrs**

#### **(A) Electronic Effects**

Electronic effects: Inductive effect, mesomeric effect (Resonance), hyperconjugation, steric effect, tautomerism; hard and soft acids and bases, acidity and basicity of organic molecules.

#### **(B) Criteria of Aromaticity**

The energy, structural and electronic criteria for aromaticity; relationship among energetic, structural and electronic criteria; Huckle's rule and molecular orbital theory, aromaticity in benzenoid, non-benzenoid compounds; aromaticity in charged ring fused-ring systems; heteroaromatic systems; annulenes: cyclobutadiene, benzene, 1,3,5,7-cyclooctatetraene, [10] annulenes-1,3,5,7,9-cyclodecapentaene isomers, and [12]-, [14]-, [16]- and [18]-annulenes; azulenes; fulvenes; fullerenes; ferrocene; anti-aromaticity; homo-aromaticity.

### **UNIT – II: Reaction Mechanism and Reactive Intermediates**

**15Hrs**

#### **(A) Reaction Mechanism**

Types of bond cleavage; general classification of organic reactions; potential energy diagrams; thermodynamic requirements; kinetic requirements; kinetic and thermodynamic control; Hammond and Marcus theories; linear free energy relationships – Hammett equation; general methods of determination of mechanism.

#### **(B) Reactive Intermediates**

General methods of generation, geometry, stability and reactivity of carbocations, carbanions, free radicals, carbenes, nitrenes and arynes.

### UNIT – III: Substitution Reactions

15 Hrs

General introduction, classification of substitution reactions.

#### (A) Nucleophilic Substitutions

##### (i) Aliphatic Nucleophilic Substitutions:

$S_N1$  and  $S_N2$  reactions: mechanism, energy profile diagram and stereochemistry, SET, Border line (mixed  $S_N1$  and  $S_N2$ ) and  $S_Ni$  mechanisms, neighbouring group participation, factors influencing nucleophilic substitution reactions: structure of the substrate, solvent, nucleophile and leaving group.

##### (ii) Aromatic Nucleophilic Substitution

Introduction,  $S_NAr$ , and benzyne mechanisms, Von Richter, Sommelet-Hauser and Smiles rearrangements.

#### (B) Electrophilic Substitutions

Introduction, The arenium ion mechanism -  $S_E2$  reaction, orientation and reactivity, energy profile diagram, ipso substitution, orientation in disubstituted benzenes, diazonium coupling, Vilsmeier reaction, Gatterman-Koch reaction, Pechmann reaction, Reimer-Tiemann reaction.

### UNIT – IV: Stereo Chemistry

15Hrs

#### (A) Molecular Representation of Organic Molecules

Wedge, Fischer, Newman and Sawhorse formula, their description, inter conversion.

#### (B) Molecular Symmetry and Chirality

Definition and classification of stereoisomers, enantiomer, diastereomer, invertomer, homomer, epimer, anomer, configuration and conformation, D-, L- and R, S nomenclature, chiral manifestation.

#### (C) Geometrical Isomerism

*Cis-trans*, *E*-, *Z*- and *Syn-anti* nomenclature, methods of determining configuration of geometrical isomers using physical, spectral and chemical methods, Stability, *cis-trans* inter conversion.

#### (D) Stereoisomerism in Molecules without Chiral Center

**Axial chirality:** Allenes, alkylidenecycloalkanes, spiranes, nomenclature.

**Atropisomerism:** Biphenyl derivatives, nomenclature

**Planar Chirality:** Ansa compounds, paracyclophanes, *trans*-cyclooctene, helicity.

#### Books Suggested:

1. Advanced Organic Chemistry-Reactions, Mechanism and structure, Jerry March, 6<sup>th</sup> Ed. (John Wiley & Sons).
2. Organic Chemistry, Paula Yurkanis Bruice, 4<sup>th</sup> Ed. (Printice Hall)
3. Organic chemistry-Clayden J. (Oxford)
4. Organic Chemsitry, Wade, L.G. Jr. 5<sup>th</sup> Ed. (Pearson)
5. Advanced Organic Chemistry: Reactions and mechanisms, Miller Bernard & Other, 2<sup>nd</sup> Ed. (Pearson)
6. Mechanism and Theory in Organic Chemistry, Thomas H. Lowry, Kathleen S. Richardson, Harper & Row, (Publishers, Inc.).
7. Stereochemistry to Organic Compounds, E.L. Eliel (John Wiley).
8. Stereochemistry to Organic Compounds, D. Nasipuri, 2<sup>nd</sup> Ed. (New Age International).
9. Stereochemistry, P.S. Kalsi, 5<sup>th</sup> Ed. (New Age International).
10. Organic Chemistry Structure and Reactivity, Ege Seyhan, 3<sup>rd</sup> Ed. (AITBS)

## 15033: PHYSICAL CHEMISTRY

### UNIT – I : Quantum Chemistry-I

### UNIT – II: Chemical Dynamics-I

### UNIT – III: Thermodynamics-I

### UNIT – IV: Electrochemistry-I

### UNIT – I : Quantum Chemistry-I

15 Hrs

#### (A) Introduction to Exact Quantum Mechanical Results

Operator algebra, Eigen values and Eigen functions, Operators for momentum and energy, Linear combination of Eigen functions of an operator. The Schrodinger wave equation and the postulates of Quantum Mechanics, Discussion of solutions of the Schrodinger equation to some model systems, viz., particle in a box, harmonic oscillator, rigid rotor, hydrogen atom. Application of the spectra of conjugated molecules.

#### (B) Approximate Methods

The Variation Theorem, Linear variation Principle, Perturbation Theory (first Order and non-degenerate), Application of Variation Method and Perturbation theory to the Helium atom.

### UNIT – II: Chemical Dynamics-I

15 Hrs

#### (A) Theories of Reaction Rates

Collision theory, steric factor. Theory of Absolute Reaction Rates-Reaction coordinate, activated complex and the transition state. Thermodynamic formulation of reaction rates, Arrhenius Equation

#### (B) Unimolecular Reactions

Lindemann, Lindemann-Hinshelwood, and RRKM theories. Termolecular reactions. Complex reactions-Rate expressions for opposing, parallel and consecutive reaction (all first order type)

#### (C) Chain Reactions

Dynamic chain, hydrogen-bromine reaction, pyrolysis of acetaldehyde, decomposition of ethane, photochemical reactions-  $\text{H}_2\text{-Br}_2$ ,  $\text{H}_2\text{-Cl}_2$  reactions, Autocatalysis,  $\text{H}_2\text{-O}_2$  reaction, explosion limits, rate expressions for chain reaction.

### UNIT – III: Thermodynamics-I

15 Hrs

#### (A) Brief Review of Thermodynamic Concepts

Enthalpy, entropy, free energy. Concept of Entropy - Entropy as a state function - Entropy change in reversible process and irreversible process - Temperature -Entropy diagrams - Entropy change and Phase change - Entropy of mixing -Entropy and disorder.

#### (B) Classical & Statistical Thermodynamics

Partial molar properties: their significance and determination of partial molar volume, fugacity and its determination. Concept of distribution, thermodynamic probability and most probable Distribution, Ensemble averaging, Postulates of ensemble averaging, canonical, grand canonical and micro-canonical ensembles, partition functions, translational, rotational, vibrational and electronic partition functions, Gibbs-Duhem equation, calculation of thermodynamic properties in terms of partition functions, Heat capacity, chemical equilibria and equilibrium constant in terms of partition functions, Entropy of monatomic gases (Sackur-Tetrad equation).

**UNIT – IV: Electrochemistry-I****15 Hrs****(A) Strong Electrolytes**

Effect of dilution on equivalent conductance-Inter ionic attraction, Debye-Huckel-Onsager treatment, derivation of Debye-Huckel-Onsager equation, Verification and limitation of Onsager equation, Bjerrum treatment of electrolytes, Debye-Falkenhagen and Wien effects.

**(B) Activity and Activity Coefficients**

Relation between different types of activity coefficients, Determination of mean ionic activity coefficients by solubility and EMF methods, Debye-Huckel Limiting law and its verification (qualitative).

**(C) Reversible electrochemical cells**

Chemical cells and concentration cells-Types of reversible electrodes-Electrode potentials. Reactions in reversible cells - Nernst equation- thermodynamic and kinetic derivation-Concentration cells with and without transference. Liquid junction potential and its determination.

**Books suggested**

1. Physical Chemistry, P. W. Atkins (ELBS)
2. Introduction to quantum Chemistry, A. K. Chandra (Tata McGraw Hill)
3. Quantum Chemistry, Ira N. Levine (Prentice Hall)
4. Atomic Structure and chemical bond, Manas Chandra.
5. Chemical Kinetics, K.J.Laidler (McGraw Hill)
6. Kinetics and Mechanism of chemical Transformations, J. Rajaraman and J. Kuriacose (McMilan)
7. Thermodynamics for Chemists, S. Glasstone
8. Chemical Thermodynamics, I. M. Klotz
9. Statistical Thermodynamics, M. Dole
10. Modern Electrochemistry, vol. I & II, J. O. M. Bockris and A. K. N. Reddy (Plenum)
11. An Introduction to Electrochemistry (3<sup>rd</sup> ed.), S. Glasstone (Associated East-West)

**15034: GENERAL CHEMISTRY****UNIT – I: Symmetry and Group Theory****UNIT – II: Errors and Statistics****UNIT – III: Microwave Spectroscopy, Infrared Spectroscopy and Raman Spectroscopy****UNIT – IV: Spectrophotometry, Flame Photometry and Atomic Absorption Spectroscopy****UNIT – I: Symmetry and Group Theory****15 Hrs**

Symmetry Elements and Symmetry operation, Definitions of a group, sub-group, Relation between orders of a finite group and its sub-group, Conjugacy Relation and classes-point symmetry group, Schonflies symbols, Representation of groups by matrices (representation for  $C_{nv}$ ,  $C_{nh}$ ,  $D_{nh}$  etc. groups to be worked out explicitly), character of a representation. The great orthogonality theorem (without proof), Character tables and their use in spectroscopy.

**UNIT – II: Errors and Statistics****15 Hrs**

Classification of errors; accuracy; precision; minimization of systematic errors; mean and median values; absolute error; relative error; mean deviation and relative mean deviation; standard deviation and relative standard deviation; variance; range; confidence interval; comparison of results: F-test and student's t-test (i. comparison of mean and

true value, ii. comparison of two means and iii. comparison of more than two means - ANOVA); Dixon's Q-test; Gaussian distribution of random errors; correlation and regression; linear-least-square fitting; significant figures and rules for computations.

### **UNIT – III: Microwave Spectroscopy, Infrared Spectroscopy and Raman Spectroscopy**

**15Hrs**

#### **(A) Microwave Spectroscopy**

Classification of molecules, rigid rotor model, effect of isotopic substitution on the transition frequencies, intensities, non-rigid rotor, Stark effect.

#### **(B) Infrared Spectroscopy**

Review of linear harmonic oscillator, vibrational energies of diatomic molecules, zero-point energy, force constant, bond strengths, anharmonicity, Morse potential energy diagram, vibration-rotation spectroscopy, PQR branches, Vibrations of simple polyatomic molecules ( $\text{CO}_2$ ,  $\text{H}_2\text{O}$  etc.), Selection rules, exclusion principle.

#### **(C) Raman Spectroscopy**

Classical and quantum theories of Raman effect, pure rotational, vibrational and vibrational – rotational Raman spectra, selection rules.

### **UNIT – IV: Spectrophotometry, Flame Photometry and Atomic Absorption Spectroscopy**

**15 Hrs**

#### **(A) Spectrophotometry**

Beer-lambert law, Photometric accuracy, Deviations from Beer-lambert law, Block-diagram of a spectrophotometer, simultaneous spectrophotometric determination of metals, Determination of ratio of metal complexes: Job's method of continuous variation, slope ratio methods.

#### **(B) Flame Photometry**

Theory and instrumentation, Interferences, background correction, applications.

#### **(C) Atomic Absorption Spectroscopy**

Theory and instrumentation, Sources of radiation (HCL and EDL), Interferences, background correction, applications.

#### **Books Suggested**

1. Symmetry and Spectroscopy molecules –K. Veera Reddy, New Age Publications, New Delhi.
2. Chemical Applications of Group Theory by Bhattacharya
3. Vogel's Text Book of Quantitative Chemical Analysis, J. Mendham, R. C. Denney, J. D. Barnes and M. J. Thomas, 4<sup>th</sup> & 6<sup>th</sup> Ed.(Pearson Education Asia).
4. Analytical Chemistry by Robert Drills
5. Quantitative Analysis by R. A. Day and A. L. Underwood.
6. Analytical Chemistry, G. D. Christian
7. Instrumental Methods of Analysis, H. W. Willard, L. L. Merritt and J. A. Dean (Affiliated East-West)
8. Principles of Instrumental Analysis, D. A. Skoog and D. M. West (Holt, Rinehart and Wilson)
9. Physical Methods in Chemistry, R. S. Drago (Saunders).
10. Introduction to molecular Spectroscopy, G. M. Barrow (McGraw Hill)
11. Basic principles of Spectroscopy, R. Chang (Mc Graw Hill)



## 15031P: INORGANIC CHEMISTRY PRACTICALS

### 1. Preparation and Purification of Inorganic Complexes

- a) Chloropentamminecobalt(III)chloride
- b) *Bis*(oxalate)cuprate(II)dehydrate
- c) *Tris*(oxalato)ferrate(III)
- d) Hexaamminenickel(II)chloride

### 2. Complex Analysis

- a) Estimation of cobalt present in chloropentamminecobalt(III)chloride
- b) Estimation of copper present in *bis*(oxalate)cuprate(II)dehydrate
- c) Estimation of iron present in *tris*(oxalato)ferrate(III)
- d) Estimation of nickel present in hexaamminenickel(II)chloride

## 15032-P: ORGANIC CHEMISTRY PRACTICALS

### 1. Systematic semi micro qualitative analysis of a binary organic mixture

Identification of method of separation and functional group present in each component and preparation of one solid derivative for the confirmation of the functional groups.

#### Books Suggested

- 1. Vogel's Text Book of Quantitative Chemical Analysis, J. Mendham, R. C. Denney, J. D. Barnes and M. J. Thomas, 4<sup>th</sup> & 6<sup>th</sup> Ed. (Pearson Education Asia).
- 2. Vogel's Text Book of Practical Organic Chemistry, B.S. Furniss, A.J. Hannaford, P.W.G. Smith, A.R. Tatchell, 5 Ed. (Longman Scientific & Technical)

## SECOND SEMESTER

### 25031: INORGANIC CHEMISTRY

#### UNIT – I: Organometallic Chemistry

#### UNIT – II: Transition Metal $\pi$ -Complexes

#### UNIT – III: Electronic Spectra of Complexes

#### UNIT – IV: Magnetic Properties of Transition Metal Complexes

#### UNIT – I: Organometallic Chemistry

15 Hrs

##### (A) Organometallic Reagents in Synthesis

Stoichiometric reactions in catalysis, Homogeneous catalytic hydrogenation, Hydroformylation (oxo reaction), Isomerisation, Zeigler-Natta polymerization of olefins, Oxopalladation reactions, Activation of small molecules by coordination.

##### (B) Fluxional Organometallic Compounds

Fluxionality and dynamic equilibria in compounds such as  $\eta^2$ -olefin,  $\eta^3$ -allyl and dienyl complexes.

#### UNIT – II: Transition Metal $\pi$ -Complexes

15 Hrs

Transition metal  $\pi$ -complexes with unsaturated organic molecules such as alkenes, alkynes, allyl, diene, dienyl, arene and trienyl complexes, General methods of preparation, Properties, Nature of bonding and structural features, Important reactions relating to nucleophilic and electrophilic attack on ligands.

#### UNIT – III: Electronic Spectra of Complexes

15 Hrs

Free Ion Terms and Energy Levels: Configurations, Terms, States and Microstates. Calculation of Microstates for  $p^2$  and  $d^2$  configuration, L-S (Russell-Saunders) Coupling Schemes, J-J Coupling scheme, derivation of terms for  $p^2$  and  $d^2$  configuration. Hole Formulation, Energy ordering of terms (Hund's Rules), Selection rules: Laporte orbital selection rule, spin selection rules. Splitting of energy levels and spectroscopic states, Orgel diagrams of  $d^1$  to  $d^9$  metal complexes. Interpretation of electronic spectra of aquo complexes of Ti(III), V(III), Cr(III), Mn(II), Fe(II), Fe(III), Co(II), Ni(II) and Cu(II). Calculation of interelectronic and spectra parameters for  $d^8$  metal complexes. Tanabe-Sugano diagrams for  $d^2$  and  $d^6$  octahedral complexes. Charge transfer ( $L \rightarrow M$  and  $M \rightarrow L$ ) spectra of metal complexes.

#### UNIT – IV: Magnetic Properties of Transition Metal Complexes

15 Hrs

Diamagnetism, paramagnetism, orbital and spin contributions, spin-orbit coupling, Hund's third rule and energies of J levels, Curie law and Curie-Weiss law, ferromagnetism and antiferromagnetism, temperature independent magnetism, magnetic susceptibility and determination of magnetic susceptibility by Gouy method, paramagnetism and crystalline fields –  $Ti^{3+}$ ,  $V^{3+}$ ,  $VO^{2+}$ ,  $Cr^{3+}$ ,  $Mn^{2+}$ ,  $Fe^{3+}$ ,  $Co^{2+}$ ,  $Ni^{2+}$  and  $Cu^{2+}$ , magnetic exchange in copper acetate and other dimers.

#### Books Suggested:

1. Advanced Inorganic Chemistry, F. A. Cotton, G. Wilkinson, M. Bochmann and R. N. Grimes, 5<sup>th</sup> Ed. (John Wiley & Sons Inc.).
2. Inorganic Chemistry: Principles of Structure and Reactivity, J. E. Huheey, E. A. Keiter and R. L. Keiter, 4<sup>th</sup> Ed.

- (Prentice Hall).
3. Inorganic Chemistry: G. Wulfsberg (University Science Books).
  4. Introduction to Ligand Fields, B. N. Figgis (Krieger Pub Co.).
  5. Concise Inorganic Chemistry, J. D. Lee, 5<sup>th</sup> Ed. (Wiley-Blackwell).
  6. Modern Inorganic Chemistry, W. L. Jolly, 2<sup>nd</sup> Ed. (McGraw-Hill).
  7. Coordination Compounds, S. F. Kettle (Springer).
  8. Magnetochemistry, R. L. Carlin (Springer-Verlag New York).
  9. Elements of Magnetochemistry R. L. Dutta and A. Syamal, 2<sup>nd</sup> Ed. (Affiliated East-West Press Pvt. Ltd).
  10. The Organometallic Chemistry of the Transition Metals, R. H. Crabtree, 3<sup>rd</sup> and 4<sup>th</sup> Ed. (Wiley Interscience).
  11. Organometallic Chemistry: A Unified Approach, R. C. Mehrotra and A. Singh, 2<sup>nd</sup> Ed. (New Age International).
  12. Principles of Organometallic Chemistry, P. Powell, 2<sup>nd</sup> Ed. (ELBS)

## **25032: ORGANIC CHEMISTRY**

### **UNIT – I: Addition and Condensation Reactions**

### **UNIT – II: Elimination, Esterification and Hydrolysis Reactions**

### **UNIT – III: Conformational Analysis**

### **UNIT – IV: Pericyclic Reactions**

### **UNIT – I: Addition and Condensation Reactions**

**15 Hrs**

#### **(A) Addition Reactions**

Introduction; addition reactions involving electrophiles (Br<sub>2</sub>, HBr, HOBr, and H<sub>2</sub>O/H<sub>2</sub>SO<sub>4</sub>); nucleophilic additions (Cannizzaro, Michael, Mannich, Grignard and Wittig reactions); free radical additions - Kharash peroxide effect; stereospecificity in addition reactions: bromination, dihydroxylation, hydroboration, hydrogenation and Sharpless asymmetric epoxidation reactions.

#### **(B) Condensation reactions**

Introduction; Aldol, Claisen, Dieckman, Perkin, Knoevenagel, Claisen-Schmidt, Benzoin and Stobbe condensation reactions.

### **UNIT – II: Elimination, Esterification and Hydrolysis Reactions**

**15 Hrs**

#### **(a) Elimination Reactions**

Introduction; type of eliminations:  $\alpha$ -,  $\beta$ - and  $\gamma$ -eliminations; Zaitsev (Saytzeff) and Hofmann rules; mechanism: E1, E2 and E1cB; competition between elimination and substitution; stereochemistry and orientation in E2 eliminations; pyrolytic syn elimination; dehydration of alcohols; dihydro-eliminations of C-C, C-O and C-N; dihalo-elimination; decarboxylative eliminations; molecular rearrangement during elimination; fragmentation reactions.

#### **(b) Esterification Reactions**

Reaction between carboxylic acid and alcohol: Fischer, Mitsunobu and Steglich esterifications; reaction between acid halide and alcohols; reaction between carboxylic acid and alkyl halides; trans esterification.

#### **(c) Hydrolysis Reactions**

General mechanism and applications of ester hydrolysis in acidic and basic conditions; hydrolysis of acid halides; hydrolysis of amides.

**UNIT – III: Conformational Analysis****15 Hrs****(A) Conformations of Acyclic Molecules**

Conformations of ethane, propane, n-butane, Physical methods for conformational analysis, 2,3-dimethylbutane, n-propyl chloride, conformation and intramolecular hydrogen bonding: ethylene glycol, Diastereomers and conformation: 2,3-dibromobutane, butane-2,3-diol and amino alcohol.

**(B) Conformations of Cyclic Systems**

Conformations of cyclohexane, mono and disubstituted cyclohexanes, cyclohexene, cyclohexanone, 2-alkyl and 3-alkylketone effect, alkylidene cyclohexane, decalin, 9-methyldecalin, decalone

**(C) Conformations of Heterocycles**

Conformations of aziridines, piperidine, 1,3-dioxanes.

**UNIT – IV: Pericyclic Reactions****15 Hrs**

Molecular orbital symmetry, frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene, allyl system and 2,4-pentadienyl systems, classification of pericyclic reactions, Electrocyclic reactions: Conrotatory and Disrotatory motions in  $4n$ ,  $4n+2$  systems, Cycloadditions: antarafacial and suprafacial additions in  $4n$  ( $2+2$  cyclo addition) and  $4n+2$  ( $4+2$  cyclo addition) systems,  $2+2$  addition of ketene, 1,3-dipolar cycloadditions and cheletropic reactions. Sigmatropic rearrangements – 1,3 and 1,5 suprafacial and antarafacial shifts of H and C, Claisen, Cope and oxy-Cope rearrangements, Ene reaction, FMO and PMO approach, Woodward-Hoffmann Correlation diagrams and Woodward-Hoffmann selection rules of electrocyclic reactions, cyclo addition reactions and sigmatropic rearrangements.

**Books Suggested:**

1. Advanced Organic Chemistry-Reactions, Mechanism and structure, Jerry March, 6<sup>th</sup> Ed. (John Wiley & Sons).
2. Modern Organic Reactions, H. O. House (Benjamin)
3. Structure and Mechanism in Organic Chemistry C. K. Ingold (Cornell University Press).
4. Organic Chemistry, Paula Yurkanis Bruice, 4<sup>th</sup> Ed. (Printice Hall)
5. Organic chemistry-Clayden J. (Oxford)
6. Organic Chemistry, Wade, L.G. Jr. 5<sup>th</sup> Ed. (Pearson)
7. Organic Chemistry, Salmons, P.W. & Others, 8<sup>th</sup> Ed. (John Wiley & Sons)
8. Advanced Organic Chemistry: Reactions and mechanisms, Miller Bernard & Other, 2<sup>nd</sup> Ed. (Pearson)
9. Mechanism and Theory in Organic Chemistry, Thomas H. Lowry, Kathleen S. Richardson, Harper & Row, (Publishers, Inc.).
10. A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, 6<sup>th</sup> Ed., (Longman).
11. Reaction Mechanism in Organic Chemistry, P.S. Kalsi, 2<sup>nd</sup> Ed. (New Age International).
12. Stereochemistry to Organic Compounds, E.L. Eliel (John Wiley).
13. Stereochemistry to Organic Compounds, D. Nasipuri, 2<sup>nd</sup> Ed. (New Age International).
14. Stereochemistry, P.S. Kalsi, 5<sup>th</sup> Ed. (New Age International).
15. Organic Chemistry Structure and Reactivity, Ege Seyhan, 3rd Ed. (AITBS)

**25033: PHYSICAL CHEMISTRY****UNIT – I: Quantum Chemistry-II****UNIT – II: Chemical Dynamics –II**

**UNIT – III: Thermodynamics-II****UNIT – IV: Electrochemistry-II****UNIT – I: Quantum Chemistry-II****15 Hrs****(A) Angular Momentum**

Angular momentum, Rotations and angular momentum, Eigen functions and Eigen values of angular momentum, Ladder operator, addition of angular momenta, Spin angular momenta, antisymmetry and Pauli Exclusion Principle, Slater determinant,

**(B) Molecular Orbital Theory**

Atomic Orbitals, Simple Molecular Orbitals, Hybrid Atomic Orbitals, Shapes and energies of Molecular Orbital Systems of Organic Molecules (Ex: Methane, Acetylene, ethylene, cyanide anion), Hückel theory of conjugated systems,  $\pi$ -bond order and charge density calculations, application to ethylene, butadiene and benzene.

**UNIT – II: Chemical Dynamics -II****15 Hrs****(A) Acid Base Catalysis: Specific Acid Catalysis**

General acid catalysis (Hydrolysis of ester and vinyl ether). Specific base catalysis and general base catalysis (the alcohol reaction and hydrolysis of acetic anhydride). Protolytic and prototropic mechanism.

**(B) Homogeneous and Heterogeneous Catalysis**

Homogeneous catalysis. Catalysis by transition metal ions and their complexes. Industrially important processes. Supported transition metal complexes as catalysts. Bimolecular reactions. Electronic theories of chemisorption and heterogeneous catalysis.

**(C) Introduction to Enzyme Catalysis**

Michaelis - Menton kinetics - effect of pH and effect of temperature on the rates of enzyme reactions.

**UNIT – III: Thermodynamics-II****15 Hrs****(A) Phase Equilibria**

Equilibrium between two phases of one component. The Clapeyron equation. The Clausius Clapeyron equation. Applications. Integrated form of Clapeyron equation.

**(B) Phase Rule**

Thermodynamic derivation of phase rule, Solid-liquid equilibria, Thermal analysis, simple eutectic, congruent fusion, incongruent fusion and systems consisting of both. Application of phase rule to three component system, Stokes and Roozeboom plots. Three component liquid systems, formation of one pair, two pairs and three pairs of partially miscible liquids, two salts and water, no chemical combination, double salt formation, one salt forms hydrate and two salts form hydrates, solid solutions.

**UNIT – IV: Electrochemistry-II****15 Hrs****(A) Irreversible Electrode Phenomenon**

Reversibility and irreversibility, Dissolution and deposition potentials, Decomposition voltage, overvoltage, diffusion overvoltage.

**(B) Batteries**

Batteries Primary and secondary batteries-Fuel cells-Proton exchange membrane fuel cells-Advantage and limitations of fuel cells working principles of UPS and its applications.

### **(C) Electrochemical Study**

General consideration, costing on electrolytic process, electrolysis parameters, principles of cell design and the addition technology of electrolysis process and typical cell design. Cyclic voltammetry and its applications.

### **Books Suggested**

1. Physical Chemistry, P. W. Atkins, (ELBS)
2. Introduction to quantum Chemistry, A. K. Chandra (Tata McGraw Hill)
3. Quantum Chemistry, Ira N. Levine, (prenticxe Hall)
4. Coulson's Valence, R. Mcweeny, (ELBS)
5. Modern Electrochemistry, vol.I & II, J. O. M. Bockris and A. K. N. Reddy (Plenum)
6. An Introduction to Electrochemistry (3<sup>rd</sup> ed.), S. Glasstone (Affiliated East-West)
7. Micelles, theoretical and applied aspects, V. Moroi (Plenum)
8. A text Book of Physical Chemistry (2<sup>nd</sup> Ed.), S. Glasstone (Macmilan)
9. Principles of Physical Chemistry, Maron and Prutton
10. Theoretical Electrochemistry, L. I. Antropov.

## **25034: SPECTROSCOPY**

### **UNIT – I: UV-Visible and IR Spectroscopy**

### **UNIT – II: Nuclear Magnetic Resonance Spectroscopy (<sup>1</sup>H NMR)**

### **UNIT – III: <sup>13</sup>C NMR spectroscopy and 2D NMR techniques**

### **UNIT – IV: Mass Spectrometry**

### **UNIT – I: UV-Visible and IR Spectroscopy**

**15 Hrs**

#### **(A) Ultraviolet and Visible Spectroscopy**

Various electronic transitions (185-800 nm), effect of solvent on electronic transitions, ultraviolet bands for carbonyl compounds, unsaturated carbonyl compounds, dienes and conjugated polyenes. Fieser-Woodward rules for conjugated dienes and carbonyl compounds, ultraviolet spectra of aromatic and heterocyclic compounds, Steric effect in biphenyls, polycyclic aromatic compounds.

#### **(B ) Infrared Spectroscopy**

Instrumentation and sample handling, FT-IR. overtones, combination bands and Fermi resonance, factors influencing vibrational frequencies, Characteristic vibrational frequencies of alkanes, alkenes, alkynes, aromatic compounds, alcohols, ethers, phenols and amines. Detailed study of vibrational frequencies of carbonyl compounds (ketones, aldehydes, esters, amides, acids, anhydrides, lactones, lactams and conjugated carbonyl compounds).

### **UNIT – II: <sup>1</sup>H NMR Spectroscopy**

**15 Hrs**

Nuclear spin, nuclear resonance, saturation, shielding of magnetic nuclei, deshielding, chemical shifts and its measurements, factors influencing chemical shift, chemical shift values and correlation for protons bonded to carbon (aliphatic, olefinic, aldehydic and aromatic) and other nuclei (alcohols, phenols, enols, carboxylic acids, amines and amides), spin-spin interactions, coupling constant (J): Types and classification (ABX, AMX, ABC etc.) of coupling constants, Karplus curve variation of coupling constant with dihedral angle, virtual coupling, chemical exchange, effect of deuteration, hindered rotation, Simplification of complex spectra: nuclear magnetic double resonance (spin decoupling), contact shift reagents, Nuclear Overhauser effect (NOE).

### **UNIT – III: <sup>13</sup>C NMR Spectroscopy and 2D NMR Techniques**

**15 Hrs**

**(A)  $^{13}\text{C}$  NMR Spectroscopy**

CW and FT techniques. Types of  $^{13}\text{C}$  NMR spectra: undecoupled, proton- decoupled and off-resonance decoupled (ORD) spectra.  $^{13}\text{C}$  chemical shifts, factors affecting the chemical shifts, chemical shifts of organic compounds. Calculation of chemical shifts of alkanes, alkenes and alkynes. Homonuclear ( $^{13}\text{C}$ - $^{13}\text{C}$  J) and heteronuclear ( $^{13}\text{C}$ -,  $^1\text{H}$  J) coupling.  $^{13}\text{C}$ -NMR spectral editing techniques: principle and applications of DEPT.

**(B) 2D NMR Techniques**

Principles of 2D NMR, classification of 2D-experiments. Correlation spectroscopy (COSY), HOMO COSY ( $^1\text{H}$ - $^1\text{H}$  COSY), COSY of *m*-dinitrobenzene, isopentyl acetate, Hetero COSY ( $^1\text{H}$ ,  $^{13}\text{C}$  COSY) Hetero COSY of isopentyl acetate and 4-methyl-2-pentanol, HMQC, HMQC of codeine, long range  $^1\text{H}$ ,  $^{13}\text{C}$  COSY (HMBC), HMBC of codeine and NOESY, NOESY of 9-benzylanthracene, 2-D INADEQUATE experiments.

**UNIT-IV: Mass Spectrometry****15 Hrs**

Introduction, principle, instrumentation, single & double focusing mass spectrometers, ionization methods: EI, CI, FDI, PDI, LDI, FAB, TSI and ESI, mass analyzers: MSA, ESA, QMA, ITA, TOF, FT and tandem, molecular-ion peak, nitrogen rule, base peak, metastable ion, isotopic abundance, high resolution mass spectrometry (HRMS), index of hydrogen deficiency (IHD), general methods of mass spectral fragmentation, Mc. Lafferty rearrangement, ortho effect, factors affecting fragmentation, mass spectral fragmentation patterns of various classes of organic compounds: alkanes, alkenes, alkynes, aromatics, alcohols, alkyl halides, ethers, aldehydes, ketones, carboxylic acids, esters, amines, amides, nitriles, nitro compounds. mass spectral problems with respect to structure determination.

**Books suggested**

1. Organic spectroscopy, W. Kemp, 5<sup>th</sup> Ed., (ELBS.2)
2. Spectroscopy of organic compounds, R.M. Silverstein and others, 5<sup>th</sup> Ed., (John Wiley)
3. Spectrometric Identification of organic compounds, R.M. Silverstein, F.X. Webster and D.J. Kiemle, 7<sup>th</sup> Ed., (Wiley)
4. Introduction to Spectroscopy, A guide for students of organic chemistry, Donald L. Pavia, Gary M. Lamp man and George S. Kriz, 3<sup>rd</sup> Ed., (Thomson).
5. Spectroscopic methods in Organic Chemistry, DH Williams & I Flemming, (TMH)
6. Spectroscopy of organic compounds, P. S. Kalsi, (Wiley)
7. Nuclear Magnetic Resonance Spectroscopy An introduction to Principles, Applications and experimental methods, Joseph B. Lambert and Eugene P. Mazzola, (Pearson Education Inc. Prentice – Hall).
8. A Complete Introduction to Modern NMR Spectroscopy, Roger S. Macomber, (John Wiley & Sons, Inc.).

**25031P: ORGANIC CHEMISTRY PRACTICALS**

**(1) Estimations:** Estimation of (a) glucose, (b) phenol, (c) aniline and (d) aspirin

**(2) Isolation and identification of Natural Products:**

- (a) Isolation of caffeine from tea leaves
- (b) Isolation of eugenol from cloves
- (c) Isolation of casein and lactose from milk powder
- (d) Isolation of piperine from black pepper (A demo on soxhlet extraction)

**25032P: PHYSICAL CHEMISTRY PRACTICALS**

- (1) Determination of critical solution temperature of phenol-water system and study the effect of electrolyte on CST.
- (2) Determination of eutectic composition and temperature of simple eutectic system (Urea-benzoic acid).
- (3) Determination of congruent composition and temperature of binary system (diphenylamine – benzophenone system)

- (4) Determination of rate constant of acid hydrolysis of an ester and investigate the effect of catalyst concentration, reactant concentration and temperature.
- (5) Conductometry.
  - (a) Determination of cell constant
  - (b) Verification of Onsager equation
  - (c) Determination of dissociation constant of a weak acid
  - (d) Titration of a strong acid with a strong base
  - (e) Titration of a weak acid with a strong base
- (6) Potentiometry
  - (a) Titration of a strong acid with a strong base
  - (b) Titration of a weak acid with a strong base
  - (d) Titration of ferrous ammonium sulphate with potassium dichromate.
- (7) Nuclear techniques
  - (a) Geiger Muller Counter
  - (b) Gamma Ray Spectrometer

### Books Suggested

1. Adapted from Introduction to Organic Laboratory Techniques: A Microscale Approach. Pavia, Lampman, Kriz, and Engel. (1999) Saunders College Publishing.
2. Text book of practical organic chemistry including qualitative organic analysis by A.I. Vogel (Longman).
3. Findlay's Practical Physical Chemistry by J.A. Kitchener, 8<sup>th</sup> Ed. (Longmans).
4. Ikan, R. Natural Products, A Laboratory Guide, 2nd ed.; Academic Press: New York, 1991.
5. Pharmaceutical drug analysis by Ashutoshkar.
6. Quantitative analysis of drugs in pharmaceutical formulations by P D Sethi.
7. Practical pharmaceutical chemistry part-1 and part-2 by A H Beckett and J B Stenlake.
8. Practical organic chemistry by Mann & Saunders.
9. Text book of practical organic chemistry including qualitative organic analysis by A.I. Vogel (Longman).

## 25035: BASICS OF CHEMISTRY

### UNIT – I: Basics of Organic Chemistry

### UNIT – II: Basic Parameters in Sample Preparation

### UNIT – III: Basics of Bioinorganic Chemistry

### UNIT – IV: Basics of Polymer Chemistry

### UNIT – I: Basics of Organic Chemistry

15 Hrs

Hybridization in organic compounds; dipole moment; inductive effect; electromeric effect; conjugation and resonance; homolysis; heterolysis; types of organic reactions; isomerism; introduction to reactive intermediates; classification of isomerism; stereochemistry of organic compounds – *E* & *Z* and *R* & *S* nomenclature

### UNIT – II: Basic Parameters in Sample Preparation

15 Hrs

Definition and calculation of substance in moles and millimoles; solutions and their concentrations: definition of solution, solute and suspension, weight percentage, volume to volume percentage, mole fraction, mole percentage, molarity, molality, normality; density and specific gravity; conversion of weight/moles to volume using density; compound empirical and molecular formulae.

### UNIT – III: Basics of Bioinorganic Chemistry

15 Hrs



Essential and trace elements – role of metal ion in biological process;  $\text{Na}^+/\text{K}^+$  pump; photosynthesis – structure of chlorophyll, photosynthetic mechanism in bacteria and in green plants (Z-scheme, PS-I & PS-II); respiration (transport and storage of dioxygen) – structure and function of myoglobin, hemoglobin, hemerythrin and model systems.

#### UNIT – IV: Basics of Polymer Chemistry

15 Hrs

**Terminology:** monomers, repeat units, degree of polymerization, linear, branched and network polymers, classification of polymers.

**Synthetic methods:** Condensation, addition, radical chain, ionic and coordination, copolymerization.

**Applications:** biomedical and industrial applications

#### Books Suggested

1. Organic Chemistry, Paula Yurkanis Bruice, 4<sup>th</sup> Ed. (Printice Hall).
2. Mechanism and Theory in Organic Chemistry, Thomas H. Lowry, Kathleen S. Richardson, Harper & Row, (Publishers, Inc.).
3. Analytical Chemistry, G. D. Christian, 5<sup>th</sup> Edition, John Wiley & Sons.
4. Bioinorganic Chemistry, R. W. Hey, Ellis Horwood Ltd., Chichester, New York
5. Bioinorganic Chemistry, K. Hussain Reddy, New Age International Publisher, New Delhi.
6. Text Book of Polymer Science, F. W. Billmeyer, Jr. (Wiley Inter Science).
7. Polymer Chemistry, Gowarikar.

## 35031: INORGANIC CHEMISTRY

### UNIT – I: Electron Spin Resonance and Mössbauer Spectroscopy

#### UNIT – II: Bioinorganic Chemistry

#### UNIT – III: Photoelectron Spectroscopy

#### UNIT – IV: Introduction to Nanomaterials

### UNIT – I: Electron Spin Resonance and Mössbauer Spectroscopy

15 Hrs

#### (A) Electron Spin Resonance Spectroscopy

Introduction, principle, instrumentation, selection rules, g-factor and its significance, hyperfine and super hyperfine coupling, zero-field splitting including Kramer's degeneracy, application of ESR to free radicals and transition metal complexes, evidence for covalence in complexes, ex. Cu(II)bissalicylaldimine, bis-acetylacetonatovanadyl and hexachloroiridium(IV) complexes.

#### (B) Mössbauer Spectroscopy

Basic principles, isomer shift, quadrupole shift and spectrum display, applications: bonding and structures of  $\text{Fe}^{2+}$  and  $\text{Fe}^{3+}$  compounds including those of intermediate spin and  $\text{Sn}^{2+}$  and  $\text{Sn}^{4+}$  compounds, nature of metal-ligand bond, coordination number, unequivalent mössbauer atoms.

### UNIT – II: Bioinorganic Chemistry

15 Hrs

#### (A) Transport and Storage of Dioxygen:

Metal complexes as oxygen carriers, heme proteins – structure and functions of hemoglobin and myoglobin, non-heme proteins – hemoerythrin and hemocyanin, model synthetic complexes of iron, cobalt and copper.

#### (B) Electron Transfer in Biology:

Structure and functions of metalloproteins in electron transfer process, catalase, peroxidase, cytochromes and iron-sulfur proteins, synthetic models.

### UNIT – III: Photoelectron Spectroscopy

15Hrs

Photoelectric effect – Koopmans theorem ionization energy, block diagram of photoelectron spectrometer: sources of radiation, monochromator, detectors, shake-up and shake-off features. Ultraviolet photoelectron spectroscopy, application of UPS to  $\text{O}_2$  and  $\text{N}_2$  molecules, Electron spectroscopy of chemical analysis, Applications of XPS to qualitative analysis-chemical shift-application to surface studies and structural analysis.

### UNIT – IV: Introduction to Nanomaterials

15Hrs

Basic chemistry for nanoscience, chemical routes for synthesis of nanomaterials: chemical precipitation and co-precipitation, metal nanocrystals by reduction, sol-gel synthesis, microemulsions or reverse micelles, solvothermal synthesis, microwave heating synthesis, sonochemical synthesis, characterization of nanomaterials: X-ray diffraction (XRD), Scanning Electron Microscopy (SEM), Transmission Electron Microscopy (TEM), Atomic Force Microscopy (AFM).

#### Books Suggested

1. Instrumental methods of analysis, H. W. Willard, L. L. Merritt and J. A. Dean.
2. Advanced Inorganic Chemistry, F. A. Cotton, G. Wilkinson, M. Bochmann and R. N. Grimes, 5<sup>th</sup> Ed. (John Wiley & Sons Inc.).
3. Inorganic Chemistry: Principles of Structure and Reactivity, J. E. Huheey, E. A. Keiter and R. L. Keiter, 4<sup>th</sup> Ed (Prentice Hall).
4. Inorganic Chemistry: G. Wulfsberg (University Science Books).
5. Concise Inorganic Chemistry, J. D. Lee, 5<sup>th</sup> Ed. (Wiley-Blackwell).
6. Modern Inorganic Chemistry, W. L. Jolly, 2<sup>nd</sup> Ed. (McGraw-Hill).

7. Introduction to Photoelectron Spectroscopy, P. K. Ghosh
8. Nanochemistry: A Chemical Approach to Nanomaterials; G.A. Ozin, A.C. Arsenault and L. Cademartiri (RSC, London).
9. Nanocomposite Science and Technology; P.M. Ajayan, L.Z. Schadler and P.V. Brown (Wiley).
10. Characterization of Nanophase Materials; Z.L. Wang (ed.) (Wiley-VCH).

## 35032: ORGANIC CHEMISTRY

### UNIT – I: Molecular Rearrangements

### UNIT – II: Photochemistry

### UNIT – III: Asymmetric Synthesis

### UNIT – IV: Green Chemistry

#### UNIT – I: Molecular Rearrangements

15 Hrs

Introduction, types of molecular rearrangements, migratory aptitude, rearrangements to electron deficient carbon: pinacol-pinacolone, Wagner-Meerwein, Demjanov Arndt-Eistert synthesis and benzil-benzilic acid rearrangements; rearrangements to electron deficient nitrogen: Beckmann, Hofmann, Curtius, Schmidt and Lossen rearrangements; rearrangements to electron deficient oxygen: Baeyer-Villiger and Dakin rearrangements; rearrangements to electron rich carbon: Favorskii and Neber rearrangements.

#### UNIT – II: Photochemistry

15Hrs

Photochemical energy, Frank-Condon principles, Jablonski diagram, singlet and triplet states, photosensitization, quantum efficiency and quantum yield; Photochemistry of carbonyl compounds:  $n \rightarrow \pi^*$  and  $\pi \rightarrow \pi^*$  transitions, Norrish type-I and Norrish type-II cleavages, Paternò-Büchi reactions, photoreduction, Rearrangement of cyclohexenones, cyclohexadienones; photochemistry of unsaturated systems (olefins): *Cis-trans* isomerization, benzene and its derivatives, oxa-di- $\pi$ -methane rearrangement; photochemistry of benzene and its derivatives, photo Fries rearrangement of phenyl esters and anilides; photolysis of nitrite esters: Barton reaction.

#### UNIT – III: Asymmetric Synthesis

15Hrs

##### (A) Introduction and terminology

Topicity in molecules: homotopic, heterotopic (enantiotopic and diastereotopic), prochirality nomenclature; Substitution and addition criteria; Pro-R, Pro-S, Re- and Si-faces; stereoselective reactions: enantioselectivity and diastereoselectivity; optical purity: enantiomeric excess and diastereomeric excess.

##### (B) Strategies in Asymmetric Synthesis

##### (i) Chiral substrate controlled asymmetric synthesis

Nucleophilic additions to chiral carbonyl compounds. 1,2-asymmetric induction, Cram's rule and Felkin-Anh model.

##### (ii) Chiral auxiliary controlled asymmetric synthesis

$\alpha$ -Alkylation of chiral enolates, azaenolates, imines. Use of chiral auxiliaries in Diels-Alder reaction and Aldol reactions.

##### (iii) Chiral reagent controlled asymmetric synthesis

Asymmetric reductions using BINAL-H. Asymmetric hydroboration using  $(IPC)_2BH$  and  $IPCBH_2$ .

##### (iv) Chiral catalyst controlled asymmetric synthesis

Sharpless and Jacobsen asymmetric epoxidations; asymmetric hydrogenations using chiral Wilkinson bisphosphine and Noyori catalyst; enzyme mediated enantioselective synthesis.

#### UNIT – IV: Green Chemistry

15 Hrs

Concept of green chemistry, principles of green chemistry and green synthetic methods – organic reactions in aqueous media: advantages and applications in pinacol coupling, Mukaiyama aldol reaction, and Trost-Tsuji reaction; ionic liquids in organic synthesis: introduction, composition, and application in stereoselective halogenation, Friedel-Craft reaction and hydroformylation; microwave assisted reactions: principle, conditions, advantages over conventional heating, and application in Fischer indole synthesis, Paal-Knorr pyrrole synthesis, Baylis-Hillman and benzil-benzilic acid rearrangement; phase transfer catalysis: introduction, types of phase transfer catalysts, mechanism of catalytic action, and application in benzoin condensation, Wittig, Wittig-Horner and Michael addition reactions; ultrasound assisted synthesis: advantages, applications in the synthesis of Diels-Alder, hydroboration and Reformatsky reactions.

#### **Books Suggested:**

1. Green Chemistry: an introductory text; M. Lancaster; 2<sup>nd</sup> Ed. (RSC).
2. Organic Synthesis: Special Techniques; V.K. Ahluwalia and R. Aggarwal; 2<sup>nd</sup> Ed. (Narosa)
3. Advanced Organic Chemistry-Reactions, Mechanism and structure, Jerry March, 6<sup>th</sup> Ed. (John Wiley & Sons).
4. Guide book to Organic Synthesis, R. K. Machie and D.N.Smith, (ELBS).
5. Advanced Organic Chemistry: Part A & B, F. A Carey and R. J. Sundberg, 5<sup>th</sup> Ed., Springer, 2007.
6. Click Chemistry: Journal of American Chemical Society (2008); Volume. 130; Pages. 5062 – 5064, and Chemical Society Reviews (2007); Vol. 36; Pages. 1249 – 1262.
7. Handbook of Metathesis; R. H. Grubbs (Wiley).
8. Application of Ionic Liquids in Organic Synthesis; Aldrichimica Acta; Volume. 35; No. 3; Pages. 75 – 83.
9. Organic Reactions in Aqueous Media with a Focus on Carbon-Carbon Bond Formation: A Decade Update; Chemistry reviews (2005); Volume. 105; Pages. 3095 – 3165.
10. Fundamentals of Photochemistry, K. K. Raotagi-Mukhergi, (Wiley Eastern).
11. Essential of Molecular Photochemistry, A. Gilbert and J. Baggott (Blackwell scientific Publications).
12. Stereoselective Synthesis, M. Nógrádi, 2<sup>nd</sup> Ed., 1995.
13. Asymmetric organic reactions, J. D. Morrison and H. S. Moscher.
14. Principles of Asymmetric synthesis, R. E. Gawley and J. Aube, 2<sup>nd</sup> Ed., Elsevier, 2012.

### **35033: PHYSICAL CHEMISTRY**

#### **UNIT – I: Surface Chemistry**

#### **UNIT – II: Polymers - Basics and Characterization**

#### **UNIT – III: X-Ray Techniques**

#### **UNIT – IV: Nuclear Techniques**

#### **UNIT – I: Surface Chemistry**

**15 Hrs**

Structural and theoretical treatment of liquid interfaces, thermodynamics of binary system, Gibbs equation and verification of Gibbs equation by microtome method and tracer method, spreading of one liquid on another, states of monomolecular films, the surface area of solids, mixed films, Gibbs adsorption isotherm, the Langmuir adsorption isotherm, BET adsorption isotherm, estimation of surface area (BET equation, theoretical concept), adsorption time. Non equilibrium thermodynamics (entropy production in irreversible process), membrane transport in biochemical reactions.

#### **UNIT – II: Polymers - Basics and Characterization**

**15 Hrs**

##### **(A) Basic Concepts**

Monomers, repeat units, degree of polymerization, linear, branched and network polymers, classification of polymers.

##### **(B) Polymerization Methods**

Condensation, addition, radical chain, ionic and coordination, copolymerization, controlled free radical polymerization, viz. ATRP.

**(C) Average Molecular Weight Concepts**

Number, weight and viscosity average molecular weights, polydispersity and molecular weight distribution, measurement of molecular weight: end group, viscosity, light scattering, osmotic and ultracentrifugation methods.

**UNIT – III: X-Ray Techniques**

**15 Hrs**

**(A) X-ray Diffraction**

Bragg conditions, Miller Indices, Laue method, Bragg method, Description of procedure for Debye Scherrer method of X-ray structural analysis of crystals, Index reflections, identification of unit cells from systematic absences in diffraction pattern-structure of simple lattices and X-ray intensities-structure factor and its relation to intensity and electron density.

**(B) X-ray Fluorescence Spectroscopy**

Principle, energy dispersive X-ray fluorescence (EDXRF), wavelength dispersive X-ray fluorescence (WDXRF), applications.

**UNIT – IV: Nuclear Techniques**

**15 Hrs**

Basic concepts of nuclear chemistry, radioactive decay and equilibrium, nuclear reactions, Q value, cross sections, types of nuclear reactions; radioactive techniques: counting techniques such as G. M. ionization and proportional counter, isotopic dilution, neutron activation analysis, radiometric titration; radiopharmaceuticals: radioimmunoassay, immunoradiometric assay, classification of radiopharmaceuticals, labeled compounds preparation, PET studies.

**Books Suggested**

1. Physical methods in Chemistry, R. S. Drago (Saunders College).
2. Principles of Physical Chemistry by Samuel H. Maron and Carl F. Prutton. The Mac Millan Company, New York.
3. Advanced Physical Chemistry by GurudeepRaj, Goel Publishers House, Meerut.
4. An introduction to Electrochemistry-4th edn: By Samuel Glasstone Affiliated East West Press Pvt. Ltd., New Delhi.
5. Electrochemistry by M. S. Yadav Anmol Publications, New Delhi.
6. Essentials of Nuclear Chemistry, 4th Ed., 1995, H. J. Harnikar (Weily Eastern)
7. Electrochemistry by S. Glasstone.
8. Text Book of Polymer Science, F. W. Billmeyer, Jr. (Wiley Inter Science)
9. Polymer Chemistry, Gowarikar.

**35034: CHROMATOGRAPHY & MEDICINAL CHEMISTRY**

**UNIT – I: Chromatography**

**UNIT – II: Basic principles of Pharmacology**

**UNIT – III: Drug Design and Lead Modification**

**UNIT – IV: SAR and QSAR Studies**

**UNIT – I: Chromatography**

**15 Hrs**

Definition, classification, partition or distribution coefficient, partition ratio, efficiency, resolution, plate height, plate number, theories of chromatography: plate theory, rate theory, band broadening; principle and applications of paper chromatography, thin layer chromatography, column chromatography, size exclusion chromatography, ion exchange chromatography.

High Performance Liquid Chromatography (HPLC): Principle, Instrumentation and Applications.

Gas Chromatography (GC): Principle, Instrumentation, Detectors and Applications of GC.

## **UNIT – II: Basic Principles of Pharmacology**

**15 Hrs**

### **(A) Definitions**

Disease, drug, bioassay, pharmacokinetics and pharmacodynamics. Stages involved in drug discovery, Formulation, Drug dosing, Routes of drug administration.

### **(B) Pharmacokinetics**

Absorption, Distribution, Metabolism and Excretion of drugs (**ADME**), Bioavailability, Drug delivery.

### **(C) Pharmacodynamics**

Nature of drug – receptor interactions, Theories of drug action: Occupancy theory, Rate theory, Induced-fit theory, and Macromolecular perturbation theory. Drug synergism and antagonism, drug toxicity, clinical trials.

## **UNIT – III: Drug Design and Lead Modification**

**15 Hrs**

### **(A) Drug design**

Lead discovery, Existing drugs as leads (me too drugs), Pharmacophore, Principles of design of agonists, antagonists and enzyme inhibitors, Design of salbutamol, cimetidine and captopril. Drug discovery without lead – serendipity- Penicillin and Librium as examples.

### **(B) Lead modification strategie**

Bioisosterism, variation of alkyl substituents, chain homologation and branching, variation of aromatic substituents, extension of structure, ring expansion and ring contraction, ring variation, variation and position of hetero atoms, ring fusion, simplification of the lead, rigidification of lead. Discovery of oxaminquine.

## **UNIT – IV: SAR and QSAR Studies**

**15 Hrs**

### **(A) Structure-Activity Relationship (SAR) studies**

SAR in sulfa drugs, benzodiazepines and taxol analogs; Structure pruning techniques with morphine as example, principles of prodrug design.

### **(B) Quantitative Structure-Activity Relationship (QSAR)**

Introduction to QSAR, physicochemical properties – lipophilicity: partition coefficient (P) and the lipophilicity substituent constant ( $\pi$ ), electronic effects: Hammett constants ( $\sigma$ ), steric effects: Taft's constant ( $E_s$ ), Hansch analysis, Craig's plot, Topliss scheme, Free Wilson approach, Lipinski rule of five.

### **Books Suggested**

1. Physical and Chemical Methods of Separation, E. W. Berg (McGraw Hill).
2. Separation Process Principles, J. D. Seader and E. J. Henley (John Wiley & Sons Inc).
3. Instrumental Methods of Analysis, H. W. Willard, L. L. Merritt and J. A. Dean (Affiliated East-West)
4. Vogel's Text Book of Quantitative Chemical Analysis, J. Mendham, R. C. Denney, J. D. Barnes and M. J. Thomas, 4<sup>th</sup> & 6<sup>th</sup> Ed. (Pearson Education Asia).
5. Principles of Instrumental Analysis, D. A. Skoog and D. M. West (Holt, Rinehart and Wilson)
6. Medicinal Chemistry and Pharmaceutical Chemistry, H. Singh and Kaur.
7. An Introduction to Medicinal Chemistry, 4<sup>th</sup> Ed., G. L. Patrik.
8. Biochemical Approach to Medicinal Chemistry, Thomas Nogrady.
9. Principles of Medicinal Chemistry, William Foye.
10. Medicinal Chemistry, Ashutosh Kar.
11. Medicinal chemistry An introduction by Garreth Thomas.
12. Berger's Medicinal Chemistry, Vols. 1-5, Manfred E. Wolf.

### 35031P: Multistep Synthesis of Organic Compounds:

1. Benzanilide from Benzophenone  
Benzophenone  $\rightarrow$  Benzophenoneoxime  $\rightarrow$  Benzanilide
2. Benzilic acid from benzoin  
Benzoin  $\rightarrow$  Benzil  $\rightarrow$  Benzilic acid
3. *p*-Bromoaniline from Aniline  
Aniline  $\rightarrow$  Acetanilide  $\rightarrow$  *p*-Bromoacetanilide  $\rightarrow$  *p*-Bromoaniline
4. Symmetrical Tribromo Benzene from aniline:  
Aniline  $\rightarrow$  Tribromoaniline  $\rightarrow$  Tribromobenzene
5. Flavone from *o*-hydroxy acetophenone  
*o*-hydroxy acetophenone  $\rightarrow$  *o*-benzoyl acetophenone  $\rightarrow$  *o*-hydroxy- dibenzoylmethane  $\rightarrow$  Flavone
6. 2-phenylindole from phenylhydrazine  
Acetophenone + phenylhydrazine  $\rightarrow$  acetophenone phenylhydrazone  $\rightarrow$  2-phenylindole
7. 3-(2-aminothiazol-4-yl)-2H-chromen-2-one from 2-hydroxybenzaldehyde and ethyl acetoacetate  
2-hydroxybenzaldehyde + ethyl acetoacetate  $\rightarrow$  3-acetyl-2H-chromen-2-one  $\rightarrow$  3-(2-bromoacetyl)-2H-chromen-2-one  $\rightarrow$  3-(2-aminothiazol-4-yl)-2H-chromen-2-one  
(or)  
2-hydroxybenzaldehyde + ethyl acetoacetate  $\rightarrow$  3-acetyl-2H-chromen-2-one  $\rightarrow$  3-(2-aminothiazol-4-yl)-2H-chromen-2-one

### 35032P: Spectral Identification of Organic Compounds (UV, IR, $^1\text{H}$ - and $^{13}\text{C}$ - NMR and Mass)

1. Composite spectral problems in three modes, 10 examples in each mode

#### Books Suggested

1. Modern Organic Synthesis in the Laboratory *A Collection of Standard Experimental Procedures*, Jie Jack Li, Chris Limberakis, Derek A. Pflum
2. Practical organic chemistry by Mann & Saunders
3. Text book of practical organic chemistry by Vogel
4. Spectrometric Identification of organic compounds, R.M. Silverstein, F.X. Webster and D.J. Kiemle, 7<sup>th</sup> Ed., (Wiley).

### 35031N: DRUG DISCOVERY, DESIGN AND DEVELOPMENT

UNIT – I: Basic Principles of Pharmacology

UNIT – II: Lead Discovery and Optimization

UNIT – III: SAR and QSAR Studies

UNIT – IV: Common Drugs

UNIT – I: Basic Principles of Pharmacology

15 Hrs

**Definitions:** disease, drug, bioassay, pharmacokinetics and pharmacodynamics, stages involved in drug discovery, formulation, drug dosing, routes of drug administration,

**Pharmacokinetics:** absorption, distribution, metabolism and excretion of drugs (ADME), drug delivery.

**Pharmacodynamics:** nature of drug - receptor interactions, theories of drug action: occupancy theory, rate theory, induced-fit theory, macromolecular perturbation theory.  
Drug synergism and antagonism, drug toxicity, clinical trials.

#### **UNIT – II: Lead Discovery and Optimization**

**15 Hrs**

**Lead discovery:** existing drugs as leads (me too drugs), pharmacophore. Principles of design of agonists e.g. salbutamol, antagonists e.g. cimetidine and enzyme inhibitors e.g. captopril. Drug discovery without lead – serendipity-penicillin and librium as examples.

**Lead optimization:** Bioisosterism, variation of alkyl substituents, chain homologation and branching, variation of aromatic substituents, extension of structure, ring expansion and ring contraction, ring variation, variation and position of hetero atoms, ring fusion, simplification of the lead, rigidification of lead, conformational blockers, discovery of oxamniquine.

#### **UNIT – III: SAR and QSAR Studies**

**15 Hrs**

**Structure Activity relationship (SAR):** SAR in sulfa drugs, benzodiazepines, and taxol analogs, principles of prodrug design

**Quantitative Structure Activity relationship (QSAR):** Introduction to QSAR, physicochemical properties – lipophilicity: partition coefficient (P) and the lipophilicity substituent constant ( $\pi$ ), electronic effects: Hammett constant ( $\sigma$ ), steric effects: Taft's constant ( $E_s$ ), Hansch analysis, Craig's plot, Topliss scheme, free Wilson approach, Lipinski rule of five.

#### **UNIT – IV: Common Drugs**

**15 Hrs**

Structure, uses, mechanism of action of antibacterial agents: sulfamethoxazole, penicillin G, antiviral agents: acyclovir, indinavir, anticancer agents: mechlorethamine, methotrexate, antifungal agents: fluconazole, griseofulvin, gastrointestinal agents: ranitidine, omeprazole, metoclopramide, cardiovascular agents: amrinone, procainamide, captopril, propranolol, methyl dopa, anticoagulants: warfarin, central nervous system agents: paracetamol, betamethasone, chlorpromazine, levodopa, diazepam, phenytoin, procaine.

#### **Books Suggested**

1. Medicinal Chemistry and Pharmaceutical Chemistry, H. Singh and Kaur.
2. An Introduction to Medicinal Chemistry, 4<sup>th</sup> Ed., G. L. Patrik.
3. Fundamentals of Medicinal Chemistry, Gareth Thomas.
4. Biochemical Approach to Medicinal Chemistry, Thomas Nogrady.
5. Principles of Medicinal Chemistry, William Foye.
6. Medicinal Chemistry, Ashutosh Kar.
7. Medicinal Chemistry, R. R. Nadendla.
8. Berger's Medicinal Chemistry, Vols. 1-5, Manfred E. Wolf.



## FOURTH SEMESTER

### 45031: REAGENTS IN ORGANIC SYNTHESIS

#### UNIT – I: Oxidations

#### UNIT – II: Reductions

#### UNIT – III: Non-Metallic Reagents in Organic Synthesis

#### UNIT – IV: Metallic Reagents in Organic Synthesis

#### UNIT – I: Oxidations

15 Hrs

- (a) Alcohols to carbonyls: Chromium (VI) Oxidants: dimethyl sulfoxide oxidation, periodate oxidation, Oppenauer oxidation, oxidation with manganese dioxide, DDQ, oxidation with silver carbonate.
- (b) Alkenes to epoxide: peroxide induced epoxidations.
- (c) Alkenes to diols: oxidation with potassium permanganate, osmium tetroxide, Prévost oxidation, Woodward modification.
- (d) Oxidation of alkyl or alkenyl fragments: selenium dioxide.

#### UNIT – II: Reductions

15 Hrs

- (a) Nucleophilic metal hydrides:  $\text{LiAlH}_4$ ,  $\text{NaBH}_4$ , Red-Al and alkoxy aluminates.
- (b) Electrophilic metal hydrides:  $\text{BH}_3$ ,  $\text{AlH}_3$  and DIBAL.
- (c) Non-metallic reductions: Diimide reduction and Wolf-Kishner reduction.
- (d) Dissolving metal reductions: Birch reduction and Clemmensen reduction.
- (e) Heterogeneous catalytic hydrogenations.

#### UNIT – III: Non-Metallic Reagents in Organic Synthesis

15 Hrs

Electronic structure and bonding in Boron, Phosphorus and Sulphur compounds – Their reactivity and applications in Organic Synthesis.

##### (A) Boron Reagents

Organoboranes in the formation of C-C bonds, alcohols, amines, halogen and carbonyl compounds, Free radical reactions of Organoboranes: simple boranes and hindered boranes.

##### (B) Phosphorus Reagents

Formation of C-C double bonds (Wittig reaction, Horner-Wordsworth-Emmons reaction), Functional group transformations, Reactivity as electrophiles and nucleophiles.

##### (C) Sulphur Reagents

Sulphur ylides: stabilized and non-stabilized, Preparation and reactivity, sulphonylcarbanions.

##### (D) Silicon reagents

Reactions involving  $\beta$ -carbocations and  $\alpha$ -carbanions, utility of trimethylsilyl halides, cyanides and triflates.

#### UNIT– IV: Metallic Reagents in Organic Synthesis

15Hrs

##### (A) Organometallic Reagents:

Grignard reagents, organolithium, organozinc, organocopper and organonickel reagents in Organic synthesis.

##### (B) Metal Mediated Cross-Coupling Reactions:

Suzuki, Heck, Stille, Sonogishira, Buchwald-Hartwig and Negishi-Kumada coupling reactions.

**Books Suggested:**

1. Modern Synthetic Reactions, H. O. House, 2<sup>nd</sup> Ed., (W.A. Benjamin)
2. Modern Methods of Organic Synthesis, W. Carruthers, 3<sup>rd</sup> Ed., (Cambridge University Press).
3. Principles of Organic Synthesis, R. O. C. Norman and J. M. Coxon, (Blakie Academic and Professional).  
Advanced Organic Chemistry: Part A & B, F. A Carey and R. J. Sundberg, 5<sup>th</sup> Ed., Springer, 2007.
4. Guide book to Organic Synthesis, R. K. Machie and D.N.Smith, (ELBS).
5. Principles of organometallic chemistry, P.Powell, (ELBS).
6. Organo transition metal chemistry-Applications to organic synthesis, S.G.Davis, Pergmon.
7. Multi-component Reactions: J. Zhu and H. Bienaymé (Wiley-VCH).
8. Strategies for organic drug synthesis and design By Daniel Lednicher.

**45032: DESIGNING OF ORGANIC SYNTHESIS****UNIT – I: Basics of Organic Synthesis and Disconnection Approach – I****UNIT – II: Disconnection Approach – II****UNIT – III: Disconnection Approach – III and Other Synthetic Strategies****UNIT – IV: Methods in Organic Synthesis****UNIT – I: Basics of Organic Synthesis and Disconnection Approach - I****15 Hrs****(A) Basics in Organic Synthesis**

Classification of organic reactions; carbon-carbon single bond formation reactions; carbon-carbon double bond formation reactions; functionalization; functional group interconversion; organic synthesis: reason for organic synthesis and total (complete), partial (semi), formal, linear and convergent synthesis; introduction to synthetic strategies.

**(B) Disconnection Approach - I**

**(i) Introduction:** Terminology: retrosynthetic analysis (disconnection approach), target, synthon, synthetic equivalent (reagent), functional group interconversion (FGI), functional group addition (FGA), functional group elimination (removal); synthesis of aromatic compounds: benzocaine, *p*-methoxytoluene, BHT, isobutylbenzene, trifluralin B, phenols, saccharine and *o*-cyanotoluene.

**(ii) Protecting groups:** Introduction and protective groups for phenols and alcohols, amines, ketones and aldehydes and carboxylic acids.

**UNIT – II: Disconnection Approach – II****15 Hrs**

**(a)** Importance of order of events; one group C-X disconnections; chemoselectivity; two group C-X disconnections; reversal of polarity (umpolung); cyclization reactions.

**(b)** One group C-C disconnections – synthesis of alcohols and carbonyl compounds; regioselectivity; olefin synthesis; use of alkynes in synthesis.

**(c)** Two group C-C disconnections: Diels-Alder reaction; 1,3-difunctionalized compounds – 1,3-dicarbonyl,  $\beta$ -hydroxy carbonyl and  $\alpha,\beta$ -unsaturated compounds, 1,5-dicarbonyl compounds – Michael addition and Robinson annulation, synthesis 1,2- and 1,4-dicarbonyl compounds – reconnection.

**UNIT – III: Disconnection Approach – III and Other Synthetic Strategies****15 Hrs****(A) Disconnection Approach - III**

General strategy; retrosynthetic analysis of target molecules: simple targets – ibogamine, salbutamol, propoxycaine, ibuprofen and dinocap, complex targets - longifolene, (+)-disparlure and penicillin V.

**(B) Other approaches to Synthetic Strategies**

- (i) Biomimetic approach: introduction, Robinson's tropinone synthesis, Johnson polyene cyclization
- (ii) Chiral template approach: introduction, synthesis of reserpine
- (iii) Retro-mass spectral approach – introduction, Kametani's mass spectral analysis of tetrahydroisoquinoline alkaloids.

**UNIT – IV: Methods in Organic Synthesis****15 Hrs**

Enamines – Introduction, generation, Stork enamine reaction, applications of enamines in organic synthesis; Multi component reactions (MCR) – Introduction, Strecker synthesis, Ugi reaction, Mannich reaction, Biginelli reaction, and Hantzsch synthesis; Tandem Synthesis – Definition, advantages, polyene cationic cyclizations, conjugate addition-aldol reaction, Mannich-cation olefin cyclization, Knoevenagel-hetero-Diels-Alder reaction.

**Books Suggested:**

1. Designing Organic Syntheses: A Programmed Introduction to the Synthon Approach, S. Warren, John Wiley & Sons.
2. Organic Synthesis: Strategy and Control, P. Wyatt and S. Warren, John Wiley & Sons.
3. Organic Synthesis: The Disconnection Approach, 1<sup>st</sup> & 2<sup>nd</sup> Ed.s, S. Warren and P. Wyatt, John Wiley & Sons.
4. Organic Synthesis: Concept, Methods and Starting Materials, J. Fuhrhop and G. Perzillin, (Verlage VCH) 2<sup>nd</sup> Ed., 1994.
5. Organic Synthesis, M. B. Smith, 4<sup>th</sup> Ed., Elsevier, 2017.
6. Advanced Organic Chemistry: Part A & B, F. A Carey and R. J. Sundberg, 5<sup>th</sup> Ed., Springer, 2007.
7. Some Modern Methods of Organic Synthesis, W. Carruthers, 3<sup>rd</sup> Ed., (Cambridge Univ. Press).
8. Introduction to Strategies for Organic Synthesis, L. S. Starkey, John Wiley & Sons, 2012.
9. Organic Chemistry, Paula Yurkanis Bruice, 4<sup>th</sup> Ed. (Printice Hall).
10. Modern Synthetic Reactions, H. O. House, 2<sup>nd</sup> Ed., (W.A. Benjamin).
11. Multi-component Reactions: J. Zhu and H. Bienaymé (Wiley-VCH).

**45033: CHEMISTRY OF HETEROCYCLIC COMPOUNDS****UNIT – I: Nomenclature, Aromaticity and Reactivity of Heterocyclic Compounds****UNIT – II: Three- and Four-membered Heterocyclic Compounds****UNIT – III: Five-membered Heterocyclic Compounds with Two Heteroatoms****UNIT – IV: Benzofused Five- and Six-membered Heterocyclic Compounds****UNIT – I: Nomenclature, Aromaticity and Reactivity of Heterocyclic Compounds****15 Hrs****(A) Nomenclature of Heterocycles**

Systematic nomenclature (Hantzsch-Widman system); trivial system; fusion nomenclature system; replacement nomenclature system; Monocyclic heterocycles, fused heterocycles, spiroheterocycles; bridged heterocycles; bicyclic systems; polycyclic systems; heterocyclic ring assemblies.

**(B) Aromaticity of Heterocycles**

Chemical behavior of aromatic heterocycles; five and six-membered aromatic heterocycles and mixed aromatic heterocycles; relationship with carbocyclic aromatic compounds; criteria of aromaticity in heterocycles; structural and electronic criteria.

**(C) Reactivity of Heteroaromatics**

Selectivity and reactivity of heteroaromatic rings: five- and six-membered heterocyclic system.

**UNIT – II: Three- and Four-membered Heterocyclic Compounds****15 Hrs**

**(A) Three-membered Heterocycles**

Synthesis and chemical reactivity of aziridines, oxiranes, oxaziridines and thiiranes.

**(B) Four-membered Heterocycles**

Synthesis and chemical reactivity of azetidines, azetidinones ( $\beta$ -lactams), oxetanes, oxetanones ( $\beta$ -lactones) and thietanes.

**UNI – III: Five-membered Heterocyclic Compounds with Two Heteroatoms**

**15 Hrs**

Synthesis, chemical reactivity and medicinal applications of pyrazoles, imidazoles, oxazoles, isoxazoles, thiazoles and isothiazoles.

**UNIT – IV: Benzofused Five- and Six-membered Heterocyclic Compounds**

**15 Hrs**

**(A) Benzofused Five Membered Heterocycles**

Synthesis, chemical reactivity and medicinal applications of benzopyrroles, benzofurans, bezothiophenes and benzimidazoles.

**(B) Benzofused Six Membered Heterocycles**

Synthesis, chemical reactivity and medicinal applications of quinolines and Isoquinolines.

**Books Suggested:**

1. Heterocyclic Chemistry Vol.1-3, R. R. Gupta, M. Kumar and V. Gupta, Springer Verlag
2. The Chemistry of Heterocycles, T. Eicher and S. Hauptmann, Thieme
3. Heterocyclic Chemistry, J.A.Joule, K. Mills and G. F. Smith, Chapman and Hall
4. Heterocyclic Chemistry, T.L.Gilchrist, Longman Scientific Technical
5. Heterocyclic Chemistry, Raj.K. Bansal.
6. An Introduction to the Heterocyclic Compounds, R. M. Acheson, John Wiley.
7. Comprehensive Heterocyclic Chemistry, A. R. Katritzky and C. W. Rees, eds., Pergamon Press
8. Principles of Modern Heterocyclic Chemistry, L. A. Paquette.
9. Enzyme structure and mechanism by Fersht and Freeman.
10. Bio-Organic chemistry by Hengan Dugas
11. Nucleic acids in Chemistry and Biology by G M Blackburn MI Gait
12. Lehninger Principles of Biochemistry by D L Nelson and M M Cox.

**45034: CHEMISTRY OF NATURAL PRODUCTS**

**UNIT – I: Terpenoids**

**UNIT – II: Alkaloids**

**UNIT – III: Steroids and Prostaglandins**

**UNIT – IV: Flavonoids and Isoflavonoids**

**UNIT – I: Terpenoids**

**15 Hrs**

Occurrence, isolation, general methods of structure determination, isoprene rule; structure determination, stereochemistry, biosynthesis and synthesis of camphor, farnesol, zingiberene, cadinene, abietic acid and lanosterol.

**UNIT – II: Steroids and Prostaglandins**

**15 Hrs**

**(A) Steroids**

Occurrence, nomenclature, basic skeleton, Diel's hydrocarbon and stereochemistry of steroids; isolation, structure determination of cholesterol, structure determination and synthesis of androsterone, testosterone, estrone and progesterone, biosynthesis of steroids.

**(B) Prostaglandins**

Occurrence, nomenclature, classification, biogenesis, physiological effects and synthesis of PGE<sub>2</sub> and PGF<sub>2</sub>.

**UNIT – II: Alkaloids**

**15 Hrs**

Introduction, isolation, general methods of structural elucidation and physiological action, degradation, classification based on nitrogen heterocyclic ring, structural elucidation, stereochemistry and synthesis of morphine, papaverine and reserpine, biosynthesis of alkaloids.

**UNIT – IV: Flavonoids and Isoflavonoids**

**15 Hrs**

Occurrence, nomenclature and general methods of structure determination; isolation, structure elucidation and synthesis of apigenin, luteolin, kaempferol, quercetin, and daidzein; biosynthesis of flavonoids and Isoflavonoids: acetate pathway and shikimic acid pathway.

**Books Suggested**

1. Natural Products: Chemistry and Biological Significance, J. Mann, R.S.Davidson, J. B. Hobbs, D. V. Banthrope and J. B. Hatrbnome, Longman, Essex.
2. Organic Chemistry, Vol. 2, I. L. Finar, ELBS.
3. Chemistry of Organic Natural Products, O. P. Agrawal, Vols. 1 &2, Goel Pubs.
4. Natural Products Chemistry K. B. G. torssell, John Wiley, 1983
5. New Trends in Natural Products Chemistry, Atta-ur-Rahman and M.I.Choudhary, Harwood Academic Publisher.
6. Chemistry of Natural products P. S. Kalsi, Kalyani Publishers
7. Biosynthesis of steroids, terpenes and acetogenins, J. H. Richards & J. R. Hendrieson
8. The biosynthesis of secondary metabolites, R. D. Herbert, Chapman & Hall
9. The Biosynthesis of Secondary Metabolite, R. D. Herbert, Second edn, Chapman and Hall 1984

**45031P: Project Work**

Students must do a research based project and submit a dissertation for evaluation. Further, a final presentation of dissertation work need to be conducted.