



# TUMKUR UNIVERSITY

## FACULTY OF SCIENCE AND TECHNOLOGY

1. **Name of the Course:** **M.Sc., Organic Chemistry**
2. **Duration of the Course:** **Two years (FOUR SEMESTERS, CBCS)**
3. **Eligibility:** A candidate must have secured 40% marks in the aggregate and studied chemistry (Cognate subject) securing 50% marks in the subject at the B.Sc. level.
4. **Admission:** As per University CBCS regulations.

### I Semester

Sl. No.	Paper	Title of the paper	Instruction Hours per Week	No. of Credits	Duration of Exam	Marks		
						Internal Assessment	Semester End Exam	Total Marks
1	CPT-1.1	Organic Chemistry-I	4	4	3Hrs	30	70	100
2	CPT-1.2	Inorganic Chemistry-I	4	4	3Hrs	30	70	100
3	CPT-1.3	Physical Chemistry-I	4	4	3Hrs	30	70	100
4	SPT-1.4.A	Medicinal Chemistry-I	4	4	3Hrs	30	70	100
	SPT-1.4.B	Green Synthesis	4	4	3Hrs	30	70	100
5	CPP-1.5 (1.1)	Practical: Organic Chemistry-1.1	4	2	4Hrs	15	35	50
6	CPP-1.6 (1.2)	Practical: Inorganic Chemistry	4	2	4Hrs	15	35	50
7	CPP-1.7 (1.3)	Practical: Physical Chemistry	4	2	4Hrs	15	35	50
8	SPP – 1.8.1 (1.4A)	Practical: Organic Chemistry – 1.8.1	4	2	4Hrs	15	35	50
	SPP – 1.8.2 (1.4B)	Practical: Organic Chemistry – 1.8.2	4	2	4Hrs	15	35	50
<b>Total Marks/Credits</b>			<b>32</b>	<b>24</b>				<b>600</b>

CPT: Core Paper Theory, CPP: CORE Paper Practical, SPT: Special Paper Theory, SPP: Special Paper Practical

**II Semester**

Sl. No.	Paper	Title of the paper	Instruction Hours per Week	No. of Credits	Duration of Exam	Marks		
						Internal Assessment	Semester End Exam	Total Marks
1	CPT- 2.1	Inorganic Chemistry-II	4	4	3Hrs	30	70	100
2	CPT- 2.2	Physical Chemistry-II	4	4	3Hrs	30	70	100
3	SPT- 2.3A	Organic Reactions & Rearrangements	4	4	3Hrs	30	70	100
	SPT- 2.3B	Group Theory & General Spectroscopy – I	4	4	3Hrs	30	70	100
4	OET – 2.4	Chemistry of Foods-I	4	4	3Hrs	30	70	100
5	CPP-2.5 (2.1)	Practical: Inorganic Chemistry	4	2	4Hrs	15	35	50
6	CPP-2.6 (2.2)	Practical: Physical Chemistry	4	2	4Hrs	15	35	50
7	SPP-2.7.1 (2.3A)	Practical: Organic Chemistry-2.7.1	4	2	4Hrs	15	35	50
	SPP-2.7.2 (2.3B)	Practical: Organic Chemistry-2.7.2	4	2	4Hrs	15	35	50
8	OEP 2.8 (2.4)	Practical: Chemistry of Foods – I	4	2	4Hrs	15	35	50
<b>Total Marks/Credits</b>			<b>32</b>	<b>24</b>				<b>600</b>

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Open Elective Theory, OEP: Open Elective Practical

## III Semester

Sl. No.	Paper	Title of the paper	Instruction Hours per Week	No. of Credits	Duration of Exam	Marks		
						Internal Assessment	Semester End Exam	Total Marks
1	CPT- 3.1	Reaction Mechanisms, Pericyclic Reactions and Biochemical Mechanisms	4	4	3Hrs	30	70	100
2	CPT- 3.2	Chemistry of Natural Products	4	4	3Hrs	30	70	100
3	SPT- 3.3A	Organic Synthesis	4	4	3Hrs	30	70	100
	SPT- 3.3B	Organic Photochemistry	4	4	3Hrs	30	70	100
4	OET – 3.4	Chemistry of Foods-II	4	4	3Hrs	30	70	100
5	CPP-3.5 (3.1)	Practical: Organic Chemistry-3.1	4	2	4Hrs	15	35	50
6	CPP-3.6 (3.2)	Practical: Organic Chemistry-3.2	4	2	4Hrs	15	35	50
7	SPP-3.7.1 (3.3A)	Practical: Organic Chemistry – 3.7.1	4	2	4Hrs	15	35	50
	SPP-3.7.2 (3.3B)	Practical: Organic Chemistry – 3.7.2	4	2	4Hrs	15	35	50
8	OEP-3.8 (3.4)	Practical: Chemistry of Foods – II	4	2	4Hrs	15	35	50
<b>Total Marks/Credits</b>			<b>32</b>	<b>24</b>				<b>600</b>

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Open Elective Theory, OEP: Open Elective Practical

## IV Semester

Sl. No.	Paper	Title of the paper	Instruction Hours per Week	No. of Credits	Duration of Exam	Marks		
						Internal Assessment	Semester End Exam	Total Marks
1	CPT- 4.1	Organometallic and Heterocyclic Chemistry	4	4	3Hrs	30	70	100
2	CPT- 4.2	Stereochemistry and Retrosynthetic Analysis	4	4	3Hrs	30	70	100
3	SPT- 4.3A	Organic Spectroscopy - II	4	4	3Hrs	30	70	100
	SPT -4.3B	Medicinal Chemistry - II	4	4	3Hrs	30	70	100
4	CPD-4.4	Practical: Core paper dissertation	4	2	-	30	70	100
5	CPP-4.5 (4.1)	Practical: Organic Chemistry-4.1	4	2	4Hrs	15	35	50
6	CPP- 4.6 (4.2)	Practical: Organic Chemistry-4.2	4	2	4Hrs	15	35	50
7	SPP-4.7(4.3A/B)	Practical: Organic Chemistry-4.7	4	2	4Hrs	15	35	50
	Project 4.8 -CPDP	Core paper dissertation Practical and Viva voce - 4.8	4	2	-	15	35	50
8	<b>Total Marks/Credits</b>	<b>32</b>	<b>24</b>	<b>24</b>				<b>600</b>

Dissertation guidance can be treated as 4 hours of Practical work per week.

CPT: Core Paper Theory, CPP: CORE Paper Practical, SPT: Special Paper Theory, SPP: Special Paper Practical, CPD – Core paper dissertation, CPDP – Core paper dissertation Practical

**Basis for Theory Internal Assessment Marks Allotment**

1 <sup>st</sup> Test for 10 marks	
2 <sup>nd</sup> Test for 10 marks: Average of two tests	: 10
Seminar	: 05
Attendance	: 05
Extra Curricular Activities	: 05
Industry or Institute visit/Extension activities	: 05
<b>Total</b>	<b>: 30 M</b>

**Attendance %**

96-100%-5 M
91-95%- 4 M
86-90%- 3 M
81-85%- 2 M
76-80%- 1 M
< 75%- 0 M

**Basis for Practical Internal Assessment Marks Allotment**

Attendance	: 05
Records	: 05
Viva/Model Preparation/Etc.	: 05
<b>Total</b>	<b>: 15</b>

**THEORY QUESTION PAPER PATTERN****M.Sc. Organic Chemistry (CBCS Scheme)****Note: Answer Question nos. 1 & 2 and any THREE of the remaining.****Max. Marks = 70**

1. Answer the following questions 8 X 2 = 16
- (a)
  - (b)
  - (c)
  - (d)
  - (e)
  - (f)
  - (g)
  - (h)
2. Write short notes on any THREE of the following 3 X 4 = 12
- (a)
  - (b)
  - (c)
  - (d)
3. 6+4+4=14
- (a)
  - (b)
  - (c)
4. 6+4+4=14
- (a)
  - (b)
  - (c)
5. 6+4+4=14
- (a)
  - (b)
  - (c)
6. 6+4+4=14
- (a)
  - (b)
  - (c)

**\*Note: Equal weightage be given to each unit while preparing question paper.**

**PRACTICAL QUESTION PAPER PATTERN****Max. Marks = 35**

1.	Experiment/Spotting	30
2.	Viva-voce	05
	<b>Total</b>	<b>35 Marks</b>

**Chairman**  
**BOS in Organic Chemistry**

**CPT-1.1: ORGANIC CHEMISTRY- I****64 Hours****UNIT-I****16h****Reaction Mechanisms-I**

Generation, structure, stability and reactivity of carbocations, carbanions, carbon free radicals, carbenes, nitrenes, nitrogen, phosphorus and sulfur ylides. Nitrile oxides and nitrile imines. Generation and reactivity of singlet and triplet oxygen. Classification of reactions and mechanisms. Thermodynamic and kinetic requirements, kinetic and thermodynamic control, Hammond postulate, Curtin-Hammett principle. Potential energy diagrams, transition states and intermediates.

Aromaticity. Huckel's rule of Aromaticity. Aromatic systems with electron numbers other than six (including azulene, tropone, tropolone and annulenes). Antiaromaticity. Aromaticity in benzenoids, meso-ionic compounds. Homo-aromaticity.

Acids and bases: Hard and soft acids and bases. Effect of structure on the strengths of acids and bases.

**UNIT-II****16h****Reaction Mechanisms-II**

Effect of structure on reactivity: Resonance, field effects and steric effects. The Hammett equation and linear free energy relationship, substituent and reaction constants. Taft equation. Nucleophilic substitution reaction at a saturated carbon: SN1, SN2, SN2i, SN1i, SNi and SET reaction mechanisms. Effect of substrate structure, attacking nucleophile, leaving group. Ambident nucleophiles and substrates. Methods of determining mechanisms: Based on the structure of products, determination of the presence of intermediates, isotopic labeling, isotope effects, cross over experiments and from stereo chemical evidences.

Mechanism and stereochemistry of eliminations-E1, E2, E1cb mechanism, cis-elimination, Hoffmann and Saytzeff eliminations, competition between elimination and substitution, Chugaev reaction.

**UNIT-III****16 h****Stereochemistry-I**

Fischer, Newman, Sawhorse and flying wedge projections and their interconversions.

Optical isomerism: Elements of symmetry and chirality. D-L conventions. CIP rules, R-S and M-P conventions. Chirality in compounds with a stereogenic centre, allenes, biphenyls, alkylidene cycloalkanes, hemispiranes and spiranes (with a stereogenic axis). Cram's and Prelog's rules.

Conformational analysis: Conformational analysis of cycloalkanes, cyclobutane, cyclopentane, cyclohexane (monosubstituted e.g., methyl, *iso*-propyl, *tert*-butyl and disubstituted cyclohexanes e.g., dialkyl, dihalo, diols), and cycloheptane. Effect of conformation on reactivity.

**UNIT-IV****16h****Stereochemistry-II**

Nomenclature and conformations of fused rings and bridged ring systems.

Prochirality: Enantiotopic and diastereotopic atoms, groups and faces.

Stereospecific and Stereoselective Synthesis: Regiospecific, Regioselective and Enantioselective synthesis.

Stereochemistry of nucleophilic substitution reactions: SN<sup>1</sup> and SN<sup>2</sup> reactions, elimination reactions: anti elimination, syn elimination, and stereoelectronic factors and addition reactions and influence of Markovnikov Orientation on stereochemical studies.

Stereoselectivity in cyclic compounds, enantio-selectivity, diastereo-selectivity, enantiomeric and diastereomeric excess, stereoselective aldol reactions. Asymmetric synthesis, use of chiral auxiliaries, chiral reagents and catalysts, asymmetric hydrogenation, asymmetric epoxidation and asymmetric dihydroxylation.

Stereochemistry of six membered rings. Determination of stereochemistry organic compounds using NMR.

**Reference Books**

1. Advanced Organic Chemistry Reactions, Mechanism and Structure, Jerry March, John Wiley
2. Advanced Organic Chemistry, F A Carey and R J Sundberg Plenum, (1990).
3. A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, Longman, (2000).
4. Structure and mechanism of Organic Chemistry, C K Ingold, Cornell University Press
5. Organic Chemistry, R T Morrison and R N Boyd, Prentice-Hall, (1998).
6. Modern Organic Reactions, H O House, Benjamin, (1972).
7. Principles of Organic Synthesis, R O C Norman and J M Coxon, Blackie Academic and Professional, (1996).
8. Stereochemistry of Organic Compounds, D Nasipuri, New-Age International, (1999).
9. Stereochemistry of Carbon Compounds, E L Eliel, S H Wilen and L N Mander, John Wiley, (1994).
10. Stereochemistry, Potapov, MIR, Moscow, 1984.
11. Stereochemistry of carbon compounds - E. L. Eliel
12. Stereochemistry of carbon compounds - E. L. Eliel and S. H. Wilen
13. Organic Chemistry – J. Clayden, N. Greeves, S. Warren and P. Wothers 1st. Ed.
14. Stereochemistry of organic compounds – Nasipuri
15. Stereochemistry of organic compounds-Kalsi
16. Organic stereochemistry – Jagdamba Singh



**CPT-1.2 INORGANIC CHEMISTRY – I****64 Hours****UNIT-I****16h**

**Chemical Bonding:-** VSEPR model, shapes of molecules- $\text{ClF}_3$ ,  $\text{ICl}_4^-$ ,  $\text{TeF}_5^-$ ,  $\text{I}_3^-$ ,  $\text{TeCl}_6^{2-}$ ,  $\text{XeF}_6$ ,  $\text{SbCl}_6^{3-}$ ,  $\text{IF}_7$ ,  $\text{ReF}_7$ ,  $\text{XeF}_8^{2-}$ ,  $\text{TaF}_8^{3-}$ ; Bent rules and energetics of hybridization; electronegativity and partial ionic character; Bonds- Multicenter, Synergic and Agostic bonding. Lattice energy: Born-Landé equation, Kapustinskii equation; polarizability and partial covalent character, radius-ratio rules, structures of simple solids, Zintl- isoelectronic relationship in solids. Molecular orbital theory: LCAO and MO diagrams of heteronuclear diatomic ( $\text{CO}$ ,  $\text{NO}$ ,  $\text{HF}$ ,  $\text{ICl}$ ) and triatomic molecules ( $\text{CO}_2$  and  $\text{NO}_2^-$ ).

**UNIT-II****16h**

**Chemistry of main group elements-** Structure and bonding in boranes, carboranes, metallocarboranes, Wade's rules, borazines, phosphazenes, S, N- compounds. **Silicates-** Classification, structures, isomorphous replacement, pyroxenes, layered and vitreous silicates, zeolites and molecular sieves.

**UNIT-III****16h**

**HSAB concept:** Basis of HSAB concept, acid-base strength, hardness and softness, symbiosis, applications of HSAB concept; Acid- base concept in non-aqueous media, reactions in  $\text{BrF}_3$ ,  $\text{N}_2\text{O}_4$ , anhydrous  $\text{H}_2\text{SO}_4$ ,  $\text{CH}_3\text{COOH}$ . Isopoly and heteropoly acids of W, Mo and V; preparations, properties, structure and applications.

**Stereoisomerism-** Chirality, optical activity- CD, ORD, Cotton effect, absolute configuration of metal complexes, magnetic circular dichroism.

**UNIT-IV****16h**

**Lanthanide series:** Review on electronic structure, oxidation states, spectral and magnetic properties, lanthanide contraction, abundance and extraction. Lanthanides as shift reagents.

**Separation of lanthanides:** Solvent extraction and ion-exchange. Chemical properties of compounds of lanthanides in II, III, and IV oxidation states.

**Actinides:** Review on Electronic structure and position in the periodic table, oxidation states, occurrence and synthesis of the elements. Spectral and magnetic properties of compounds of actinides in comparison with those of lanthanides and d-block elements. Trans actinides Chemistry of Trans –uranium elements.

**Reference Books**

1. Basic Inorganic Chemistry- F. A. Cotton, G. Wilkinson and P. L. Gaus; John Wiley and sons. Inc, 6<sup>th</sup> edition (1999).
2. Advanced Inorganic Chemistry, 6th edition; F. A. Cotton and G. Wilkinson.
3. Inorganic Chemistry IV edition; J. E. Huheey, E. A. Keiter and R. L. Keiter, Addison; Wesley (1993).
4. Inorganic Chemistry, II edition, D. F. Shriver, P. W. Atkins and C. H. Langford, ELBS; Oxford University Press, 1994.
5. Concise Inorganic Chemistry, 5th edition; J. D. Lee (1996).
6. Inorganic Chemistry, 3rd Edition; Gary. L. Miessler and Donald . A. Tarr (2007).

**CPT-1.3: PHYSICAL CHEMISTRY-I****64 Hours****UNIT-I****16h****Thermodynamics-I**

**Concepts of entropy and free energy:** Entropy as measure of randomness and unavailable energy. Entropy changes in reversible and irreversible process and during various processes. Variation of entropy with T and P. Helmholtz and Gibbs free energies. Thermodynamic criteria of equilibrium and spontaneity. Variation of free energy with temperature and pressure. Maxwell's relations, Von't Hoff's reaction isotherm and isochore, Gibbs-Helmholtz equation. Determination of free energy changes. Nernst heat theorem and third law of thermodynamics- calculation of absolute entropies and residual entropy.

**Partial molar Properties:** Physical significance, Partial molar volume and partial molar free energy (chemical potential). Determination of partial molar quantities by intercept method and slope methods. Physical significance of chemical potential. Variation of chemical potential with temperature and pressure. Formulation of the Gibbs Duhem equation. Derivation of Duhem- Margules equation.

**UNIT-II****16h****Quantum Mechanics-I**

**Quantum Chemistry:** A brief review of wave-particle duality and Heisenberg Uncertainty principle. Concept of operators (operator-operand): algebra of operators, commutative and non- commutative operators, linear operator, Laplacian operator, Hamiltonian operator. Eigen value, eigen function, well behaved function, Hermitian operator and its characteristics. Schrodinger wave equation for particles. Wave function: significance of  $\psi^2$  and  $\psi\psi^*$ . Postulates of quantum mechanics. Application of Schrodinger equation to a particle trapped in a potential field (one dimension and three dimensions). Concept of Degeneracy. Wave equation for H atom: separation and solution of R,  $\theta$  and  $\phi$  equations (Rigorous treatment not required), radial and angular distributions, quantum numbers. Application of Schrodinger equation to rigid rotor and simple harmonic oscillator.

**UNIT-III****16h****Chemical Dynamics-I**

**A.** Macroscopic and microscopic kinetics, Review of theories of reaction rate-Collision theory and Transition state theory, Comparison of collision theory with transition state theory, Arrhenius equation- characteristics, Significance of energy of activation, Temperature coefficient and its evaluation. Thermodynamical formulation of reaction rates (Wyne-jones and Eyring treatment), Reaction between ions in solutions – Influence of ionic strength on reaction rates (primary and secondary salt effects).

**B.** Concept of Steady state kinetics, Chain reactions–chain length and chain inhibition, comparison of photochemical and thermal reactions, Mechanisms of thermal and photochemical reactions between hydrogen-bromine and hydrogen-chlorine. Comparative study of thermal and photochemical hydrogen-halogen reactions. Pyrolysis of acetaldehyde, Decomposition of ethane.

C. Kinetics of fast reactions- Introduction, Study of reactions by relaxation method (Temperature and pressure jump), flow method (Plug flow method and Stopped flow method), Flash photolysis and Shock tube method.

#### UNIT-IV

16h

#### **Chemical Dynamics-II**

D. Kinetics of homogeneous catalysis-kinetics of auto catalytic reactions, kinetics of acid-base catalyzed reactions. Comparison of enzyme catalyzed and chemical catalyzed reactions, Mechanism (Lock and Key theory), Kinetics of enzyme catalyzed reactions – Henri-Michaelis- Menten mechanism, Significance of Michaelis-Menten constant, Lineweaver-Burk plot. Effect of enzyme concentration, pH, Temperature, Activators and Inhibitors on enzyme activity.

E. Theories of uni-molecular reactions: Lindemann theory, and Hinshelwood theory.

F. **Surface reactions**-Unimolecular and biomolecular surface reactions: mechanism, inhibition and activation energy.

#### **Reference**

1. Physical Chemistry, P. W. Atkins, Julio de Paula, ELBS, 7<sup>th</sup> edition, (2002).
2. Physical Chemistry: A Molecular Approach, McQuarie and Simon, Viva, New Delhi, (2001).
3. Introduction to Quantum Chemistry, A. K. Chandra, Tata McGraw Hill, (1988).
4. Quantum Chemistry, Ira. N. Levine, Prentice Hall, New Jersey, (1991).
5. Chemical Kinetics- K. J. Laidler, McGraw Hill. Inc. New York (1988).
6. Principles of Chemical Kinetics – House J. E. Wm C Brown Publisher, Boston, (1997).
7. Kinetics and Mechanism – A. A. Frost and R. G. Pearson, John-Wiley, New York, (1961).
8. Chemical Kinetic Methods – C. Kalidas, New Age International Publisher, New Delhi (1995)
9. S.H. Maran and C. F. Pruton, 4<sup>th</sup>Edn., Oxford, & IBH publishing Co. Pvt. Ltd. New Delhi (1965).
10. Physical Chemistry- P. Atkins and J. D. Paula, 9<sup>th</sup>Edn., Oxford University Press (2010).
11. Principles of Physical Chemistry, Puri, Sharma and Pathania, Vishal Publishing Co.
12. Essentials of Physical Chemistry, Arun Bahl, B. S. Bahl and G. D. Tuli, S. Chand Publishing Co.
13. A text book of Physical Chemistry, Vol. 1-6, K.L. Kapoor, Macmillan Publishers India Limited.

**SPT-1.4 A: MEDICINAL CHEMISTRY-I****64 Hours****UNIT-I****16h**

**Concepts of Medicinal Chemistry:** Important terminology in medicinal Chemistry, Drug, Pharmacy, Pharmaceutics, Toxicology, Pharmacodynamics agents, Pharmacophore, pharmacodynamics, metabolites and anti-metabolites, chemotherapy.

Mechanism of chemotherapeutic actions: 1) Biological defenses. 2) Chemical defenses.

a) Surface active agents; b) Metabolic antagonism. Assay of Drugs: Chemical Assay, Biological Assay, Immunological Assay, LD<sub>50</sub>, ED<sub>50</sub>, IC<sub>50</sub> and ID<sub>50</sub>.

**Classification and nomenclature of Drugs**

Classification of drugs on the basis of therapeutic action. Nomenclature of Drugs. Difference between drugs and medicines.

**UNIT-II****16h****Drug Discovery**

Introduction. Procedure followed in Drug Design. a) Drug Discovery without a lead b) Lead Discovery. Lead Modification: Drug Design and Development

Identification of active part: The pharmacophore b) Functional group modification, c) Structure-activity relationship d) Structure modification to increase potency and the therapeutic index: 1. Homologation; 2. Chain branching; 3. Ring-chain transformation; 4. Bio-isosterism Structural Modification to increase oral Bioactivity.

1) Electronic Effect; 2) The Hammett equation; 3) Lipophilicity effect.

**Concept of Prodrugs and soft drugs.**

- a) Prodrugs: i) Prodrugs designing, types of prodrugs; ii) Prodrug formation of compounds containing various chemical groups, Prodrugs and Drug delivery system
- b) Soft drugs: i) soft drug concept; ii) Properties of soft drugs.

**UNIT-III****16h****Drug Absorption:**

Drug Entry into the Bloodstream, Oral, Injection, Transdermal, Other Routes, Topical, Distribution: Drug Transport, Blood, Crossing Membranes, Blood–Brain Barrier, Pharmacodynamics: At the Drug Target, Metabolism and Elimination: Drug Removal, Kidneys and Liver.

**Enzymes as Drug Targets**

Introduction, Definition, Structure, Case Study Use of  $\alpha$ -Helices to Cross Cell Membranes, Types, Mode of Action, Kinetics, Single Substrate, Multiple Substrates, Inhibitors, Reversible and Irreversible, Pharmaceutical Concerns, Mutational Resistance to Inhibitors, Concentration Effects, Metabolism of Drugs.

**Receptors as Drug Targets**

Receptors, Similarities and Differences from Enzymes, Classification, Ligand-Gated Ion Channels, G-Protein–Coupled Receptors, Tyrosine Kinase–Linked Receptors, Nuclear Receptors, Types of Ligands, Agonists, Antagonists, Inverse Agonists, Receptor Theories, Occupancy Theory, Allosteric Theory, Rate Theory, Drug-Target Residence Time.

**UNIT-IV****16h*****In-silico* and Computer Aided Drug design**

Introduction to Molecular Modeling, Lipinski's rule of five, Protein preparation, Ligand preparation, Molecular Mechanics, force fields (Potential energy function), Energy Minimization Methods, Conformational Analysis. Concepts of Virtual Screening, Drug likeliness, Screening-Counting Schemes, Functional Group Filters, Topological Drug Classification-Pharmacophore Point Filter-Focused Screening Libraries for Lead Identification, Pharmacophore Screening, Structure-Based Virtual Screening, Protein Structures, Computational Protein-Ligand Docking Techniques with the help of docking servers, Types-Rigid Docking, Flexible or induced fit Docking, *in silico* De Novo design.

**Reference Books**

1. Gringauz, A. Introduction to Medicinal Chemistry: How Drugs Act and Why? John Wiley & Sons (1997).
2. Medicinal Chemistry an Introduction-Gareth Thomas 2nd Ed. Wiley
3. An introduction to Medicinal Chemistry-Graham L. Patrick 5th Ed. Oxford
4. Introduction to Medicinal Chemistry-Alex Gringauz (Wiley)
5. Medicinal Chemistry-Ashutosh Karr
6. Medicinal Chemistry the Modern Drug Discovery Process- Erland Stevens, 2014 by Pearson Education.
7. Quintessence of Medical pharmacology-Sujit K. Choudhary, New Central book agency
8. Principles of Medicinal chemistry Vol I & II- S.S Kadam, K.R. Mahadik, K.G. Bothara, Nirali Prakshan.
9. Drug design volumes by Ariens
10. Principles of Drug design by Smith
11. Strategy of Drug design by Brucell
12. The Organic Chemistry of the Drug design and Drug action by Richard B.Silverman

**SPT-1.4 B-GREEN SYNTHESIS****64 Hours****UNIT-I****16h****Use of ultrasound and Microwaves in Organic Synthesis**

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

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

**UNIT-II****16h**

**Ionic-liquids:** Introduction, structure, synthesis and applications of some important ionic liquids in organic synthesis.

**Polymer supported reagents in organic synthesis**

Introduction- properties of polymer support, advantages of polymer supported reagents and choice of polymers. Applications: Substrate covalently bound to the support: Synthesis of oligosaccharides, Dieckmann cyclisation. Preparation of polymer bound aldehyde and application in aldol reactions. Synthesis of polystyryl boronic acid and use in diol protection reaction. Reagent linked to a polymeric material: Preparation of sulfonamide polymer and application in diazo transfer reaction. Synthesis of polymer bound per acid and its applications.

Polymer supported catalytic reactions: Preparation of polymer supported  $AlCl_3$  and application in etherification and acetal formation reactions.

**UNIT-III****16h****Phase transfer catalysis and Crown ethers**

Phase transfer catalysis: Introduction, definition, mechanism of phase transfer catalysis. Types of phase transfer catalysts and reactions and their advantages. Preparation of catalysts and their application in substitution, elimination, addition, alkylation, oxidation and reduction reactions.

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

**UNIT-IV****16h****Multi-component Reactions**

Studies on the mechanistic aspects and applications of the following reactions in organic synthesis: Passerini-Ugi, Hantzsch, Biginelli, Doebner-Miller, Ritter, Jacobson, Betti, Robinson-Schopf, Barbier, Baylis-Hillman, Ivanov and Suzuki coupling reaction.

**Reference Books**

1. Modern Organic Reactions-H.O.House.
2. Organic Synthesis-R.E.Ireland (Prentice Hall India), 1969.
3. Art in Organic Synthesis-Anand, Bindra & Ranganath-(Wiley New Delhi), 1970.
4. Advanced Organic Chemistry-IV-Ed. Part A &B-F.J.Carrey & R.J.Sundberg(Kluwer) 2001.
5. Modern Methods of Organic Synthesis-N.Carruthers(Cambridge University), 1996.

**SECOND SEMESTER**  
**CPT-2.1: INORGANIC CHEMISTRY- II**

64 hours

**UNIT-I**

16h

**Metal-Ligand equilibria in solution-** Step-wise and overall formation constant and their relationship, trends in step-wise constant, kinetic and thermodynamic stability of metal complexes, factors affecting the stability of metal complexes with reference to the nature of the metal ion and ligand, chelate effect, macrocyclic effect and their thermodynamic origin. Determination of binary formation constant by pH metry, spectrophotometry, polarography and ion exchange methods.

**Structure and bonding-** Structure and bonding in hydride, dihydrogen, dioxygen, isocyanide, CO, NO, N<sub>2</sub> and tertiary phosphine complexes of transition metals.

**UNIT-II**

16h

**Metal-ligand bonding-** Stereoisomerism- coordination numbers 3 to 8. Crystal field theory, salient features, spectrochemical series, splitting of d-orbitals in tetragonal, square planar, trigonal-bipyramidal and square-pyramidal geometry, applications of CFT- colors of transition metal complexes, magnetic properties of octahedral complex, distortion of octahedral complex, CFSE and their uses, factors affecting CFSE, limitations of CFT, experimental evidence for metal-ligand covalent bonding in complexes, nephelauxetic effect, Ligand Field Theory, MO theory: tetrahedral and octahedral complexes (including  $\pi$ -bonding), angular overlap model. Stereochemical non-rigidity, self-assembly in supramolecular chemistry.

**UNIT-III**

16h

**Electronic spectra of coordination compounds-** Spectroscopic ground states, selection rules, term symbols for d<sup>n</sup> ions, Racah parameters, Orgel, Correlation and Tanabe-Sugano diagrams, spectra of 3d metal-aqua complexes of trivalent V, Cr, divalent Mn, Co and Ni, CoCl<sub>4</sub><sup>2-</sup>, calculation of Dq, B and  $\beta$  parameters, CT spectra. Spectral properties of Lanthanide and Actinide metal complexes.

**UNIT-IV**

16h

**Magnetic properties of coordination compounds-** Types of magnetic behaviour, magnetic susceptibility and its determination- Gouy, Faraday, VSM method. Diamagnetic correction, orbital contribution, spin-orbital coupling, ferro- and anti-ferromagnetic coupling, spin-crossover. Magnetic properties of Lanthanide and Actinide metal complexes.

**Photochemical reactions of transition metals complexes:** Basic photochemical processes, Kasha's rule, quantum yield, Jablonski diagrams, photo substitution reactions, photo-redox reactions, ligand photoreactions and solar energy conversion.

**Reference Books**

1. Advanced inorganic chemistry, (5<sup>th</sup> edition)- F.A. Cotton and G. Wilkinson: John Wiley and sons 1988.
2. Inorganic chemistry (3<sup>rd</sup> edition)-J.E. Huheey: Harper and Row, N.Y. 1983
3. Modern aspects of Inorganic chemistry (4<sup>th</sup> edition)-H.J., Emeleus and A.G. Sharpe: UBS 1989.
4. Coordination chemistry-S.F.A. Kettle, (1969)-Thomas Nelson and Sons Ltd., London.

5. Physical Inorganic Chemistry-A Coordination Chemistry Approach- S.F.A. Kettle, Spektrum, Oxford, 1996.
6. Symmetry and spectroscopy of molecules, K. Veera Reddy, New-Age International, 2009.
7. Group theory and its chemical applications, P. K. Bhattacharya, Himalaya Publishers, Students Edition.
8. Spectroscopy by B P Stranghan and S Walker, John Wiley and Sons, Inc., New York, Vol. I and 2 , 1976
9. Organic spectroscopy by Willaa Kemp, ELBS Society, MacMillan, 1987.
10. Application of absorption spectroscopy of organic compounds by JohnR. Dyer, Prentice-Hall of India Pvt. Ltd., New Delhi.1974.
11. Organic spectroscopy by V.R. Dhani, Tata McGrow-Hill Publishing company Ltd., New Delhi, 1995.
12. Spectrometric identification of organic compounds, 4<sup>th</sup> edition, Robert M, Silverstein, G. Clayton Bassler and Terence C. Morrill, John Wiley and Sons Inc., New York, Vol.1, 1981.
13. Analytical Chemistry Principles, John H. Kennedy, 2<sup>nd</sup> edition, Saunders College Publishing, California, 1990.
14. Instrumental method of analysis, Hobart H, Willard, Lynne L, Merritt, Jr., John A. dean and franmk A Settle, Jr., 6<sup>th</sup> edition, CBS Publishers and Distributors, Delhi, 1986.
15. Physical methods for chemists by R.S. Drago, Sunders College publishing, New York.
16. Quantitative Analysis, R. A Day and A./L Underwqood, 6<sup>th</sup> edition, prentice Hall, Inc., 1999.
17. Principles of instrumental Analysis, D.A.Skoog, F.J Holler and T.A. Nieman, 5<sup>th</sup> edition, Thomson Asis Pvt. Ltd. Singapore, 1998.



**CPT-2.2: PHYSICAL CHEMISTRY- II****64 Hours****UNIT-I****16h****Thermodynamics-II**

**Fugacity:** Relation between fugacity and pressure, determination of fugacity of gases. Variation of fugacity with temperature and pressure. Activity and activity coefficients. Variation of activity with temperature and pressure. Determination of activity coefficients by electrical methods.

**Thermodynamics of dilute solutions:** Raoult's law, Henry's law. Ideal and non-ideal solutions. Discussion and thermodynamic derivation of the laws of osmotic pressure, cryoscopy and ebullioscopy. Determination of molecular weights. Thermodynamic treatment using the concept of chemical potentials.

**Phase Rule Studies:** Thermodynamic derivation of phase rule; application of phase rule to the two component systems: simple eutectic type, compound formation with congruent melting point and incongruent melting points, systems involving the formation of a continuous series of solid solutions. Application of phase rule to three component systems: Systems of three liquids and systems of two salts and a liquid.

**UNIT-II****16h****Statistical Thermodynamics**

Introduction, thermodynamic probability, relation between entropy and thermodynamic probability, principle of equipartition of energy, Maxwell-Boltzmann distribution equation, partition function and its significance. Derivation of translational, rotational, vibrational and electronic partition functions for a molecule. Evaluation of internal energy, enthalpy, Helmholtz and Gibbs free energies, equilibrium constant, partition functions of atoms and diatomic molecules. Evaluation of molecular entropies, entropy of monatomic gas (Sackur-Tetrode equation).

**Distribution equations** – Bose-Einstein and Fermi-Dirac distribution equations.

**Heat capacity of solids:** Einstein and Debye heat capacity equations, Debye-characteristic temperature and its significance.

**UNIT-III****16h****Electrochemistry-I**

Electrochemistry of solutions: Ionic atmosphere, Debye-Huckel theory for the problem of activity coefficient, Debye-Huckel limiting Law, Debye-Huckel equation for appreciable concentration, Debye-Huckel Onsager conductance equation and its extension to ion solvent-interactions, Debye-Huckel Bjerrum mode, Ion association, triple ions, triple ions and conductance minima. Thermodynamics of electrified interface, derivation of electro capillary Lippmann's equation, surface excess, thermodynamic aspects of surface excess. The method of determination and measurement of interfacial tension as a function of applied potential difference across the interface.

**UNIT-IV****16h****Quantum Chemistry-II**

**Approximate methods** –Necessity of approximate methods, Perturbation method: first order and second order corrections for wave functions and energies, application to He – atom (first order correction only) – calculation of first ionization potential and binding energy. Variation theorem-statement and proof. Application of variation theorem to a particle in one dimensional box, H and He – atoms.

**Chemical Bonding in diatomics:** Covalent bond-Valence bond and molecular orbital approaches with comparison. Secular equations and secular determinants. Molecular orbital theory applied to homonuclear and heteronuclear diatomic molecules. Introduction to Huckel molecular orbital theory of conjugated systems and its applications.

### Reference Books

1. Introduction to electrochemistry by S. Glasstone.
2. Modern Electrochemistry Vol I and II by J.O.M. Bockr's and A.K.N. Reddy, Plenum Press, New York (1970).
3. Electrochemistry –Principles and applications by E.G. Potter.
4. Electrochemistry by Reiger, Prince Hall (1987).
5. Physical Chemistry, P. W. Atkins, Julio de Paula, ELBS, 7<sup>th</sup> edition, (2002).
6. Physical Chemistry: A Molecular Approach, McQuarie and Simon, Viva, New Delhi, (2001).
7. Introduction to Quantum Chemistry, A. K. Chandra, Tata McGraw Hill, (1988).
8. Quantum Chemistry, Ira. N. Levine, Prentice Hall, New Jersey, (1991).
9. Physical Chemistry- P. Atkins and J. D. Paula, 9<sup>th</sup>Edn., Oxford University Press (2010).
10. Principles of Physical Chemistry, Puri, Sharma and Pathania, Vishal Publishing Co.
11. Essentials of Physical Chemistry, Arun Bahl, B. S. Bahl and G. D. Tuli, S. Chand Publishing Co.
12. A text book of Physical Chemistry, Vol. 1-6, K.L. Kapoor, Macmillan Publishers India Limited.

**SPT-2.3 A: ORGANIC REACTIONS AND REARRANGEMENTS****64 Hours****UNIT-I****16h****Aromatic Substitution Reactions**

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

**Nucleophilic substitution reactions:** The  $S_NAr$ ,  $S_N1$ , benzyne and  $SR_N1$  mechanisms. Reactivity: effect of substrate structure, leaving group and attacking nucleophile. Goldberg reaction, Bucherer reaction, Schiemann reaction, Von Richter reaction.

**UNIT-II****16h****Addition Reactions**

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

**Addition to carbon-heteroatom multiple bonds:** Mechanism of metal hydride reduction ( $NaH$ ,  $LiH$ ,  $LiAlH_4$ ,  $NaBH_4$ ) of saturated and unsaturated carbonyl compounds, acids, esters and nitriles. Addition of Grignard reagents and organolithium reagents to carbonyl compounds and unsaturated carbonyl compounds. Conversion of aldehydes to nitriles. Hydrolysis of nitriles and addition of amines to isocyanates. Formation of xanthates. Wittig reaction. Addition of amines, alcohols, water,  $NaHSO_4$ .

**UNIT-III****16h****Organic Named reactions:**

Reactions, Mechanisms and synthetic uses of the following: Stobbe condensation, Darzen condensation, Cannizzaro reaction, Chichibabin reaction, Benzoin condensation, Claisen-Schmidt condensation, Claisen reaction, Simon-Smith reaction, Stark Enamine reactions, Sharpless asymmetric epoxidation, Prin's reaction, Knoevenagel reaction, Sandmeyer reaction, Ullmann reaction, Mitsunobu reaction, Robinson annulation, Dieckmann condensation and Mannich reaction, Van-braun reaction, Heck reaction, Suzuki reaction.

**UNIT-IV****16h****Organic Named Rearrangements:**

Reactions, Mechanisms and synthetic uses of the following: Wagner-Meerwein, Pinacol-Pinacolone, Fries, Wolff, Beckmann, Hofmann, Curtius, Lossen and Schmidt rearrangements. Benzil-benzilic acid rearrangement, Arndt-Eistert reaction, Tiffeneau-Demjanov reaction, Fritsch-Buttenberg-Wiechell rearrangement. Stevens, Wittig, Favorskii rearrangements, Dienone-phenol, Baker-Venkatraman rearrangement, Baeyer-Villiger oxidation, Neber rearrangement, Benzidine rearrangement and allylic rearrangement.

**Reference Books**

1. Advanced Organic Chemistry – Reactions, Mechanism and Structure, Jerry March, John Wiley (2008).
2. Advanced Organic Chemistry, F. A. Carey and R. J. Sundberg, Plenum (1990).
3. A Guide Book to Mechanism of Organic Chemistry, Peter Sykes, Longman (2000).
4. Structure and Mechanism of Organic Chemistry, C. K. Ingold, Cornell University Press.
5. Organic Chemistry, R. T. Morrison and R. N. Boyd, Prentice-Hall (1998).
6. Modern Organic Reactions, H. O. House, Benjamin (1972).
7. Principles of Organic Synthesis, R. C. Norman and J. M. Coxon, Blackie Academic and Professional (1996).
8. Stereochemistry of Organic Compounds, D. Nasipuri, New-Age International (1999).
9. Stereochemistry of Carbon Compounds, E. L. Eliel, S. H. Wilen and L. N. Mander, John Wiley (1994).
10. Organic Chemistry, Volumes I and II, I L Finar, Longman. (1999).
11. Physical Chemistry, P. W. Atkins, Julio de Paula, ELBS, 7<sup>th</sup> edition, (2002).
12. Physical Chemistry: A Molecular Approach, McQuarrie and Simon, Viva, New Delhi.
13. Kinetics and Mechanism – A. A. Frost and R. G. Pearson, John-Wiley, New York.
14. Chemical Kinetic Methods – C. Kalidas, New Age International Publisher, New Delhi.
15. S.H. Maran and C. F. Pruton, 4<sup>th</sup>Edn., Oxford, & IBH publishing Co. Pvt. Ltd. New Delhi (1965).
16. Physical Chemistry- P. Atkins and J. D. Paula, 9<sup>th</sup>Edn., Oxford University Press (2010).
17. Biochemistry, - Geoffrey Zubay, 2<sup>nd</sup>Edn., Macmillan Publishing Co. New York (1981).
18. Surface Chemistry: Theory and Applications, J. J. Bikerman, Academic Press. New York (1972).

**SPT-2.3 B: GROUP THEORY AND GENERAL SPECTROSCOPY-I****64 Hours****UNIT-I****16h****Symmetry and Group Theory in Chemistry**

Definition of groups, subgroups, cyclic groups, conjugate relationships, classes, simple theorems in group theory. Symmetry elements and symmetry operations, point groups, Schönflies notations, representations of groups by matrices, reducible and irreducible representations, characters of representations. Great Orthogonality Theorem (without proof) and its applications, character tables and their uses (representations for the  $C_n$ ,  $C_{nv}$ ,  $C_{nh}$ ,  $D_{nh}$  etc groups to be worked out explicitly). Mulliken symbols for irreducible representations Direct products, Applications of group theory to quantum mechanics- identifying non-zero matrix elements, derivation of the ortho normalization conditions.

**UNIT-II****16h****Microwave Spectroscopy**

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

**Infrared Spectroscopy-I**

Vibrations of molecules, harmonic and anharmonic oscillators-vibrational energy expression, energy level diagram, vibrational wave functions and their symmetry, selection rules, expression for the energies of spectral lines, computation of intensities, hot bands, effect of isotopic substitution, Diatomic vibrating rotor, Born-Oppenheimer approximation, vibrational-rotational spectra of diatomic molecules, P, Q and R branches, breakdown of the Born-Oppenheimer approximation.

**UNIT-III****16h****Infrared Spectroscopy-II**

Vibrations of polyatomic molecules: Normal co-ordinates, translations, vibrations and rotations, vibrational energy levels and wave functions, fundamentals, overtones and combinations. Vibration-rotation spectra of polyatomic molecules- parallel and perpendicular vibrations of linear and symmetric top molecules. Techniques and instrumentation, FT-IR.

**Raman Spectroscopy**

Classical theory of the Raman effect, polarizability as a tensor, polarizability ellipsoids, quantum theory of the Raman effect, Pure rotational Raman spectra of linear and asymmetric top molecules, vibrational Raman spectra, Raman activity of vibrations, rule of mutual exclusion, rotational fine structure- O and S branches, Polarization of Raman scattered photons. Structural determination from Raman and IR spectroscopy- $AB_2$  and  $AB_3$  molecules, techniques and instrumentation.

**UNIT-IV****16h****Electronic Spectroscopy**

Born-Oppenheimer approximation, vibrational coarse structure, intensities by Franck-Condon principle, Dissociation energy, rotational fine structure, Fortrat diagram, pre-dissociation.

Electronic structure of diatomic molecules- basic results of MO theory, classification of states by electronic angular momentum-and molecular orbitals, selection rules, spectrum of singlet and triplet molecular hydrogen. Electronic spectra of polyatomic molecules- localized MOs, spectrum of HCHO, change of shape on excitation. Decay of excited states-radiative (fluorescence and phosphorescence) and non-radiative decay, internal conversion.

### Reference

1. Chemical Applications of Group Theory, F. A. Cotton, Wiley Eastern (1976).
2. Molecular Symmetry, D. S. Schonland, Van Nostrand (1965).
3. Chemical Applications of Group Theory, 3rd edition, F.A. Cotton, John Wiley and Sons (2006).
4. Molecular Symmetry and Group Theory – Robert L Carter, John Wiley and Sons (2005).
5. Symmetry in Chemistry - H. Jaffe and M. Orchin, John Wiley, New York (1965).
6. Introduction to Molecular Spectroscopy, C. N. Banwell, TMH Edition (1994).
7. Introduction to Molecular Spectroscopy, G. M. Barrow, McGraw Hill (Int. Students Edition) (1988).
8. Molecular Spectroscopy, J. D. Graybeal, McGraw Hill (Int. Students Edition) (1990).
9. Spectroscopy, Vols. 1-3, B. P. Straughan and W. Walker, Chapman Hall (1976).
10. Spectroscopy of organic compounds, P. S. Kalsi, new age international publishers, New Delhi.
11. Spectroscopy Vol I and II by B. P. Straughan and S. Walker, John wiley and sons Inc, New York. (1976).
12. Introduction to Spectroscopy - Pavia, Lampman and Kriz, 3rd edition, Thomson.
13. Organic Spectroscopy, William Kemp, English Language Book society, Macmillan, 1987.

**OET-2.4: CHEMISTRY OF FOODS - I****64 Hours****UNIT-I****16h**

Food Classification, Chemical composition and nutritional value of common food stuffs, properties of foods.

Food preservation and processing: Food deterioration, methods of preservation and processing by heat, cold, chill storage, deep freezing, drying, concentration, fermentation and radiation.

Food quality: Sensory evaluation, objective methods, non-nutritional constituents and food safety.

**UNIT-II****16h**

Food additives properties & uses: classification of food additives, Antioxidants (Ascorbic acid, Citric acid, Tocopherols, Butylated hydroxyl anisole (BHA), Tertiary butyl hydroquinone, colouring agents (Chlorophyll, Caramel, Curcumin or turmeric, Indigo carmine), flavours (Diacetyl, Vanilla extracts, Vanillin, Ethyl vanillin), emulsifiers (Methyl cellulose, Carboxymethyl cellulose, Gellan gum), Artificial sweeteners (Aspartame, Acesulfame K, Sucralose), leavening agents (Baking powder, Ammonium bi-carbonate, Ammonium carbonate), thickeners (Alginic acid and their salts) and preservatives (Sorbic acid and its sodium, potassium and calcium salts, Benzoic acid).

**UNIT-III****16h**

Pigments and colours: Importance & perception of color in foods, Chlorophylls, myoglobin and haemoglobin, anthocyanins, flavonoids, tannins, betalains, quinones, xanthenes, carotenoids properties & uses. Chemical analyses of pigments in foods: extraction, concentration, semi-purification and measurement.

**UNIT-IV****16h**

Vitamins: Classification, functions requirements, distribution in foods, loss during processing, effects of deficiency and characteristic properties of vitamins – B<sub>1</sub>( Thiamine), B<sub>2</sub>(Riboflavin), B<sub>3</sub> (Pantothenic acid ), B<sub>6</sub> (pyridoxine), B<sub>12</sub> (Cyanocobalamin), H(Biotin), P(Ruti), C (ascorbic acid), A (Retinol), D (Calciferol), E (Tocopherol), K (naphthoquinone), Folic acid (PGA) and Niacin.

**Reference Books**

1. Food Chemistry by L.W. Aurand and A.E. woods the AVI Publising Inc.
2. Food Chemistry by L.H. Meyer, Affiliated East- West press Ltd, New Delhi.
3. Foods- Facts and principles by N. ShakuntalaManay, M. ShdaksharaSwamy.
4. Principles of Food Chemistry by John M. deMan.

**THIRD SEMESTER**  
**CPT-3.1: REACTION MECHANISMS, PERICYCLIC REACTIONS AND**  
**BIOCHEMICAL MECHANISMS**

64 Hours

**UNIT-I**

16h

**Aliphatic nucleophilic and electrophilic substitution reactions**

Nucleophilic substitution reactions: Substitution at allylic carbon (allylic rearrangement), trigonal carbon (hydrolysis of esters and amides, use of DCC in the formation of anhydrides), vinylic carbon. Neighboring group participation and  $S_Ni$  reactions.

**Electrophilic substitution reactions:**  $S_E2$ ,  $S_E1$  and  $S_{Ei}$  mechanisms. Hydrogen exchange, migration of double bonds,  $\alpha$ -halogenation of aldehydes, ketones and acids. Aliphatic diazonium coupling, nitrosation at carbon bearing active hydrogens, diazo transfer reaction, carbene and nitrene insertion, decarboxylation of aliphatic acids, haloform reaction, Haller-Bauer reaction.

**UNIT-II**

16h

**Free-radical chemistry**

Generation of free-radicals: Thermal homolysis of peroxides, per-esters and azo compounds, photochemical methods. Free radical reactions: Free-radical mechanisms in general. Free-radical substitution mechanisms. Mechanisms at an aromatic substrate. Neighboring group assistance in free-radical reactions. Reactivity for aliphatic substrates, reactivity at a bridgehead, reactivity in aromatic substrates, reactivity in the attacking radical. Halogenation at an alkyl carbon and an allylic carbon, hydroxylation at an aliphatic carbon, hydroxylation at an aromatic carbon, oxidation of aldehydes to carboxylic acids, formation of hydroperoxides and peroxides. Gomberg-Bachmann reaction, Meerwein arylation, Kolbe reaction and Hunsdiecker reaction.

**UNIT-III**

16h

**Pericyclic reactions-I**

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

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

Cycloadditions: The frontier orbital description of cycloadditions,  $[2+2]$   $[3+2]$  and  $[4+2]$  cycloadditions, analysis by FMO and correlation diagram method. Antarafacial and suprafacial additions,  $[\pi m_s + \pi n_a]$  and  $[\pi m_s + \pi n_s]$ -cycloadditions.  $[\omega 2_a + \pi 2_s]$  and  $[\pi 4_s + \omega 2_s]$ -cheletropic reactions, 1,3-dipolar cycloadditions.

**Pericyclic reactions-II**

Regio, enantio and Endo selectivities in Diels-Alder reactions. Retro Diels-Alder reaction. Sigmatropic rearrangements: Classification, Orbital description, suprafacial and antarafacial shifts of H, sigmatropic shifts involving carbon moieties.  $[i, j]$ -sigmatropic rearrangements (including Walk, Cope, oxy and aza-Cope rearrangements).



**UNIT-IV****16h****Biochemical mechanisms**

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

- i). Thiamine pyrophosphate (TPP) in decarboxylation of keto-acids and in the formation of -ketols.
- ii). Pyridoxal phosphate (PLP) in transamination, decarboxylation, dealdolisation and elimination reactions of amino acids.
- iii). Lipoic acid in the transfer of acyl group reactions.
- iv). Coenzyme A (CoASH) in the transfer of acyl group.
  - v). Biotin
- vi). Vitamin K<sub>2</sub> coenzyme in carboxylation reactions. vii). Tetrahydrofolic acid (H<sub>4</sub>F) in one-carbon transfer reactions.
- viii). Vitamin B<sub>12</sub> coenzymes in molecular rearrangement reactions and in the synthesis of methionine and methane.
- ix). Nicotinamide and
- x). Flavin coenzymes in biological redox reactions.

**Reference Books**

1. Advanced Organic Chemistry – Reactions, Mechanism and Structure, Jerry March, John Wiley (2008).
2. Understanding organic reaction mechanisms, A. Jacob, Cambridge Univ. Press, 1997.
3. Introduction to organic chemistry A. Streitwieser, Jr and C. H. Heathcock, Macmillan, 1985.
4. Physical and mechanistic organic chemistry, R.A.Y. Jones, 1<sup>st</sup> Edn. Cambridge Univ. Press, 1979.
5. Mechanisms of molecular migrations, Vols I and II, B. S. Thiagarajan, 1<sup>st</sup> Edn. Pergamon Press, Oxford, 1979.
6. P. J. Garratt in Comprehensive organic chemistry, D. Barton and W. D. Ollis, 1<sup>st</sup> Edn. Pergamon Press, Oxford, 1979.
7. Radicals in organic synthesis, B. Giese, Pergamon Press, 1986.
8. Gringauz, A. Introduction to Medicinal Chemistry: How Drugs Act and Why? John Wiley & Sons (1997).
9. Dugas, H. & Penny, C. Bioorganic Chemistry: A Chemical Approach to Enzyme Action, Springer Verlag (1998).

**CPT-3.2: CHEMISTRY OF NATURAL PRODUCTS****64 Hours****UNIT-I****16h****Terpenoids and Carotenoids**

Classification, nomenclature, occurrence and isolation. Isoprene rules. Stereochemistry of citral, farnesol, limonene, 1,8-cineole, menthols and borneols. Correlation of configurations of terpenoids.

Structure elucidation of camphene, (-)pinene, (-)caryophyllene, and (-)santonin.

Synthesis and biosynthesis of the following: Linalool and (-)terpineol. Commercial synthesis of camphor. Biosynthesis of squalene and cyclisation of squalene into (-)lanosterol and friedelene. Carotenoids: Methods of isolation. Structural relationship of  $\alpha$ -,  $\beta$ - and  $\gamma$ -carotenes. Structure elucidation and synthesis of  $\beta$ -carotene.

**UNIT-II****16h****Alkaloids**

Definition, nomenclature, occurrence, isolation & classification.

Structural elucidation and synthesis of the following alkaloids: Ephedrine, Cinchonine & Morphine.

**Steroids**

Occurrence. Nomenclature, basic skeleton, Diels hydrocarbon and stereochemistry. Isolation, structure and structural elucidation of sterols and bile acids (determination of ring size, nature of side chain, position of angular methyl and stereochemistry of ring junctions).

**UNIT-III****16h****Porphyryns and vitamin B<sub>12</sub>**

Structure elucidation and synthesis of haemin, chlorophyll-a and vitamin-B<sub>12</sub> (synthesis of Vitamin-B<sub>12</sub> from coobyric acid).

**Nucleic acids**

Introduction, components of nucleic acids, nucleosides, nucleotides and oligonucleotides.

Structure elucidation and synthesis of nucleosides and nucleotides.

Chemical synthesis of oligo-nucleotides: Protecting groups for hydroxy group in sugar, amino group in the base and phosphate functions.

Methods of formation of inter nucleotide bonds: DCC, phosphodiester approach, phosphotriester approach, phosphite triester and phosphoramidite methods. Solid-phase synthesis of oligonucleotides.

**UNIT-IV****16h****Prostaglandins**

Introduction, nomenclature, classification and biological role of prostaglandins. Structure elucidation and stereochemistry of PGE<sub>1</sub>, PGE<sub>2</sub> and PGE<sub>3</sub>.

Synthesis of PGE<sub>1</sub> and PGE<sub>2</sub> by Corey's and Stork's approaches. Synthesis of PGE<sub>3</sub> by Upjohn's approach.

Synthesis of prostacyclin I<sub>2</sub> and thromboxane B<sub>2</sub>. Biosynthesis of prostaglandins.

**Insect pheromones**

Introduction, classification and Pheromones in pest control.

Syntheses of (one synthesis should be stereoselective synthesis)

- i) Grandisol (component of boll weevil pheromone)
- ii) Bombykol (sex pheromone of silkworm moth).
- iii) Brevicommin (pheromone from *Dendroitis brevicomis*)

**Reference Books**

1. Natural products: Their chemistry and biological significance-J. Mann, S. Davidson, J. B. Hobbs, D. V. Banthorpe & J. B. Harborne, Longman, UK, 1994.
2. Terpenes, J. Verghese, Tata McGraw-Hill, New Delhi, 1982.
3. Chemistry of terpenes and terpenoids, A. Newman, Academic Press, London, 1975.
4. Handbook of naturally occurring compounds Vol. II: Terpenes, T. K. Davon, I. Scott, Academic Press, NY, 1972.
5. Natural products chemistry Vol. I & II, K. Nakanishi, T. Goso, S. Ito, S. Natori & S. Nozoe, Academic Press, NY, 1974.
6. Total synthesis of natural products Vol. I & VI, Apsimon, John Wiley, NY, 1973-1981.
7. Organic chemistry Vol.II, I. L. Finar, 6<sup>th</sup> Edn. Longman, 1992.
8. Chemistry of natural products Vol. I & II, O. P. Aggarwal, Goel Publishing House, 6<sup>th</sup> Edn. 1982.
9. Total synthesis of natural products: The chiral approach Vol.III, S. Hanessian Pergamon Press, 1983.
10. Total synthesis of steroids, Akhaun & Titov, Jerusalem, 1969.
11. Medicinal natural products: A biosynthetic approach, P. M. Dewick. John Wiley, Chichester, 1997.
12. The colours of life: An introduction to the chemistry of porphyrins and related compounds, L. R. Milgrom, Wiley Chichester, 1995.
13. Interpretation of the UV spectra of natural products, A.I. Scott, Pergamon Press, Oxford, 1964.
14. Spectral data of natural products Vol. I- K.Yamaguchi, Elsevier Publishing Co, London, 1970.

**SPT-3.3A ORGANIC SYNTHESIS****64 Hours****UNIT-I****16h****C-C and C-N bond forming reactions**

Darzen's reaction, Use of acetylides in C-C bond formation reactions. Acid-catalyzed self-condensation of olefins, Prin's reaction, Shapiro reaction, Dieckmann cyclization, Robinson annulations, Hofmann-Martius reaction, Acyloin condensation and Houben-Hoesch reaction. Stork-enamine synthesis, Meyer synthesis. Use of nucleophilic nitrogen and electrophilic carbon (NH<sub>3</sub>, amines and nitrite as nucleophiles in substitution, NH<sub>3</sub> and amines in addition to ketones and aldehydes). Electrophilic nitrogen and nucleophilic carbon (nitration, nitrosation) for the bond formation reactions (including Skraup synthesis, Mitsunobu reaction, N-Nitroaromatic amine rearrangement, Fisher-Hepp reaction. Japp- Klingemann reaction).

**UNIT-II****16h****Reagents in organic synthesis**

Use of the following in organic synthesis and functional group transformations.

Aluminium *iso*-propoxide, NBS, Lithium diisopropylamide (LDA), dicyclohexyl carbodimide (DCC), dichlorodicyanoquinone (DDQ), Corey-Chaykovsky reagent, Raney-Nickel, diazomethane, TMS-chloride, 1,3-Dithiane (reactivity and umpolung), PPA, Yamaguchi reagent. Woodward and Prevost hydroxylation. Functional group transformations: Nitro to keto group (Neff reaction), alcohol to aldehyde.

**Oxidations-I** Oxidation with Cr (VI) oxidants (CrO<sub>3</sub>, K<sub>2</sub>Cr<sub>2</sub>O<sub>7</sub>, PCC, PDC), Mn (VII)

oxidants (Jones reagent, MnO<sub>2</sub>, KMnO<sub>4</sub>), OsO<sub>4</sub>, SeO<sub>2</sub>, Pb(OAc)<sub>4</sub>, HIO<sub>4</sub>, Ag<sub>2</sub>O, DMSO.

**UNIT-III****16h****Oxidations-II**

Ozone, peroxides (H<sub>2</sub>O<sub>2</sub>, *t*-BuOOH, dibenzoylperoxide) and peracids (Preparation, properties and applications of CF<sub>3</sub>COOOH, *m*-CPBA, momoperphthalic acid) as oxidizing agents. Dess-Martin oxidation.

**Reductions**

Complex metal hydrides, dissolving metal reductions (including Birch, Benkeser, Clemmensen reductions), diimide reduction, catalytic hydrogenation (homogeneous and heterogeneous), Leukart reaction (reductive amination), Wolf-Kishner reduction, McMurry reaction, Pummer, Willgerdot, Corey-Bakshi-Shibata and Tishchenko reactions.

**UNIT-IV****16h****Asymmetric Synthesis**

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

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

Acyclic stereoselection: Addition of nucleophiles to carbonyl compounds (1,2- 1,3- and 1,4-asymmetric induction). Asymmetric aldol condensation .Addition of allylmetal and allylboranes to carbonyl group.

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

Enantioselective synthesis: Reduction with chiral hydride donors [(S)-PBMgCl, (-)-<sup>i</sup>BOAlCl<sub>2</sub>, alpine-borane, (S)-BINAL-H, (R,R)-DIOP, and (S,S)-CHIRAPHOS). Enantioselective alkylation of ketones *via* hydrazones. Enantioselective alkylation with chiral PTC. Enantioselective Michael addition. Enantioselective intramolecular aldol condensation. Use of (+) and (-)-DET in asymmetric epoxidation.

Polymer-bound chiral catalysts in asymmetric induction, Asymmetric amplification.

### Reference

1. Advanced organic chemistry, J. March, 4<sup>th</sup> Edn. John Wiley, 2008. Organic synthesis, R.E.Ireland, Prentice-hall India, New Delhi, 1975.
2. Understanding organic reaction mechanisms, A. Jacob, Cambridge Univ Press, 1997.
3. Introduction to organic chemistry, A. Streitwieser, Jr and C. H. Heathcock, Macmillan, 1985.
4. Physical and mechanistic organic chemistry, R. A.Y. Jones, 1<sup>st</sup> Edn. Cambridge Univ Press, 1979.
5. Modern synthetic reactions, H. O. House, W. A. Benjamin, California, 2<sup>nd</sup> Edn. 1972.
6. Some modern methods of organic synthesis, W. Carruthers, Cambridge Univ. Press, London, 2<sup>nd</sup> Edn. 1978.
7. Mechanisms of molecular migration, Vols I & II, B.S. Thyagarajan, Pergamon Press, Oxford, 1979.
8. Comprehensive organic chemistry, D. Barton and W. D. Wallis, Pergamon Press, Oxford, 1983.
9. Organic chemistry Vol. II, I. L. Finar 6<sup>th</sup> Edn. Longman, 1992.
10. Organic reaction Mechanisms, 3<sup>rd</sup> Edn., V. K. Ahluwalia and R. K. Prashar, Narosa, New Delhi, 2005.

**SPT-3.3B: ORGANIC PHOTOCHEMISTRY****64 Hours****UNIT-I****16h****Photochemistry:**

Importance of Photochemistry, Laws of Photochemistry: Grothus –Draper Law, Stark-Einsteins Law, Laws of light absorption, Quantum yield and numerical problems. Photochemistry and spectroscopy, units and dimensions. Electronic energy states of atoms, term symbols for atoms, energy levels for the electronic configuration of carbon and oxygen illustrating spin orbit coupling and Hund's rules, inverted multiplets as applied to simple atoms and also for inner transition metals, Laporte's selection rules. Physicochemical Properties of electronically excited molecules: Nature of changes on electronic excitation: acidity, dipole moment, redox potentials etc. Fates of excited species, Electronic, vibrational, rotational energies-potential energies diagram. Shapes of absorption band and Franck Condon principle.

**UNIT-II****16h**

Quantum mechanical formulation of Franck Condon, crossing of potential energy surfaces, Non crossing rule of Teller for potential energy surface. Emission spectra, fluorescence and phosphorescence.

Environmental effect on absorption and emission spectra, solvent red and blue shift in absorption spectra. Experimental techniques to determine the intermediates in photochemical reactions.

Classification of photochemical reactions, Rate constants and life times of reactive energy state Effect of light intensity on the rate of photochemical reaction Photo-fragmentation, photo-dissociation-Gas phase photolysis.

**UNIT-III****16h**

Photosensitized reaction, photo-fragmentation in liquid phase, photo-degradation of polymers, Isomerization and other rearrangement reactions. Atmospheric photochemistry

**Some current topics in photochemistry:**

Semiconductors: Bonding and conductivity, mechanism of conductivity, energy bands in semiconductors, impurity semiconductors.

Photo voltaic effect: p-n junction solar cells, silicon cells, Ga-As solar cells, schottky barrier solar cells.

Photo-electrochemistry: Introduction, efficiency of conversion of light to chemical and electrical energy, frequently measured quantities. Photo-splitting of water using colloidal suspensions Photo-catalysis: Photo-cleavage of waste which are environmentally hazardous by using TiO<sub>2</sub>, Photo-oxidation and photo-reduction reactions

**UNIT-IV****16h****Photochemistry**

Physical and Chemical processes, Jablonski diagram. Photosensitization, quantum efficiency, quantum and chemical yields.

Photochemistry of functional groups:

Olefins: *Cis-trans* isomerism, [2+2]-cycloaddition, rearrangements. Reaction of conjugated olefins; di- $\pi$ -methane rearrangements (including oxa and aza-di- $\pi$ -methane rearrangements).

Ketones: Excited state of C=O. Norrish type-I and type-II cleavages.  $\alpha$ - $\beta$ -unsaturated ketones.

[2+2] addition. Rearrangement of cyclohexadienones (application in the synthesis of some important natural products).

Aromatic compounds: Photo-rearrangement of benzene and its derivatives, cycloaddition of benzene.

Photochemical oxidations and reductions: Cycloaddition of singlet molecular oxygen {[2+2], [4+2]-additions}. Oxidative coupling of aromatic compounds, photo-reduction by hydrogen abstraction.

### Reference Books

1. Advances in Photochemistry - Rohatgi Mukherjee.
2. Principles and applications of Photochemistry - R.P. Wayne, Elsevier, New York., 1970.
3. Dupey and Chapmann, Molecular reactions and photochemistry, Prentice Hall - International, Tokyo, 1972.

**OET-3.4: CHEMISTRY OF FOODS - II****64 Hours****UNIT-I****16h**

Enzymes: Classification, specificity, factors effecting the rate of enzyme catalyzed reactions, enzyme inhibitors, enzymic browning, enzymes in food processing - carbohydrase, proteases, lipases, oxidoreductases

**UNIT-II****16h**

Carbohydrates: Classification, reactions of simple sugars; Oxidation, reduction, condensation with phenyl hydrazine, action of alkalis, action of acids, formation of esters, formation of colored products. Function of sugars in foods - Browning reaction (non-enzymic).

Polysaccharides: Brief study of the chemistry - starch dextrin, glycogen, cellulose, hemicelluloses, pectic substances, gums. Sweetness of sugars, relation of structure to sweetness.

**UNIT-III****16h**

Proteins and amino acids: Amino acids - classification, structure & physical & chemical properties. Peptides (Oxytocin), properties of peptides.

Food proteins - classification, protein structure, properties of proteins, denaturation, protein gels, proteolytic enzymes. Biological importance of proteins.

**UNIT-IV****16h**

Lipids: Classification, role of lipids, fatty acids and glycerol derived from oils and fats, Physical properties - polymorphism, reactions of fats, rancidity, reversion, polymerization, saponification, addition, hydrogenation, phospholipids, lipid metabolism.

**Reference:**

1. Food Chemistry by L.W. Aurand and A.E. woods the AVI Publising Inc.
2. Food Chemistry by L.H. Meyer, Affiliated East- West press Ltd, New Delhi.
3. Foods- Facts and principles by N. ShakuntalaManay, M. ShdaksharaSwamy.
4. Principles of Food Chemistry by John M. deMan.
5. Principles of Food Science, Part I, Food Chemistry edited by Owen R.Fennama , Mareal Dekker, Inc., New York.
6. Hand book of Food and Nutrition by M. Swaminathan



**FOURTH SEMESTER****CPT-4.1: ORGANOMETALLIC AND HETEROCYCLIC CHEMISTRY****64 Hours****UNIT-I****16h****Organometallic Compounds in Organic Synthesis-I**

Chemistry of Organo-transition metal complexes: General introduction. 18 and 16-Electron rules. Complexation and De-complexation Reactions:  $\sigma$ -Bonded systems including  $\eta^1$  ligands.  $\pi$ -Bonded systems involving dihapto to octahapto ligands such as olefins, acetylenes, allylmoieties, butadiene, cyclobutadiene, arenes, cyclopenta, cyclohexa and cycloheptadienyl moieties; cyclohepta, cyclooctatrienes, and cyclooctatetraene moieties.

Use of organo-transition metal complexes as protecting and stabilizing groups: Protection of olefins, acetylenes and dienes. Stabilization of cyclobutadienes and norbornadienones.

Organo-metallics as electrophiles and nucleophiles: Nucleophilic addition to  $\eta^2$ ,  $\eta^5$  and  $\eta^6$  complexes. Electrophilic addition to  $\eta^4$ ,  $\eta^6$  and carbene complexes.

Organo-metallics in coupling and cyclization reactions: Coupling and cyclization of organic nucleophiles with olefins (including Heck reaction), and coupling of olefins with acetylenes (including Felkin's reaction).

Organo-metallics in isomerization, oxidation and reduction reactions: Isomerization of olefins, allylic alcohols and allylic ethers. Oxidation of olefins (including Wacker's process and epoxidation), reduction of olefins and  $\alpha,\beta$ -unsaturated compounds (including Wilkinson's reaction).

**UNIT-II****16h****Organometallic Compounds in Organic Synthesis-II**

Carbonylation reactions: Use of zirconium complexes in the synthesis of esters, acids, aldehydes or acyl halides from alkyl halides. In the hydroformylation of olefins and dienes.

Use of iron complexes for the insertion of CO group into organic molecules such as dienes, alkyl halides and vinyl epoxides. Use of cobalt complexes in the synthesis of ketones from epoxides, lactones from allylic alcohols and in the hydroformylation of olefins.

Use of palladium complexes for the carbonylation of alkyl halides, dienes and allenes.

Application of the following organo-metallics in Organic Synthesis: Organo-zincs: Preparation, reaction with compounds containing acidic protons, reaction with C-C multiple bonds, trans-metallation, addition reactions of zinc reagents with carbonyl compounds. Simmons-smith, and Reformatsky reaction.

Organo-lithiums: Preparation. Deprotonation reactions, Nucleophilic-addition reactions.

Reactions with imines, nitriles and isonitriles. Organo-copper reagents: (Gilman reagents-lithium dialkyl cuprates): Preparation, reactions with alkyl, allyl, vinyl, benzyl and aryl halides, aldehydes, ketones (including  $\alpha$ ,  $\beta$ -unsaturated carbonyl compounds) and epoxides.

organoboranes: isomerization reactions, oxidation, protonolysis, carbonylation, cyanidation.

Organosilicon compounds: Introduction, preparations and reactions, Peterson reaction.

Organophosphorous compounds: Nomenclature, synthesis and reactions of trialkyl phosphine, triarylphosphine, trialkyl phosphite, organomagnesium (Grignard reagent), organomanganese.

**Organononmetallic Compounds**

Organofluorine and Organosulphur compounds: Introduction. Preparations, reactions, mechanism and synthetic applications of important fluorine, sulphur containing reagents.

**UNIT-III****16h****Heterocyclic Chemistry-I**

Small Ring Heterocycles: Synthesis, reactivity, Properties and Reactions of three and four membered heterocycles: Oxirane, thirane, aziridine, azetidines, oxetane and thietanes

Five membered heterocycles: Synthesis, reactivity, aromatic character and importance of following heterocyclic rings: Furan, Pyrrole, Thiophene, Pyrazole, Imidazole, thiadiazoles and oxazoles. Condensed five and six membered heterocycles Synthesis, reactivity: Benzofuran, Benzothiophene, Benzooxazoles, Benothiazoles, Benzimidazoles, Indole, Isoquinoline and Quinoline. Synthesis, reactivity, aromatic character and biological importance of following heterocycles: 1,2,3-triazole, 1,2,4-triazole, 1,2,4-oxadiazole, 1,3,4-oxadiazole, 1,2,5-oxadiazole.

**UNIT-IV****16h****Heterocyclic Chemistry-II**

Six membered heterocycles: Synthesis, reactivity, aromatic character and importance of following heterocyclic rings: Pyridine, Pyrimidine, Pyrazine, Diazines, Triazines, Tetrazines and Thiazines.

Seven and large membered heterocycles: Synthesis and reactions of azepanes, oxepines, thiepinines, diazepines, thiazepines, azocines, diazocines, dioxocines and dithiocines.

Synthesis of 5- and 6- membered Heterocycles containing P, As, Sb and Bi.

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

**Reference Books**

1. Organic Reactions and Their Mechanisms-P.S. Kalsi (New Age, New Delhi),1996.
2. Organic Chemistry-Vol. -I & II-Mukherji, Singh and Kapoor. (Wiley Eastern, New Delhi) 1985.
3. An Introduction to the Chemistry of Heterocyclic Compounds-Acheson (Wiley -Eastern) 1987.
4. Heterocyclic Chemistry-J. Joule & G. Smith, (Van-Nostrand, ELBS), 1978.
5. Organic Chemistry-P.Y. Bruice (Pearson Education, New Delhi) 2002.
6. F. A. Carey and Sundberg, Advanced Organic Chemistry-Part A and B, 3rd edition, Plenum Press, New York,1990.
7. Comprehensive Organic Synthesis-B. M. Trost and I. Fleming series, Pergamon
8. Heterocyclic Chemistry -T. Gilchrist
9. An introduction to the chemistry of heterocyclic Compounds-R M Acheso
10. Heterocyclic Chemistry- J A Joule and K Mills
11. Principles of modern heterocyclic chemistry- A Paquette
12. Heterocyclic Chemistry- J A Joule and Smith
13. Handbook of Heterocyclic Chemistry- A R Katritzky, A F Pozharskii
14. Heterocyclic Chemistry-II- R R Gupta, M Kumar, V Gupta, Springer (India) pvt

**CPT-4.2 STEREOCHEMISTRY AND RETROSYNTHETIC ANALYSIS****64 Hours****UNIT-I****16h****Optical activity in the absence of chiral atoms**

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

**Optical activity due to the presence hetero atoms**

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

**Transannular reactions**

Conformational analysis of medium rings. Transannular reactions: Hydrolysis of medium ring epoxides and bromination of C<sub>8</sub>-C<sub>10</sub> cyclic dienes.

**UNIT-II****16h****Determining absolute and relative configuration**

Chemical correlation of configuration: Methods without involving the chiral centre. Chemical transformation involving the chiral centre. Chemical correlation involving diastereomers.

Methods based on comparison of optical rotation: Distance rule, Rule of shift, Rule of optical superposition, Mill's rule, Method based on molecular rotation difference. The method of quasi-racemate.

Use optical rotatory dispersion curves:  $\alpha$ -axial halo-ketone rule and its applications, octant rule (application of these rules in the determination of absolute configuration of substituted cyclohexanones, decalones and cholestanones). Method based on anomalous X- ray scattering.

**Retrosynthetic Analysis:**

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

**UNIT-III****16h**

**Protecting groups:** Principle of protection of alcohols, amines, acids and carbonyl groups.

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

Synthesis of alcohols, carbonyl compounds and alkenes. Use of acetylides and aliphatic nitro compounds in organic synthesis. Diels-Alder reaction, 1,3-difunctionalised compounds,  $\alpha$ ,  $\beta$ -unsaturated compounds, carbonyl compounds condensations, 1,5-di-functionalised compounds. Micheal addition and Robinson annulation.

**UNIT-IV****16h**

**Ring Synthesis:** Synthesis of saturated heterocycles: 3-, 4-, 5- and 6-membered rings.

**Named Reactions in Heterocyclic Synthesis:** Castro-Stephens Coupling, Heine Reaction, Paterno-Büchi Reaction, Biginelli reaction, Hantzsch dihydropyridine synthesis, von Pechman reaction and Hofmann-Löffler-Freytag reaction.

**Synthesis of some complex molecules using disconnection approach:** Aromadendrene, longifloene, cortisone, reserpine, vitamin-D, juvabione, fredericamycin-A and Lycorane.

**Reference Books**

1. Stereochemistry of carbon compounds, E. L. Eliel, S. H. Wilen and L. N. Mander, John Wiley & Sons, 1994.
2. Stereochemistry, Potapov, MIR, Moscow, 1984.
3. Stereochemistry, Nasipuri, D, New Age, 1999.
4. Advanced organic chemistry, J. March, 4<sup>th</sup> Edn. John Wiley, 2008.
5. Organic Chemistry, R. E. Ireland Prentice-Hall India, New Delhi, 1975.
6. Some modern methods of Organic Synthesis, W. Caruthers, Cambridge Uni. Press London, 2<sup>nd</sup> Edn., 1998.
7. Stereochemistry of organic compounds- Principle and applications, D. Nasipuri, 2<sup>nd</sup> Edn., New Age International Publishers, 2001.
8. Organic synthesis: The synthon approach, S. Warren, John Wiley & Sons, New York, 1<sup>st</sup> Edn. 1983.
9. Designing organic synthesis: A disconnection approach, S. Warren, John Wiley & Sons, New York, 2<sup>nd</sup> Edn. 1987.
10. Organic synthesis, C. Willis and M. Wills, Oxford University Press, 1995.
11. Organic synthesis: Concepts, methods and starting materials, J. Furhlop and G. Penzillin, Verlag VCH.
12. Principles of organic synthesis, R. Norman and J. M. Coxon, Blackie Academic & Professional.
13. Advanced organic chemistry Part B, F. A. Carrey and J. Sundberg, Plenum Press, 1999.
14. Organic chemistry Vol. 2, 6<sup>th</sup>Edn., I. L. Finar, Longman,1992.
15. Strategic Applications of Named Reactions in Organic Synthesis - Laszlo Kurti and Barbara Czako, Elsevier Academic Press.

**SPT-4.3A: ORGANIC SPECTROSCOPY-II****64 hours****UNIT-I****16h**

**UV Visible spectroscopy:** Quantitative aspects of absorption – Beer's law, Technology associated with absorption measurements. Limitations of the law – real, chemical, instrumental and personal. Theory of molecular absorption. Vibration rotation fine structure of electronic spectra. Types of absorption bands-  $n$  to  $\pi^*$ ,  $\pi$  to  $\pi^*$ ,  $n$  to  $\sigma^*$  and  $\sigma$  to  $\sigma^*$ , C-T and ligand field. Woodward's empirical rules for predicting the wavelength of maximum absorption for olefins, conjugated dienes, cyclic trienes and polyenes,  $\alpha,\beta$ - unsaturated aldehydes and ketones, benzene and substituted benzene rings. Applications: Qualitative and quantitative analysis of binary mixtures, measurements of dissociation constants of acids and bases, determination of molecular weight, determination of stoichiometry and stability of the complexes. Photometric titrations and kinetic studies.

**Vibrational Spectroscopy**

Sampling techniques, Group frequencies, factors affecting group frequencies, Bond-order, Mass effect, Conjugation, Inductive, resonance, steric effects. Intra-molecular interactions. Application of IR in the study of H-bonding, stereoisomerism and tautomerism. Complementarity of IR and Raman. Identification of Tautomerism. Identification of the following Amides, Amines, Esters, Halides, Nitro compounds, etc., problems using UV and IR.

**UNIT-II****16h****Nuclear magnetic resonance spectroscopy-I**

Introduction, Magnetic properties of nuclei- Resonance condition. Nuclear spin, population of nuclear spin levels and NMR isotopes, Relaxation methods. Instrumentation and sample handling, FT-NMR. Chemical shift. Mechanism of shielding and deshielding in Alkanes, Alkyl halides, Alkenes, Aromatic compounds, Carbonyl compounds and Annulenes. Pascal's triangle-low and high resolution, spectrum of ethanol. Karplus Curve, Diamagnetic and paramagnetic effects and magnetic anisotropy. Equivalence of protons-chemical and magnetic equivalence. Spin-systems: First order and second order coupling of AB systems, Simplifications of complex spectra's. Problems. Spin-spin interactions: AX, AX<sub>2</sub>, AX<sub>3</sub>, AMX, AB types. Vicinal, geminal and long range coupling-Spin decoupling. Chemical shift reagents and deuterium exchange. Stereochemistry and hindered rotations. Temperature effects.

**UNIT-III****16h****Nuclear magnetic resonance spectroscopy-II**

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

<sup>13</sup>C NMR Spectroscopy: Range and factors affecting chemical shifts of alkanes, alkyl halides, alkenes, alcohols, ethers, alkynes, carbonyl compounds and aromatics.

Multiple resonance spectroscopy: Introduction to 2D-techniques: DEPT, COSY, HETCOR, and INADEQUATE. Explanation of the principle, applications to structure elucidation and stereochemistry of simple organic molecules.

Dynamic NMR. NMR spectroscopy of other nuclei with spin  $I = \frac{1}{2}$ . Introduction to <sup>15</sup>N, <sup>19</sup>F, <sup>29</sup>Si and <sup>31</sup>P NMR spectroscopies. Chemical shift values for <sup>15</sup>N, <sup>19</sup>F, <sup>29</sup>Si and <sup>31</sup>P containing compounds.

**UNIT-IV****16h****Mass spectrometry and Composite Problems:**

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

**Reference**

1. Applications of absorption spectroscopy to organic compounds, J. R. Dyer, Prentice-Hall, New Delhi, 1969.
2. Organic spectroscopy, P. Laszlo and P. Stang, Harper & Row, New York, 1971.
3. Organic spectroscopy, W. Kemp, ELBS London, 2000.
4. Spectrometric identification of organic compounds, R. M. Silverstien, and W. P. Weber, 2005.
5. Introduction to spectroscopy, 3<sup>rd</sup> Edn., D. L. Pavia, G. M. Laupman and G. S. Kriz, Harcourt College Publishers, 2001.
6. Organic mass spectroscopy, K. R. Dass & E. P. James, IBH New Delhi, 1976.
7. Interpretation of organic mass spectra, F. W. McLafferty, W. A. Benjamin, London, 1973.
8. Practical Organic Mass Spectroscopy, 2<sup>nd</sup> Edn. J R Chapman, John Wiley, NY, 1993.
9. The IR Spectra of complex molecules, Vols. I and II, L J Bellamy, Chapman and Hall, London, 1975.
10. Spectroscopic techniques for Organic Chemists, J W Cooper, John Wiley, NY, 1980.
11. Biomolecular NMR Spectroscopy, J N S Evans, Oxford Univ. 1995.
12. Mass spectrometry a foundation course, K Downard, RSC, Cambridge, 2004.
13. Mass spectrometry of organic compounds, H. Budzikiewicz, Djerassi C. and D. H. Williams, Holden-Day New York, 1975.
14. Modern NMR techniques and their Applications, Ed. A I Popov, Marcel Deckker, 1991.
15. Modern structural theory of organic compounds, L. N. Ferguson, Prentice-Hall, New Delhi, 1973.
17. Fundamentals of molecular spectroscopy, 4<sup>th</sup> edn., C. N. Banwell and E. M. McCash, Tata McGraw-Hill, New Delhi, 1999.

**SPT-4.3B MEDICINAL CHEMISTRY-II****64 Hours****UNIT-I****16h**

Introduction, classification, mode of action and SAR of following agents:

**Anti-infective agents:** furazolidon and nitrofurazone.

**Sulfonamides:** sulfisoxazoles and sulfamethoxazoles

**Antibiotics:** Penicillin G, cephalosporins, and tetracyclins.

**Antitubercular and Antileprotic agents:** isoniazid, ethambutol, clofazimine and dapson.

**Analgesic agents:** phenylbutazone and diclofenac sodium.

**Antimalarials:** Chloroquine and mefloquine. Synthesis of Penicillin G, sulfamethoxazole and Chloroquine

**UNIT-II****16h**

Introduction, classification, mode of action and SAR of following agents: **Antipyretics, analgesics and non-steroidal anti-inflammatory drugs:** Aspirin, paracetamol, phenacetin, novalgine, phenylbutazone and ibuprofen.

**Anti-diabetics:** Sequence of A- & B- chains of insulin, glibenclamide, metformin, ciglitazone.

**Anti-histamines:** Methapyrilene, chlorpheniramine.

**Anti-virals:** Acyclovir, amantidine, rimantidine and zidovudine.

Synthesis of ibuprofen, chlorpheniramine and zidovudine

**UNIT-III****16h**

**Anti-neoplastic agents:** Introduction, cancer chemotherapy, special problems, role of alkylating agents and anti-metabolites in treatment of cancer. Mention of carcinolytic antibiotics and mitotic inhibitors. Synthesis of mechlorethamine, cyclophosphamide, melaphan, uracil mustards and 6-mercaptopurine. Recent development in cancer chemotherapy. Hormone and natural products.

**Cardiovascular drugs:** Introduction, cardiovascular diseases, drug inhibitors of peripheral sympathetic function, central intervention of cardiovascular output. Direct acting arteriolar dilators. Synthesis of amyl nitrite, sorbitrate, diltiazem, quinidine, verapamil, methyl dopa, atenolol, oxyprenol.

**UNIT-IV****16h****Psychoactive drugs-chemotherapy of the mind**

Introduction, neurotransmitters, CNS depressants, general anaesthetics, mode of action of hypnotics, sedatives, anti-anxiety drugs, benzodiazepines, buspirone, neurochemistry of mental diseases. Antipsychotic drugs- the neuroleptics, antidepressants, butyrophenones, serendipity and drug development, stereochemical aspects of psychotropic drugs. Synthesis of chlorpromazine, diazepam, oxazepam, chlorazepam, alprazolam, phenytoin, ethosuximide, trimethadione, barbiturates, thiopental sodium, glutethimide.

**Reference Books**

1. Burgers medicinal chemistry M. E. Welly Medicinal Chemistry M.E. Walffed John Willey and sons, Vo 1, 2 and 3.
2. Wilson and Giswold's, Text Book of Organic and Medicinal Chemistry.
3. William. O. Foye, Principles of Medicinal chemistry, Lea and Febiger, Philadelphia.
4. Martindale, the extra pharmacopoeia, J.E. Reynolds. The Pharmaceuticals Press, London.
5. A. M. Beckett and J.B. Stanlake and Garrel, Practical Pharmaceutical chemistry, the Sthalone Press, University of London, London.
6. B.D. Furniss, A.J. Hannaford, V.Regers, P.W.G. Smith and A.R. Tachell, Vogel's textbook of practical organic chemistry, including quantitative analysis

**ORGANIC CHEMISTRY PRACTICALS****I-SEM****CPP-1.5 (1.1) PRACTICAL: ORGANIC CHEMISTRY**

1. Cannizarro reaction: Benzaldehyde.
2. Fries rearrangement: Phenyl acetate.
3. Friedel-Crafts reaction: Benzene and Acetyl chloride.
4. Sandmeyer reaction: 4-Chlorotoluene from 4-toluidine.
5. Pechmann reaction: Resorcinol and ethylacetoacetate.
6. Oxidation of Cyclohexanol.
7. Preparation of S- Benzylisothiuronium chloride.
8. Synthesis of *p*-iodonitrobenzene
9. Synthesis of N-Phenyl-2,4-dinitroaniline.
10. Synthesis of 2,4,6-tribromoaniline.
11. Synthesis of 2,4-dichlorophenoxyacetic acid.

**CPP-1.6 (1.2) PRACTICAL: INORGANIC CHEMISTRY****Volumetric analysis**

1. Volumetric estimation of Ca and Mg in Dolomite solution.
2. Volumetric estimation of Cu in Cu and Ni (German Silver).
3. Volumetric estimation of Fe in Cu and Fe solution.
4. Volumetric estimation of Zn in Cu and Zn solution.
5. Volumetric estimation of Ni in Ni and Zn solution.

**Gravimetric analysis**

1. Gravimetric determination of Fe in iron ore as Fe<sub>2</sub>O<sub>3</sub>.
2. Gravimetric determination of Ni in Cu and Ni solution.
3. Gravimetric determination of Fe in Fe and Cr solution.
4. Total gravimetric estimation of Fe and Al.
5. Gravimetric estimation of Cu in Cu and Fe solution.
6. Gravimetric estimation of Cu in Cu and Zn solution.

**CPP-1.7(1.3) PRACTICAL: PHYSICAL CHEMISTRY**

1. Study the hydrolysis of methyl acetate in presence of two different concentrations of HCl and report the relative strength.
2. Study the hydrolysis of methyl acetate in the presence of HCl at different temperatures and report the energy of activation.
3. Study of kinetics of autocatalytic reaction between KMnO<sub>4</sub> versus oxalic acid.
4. Evaluation of Arrhenius parameter for the reaction between K<sub>2</sub>S<sub>2</sub>O<sub>8</sub> versus KI (first order)
5. Study the primary salt effect on the kinetics of ionic reactions.
6. To determine conductometrically the second order rate constant for the hydrolysis of ethyl acetate by sodium hydroxide.
7. To investigate the reaction between potassium persulphate and potassium iodide by colorimetric measurement
8. Kinetics of saponification of ethyl acetate by conductivity method and study the effect of dielectric constant of the medium (Using methanol).
9. To determine the partial molal volumes of sodium chloride in aqueous solutions.
10. To determine the partial molal volumes of potassium chloride in aqueous solutions.
11. Determine the partial molar volume of methanol in dilute aqueous solutions.



12. Determine the partial molar volume of ethanol in dilute aqueous solutions.
13. Determination of heat of neutralization of strong acid by strong base by using a calorimeter.
14. Determination of heat of neutralization of weak acid by strong base by using a calorimeter.
15. Determination of heat of solution of a salt by using a calorimeter.

#### **SPP-1.8(1.4A) PRACTICAL: ORGANIC CHEMISTRY -A**

1. Preparation of p-bromoaniline from acetanilide.
2. Preparation of p-nitroacetanilide from acetanilide.
3. Preparation of aspirin.
4. Synthesis of PABA
5. Preparation of Methyl Salicylate.
6. Preparation of methyl benzoate.
7. Synthesis of sulfanilamide.
8. Preparation of ascodan.
9. Preparation of benzocaine.
10. Preparation of nitro ferfural

#### **SPP-1.8(1.4B) PRACTICAL: ORGANIC CHEMISTRY -B**

##### **Green Synthesis of the following compounds**

1. Acetylation of primary amine (preparation of acetanilide)
2. Base catalyzed aldol condensation (synthesis of dibenzalpropanone)
3. Halogen addition to c=c bond (bromination of trans-stilbene)
4. [4+2] cycloaddition reaction (diels-alder reaction between furan and maleic acid)
5. Rearrangement reaction - (benzil - benzoic acid rearrangement)
6. Conversion of acetophenone to hydroxypropylbenzene
7. Conversion of Chlorobenzaldehyde to Chloro-benzylalcohol
8. Conversion of p-nitrobenzaldehyde to p-nitrobenzylalcohol
9. Synthesis of 4-methoxyacetophenonephenylpropenone from 4-methoxyacetophenone and benzaldehyde
10. Synthesis of acetophenone-4-nitrophenylpropenone from acetophenone and p-nitrobenzaldehyde
11. Synthesis of 4-chloroacetophenone-4-methoxyphenylpropenone from 4-chloroacetophenone and 4-methoxybenzaldehyde.

##### **Reference Books**

1. Mechanisms of molecular migration, Vols I & II, B.S. Thyagarajan, Pergamon Press, Oxford, 1979.
2. Comprehensive organic chemistry, D. Barton and W. D. Wallis, Pergamon Press, Oxford, 1983.
3. Organic chemistry Vol. II, I. L. Finar 6<sup>th</sup> Edn. Longman, 1992.
4. Organic reaction Mechanisms, 3<sup>rd</sup> Edn., V. K. Ahluwalia and R. K. Prashar, Narosa, New Delhi, 2005.
5. Vogel's Text book of Qualitative Chemical Analysis, J. Bassett, G. H. Jeffery and J. Mendham, ELBS (1986).
6. Inorganic Semimicro Qualitative Analysis, V. V. Ramanujam; The National Pub. Co. (1974).

7. Practical Inorganic Chemistry, G. Marr and B. W. Rockett, Von Nostrand Reinhold Co., London (1972).
8. Findlays practical physical chemisty revised by P. B. Levitt, Longman's London (1966).
9. Experiments in Physical Chemistry by Shoemaker and Garland, McGraw Hill International Edn. (1966)
10. Advanced Practical Physical Chemistry by J. B. Yadav, Goel Publications Meerut (1988)
11. Senior Practical Physical Chemistry by B. C. Kosla, Simla Printers New Delhi (1987)
12. Experimental Physical Chemistry by Daniel et al., McGraw Hill, New York (1962).
13. Practical Physical Chemistry by A.M James and P. E. Pritchard, Longman's Group Ltd (1968)
14. Experimental Physical Chemistry by Wilson, New combe & others, Pergamon Press, New York (1962)
15. Experimental Physical Chemistry by R. C. Behra and B Behra, Tata McGraw, New Delhi (1983)
16. Experimental Physical Chemistry by V. D. Atavale and Parul Mathur, New Age International, New York (2001)
17. Physical Chemistry Laboratory Principles and Experiments by H. W. Salberg J. I. Morrow, S. R. Cohen and M. E. Green Macmillan publishing Co .new York.

**II –SEM****CPP-2.5(2.1) PRACTICAL: INORGANIC CHEMISTRY**

1. Preparation of any Four of the following complexes and determination of the purity of the prepared sample and structural study of the prepared complexes using physical methods such as magnetic susceptibility measurements, absorption spectra etc.
  - a) Chloropentaammine Cobalt (III) Chloride
  - b) nitropentaammine Cobalt (III) Chloride
  - c) nitritopentaammine Cobalt (III) Chloride
  - d) Hexamine Cobalt (III) Chloride
  - e) mercury tetrathiocyanato cobaltate (II)
  - f) Hexemine nickel (II) chloride
  - g) tris –(thiourea) copper (I) sulphate
  - h) Potassium tris (Oxalato) ferrate (III)
2. Determination of ionisable chloride by ion exchange method.
3. Stabilization of an unstable oxidation state by complexation: Preparation of Manganese (III) acetyl acetate
4. Preparation of EDTA complex of Mn (III).
5. Determination of the composition of a complex of iron-phenanthroline by
  - a) Mole -ratio method
  - b) Job's method
  - c) Slope ratio method
6. Determination of the stability constant of a complex
  - a) Turner-Aderson method (iron-T iron or iron-phenanthroline complex)
  - b) Bjerrum's method (copper sulphosalicylic acid)
  - c) Kinetic method (KI<sub>3</sub> complex)
7. Preparation and kinetics of the acid hydrolysis of potassium trisoxalato cobaltate (III) trihydrate
8. Preparation and photolysis of potassium trisoxalato ferrate(III).
9. Preparation and screening of copper complex for its fungicidal and bactericidal activity.
10. Demonstration Experiments
  - a) Recording and interpretation of IR and NMR spectra of complexes
  - b) Interpretation of a simple x-ray powder photograph
  - c) TGA of calcium Oxalate monohydrate
  - d) DTA studies of copper sulphate penta hydrate
  - e) Spectrochemical series- evaluation of Dq value.

**SUGGESTED BOOKS**

1. A Text Book of quantitative Inorganic Analysis- 5<sup>th</sup> edition- A. I. Vogel.
2. Experimental inorganic chemistry- G. Palmer
3. Inorganic synthesis- O. Glemser.
4. Experimental Inorganic/Physical chemistry- Mounir A. Malati.
5. Instrumental analysis manual- Modern experiments for Laboratory- G G. Guilbault and L.G. Hargis

**CPP-2.6(2.2) PRACTICAL: PHYSICAL CHEMISTRY**

1. Verification of Beer's Law for  $\text{Cu}^{2+}$  ions
2. Verification of Beer's Law for  $\text{Fe}^{2+}$  ions
3. Estimation of  $\text{Fe}^{2+}$  ions concentration in the given solution by titration of FAS versus  $\text{KMnO}_4$  through colorimetric method.
4. Estimation of  $\text{Fe}^{2+}$  ions concentration using EDTA through colorimetric method
5. Verification of Freundlich and Langmuir isotherm for adsorption of oxalic/acetic acid on activated charcoal.
6. Study of phase diagram of a three component liquid-liquid-liquid systems.
7. Study of phase diagram of a three component solid-solid-liquid systems.
8. Determine the degree of association and association constant of benzoic acid in benzene/toluene.
9. Phase diagram of two component systems and determination of  $E_c$ ,  $E_T$  and the determination of the composition of given unknown.
10. Determination of the equivalent conductance of a weak acid at different concentrations and verification of Ostwald's dilution law.
11. Determination of equivalent conductance of a strong electrolyte at different concentrations and examine the validity of the Onsager's theory as limiting law at high dilutions.
12. Determination of the activity co-efficient of zinc ions in the solution of 0.002 M Zinc sulphate using Debye-Huckel limiting law.
13. Conductometric titrations of a mixture of  $\text{HCl}$ ,  $\text{CH}_3\text{COOH}$  and  $\text{CuSO}_4$  and  $\text{NaOH}$ .
14. Determination of the dissociation constant of an acid at different dilution by conductance measurements.
15. Compare the relative strength of acetic acid and mono chloroacetic acid by conductance method.
16. Determine the electrode potentials of Zn and Ag electrodes in 0.1M and 0.001M solutions at 298 K and find the standard potentials for these electrodes and test the validity of Nernst equation.
17. Determine the dissociation constant of weak acids by potentiometric method.
18. Determination of redox potential and estimation of  $\text{Fe}^{2+}$  ions by potentiometric method.
19. Potentiometric titration of a mixture of halides ( $\text{KCl} + \text{KI}$  and  $\text{KCl} + \text{KBr} + \text{KI}$ ) against  $\text{AgNO}_3$
20. Potentiometric titration of  $\text{KI}$  Vs  $\text{KMnO}_4$  solution.
21. Conductometry – to determine the degree of hydrolysis and hydrolysis constant of aniline hydrochloride.

**SUGGESTED BOOKS**

1. Practical Physical chemistry – A.J. Findlay.
2. Experimental Physical Chemistry – F. Daniels et al.
3. Selected Experiments in Physical Chemistry – Latham.

4. Experiments in Physical Chemistry – James and Prichard.
5. Experiments in Physical Chemistry – Shoemaker.
6. Advanced Physico – Chemical experiments – J. Rose.
7. Practical Physical Chemistry. - S.R. Palit.
8. Experiments in Physical Chemistry – Yadav, Geol Publishing House.
9. Experiments in Physical Chemistry – Palmer.
10. Experiments in Chemistry – D.V. Jahagirdar, Himalaya Publishing House, Bombay, (1994)
11. Experimental physical chemistry, R. C. Das and B. Behera, Tata McGraw-Hill Publishing Company Limited, 1983.
12. Experimental Physical Chemistry, V. D. Athawale and Parul Mathur, New Age International (p) Limited, Publishers, New Delhi, 2001.

#### **SPP-2.7.1(2.3A) PRACTICAL: ORGANIC CHEMISTRY-A**

**Qualitative analysis:** Systematic analysis and identification of organic compounds.

#### **SPP-2.7.2(2.3B) PRACTICAL: ORGANIC CHEMISTRY-B**

##### **ISOLATION**

1. Isolation of piperine from pepper
2. Isolation of caffeine from tea
3. Isolation of cysteine from hair
4. Isolation of hesperidiene from orange peel
5. Isolation of azaleic acid from castor oil
6. Isolation and spectroscopic characterization of Lycopene
7. Isolation of lipids from egg yolks
8. Extraction of nicotine from tobacco leaves
9. Isolation of casein from milk
10. Isolation of lycopene from tomato
11. Isolation of  $\beta$ -carotene from carrots.

#### **OEP-2.8 (2.4) PRACTICAL: CHEMISTRY OF FOODS - I**

1. Determination of Water Activity of different foods
2. Determination of viscosity of liquid foods
3. Determination of Specific gravity & refractive index for different foods
4. Odors and Physical State of Lipids and Fatty Acids
5. Determination of Water-Absorbing Capacity
6. Determination of Oxidative Rancidity
7. Quantitative Determination of Protein in Foods by the Biuret Method
8. Determination of total dissolved solids

##### **Reference Books**

1. Practical Inorganic Chemistry, G. Marr and B. W. Rockett, Von Nostrand Reinhold Co., London (1972).
2. Findlays practical physical chemistry revised by P. B. Levitt, Longman's London (1966).
3. Experiments in Physical Chemistry by Shoemaker and Garland, McGraw Hill International Edn. (1966)

4. Advanced Practical Physical Chemistry by J. B. Yadav, Goel Publications Meerut (1988)
5. Senior Practical Physical Chemistry by B. C. Kosla, Simla Printers New Delhi (1987)
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9. Comprehensive organic chemistry, D. Barton and W. D. Wallis, Pergamon Press, Oxford, 1983.
10. Organic chemistry Vol. II, I. L. Finar 6<sup>th</sup> Edn. Longman, 1992.
11. Organic reaction Mechanisms, 3<sup>rd</sup> Edn., V. K. Ahluwalia and R. K. Prashar, Narosa, New Delhi, 2005.
12. Vogel's Text book of Qualitative Chemical Analysis, J. Bassett, G. H. Jeffery and J. Mendham, ELBS (1986).
13. Principles of Food Chemistry by John M. deMan.
14. Principles of Food Science, Part I, Food Chemistry edited by Owen R. Fennema, Marel Dekker, Inc., New York.

**III –SEM****CPP-3.5(3.1) PRACTICAL: ORGANIC CHEMISTRY****Preparation (Two and three stages)**

1. Preparation of 2,4-Dinitrophenylhydrazine from chloronitrobenzene.
2. Preparation of Anthranilic acid from phthalic acid.
3. Preparation of Benzanilide from benzophenone.
4. Preparation of Benzilic acid from benzoin.
5. Synthesis of Acridone.
6. Synthesis of Hydantoin.

**CPP 3.6(3.2) PRACTICAL: ORGANIC CHEMISTRY****Quantitative analysis**

1. Titrimetric estimation of amino acids.
2. Saponification value of oil.
3. Estimation of glucose by Feighling's method.
4. Estimation of keto group.
5. Estimation of phenols.
6. Iodine value of oil (chloramine-T method).
7. Estimation of creatinine
8. Estimation of Tannin
9. Estimation of HMF in Honey

**SPP-3.7.1(3.3A) PRACTICAL: ORGANIC CHEMISTRY****Preparations**

1. Preparation of NBS from succinic acid and its application in allylic bromination reactions.
2. Preparation of benzpinacolone from benzophenone.
3. Generation of benzyne and its trapping with tetracyclone.
4. Preparation of 2-phenylindole from phenylhydrazine
5. Anthrone from Anthracene.
6. Synthesis of stilbene.
7. Synthesis of benzocaine from 4-nitrobenzoic acid.
8. Preparation of tetraphenyldihydrophthalic anhydride from N-phenylglycine.
9. Preparation of PAS from p-nitro salicylic acid.
10. Preparation of sulfanilamide from acetanilide
11. Preparation of cinnamic acid from perkin reaction.
12. Preparation of mefenamic acid from anthranilic acid.

**SPP-3.7.2(3.3B) PRACTICAL: ORGANIC CHEMISTRY****Qualitative Analysis**

Separation of a binary mixture of organic compounds and identification of the separated components by systematic qualitative organic analysis. (8 different mixtures)

**OEP-3.8(3.4) PRACTICAL: CHEMISTRY OF FOODS - II**

1. Determination of Water soluble vitamins: (B1, B2, B3, B12, C and folic acid) (Visible spectrophotometric technique).
2. Methods of determination of fat soluble vitamins: (A, D, E and K) (visible spectrophotometric technique).
3. Estimation of Vitamin –C in fruit juice by titrimetric method.
4. Estimation of glucose by DNS method.
5. Estimation of glucose by Benedict's titrimetric method.
6. Estimation of total carbohydrates by anthrone method.
7. Estimation of iron in apple juice by phenanthroline method.
8. Determination of iodine value of oil.
9. Separation of amino acids by paper chromatography.

**Reference Books**

1. Understanding organic reaction mechanisms, A. Jacob, Cambridge Univ Press, 1997.
2. Introduction to organic chemistry, A. Streitweiser, Jr and C. H. Heathcock, Macmillan, 1985.
3. Physical and mechanistic organic chemistry, R. A.Y. Jones, 1<sup>st</sup> Edn. Cambridge Univ Press, 1979.
4. Modern synthetic reactions, H. O. House, W. A. Benjamin, California, 2<sup>nd</sup> Edn. 1972.
5. Some modern methods of organic synthesis, W. Carruthers, Cambridge Univ. Press, London, 2<sup>nd</sup> Edn. 1978.
6. Mechanisms of molecular migration, Vols I & II, B.S. Thyagarajan, Pergamon Press, Oxford, 1979.
7. Comprehensive organic chemistry, D. Barton and W. D. Wallis, Pergamon Press, Oxford, 1983.
8. Organic chemistry Vol. II, I. L. Finar 6<sup>th</sup> Edn. Longman, 1992.
9. Organic reaction Mechanisms, 3<sup>rd</sup> Edn., V. K. Ahluwalia and R. K. Prashar, Narosa, New Delhi, 2005.
10. Vogel's Text book of Qualitative Chemical Analysis, J. Bassett, G. H. Jeffery and J. Mendham, ELBS (1986).
11. Principles of Food Chemistry by John M. deMan.
12. Principles of Food Science, Part I, Food Chemistry edited by Owen R. Fennema, Marel Dekker, Inc., New York.
13. Hand book of Food and Nutrition by M. Swaminathan



**IV –SEM****CPP-4.5(4.1) PRACTICAL: ORGANIC CHEMISTRY**

1. Preparation of 2,4,5-triphenyloxazole from benzoin
2. Biosynthesis of ethanol from sucrose.
3. Synthesis of Methyl Red
4. Synthesis of 1-bromo-2-naphthol from 2-naphthol
5. Synthesis of Hippuric acid
6. 1,2,3,4- Tetrahydrocarbazole
7. Diels-Alder reaction of anthracene with maleic anhydride
8. Synthesis of 2,3-diphenylquinoxaline
9. Synthesis of Substituted 4-amino-5-mercapto-1,2,4-triazoles
10. Synthesis of Benzimidazoles
11. Synthesis of Benzofuran
12. Synthesis of Quinoxalines
13. Synthesis of 7-hydroxy-4-methyl-coumarin
14. Synthesis of Thiobarbituric acid
15. Synthesis of Indole derivative from phenyl hydrazine
16. Synthesis of 1,3-oxazolone derivative from benzoyl glycine

**CPP-4.6(4.2) PRACTICAL: ORGANIC CHEMISTRY****Quantitative Analysis**

1. Estimation of Nitro group by reduction using  $\text{SnCl}_2$ .
2. Estimation of Nitrogen by Kjeldahl's method.
3. Estimation of an acid in presence of an amide.
4. Estimation of an ester in the presence of an acid.
5. Estimation of amine group by acetylation method
6. Estimation of OH group by acetylation method
7. Estimation of amide group
8. Estimation of equivalent weight of an acid group by titrimetric method.
9. Estimation of methyl ketone
10. Estimation of fat or an oil
11. Estimation of sulphur in an organic compound

**SPP-4.7(4.3A/B) PRACTICAL: ORGANIC SPECTROSCOPY AND  
MEDICINAL CHEMISTRY - II****Instrumental Methods in Organic Analysis and Spectral Interpretation****A. Estimation of different class of drugs using instrumental methods**

(A minimum of 06 drug sample analysis has to be done).

1. Assay of Ibuprofen
2. Assay of Diclofenac
3. Assay of Analgin
4. Assay of Ephedrine hydrochloride
5. Assay of Benzocaine
6. Assay of sulfadiazine

7. Assay of ascorbic acid
8. Assay of Benzyl penicillin
9. Assay of Dapsone
10. Assay of Aspirin
11. Assay of paracetamol

**B. Recording/predicting/downloading from web sites the UV, IR, NMR and GC- MS/mass spectra of the compounds prepared in Organic Practical's and Structural elucidation of organic compounds with the help of spectra provided by the instructors/examiners. (A minimum of 10 spectral analyses has to be done).**

### Reference Books

1. Advanced organic chemistry, J. March, 4<sup>th</sup> Edn. John Wiley, 2008.
2. Organic synthesis, R.E.Ireland, Prentice-hall India, New Delhi,1975.
3. Understanding organic reaction mechanisms, A. Jacob, Cambridge Univ Press, 1997.
4. Introduction to organic chemistry, A. Streitweiser, Jr and C. H. Heathcock, Macmillan, 1985.
5. Physical and mechanistic organic chemistry, R. A.Y. Jones, 1<sup>st</sup> Edn. Cambridge Univ Press, 1979.
6. Modern synthetic reactions, H. O. House, W. A. Benjamin, California, 2<sup>nd</sup> Edn. 1972.
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11. Vogel's Text book of Qualitative Chemical Analysis, J. Bassett, G. H. Jeffery and J. Mendham, ELBS (1986).
12. Vogel's text book of Quantitative Chemical Analysis, 5<sup>th</sup> Edition, J. Bassett, G. H. Jeffery and J. Mendham, and R. C. Denny, Longman Scientific and Technical (1999).
13. Introduction to Molecular Spectroscopy, C. N. Banwell, TMH Edition (1994).
14. Introduction to Molecular Spectroscopy, G. M. Barrow, McGraw Hill (Int. Students Edition) (1988).
15. Burgers medicinal chemistry M. E. Welly Medicinal Chemistry M.E. Walffed John willey and sons, Vo 1, 2 and 3. Wilson and Giswold's, Text Book of Organic and Medicinal Chemistry.

M.Sc., OC Syllabus

**CORE PAPER DISSERTATION PRACTICAL**

**(32 H)**

**CHAIRMAN (BOS in OC)**