

Address : UNIREG
Telephone No. : 2419677/2419361
Fax : 0821-2419363/2419301

e-mail : registrar@uni-mysore.ac.in
www.uni-mysore.ac.in

UNIVERSITY OF MYSORE



Estd. 1916

VISHWAVIDYANILAYA KARYA SODHA
CRAWFORD HALL, POST BOX NO. 406
MYSORE-570 005

No.AC.2(S)/401/13-14

Dated: 24-05-2014

NOTIFICATION

Sub: Restructuring the Curriculum of Organic Chemistry (PG) programme.

Ref: 1. Proceedings of Faculty of Science & Technology Meeting held on 14-02-2014.
2. Proceedings of the Meeting of Academic Council held on 29-03-2014.

The Board of Studies in **Organic Chemistry (PG)** at its meeting held on 07-12-2013 has resolved to restructuring the existing syllabus of Organic Chemistry (PG) to be effective from the academic year 2014-15 onwards.

The Faculty of Science and Technology and the Academic Council at their meetings held on 14-02-2014 and 29-03-2014 respectively approved the above proposals and the same is hereby notified.

The copy of restructuring the existing syllabus of Organic Chemistry (PG) is annexed herewith.

To

1. The Registrar (Evaluation), University of Mysore, Mysore.
2. The Chairperson, BOS/DOS in Chemistry, MGM.
3. The Dean, Faculty of Science & Technology, DOS in Zoology, MGM.
4. The Principals of the Affiliated Science Colleges.
5. The Deputy/Assistant Registrar (Evaluation), University of Mysore, Mysore.
6. Sri Narasimha Murthy, Statistician, E.B. UOM, Mysore.
7. The Supdt AC.1 & AC.2, A.B., Academic Section / PMEB, UOM., Mysore.
8. The P.A. to the Vice-Chancellor/Registrar/Registrar (Evaluation), UOM., Mysore.
9. The Case Worker, AC.7, Academic Section, University of Mysore, Mysore.
10. The Section Guard File(Supdt.AC.2), A.B., A.C., UOM.
11. The Schedule File.

Jay S. Sampath
REGISTRAR
UNIVERSITY OF MYSORE
MYSORE

UNIVERSITY OF MYSORE

Established



1916

**SYLLABUS FOR M. Sc. DEGREE COURSE
(CHOICE BASED CREDIT SEMESTER SCHEME)**

ORGANIC CHEMISTRY

2014-15

M. Sc Course in Organic Chemistry
Syllabus

	Title of the paper	Credits	L	T	P	Duration of examination in hour	Marks in the examination	
	I Semester						theory	practical
	Hard core papers							
OCI HCT: 1.1	Concepts and Models of Inorganic Chemistry	4	2	0	2	3	70+30, (70+30)	
OCO HCT: 1.2	Reaction Mechanism	4	2	0	2	3	70+30 (70+30),	
OCP HCT: 1.3	Physical Chemistry - I	4	2	0	2	3	70+30 (70+30),	
OCG HCT: 1.4	Symmetry, Group Theory and Chemical Spectroscopy	3	3	0	0	3	(70+30),	
	Soft core papers							
OCA SCT: 1.51	Fundamentals of Chemical Analysis	4 ^a	2	0	2	3	70+30 (70+30),	
OCI SCT: 1.52	chemistry of selected elements	2	2	0	0	3	(70+30),	
OCO SCT: 1.53	Vitamins, green chemistry and medicinal chemistry	2	2	0	0	3	(70+30),	
OCP SCT: 1.54.	biophysical chemistry and pharmacokinetics	2	2	0	0	3	(70+30),	
	Total credits	25						

II Semester

	Title of the paper	Credits	L	T	P	Duration of examination in hour	Marks in the examination	
							theory	practical
	Hard core papers							

OCI HCT: 2.1	coordination chemistry	4	2	0	2	3	70+30 (70+30),
OCO HCT: 2.2	Stereochemistry and heterocyclic chemistry	4	2	0	2	3	70+30 (70+30),
OCP HCT: 2.3	Physical Chemistry - II	4	2	0	2	3	70+30 (70+30),
OCG HCT: 2.4	Spectroscopy	3	3	0	0	3	(70+30),
Soft core papers							
OCA SCT: 2.51	Separation techniques	4 ^a	2	0	2	3	70+30 (70+30),
OCI SCT: 2.52	Industrial inorganic chemistry	2	2	0	0	3	(70+30),
OCO SCT: 2.53	Dyes & Insecticides	2	2	0	0	3	(70+30),
OCP SCT: 2.54.	Nanomaterials, semi conductors and super conductors	2	2	0	0	3	(70+30),
Total credits		25					
OPEN ELECTIVE							
OCO OET 2.61	Applications of synthetic products	3	3	0	0		(70+30),
OCO OET 2.62:	Natural and synthetic products	3	3	0	0		(70+30),

III Semester

	Title of the paper	Credits	L	T	P	Duration of examination	Marks in the examination
--	--------------------	---------	---	---	---	----------------------------	-----------------------------

							in hour	
								theory practical
Hard core papers								
OCO HCT: 3.1	Reagents in organic synthesis	4	2	0	2	3		70+30 (70+30),
OCO HCT: 3.2	Synthetic organic chemistry	4	2	0	2	3		70+30 (70+30),
OCO HCT: 3.3	Photochemistry, Pericyclic reactions and heterocyclic chemistry	3	3	0	0	3		(70+30),
		Soft core papers						
OCO SCT 3.41	Carbohydrates, proteins and nucleic acids	3	3	0	0	3		(70+30),
OCO SCT 3.42:	Metals in Organic chemistry and Food Analysis	3	3	0	0	3		(70+30),
OCO SCT 3.43	Enzymes functions and their kinetics	3	2	0	2	3		(70+30),
	Total credits	20						700
	OPEN ELECTIVE							
OCO OET 3.61	Applications of synthetic products	3	3	0	0			(70+30),
OCO OET 3.62:	Natural and synthetic products	3	3	0	0			(70+30),

IV Semester

	Title of the paper	Credits	L	T	P	Duration of examination in hour	Marks in the examination	
							theory	practical
Hard core papers								
OCO HCT 4.1	Lipids, Porphyrins, anthocyanins and flavonoids	4	2	0	2	3	70+30 (70+30),	
OCO HCT:4.2	molecular rearrangements, retrosynthesis, and organo metallic compounds	3	3	0	0	3	70+30 (70+30),	
OCO HCT: 4.3	Dissertation	4	4	0	0	3	(70+30),	
		Soft core papers						
OCO SCT 4.41	Advanced Medicinal chemistry	3	3	0	0	3	(70+30),	
OCO SCT 4.42:	Steroids, Alkaloids and Polymer Chemistry	3	3	0	0	3	(70+30),	
OCO SCT 4.43	Industrial Chemicals	3		0	0	3	(70+30),	
Total credits		20					700	

GENERAL REQUIREMENTS

1. All hard core papers are compulsory.

2. Twenty soft core credits have to be taken in four semesters.
3. The students who have studied or opted as hard core/soft core subjects in any other or in the respective departments, are not eligible for opting these subjects.
4. Minimum of 10 students are eligible to study open electives in the department.
5. Open elective subjects are only for students of departments other than chemistry and organic chemistry.
6. Admission rules and regulations are laid down as per the University of Mysore.
7. **DISSERTATION:** Preparation of dissertation on the topic assigned. This include literature collection, identification of objectives, methodology followed, analytical instruments used, data collected, analysis of data, data synthesis and conclusions. The material collected has to be submitted in a bound volume from one month before the commencement of practical examination. A certificate has to be enclosed stating that the material collected and presented in the Dissertation has not been submitted for the award of any Dissertation/Degree in this University or in any other University signed by the candidate and the guide.

Chairman
BOS in Organic chemistry

FIRST SEMESTER

OCI HCT: 1.1. CONCEPTS AND MODELS OF INORGANIC CHEMISTRY

UNIT – I

Chemical Periodicity: Review of periodic properties.

Structures and energetics of ionic crystals: Introduction, MX (NaCl, CsCl, ZnS) and MX₂ (fluorite, rutile, β-cristobalite and cadmium iodide) types. The perovskite and spinel structures. Thermodynamics of ionic crystal formation. Lattice energy, Born-Haber cycle, Born-Lande equation. Applications of lattice energetics. Radius ratio rules.

Structures and energetics of inorganic molecules: Introduction, Energetics of hybridization. VSEPR model for explaining structure of AB, AB₂E, AB₃E, AB₂E₂, ABE₃, AB₂E₃, AB₄E₂, AB₅E and AB₆ molecules. M.O. treatment of homonuclear and heteronuclear diatomic molecules. M.O. treatment involving delocalized π-bonding (CO₃²⁻, NO₃⁻, NO₂⁻, CO₂ and N₃⁻), M.O. correlation diagrams (Walsh) for triatomic molecules. [16 Hrs]

UNIT – II

Modern concept of acids and bases: Lux-Flood and Usanovich concepts, solvent system and leveling effect. Hard-Soft Acids and Bases, Classification and Theoretical backgrounds.

Non-aqueous solvents: Classification of solvents, Properties of solvents (dielectric constant, donor and acceptor properties) protic solvents (anhydrous H₂SO₄ and HF) aprotic solvents (liquid SO₂, BrF₃ and N₂O₄). Solutions of metals in liquid ammonia, hydrated electron. Super acids.

Inner transition elements: Spectral and magnetic properties, redox chemistry.

Applications: Lanthanides as shift reagents, high temperature super conductors.

Chemistry of trans-uranium elements.

[16 Hrs]

References:

1. Basic Inorganic Chemistry – 3rd edition. F.A. Cotton, G. Wilkinson and P.L. Gaus, John Wiley and Sons (2002).
2. Inorganic Chemistry, 3rd edition. James E. Huheey, Harper and Row Publishers (1983).
3. Inorganic Chemistry, 3rd edition. G.L. Miessler and D.A. Tarr, Pearson Education (2004).

4. Inorganic Chemistry, 2nd edition. D.F. Shriver, P.W. Atkins and C.H. Langford, Oxford University Press (1994).
5. Inorganic Chemistry, 2nd edition. C.E. Housecroft and A.G. Sharpe, Pearson Education Ltd. (2005).
6. Introduction to Modern Inorganic Chemistry, K.M. Mackay and R.A. Mackay, Blackie Publication (1989).
7. Concepts and Models of Inorganic Chemistry 3rd edition. B.E. Douglas, D.H. McDaniel and Alexander, Wiley (2001).

INORGANIC CHEMISTRY PRACTICALS-I [16 Hrs]

1. Determination of iron in haematite using cerium(IV) solution (0.02M) as the titrant, and gravimetric estimation of insoluble residue.
2. Estimation of calcium and magnesium carbonates in dolomite using EDTA titration, and gravimetric analysis of insoluble residue.
3. Determination of manganese dioxide in pyrolusite using permanganate titration.
4. Quantitative analysis of copper-nickel in alloy/mixture:
 - i. Copper volumetrically using KIO_3 .
 - ii. Nickel gravimetrically using DMG
5. Determination of lead and tin in a mixture: Analysis of solder using EDTA titration.
6. Quantitative analysis of chloride and iodide in a mixture:
 - i. Iodide volumetrically using KIO_3
 - ii. Total halide gravimetrically
7. Gravimetric analysis of molybdenum with 8-hydroxyquinoline.
8. Quantitative analysis of copper(II) and iron(II) in a mixture:
 - i. Copper gravimetrically as CuSCN and
 - ii. Iron volumetrically using cerium(IV) solution
9. Spectrophotometric determinations of:
 - a. Titanium using hydrogen peroxide
 - b. Chromium using diphenyl carbazide in industrial effluents
 - c. Iron using thiocyanate/1,10-phenanthroline method in commercial samples
 - d. Nickel using dimethylglyoxime in steel solution

10. Micro-titrimetric estimation of :
 - a) Iron using cerium(IV)
 - b) Calcium and magnesium using EDTA
11. Quantitative estimation of copper(II), calcium(II) and chloride in a mixture.
12. Circular paper chromatographic separation of: (Demonstration)
 - a. Iron and nickel
 - b. Copper and nickel

References:

1. Vogel's Text Book of Quantitative Chemical Analysis – 5th edition, J. Basset, R.C. Denney, G.H. Jeffery and J. Mendhom.
2. A Text Book of Quantitative Inorganic Analysis by A.I. Vogel, 3rd edition.
3. Spectrophotometric Determination of Elements by Z. Marczenko.
4. Vogel's Qualitative Inorganic Analysis – Svelha.
5. Macro and Semimicro Inorganic Qualitative Analysis by A.I. Vogel.
6. Semimicro Qualitative Analysis by F.J. Welcher and R.B. Halin.
7. Quantitative Chemical Analysis by Daniel C. Harris, 7th edition, (2006).

OCO HCT: 1.2. REACTION MECHANISMS

UNIT – I:

Basics of organic reactions: Meaning and importance of reaction mechanism, classification and examples for each class.

Bonding in organic systems: Theories of bonding-molecular orbital approaches. Huckel molecular orbital theory and its application to simple π -systems: ethylene, allyl, cyclopropyl, butadienyl, cyclopentadienyl, pentadienyl, hexatrienyl, cyclohexatrienyl, heptatrienyl, cycloheptatrienyl systems. Calculation of the total π -energy, and M.O. coefficients of the systems.

Aromaticity: Concept of aromaticity, Huckel's rule, Polygon rule, annulenes, heteroannulenes and polycyclic systems.

Structure and reactivity: Brief discussion on effects of hydrogen bonding, resonance, inductive and hyperconjugation on strengths of acids and bases.

Methods of determining organic reaction mechanism: Thermodynamic and kinetic requirements for reactions, kinetic and thermodynamic control. Identification of products.

Formation, structure, stability, detection and reactions of carbocations (classical and non-classical), carbanions, free radicals, carbenes, nitrenes, arynes and ylides (Sulphur, nitrogen and phosphorous). Determination of reaction intermediates, isotope labeling and effects of cross over experiments. Kinetic and stereochemical evidence, solvent effect. [16 Hrs]

UNIT – II:

Substitution reactions – Kinetics, mechanism and stereochemical factor affecting the rate of S_N^1 , S_N^2 , S_{RN}^i , S_N^i , $S_N^{1'}$, $S_N^{2'}$, S_N^{li} and SRN^1 reactions, Neighbouring group participation.

Electrophilic substitution reactions – Kinetics, mechanism and stereochemical factor affecting the rate of S_E1 & S_E2

Aromatic electrophilic substitution reactions: Mechanism of nitration, halogenation, sulphonation, Friedel-Crafts alkylation and acylation, Mannich reaction, chloromethylation, Vilsmeier Haack reaction, Diazonium coupling, Gattermann–Koch reaction, Mercuration reaction.

Aromatic nucleophilic substitution reactions: S_N^1 , S_N^2 and benzyne mechanism, Bucherer reaction, von Richter reaction.

Mechanism of Addition reactions: Addition to C-C multiple bonds involving electrophiles, nucleophiles. Markownikoff's rule and anti-Markownikoff's rule.

Additions to carbonyl compounds: Addition of water, alcohol, bisulphate, HCN and amino compounds.

Elimination reactions: Mechanism and stereochemistry of eliminations - E1, E2, E1cB. cis elimination, Hofmann and Saytzeff eliminations, competition between elimination and substitution, decarboxylation reactions. Chugaev reaction. [16 Hrs]

References:

- 1.. H. Pine, Hendrickson, Cram and Hammond, Organic Chemistry, Mc Graw Hill, New York, 1987.
2. I.L. Finar, Organic Chemistry, ELBS Longmann, Vol. I & II, 1984.

3. N.S. Issacs, Reactive Intermediates in Organic Chemistry, John Wiley and Sons, New York.1974.
4. R.K. Bansal, Organic Reaction Mechanism, Wiley Eastern Limited, New Delhi, 1993.
5. J. March, Advanced Organic Chemistry, Wiley Interscience, 1994.
6. A Guide Book to Mechanism in Organic Chemistry by Petersykes
7. F.A. Carey and Sundberg, Advanced Organic Chemistry – Part A & B, 3rd edition, Plenum Press, New York, 1990.
8. E. S. Gould, Mechanism and Structure in Organic Chemistry, Halt, Rinhart & Winston, New York, 1964.
9. S.K. Ghosh, Advanced General Organic Chemistry, Book and Alleied (P) Ltd, 1998.

ORGANIC CHEMISTRY PRACTICALS-I [64 Hrs]

Material Safety Data Sheet (MSDS): Analysis of MSDS for all chemicals, noting the hazards and biological effects in the laboratory note book before doing the experiment.

Organic Preparations: Preparations involving oxidation, reduction, dehydration, nitration, diazotization, cyclization, condensation, addition reactions. Report the yield and cost per Kg of the product synthesized and the cost from the catalogue.

1. Preparation of aniline from nitrobenzene (Reduction).
2. Preparation of p-nitroacetanilide from acetanilide.
3. Preparation of n-butyl bromide from n-butanol.
4. Preparation of p-iodonitrobenzene from p-nitroaniline.
5. Preparation of osazone derivative.
6. Preparation of penta-O-acetyl-D-glucose from glucose.
7. Preparation of *cis* and *trans* cinnamic acid.
8. Preparation of phenoxy acetic acid.
9. Preparation of hippuric acid from glycine.
10. Preparation of p-nitrobenzoic acid from p-nitrotoluene (Oxidation).
11. Preparation of 7-hydroxy-4-methyl coumarin.

12. Preparation of m-nitrobenzoic acid from methyl benzoate.
13. Preparation of aspirin.
14. Preparation of Tetrahydrocarbazole from cyclohexanone (Fischer indole synthesis).

References:

1. Manual of Organic Chemistry - Dey and Seetharaman.
2. Modern Experimental Organic Chemistry by John H. Miller and E.F. Neugil, p 289.
3. An Introduction to Practical Organic Chemistry - Robert, Wingrove etc.
4. A Text Book of Practical Organic Chemistry – A.I. Vogel, Vol.III
5. Practical Organic Chemistry - Mann & Saunders 6. Semimicro Qualitative Organic Analysis by Cheronis, Entrikin and Hodnet .

OCP HCT: 1.3. PHYSICAL CHEMISTRY - I

UNIT-I

Concepts of entropy and free energy: A brief resume of laws of thermodynamics (First and second laws). Entropy as a measure of unavailable energy. Entropy change during spontaneous process. Helmholtz and Gibbs free energies. Thermodynamic criteria of equilibrium and spontaneity. Variation of free energy with temperature and pressure. Maxwell's relations. Third law of thermodynamics - calculation of absolute entropies. Nernst heat theorem & its applications.

Partial molar properties: Partial molar volumes and their determination by intercept method and from density measurements. Chemical potential and its significance. Variation of chemical potential with temperature and pressure. Formulation of the Gibbs - Duhem equation. Derivation of Duhem-Margules equation.

Fugacity: Concept of fugacity, 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 co-efficients by vapour pressure, depression in freezing point, solubility measurements by electrical methods.

Thermodynamics of dilute solutions: Raoult's law, Henry's law. Ideal and non-ideal solutions.

[16 Hrs]

UNIT- II

Chemical Kinetics: Determination of order of reactions, complex reactions - parallel, consecutive and reversible reactions. Chain reactions - Branched chain reactions- general rate expression, explosion limits.

Theories of reaction rates: Collision theory and its limitations, Activated complex theory (postulates -derivation) and its applications to reactions in solution. Energy of activation, other activation parameters - determinations and their significance. Lindemann theory of unimolecular reactions. Qualitative account of its modifications (no derivation).

Potential energy surfaces: Features and construction, theoretical calculations of E_a .

Reactions in solution: Ionic reactions - salt and solvent effects. Effect of pressure on the rates of reactions. Cage effect with an example. Oscillatory reactions.

Fast reactions- Study of fast reactions by continuous and stopped flow techniques, relaxation methods (T-jump and P-jump methods), flash photolysis, pulse and shock tube methods.

[16 Hrs]

Reference text books

1. Physical Chemistry by P.W. Atkins, ELBS, 5th edition, Oxford University Press (1995).
2. Text Book of Physical Chemistry by Samuel Glasstone, MacMillan Indian Ltd., 2nd edition (1974).
3. Elements of Physical Chemistry by Lewis and Glasstone.
4. Fundamentals of physical chemistry – Maron and Lando (Collier Macmillan) 1974.
5. Thermodynamics for Chemists by S. Glasstone, Affiliated East-West Press, New Delhi, (1965).
6. Chemical Thermodynamics by I.M. Klotz, W.A. Benzamin Inc. New York, Amsterdam (1964).
7. Chemical Kinetics by K.J. Laidler.
8. Chemical Kinetics by Frost and Pearson.
9. Kinetics and Mechanism of Chemical Transformation by J. Rajaram and J.C. Kuriacose.
10. Chemical Kinetics by L.K. Jain.
11. Chemical Kinetics by Benson.

PHYSICAL CHEMISTRY PRACTICALS – I

[16 Hrs]

1. Study of kinetics of hydrolysis of an ester using HCl/H₂SO₄ at two different temperatures, determination of rate constants and energy of activation.
2. Study of kinetics of reaction between K₂S₂O₈ and KI, first order, determination of rate constants at two different temperatures and E_a .

3. To study the kinetics of saponification of ethyl acetate by conductivity method, determination of rate constant.
4. Conductometric titration of a mixture of HCl and CH₃COOH against NaOH.
5. Conductometric titration of sodium sulphate against barium chloride.
6. Determination of equivalent conductance at infinite dilution of a strong electrolytes and verification of Onsager equation.
7. Potentiometric titration of KI vs KMnO₄ solution.
8. Determination of dissociation constant of a weak acid by potentiometric method.
9. Potentiometric titration of AgNO₃ vs KCl.
10. To obtain the absorption spectra of coloured complexes, verification of Beer's law and estimation of metal ions in solution using a spectrophotometer.
11. Spectrophotometric titration of FeSO₄ against KMnO₄.
12. Determination of heat of solution of benzoic acid by variable temperature method (graphical method).
13. Kinetics of photodegradation of indigocarmine (IC) using ZnO/TiO₂ as photocatalyst and study the effect of [ZnO/TiO₂] and [IC] on the rate of photodegradation.
14. Determination of the molecular weight of a polymer material by viscosity measurements (cellulose acetate/methyl acrylate).
15. Analysis of a binary mixture (Glycerol & Water) by measurement of refractive index.
16. Determination of degree of association of benzoic acid in benzene by distribution method.

Reference text 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 Mc Graw Hill.

OCG HCT: 1.4. SYMMETRY, GROUP THEORY AND CHEMICAL SPECTROSCOPY

UNIT-I

Molecular symmetry and group theory: Symmetry elements and symmetry operations. Concept of a group, definition of a point group. Classification of molecules into point groups. Subgroups. Schoenflies and Hermann-Mauguin symbols for point groups. Multiplication tables (C_n , C_{2v} and C_{3v}). Matrix notation for the symmetry elements. Classes and similarity transformation.

Representation of groups: The Great Orthogonality theorem and its consequences. Character tables (C_s , C_i , C_2 , C_{2v} , C_{2h} and C_{3v}). Symmetry and dipole moment.

Applications of group theory: Group theory and hybrid orbital. Group theory to Crystal field theory and Molecular orbital theory (octahedral and tetrahedral complexes). Determining the symmetry groups of normal modes (both linear and non-linear molecules).

[16 Hrs]

UNIT – II

Microwave spectroscopy: Rotation spectra of diatomic Molecules - rigid and non rigid rotator model. Rotational quantum number and the selection rule. Effect of isotopic substitution on rotation spectra. Relative intensities of the spectral lines. Classification of polyatomic molecules based on moment of inertia - Linear, symmetric top, asymmetric top and spherical molecules. Rotation spectra of polyatomic molecules (OCS CH_3F and BCl_3). Moment of inertia expression for linear tri-atomic molecules. Applications - Principles of determination of Bond length and moment of inertia from rotational spectra. Stark effect in rotation spectra and determination of dipole moments.

Vibration spectroscopy: Vibration of diatomic molecules, vibrational energy curves for simple harmonic oscillator. Effects of anharmonic oscillation. Vibration - rotation spectra of carbon monoxide. Expressions for fundamental and overtone frequencies. Vibration of polyatomic molecules – The number of degrees of freedom of vibration. Parallel and perpendicular vibrations (CO_2 and H_2O). fundamental, overtone, combination and difference

bands. Fermi resonance. Force constant and its significance. Theory of infrared absorption and theoretical group frequency. Intensity of absorption band and types of absorptions. Correlation chart. Important spectral regions - hydrogen stretching region, double and triple bonds regions, fingerprint region. Factors affecting the group frequency – Physical state, vibrational coupling, electrical effect, hydrogen bonding, steric effect and ring strain. Applications: Structures of small molecules: XY_2 – linear or bent, XY_3 – planar or pyramidal.

[16 hrs]

UNIT – III

Raman spectroscopy: Introduction, Raman and Rayleigh scattering, Stokes and anti-Stokes lines, polarization of Raman lines, depolarization factor, polarizability ellipsoid. Theories of Raman spectra - classical and quantum theory. Rotation-Raman and vibration-Raman spectra. Comparison of Raman and IR spectra, rule of mutual exclusion principle. Vibration modes of some simple molecules and their activity in Raman.

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 π^* , π to π^* , n to σ^* and σ to σ^* , C-T and ligand field.

Woodwards empirical rules for predicting the wavelength of maximum absorption for olefins, conjugated dienes, cyclic trienes and polyenes, α,β -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.

[16 hrs]

Reference text books

1. Chemical Applications of Group Theory, 3rd edition, F.A. Cotton, John Wiley and Sons (2006).
2. Molecular Symmetry and Group Theory – Robert L Carter, John Wiley and Sons (2005).
3. Symmetry in Chemistry - H. Jaffe and M. Orchin, John Wiley, New York (1965).

4. Vibrational Spectroscopy - Theory and Applications- D.N. Sathyanarayana, New Age International Publications, New Delhi (1996).
5. Group Theory and its Chemical Applications - P.K. Bhattacharya, Himalaya Publications, New Delhi (1998).
6. Fundamentals of Molecular Spectroscopy, C.N. Banwell and E.M. McCash. 4th edition, Tata McGraw Hill, New Delhi.
7. Fundamentals of molecular spectroscopy, G. M. Barrow, MgGraw Hill, New York (International students Edition), 1974.
8. Theoretical chemistry, S. Glasstone, affiliated East-West Press Pvt. Ltd, New Delhi, 1973.
9. Introduction to Spectroscopy - Pavia, Lampman and Kriz, 3rd edition, Thomson.
10. Spectroscopy, B.P. Straughan and S. Walker, John Wiley & Sons Inc., New York, Vol. 1 and 2, 1976.
11. Vibration Spectroscopy Theory and Applications, D.N. Satyanarayana, New Age International, New Delhi.
12. Spectroscopy, B.P. Straughan and S. Salker, John Wiley and Sons Inc., New York, Vol.2, 1976.
13. Organic Spectroscopy, William Kemp, English Language Book society, Macmillan, 1987.
14. Instrumental methods of analysis, H. H. Willard, L. L. Merritt and J. A. Dean, 7th Edition, 1988.
15. Physical methods in inorganic chemistry, R. S. Drago, affiliated East-West press Pvt. Ltd., (Student Edition) 1978.

OCA SCT: 1.51 FUNDAMENTALS OF CHEMICAL ANALYSIS

UNIT – I

Analytical Chemistry - Meaning and analytical prospective, scope and function: Analytical problems and their solutions, trends in analytical methods and procedures.

Language of analytical chemistry - Analysis, determination and measurement. Techniques, methods, procedures and protocols. Classifying analytical techniques. selecting an analytical

method - accuracy, precision, sensitivity, selectivity, robustness and ruggedness. Scale of operation, equipment, time and cost. Making the final choice

Errors and treatment of analytical data: Limitations of analytical methods – Error: determinate and indeterminate errors, minimization of errors. Accuracy and precision, distribution of random errors, the normal error curve. Statistical treatment of finite samples - measures of central tendency and variability: mean, median, range, standard deviation and variance. Student's t-test, confidence interval of mean. Testing for significance - comparison of two means and two standard deviations. Comparison of an experimental mean and a true mean. Criteria for the rejection of an observation - Q-test. Propagation of errors: determinate errors and indeterminate errors.

Acid-base titrations in non-aqueous media: Role of solvent in acid-base titrations, solvent systems, differentiating ability of a solvent, some selected solvents, titrants and standards, titration curves, effect of water, determining the equivalence point, typical applications - determination of carboxylic acids, phenols and amines. [16 Hrs]

UNIT – II

Titrimetric analysis: An overview of titrimetry. Principles of titrimetric analysis. Titration curves. Titrations based on acid-base reactions - titration curves for strong acid and strong base, weak acid and strong base and weak base and strong acid titrations. Selecting and evaluating the end point. Finding the end point by visual indicators, monitoring *pH* and temperature. Quantitative applications – selecting and standardizing a titrant, inorganic analysis - alkalinity, acidity and free CO₂ in water and waste waters, nitrogen, sulphur ammonium salts, nitrates and nitrites, carbonates and bicarbonates.

Precipitation titrations: Titration curves, feasibility of precipitation titrations, factors affecting shape - titrant and analyte concentration, completeness of the reaction, titrants and standards, indicators for precipitation titrations involving silver nitrate, the Volhard, the Mohr and the Fajan's methods, typical applications.

Complexometric titrations: Complex formation reactions, stability of complexes, stepwise formation constants, chelating agents, EDTA - acidic properties, complexes with metal ions, equilibrium calculations involving EDTA, conditional formation constants, derivation of EDTA titration curves, effect of other complexing agents, factors affecting the shape of titration curves - completeness of reaction, indicators for EDTA titrations - theory of common

indicators, titration methods employing EDTA - direct, back and displacement titrations, indirect determinations, titration of mixtures. [16 Hrs]

References:

1. Fundamental of Analytical Chemistry, D.A. Skoog, D.M. West, Holler and Crouch, 8th edition, 2005, Saunders College Publishing, New York.
2. Analytical Chemistry, G.D. Christian, 5th edition, 2001, John Wiley & Sons, Inc, India.
3. Quantitative Analysis, R.A. Day and A.L. Underwood, 6th edition, 1993, Prentice Hall, Inc. New Delhi.
4. Vogel's Textbook of Quantitative Chemical Analysis, J. Mendham, R.C. Denney, J.D. Barnes and M.J.K. Thomas, 6th edition, Third Indian Reprint, 2003, Pearson Education Pvt. Ltd., New Delhi.
5. Analytical Chemistry Principles, John H. Kennedy, 2nd edition, Saunders College Publishing, California, 1990.
6. Principles and Practice of Analytical Chemistry, F.W. Fifield and Kealey, 3rd edition, 2000, Blackwell Sci., Ltd. Malden, USA.
7. Modern Analytical Chemistry, David Harvey, McGraw Hill, New Delhi, 2000.

ANALYTICAL CHEMISTRY PRACTICALS [16 Hrs]

1. Determination of total acidity of vinegar and wines by acid-base titration.
2. Determination of purity of a commercial boric acid sample, and Na_2CO_3 content of washing soda.
3. Analysis of chromate-dichromate mixture by acid-base titration.
4. Determination of replaceable hydrogen and relative molecular mass of a weak organic acid by titration with NaOH.
5. Determination of aspirin in their tablet preparations by residual acid-base titrimetry.
6. Determination of purity of aniline
7. Assay of chlorpromazine tablets by non-aqueous acid-base titration.
8. Determination of carbonate and bicarbonate in a mixture by pH-metric titration and comparison with visual acid-base titration.

9. Determination of benzoic acid in food products by titration with methanolic KOH in chloroform medium using thymol blue as indicator.
10. Analysis of water/waste water for acidity by visual, pH metric and conductometric titrations.
11. Analysis of water/waste water for alkalinity by visual, pH metric and conductometric titrations.
12. Determination of carbonate and hydroxide-analysis of a commercial washing soda by visual and pH-titrimetry.
13. Spectrophotometric determination of creatinine and phosphorus in urine.
14. Flame emission spectrometric determination of sodium and potassium in river/lake water.

References:

1. Fundamental of Analytical Chemistry, D.A. Skoog, D.M. West, Holler and Crouch 8th edition, 2005, Saunders College Publishing, New York.
2. Analytical Chemistry, G.D. Christian, 5th edition, 2001 John Wiley & Sons, Inc, India.
3. Quantitative Analysis, R.A. Day and A.L. Underwood, 6th edition, 1993, Prentice Hall, Inc. New Delhi.
4. Vogel's Textbook of Quantitative Chemical Analysis, J. Mendham, R.C. Denney, J.D. Barnes and M.J.K. Thomas, 6th edition, Third Indian Reprint, 2003, Pearson Education Pvt. Ltd., New Delhi.
5. Analytical Chemistry Principles, John H. Kennedy, 2nd edition, Saunders College Publishing, California, 1990.
6. Practical Clinical biochemistry methods and interpretations, R. Chawla, J.P. Bothers Medical Publishers (P) Ltd., 1995.
7. Laboratory manual in biochemistry, J. Jayaraman, New Age International Publishers, New Delhi, 1981.
8. Practical Clinical Biochemistry by Harold Varley and Arnold.Heinmann, 4th edition.

OCI SCT: 1.52 CHEMISTRY OF SELECTED ELEMENTS

UNIT-I

Compounds of hydrogen: The hydrogen and hydride ions, Dihydrogen and hydrogen bonding. Classes of binary hydrides: Molecular hydrides, saline hydrides and metallic hydrides.

The Group 1 elements: Occurrence, extraction and uses. Simple compounds: Hydrides, halides, oxides, hydroxides, oxoacids, nitrides, solubility and hydration and solutions in liquid ammonia. Coordination and organometallic compounds. Applications.

The Group 2 elements: Occurrence, extraction and uses. Halides, hydrides and salts of oxoacids. Complex ion in aqueous solution and complexes with amido and alkoxy ligands.

The Group 17 elements: Occurrence, recovery and uses. Trends in properties and pseudohalogens. [16 Hrs]

UNIT-II

Interhalogens: Physical properties and structures, chemical properties, cationic interhalogens, halogen complexes and polyhalides.

Compounds with oxygen: Halogen oxides, oxoacids and oxoanions.

Trends in rates of redox reactions and redox properties of individual oxidation states.

Chemistry of astatine.

The Group 18 elements: Occurrence, recovery and uses. Synthesis and structure of xenon fluorides, Reaction of xenon fluorides, xenon-oxygen compounds, Organoxenon compounds, Other compounds of noble gases.

M-M bonds: Multiple metal-metal bonds.

Cluster compounds: carbonyl and carbide clusters. [16 Hrs]

References:

1. Basic Inorganic Chemistry – 3rd edition. F.A. Cotton, G. Wilkinson and P.L. Gaus, John Wiley and Sons (2002).
2. Inorganic Chemistry, 3rd edition. James E. Huheey, Harper and Row Publishers (1983).

3. Inorganic Chemistry, 3rd edition. G.L. Miessler and D.A. Tarr, Pearson Education (2004).
4. Inorganic Chemistry, 2nd edition. C.E. Housecroft and A.G. Sharpe, Pearson Education.
5. Chemistry of the Elements – N.N. Greenwood and A. Earnshaw, Pergamon Press (1985).
6. Inorganic Chemistry - 2nd edition, D.F. Shriver, P.W. Atkins and C.H. Langford, Oxford University Press, (1994).

OCO SCT: 1.53 Vitamins, green chemistry and medicinal chemistry

UNIT – I:

Vitamins: Introduction, constitution, synthesis and biological significance of thiamine, riboflavin, pyridoxine, biotin, ascorbic acid, vitamins A₁ & A₂, E₁ and E₂, B₁₂ and K groups.

Green chemistry:

Definition and principles, planning a green synthesis in a chemical laboratory, Green preparation-Aqueous phase reactions, solid state (solvent less) reactions, photochemical reactions, Phase transfer catalyst catalyzed reactions, enzymatic transformations & reactions in ionic liquids. [16 Hrs]

UNIT – II:

Medicinal Chemistry

Chemotherapy : Definition, History, and Evolution of Chemotherapy

Classification of drugs on the basis of therapeutic action, pharmacophoric, API (active pharmaceutical ingredient) chiral drugs, development of new drugs, procedures followed in drug design, concept of lead and lead-compounds and lead modifications, molecular modeling, concept of pro-drug and soft drug, factor affecting bioactivity.

Theories of drug activity, occupancy-theory, rate theory, induced-fit theory. Quantitative structure-activity relationship, history and development of QSAR, concept of drug receptors, elementary treatment of drug receptor interactions.

Physicochemical parameters: lipophilicity, partition-coefficient, electronic ionization constant, steric, Shelton and surface activity parameters and redox potential.

Evaluation methods: Free-Wilson analysis, Hansch-analysis, relationship between Free-Wilson analysis and Hansch-analysis – LD₅₀, ED₅₀, ID₅₀, IC₅₀ (mathematical derivation of equation excluded). [16 Hrs]

References:

1. Introduction to medicinal chemistry, A Gringuage, Wiley-VCH.
2. Wilson and Gisvold's Text Book of organic medicinal and pharmaceutical chemistry, Ed Robert F. Dorge.
3. An introduction to drug design, S.S. Pandey and J.R. Dimmock, New Age International.
4. Burger's medicinal chemistry and drug discovery, Vol-1 (Chapter-9 and Ch-14), Ed.M.E. Wolff, John Wiley.
5. L. Finar, Organic Chemistry, ELBS Longmann, Vol. I & II, 1984.
6. K. Albert, L. Lehninger, D. L. Nelson, M. M. Cox, Principles of Biochemistry, CBZ publishers, 1st edition, New Delhi, 1993.
7. Harper's Biochemistry, Ed. R.Harper, 22nd edition, Prentice Hall Press, New York, 1990.
8. Harper's review of biochemistry – P. W. Martin, P. A. Mayer & V. W. Rodfwell, 5th edition, Maurzen Asian Edition, California, 1981.

OCP SCT: 1.54. BIOPHYSICAL CHEMISTRY AND PHARMACOKINETICS

UNIT – I

Biophysical chemistry: Electrophoresis - principles of free electrophoresis, zone electrophoresis, gel electrophoresis and its applications in qualitative and quantitative study of proteins. Determination of isoelectric point of a protein. Electro-osmosis and streaming potential and its biological significance. Biological significance of Donnan membrane phenomenon. Micelles and its involvement during digestion and absorption of dietary lipids. Diffusion of solutes across bio-membranes and its application in the mechanism of respiratory exchange. "Salting In" and "Salting Out" of proteins. Osmotic behaviour of cells and osmo-regulation and its application in the evolution of excretory systems of organisms. Effect of temperature and pH on the viscosity of biomolecules (albumin solution). Significance of viscosity in biological systems - mechanism of muscle contraction, detection

of intrastrand disulfide bonds in proteins, polymerization of DNA and nature of blood flow through different vessels. Effect of temperature, solute concentration (amino acids) on surface tension. Biological significance of surface tension - stability of Alveoli in lungs, interfacial tension in living cells (Danielli and Davson model). Application of sedimentation velocity and sedimentation equilibrium method for molecular weight determination of proteins.

[16 Hrs]

UNIT – II

Pharmacokinetics: Introduction, biopharmaceutics, pharmacokinetics, clinical pharmacokinetics, pharmacodynamics, toxicokinetics and clinical toxicology. Measurement of drug concentration in blood, plasma or serum. Plasma level-time curve, significance of measuring plasma drug concentrations.

One compartment open model: Intravenous route of administration of drug, elimination rate constant, apparent volume of distribution and significance. Calculation of elimination rate constant from urinary excretion data, clinical application.

Two compartment model: Plasma level-time curve, relationship between tissue and plasma drug concentrations, Apparent volumes of distribution. Drug clearance, clinical example. Plasma level-time curve for a three compartment open model.

Drug absorption: Factors affecting the rate of drug absorption - nature of the cell membrane, Route of drug administration - oral drug absorption, Intravenous infusion and intravenous solutions, Effect of food on gastrointestinal drug absorption rate.

[16 Hrs]

Reference text books

1. Introduction to Physical Organic Chemistry, R.D. Gilliom, Madison – Wesley, USA (1970).
2. Physical Organic Chemistry, Reaction Rate and Equilibrium Mechanism – L.P. Hammett, McGraw HillBook, Co., (1970).
3. Biophysical Chemistry, Principle and Technique – A. Upadhyay, K. Upadhyay and N. Nath, Himalaya Publishing House, Bombay, (1998).
4. Essentials of Physical Chemistry and Pharmacy – H. J. Arnika, S. S. Kadam, K.N. Gujan, Orient Longman, Bombay, (1992).
5. Applied Biopharmacokinetics and Pharmacokinetics - Leon Shargel, Andrew YuPrentice-Hall International, Inc (4th edition).

6. Essentials of Physical Chemistry and Pharmacy – H.J. Arnikaar, S.S. Kadam, K.N. Gujan, Orient Longman, Bombay, (1992).

SECOND SEMESTER

OCI HCT: 2.1. COORDINATION CHEMISTRY

UNIT – I

Preparation of coordination compounds: Introduction, Preparative methods - simple addition reactions, substitution reactions, oxidation-reduction reactions, thermal dissociation reactions. Geometries of metal complexes of higher coordination numbers (2-12).

Stability of coordination compounds: Introduction, trends in stepwise stability constants, factors influencing the stability of metal complexes with reference to the nature of metal ion and ligands, the Irving-William series, chelate effect.

Determination of stability constants: Theoretical aspects of determination of stability constants of metal complexes by spectrophotometric and polarographic methods.

Crystal field theory: Salient features of CFT, d-orbital splitting in octahedral, tetrahedral, square planar and tetragonal complexes, Jahn-Teller distortions, measurement of $10 Dq$ and factors affecting it. Evidences for metal-ligand covalency.

Molecular Orbital Theory: MOT to octahedral, tetrahedral and square planar complexes without and with pi-bonding. [16 Hrs]

UNIT – II

Electronic spectra: Introduction, selection rules and intensities, electronic spectra of octahedral and tetrahedral complexes, Term symbols for d^n ions, Orgel and Tanabe-Sugano diagrams, charge-transfer spectra.

Magnetic properties: Introduction, magnetic susceptibility and its measurements, spin and orbital contributions to the magnetic moment, the effects of temperature on μ_{eff} , spin-cross over, ferromagnetism, antiferromagnetism and ferrimagnetism.

Reaction and Mechanisms: Introduction. *Substitution reactions* - Inert and labile compounds, mechanisms of substitution.

Kinetic consequences of Reaction pathways - Dissociation, interchange and association.
Experimental evidence in octahedral substitution - Dissociation, associative mechanisms, the conjugate base mechanism, the kinetic chelate effect.

Substitution reactions of square-planar complexes - kinetics and stereochemistry of square-planar substitutions, evidence for associative reactions, explanations of the trans effect.

Electron-transfer processes: Inner-sphere mechanism and outer-sphere mechanism, conditions for high and low oxidation numbers. Photochemistry of Coordination Compounds: Overview and General Concepts. **[16 Hrs]**

References:

1. Physical Inorganic Chemistry - A Coordination Chemistry Approach- S.F.A. Kettle, Spektrum, Oxford, (1996).
2. Inorganic Chemistry - 2nd edition, C.E. Housecroft and A.G. Sharpe, Pearson Education Ltd., (2005).
3. Inorganic Chemistry - 3rd edition, G.L. Miessler and D.A. Tarr, Pearson Education, (2004).
4. Inorganic Chemistry - 2nd edition, D.F. Shriver, P.W. Atkins and C.H. Langford, Oxford University Press, (1994).
5. Inorganic Chemistry- 3rd edition, James E. Huheey, Harper and Row Publishers, (1983).
6. Basic Inorganic Chemistry- 3rd edition, F.A. Cotton, G. Wilkinson and P.L. Gaus, John Wiley and Sons, (2002).

INORGANIC CHEMISTRY PRACTICALS-II

[64 HOURS]

Part-I

1. Determination of bismuth, cadmium and lead in a mixture: Analysis of a low melting alloy (Wood's alloy).
2. Simultaneous spectrophotometric determination of chromium and manganese in a steel solution.
3. Gravimetric determination of copper(II) and nickel(II) using salicylaldoxime.
4. Preparation of mercurytetrathiocyanatocobaltate(II) and estimation of mercury by gravimetry.
5. Preparation of tris(oxalato)ferrate(III) and estimate the metal ion.

Part-II

Semimicro qualitative analysis of mixtures containing **TWO** anions and **TWO** cations (excluding sodium, potassium and ammonium cations) and **ONE** of the following less common cations: W, Mo, Ce, Th, Ti, Zr, V, U and Li.

References:

1. Vogel's Text Book of Quantitative Chemical Analysis – 5th edition, J. Basset, R.C. Denney, G.H. Jeffery and J. Mendhom.
2. A Text Book of Quantitative Inorganic Analysis by A.I. Vogel, 3rd edition.
3. Spectrophotometric Determination of Elements by Z. Marczenko.
4. Vogel's Qualitative Inorganic Analysis – Svelha.
5. Macro and Semimicro Inorganic Qualitative Analysis by A.I. Vogel.
6. Semimicro Qualitative Analysis by F.J. Welcher and R.B. Halin.
7. Quantitative Chemical Analysis by Daniel C. Harris, 7th edition, (2006).

OCI HCT: 2.2. STEREOCHEMISTRY AND HETEROCYCLIC CHEMISTRY

UNIT – I:

STEREOCHEMISTRY

Stereoisomerism: Projection formulae [flywedge, Fischer, Newman and sawhorse], enantiomers, diastereoisomers, mesomers, racemic mixture and their resolution, configurational notations of simple molecules, DL and RS configurational notations.

Optical isomerism: Conditions for optical isomerism: Elements of symmetry-plane of symmetry, centre of symmetry, alternating axis of symmetry (rotation-reflection symmetry). Optical isomerism due to chiral centers and molecular dissymmetry, allenes and biphenyls, criteria for optical purity.

Geometrical isomerism: Due to C=C, C=N and N=N bonds, E, Z conventions, determination of configuration by physical and chemical methods. Geometrical isomerism in cyclic systems.

Conformational analysis: Elementary account of conformational equilibria of ethane, butane and cyclohexane. Conformation of cyclic compounds such as cyclopentane, cyclohexane, cyclohexanones and decalins. Conformational analysis of 1,2-, 1,3- and 1,4-

disubstituted cyclohexane derivatives and D-Glucose, Effect of conformation on the course and rate of reactions.

Stereoselectivity: Meaning and examples of stereospecific reactions, stereoselective reactions, diastereoselective reactions, regioselective, regiospecific reactions, enantioselective reactions and enantiospecific reactions. [16 Hrs]

Unit II

Heterocyclic chemistry:

Nomenclature of heterocyclic compounds. Structure (no elucidation), reactivity, synthesis (minimum three synthesis) and reactions (minimum three reactions) of furan, pyrrole, thiophene, indole, pyridine, quinoline, isoquinoline, pyrazole, imidazole, pyrone, coumarin, chromones, pyrimidines, purines. [16 Hrs]

References:

1. E.L. Eliel and S.H. Wilen, Stereochemistry of Organic Compounds, John Wiley and Sons, New York. 1994.
2. Stereochemistry and Mechanism through Solved Problems by P.S. Kalsi.
3. Heterocyclic Chemistry – Joule & Smith
4. Basic Principles of Heterocyclic Chemistry – L.A. Pacquette
5. D. Nasipuri, Stereochemistry of Organic Compounds, 2nd edition, Wiley Eastern Limited, New Delhi, 1991.
6. Comprehensive heterocyclic chemistry –Kartritzky series, Pergamon Press, New York, 1984.

ORGANIC CHEMISTRY PRACTICALS [64 hrs]

Qualitative analysis: Separation of binary mixtures, identification of functional groups and preparation of suitable solid derivatives.

References:

1. Manual of Organic Chemistry - Dey and Seetharaman.
2. Modern Experimental Organic Chemistry by John H. Miller and E.F. Neugil, p 289.
3. An Introduction to Practical Organic Chemistry - Robert, Wingrove etc.

4. A Text Book of Practical Organic Chemistry – A.I. Vogel, Vol.III
5. Practical Organic Chemistry - Mann & Saunders

OCP HCT: 2.3. PHYSICAL CHEMISTRY - II

UNIT – I

Electrochemistry of solutions: Arrhenius theory of strong and weak electrolytes and its limitations. Factor effecting electrolytic conductance, Debye-Huckel theory - concept of ionic atmosphere. Debye-Huckel-Onsager equation of conductivity and its validity. Debye-Huckel limiting law (DHL), its modification for appreciable concentrations. A brief survey of Helmholtz-Perrin, Guoy-Chapman and Stern electrical double layer (no derivation). Determination of transference number by emf and Hittorf's methods. True and apparent transference numbers. Abnormal transference numbers, effect of temperature on transference numbers. Liquid junction potential-determination and minimization.

Irreversible electrode process: Introduction, reversible and irreversible electrodes, reversible and irreversible cells. Polarization, over voltage - concentration over voltage, activation over voltage and ohmic over voltage. Experimental determination of over voltage. Equations for concentration over potential, stationary and non-stationary surface. Polarography- Half wave potential, application in qualitative and quantitative analysis. Butler-Volmer equation, Tafel equation. Hydrogen oxygen over voltage. Effect of temperature, current density and *pH* on over voltage. [16 Hrs]

UNIT – II

Quantum Chemistry: A brief resume of black body radiation, and atomic spectra-Bohr's theory of hydrogen atom. Photoelectric and Compton effects, de-Broglie concept, uncertainty principle. Operators - algebra of operators, commutative and non-commutative operators, linear operator, Laplacian operator, Hermitian operator, Hamiltonian operator, turn over rule. Wave equation for stretched strings, Schrodinger wave equation for particles, Eigen values and Eigen functions, postulates of quantum mechanics. Application of Schrodinger equation to a free particle and to a particle trapped in a potential field (one dimension and three dimensions). Degeneracy, Wave equation for H-atom, separation and solution of R , ϕ and θ equations. Application of Schrodinger equation to rigid rotator and harmonic oscillator.

[16 Hrs]

Reference text books

1. Text Book of Physical Chemistry by Samuel Glasstone, MacMillan Indian Ltd., 2nd edition (1974).
2. Elements of Physical Chemistry by Lewis and Glasstone.
3. Physical Chemistry by P.W. Atkins, ELBS, 4th edition, Oxford University Press (1990).
4. Physical Chemistry – G.M. Barrow, McGraw Hill International Service (1988).
5. Introduction to Electrochemistry by S. Glasstone.
6. Electrochemistry –Principles and Applications by E.G. Potter.
7. Electrochemistry by Reiger, Prentice Hall (1987).
8. Modern Electrochemistry Vol. I and II by J.O.M. Bockris and A.K.N. Reddy, Pentium Press, New York (1970).
9. Quantum Chemistry – A.K. Chandra. 2nd edition, Tata McGraw Hill Publishing Co. Ltd., (1983).
10. Quantum Chemistry – Eyring, Walter and Kimball. John Wiley and Sons, Inc., New York.
11. Quantum Chemistry – I.N. Levine. Pearson Education, New Delhi, (2000).
12. Theoretical Chemistry – S. Glasstone. East West Press, New Delhi, (1973).
13. Quantum Chemistry – R.K. Prasad, New Age International Publishers, (1996).
14. Valence Theory – Tedder, Murel and Kettle.
15. Quantum Chemistry – D.A. McQuarrie.

PHYSICAL CHEMISTRY PRACTICALS – II [64 Hrs]

1. Study of kinetics of reaction between CAT and indigocarmine spectrophotometrically and determination of rate constant.
2. Kinetics of reaction between sodium formate and iodine, determination of energy of activation.
3. Determination of energy of activation for the bromide-bromate reaction.
4. Determination of dissociation constant and mean ionic activity coefficient of weak electrolytes by conductivity method.
5. Conductometric titration of oxalic acid against NaOH and NH₄OH.
6. pH titration of (a) CH₃COOH vs. NaOH and determination of K_a.
7. Potentiometric titration of a mixture of halides (KCl+KI) against AgNO₃.
8. Determination of redox potential of Fe²⁺ ions by potentiometric method.
9. Determination of activity of 0.1 M HCl by EMF method.

10. Determination of partial molar volume of NaCl-H₂O/KCl- H₂O/KNO₃/ H₂O systems.
11. G.M. Counter – determination of G.M. plateau and dead time.
12. Verification of inverse square law using gamma emitter.
13. Determine the concentration of KI potentiometrically by calibration method.
14. To study the kinetics of reaction between acetone and iodine - determination of order of reaction w.r.t. iodine and acetone.
15. To determine the eutectic point of a two component system (Naphthalene-*m*-dinitrobenzene system).
16. Coulometric titration I₂ vs Na₂S₂O₃.

Reference text 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 Mc Graw Hill.

OCG HCT: 2.4. SPECTROSCOPY

UNIT - I

NMR Spectroscopy: Magnetic properties of nuclei (magnetic moment, g factor, nuclear spin), effect of external magnetic field on spinning nuclei, Larmor precession frequency, resonance conditions, population of nuclear magnetic energy levels, relaxation processes, relaxation time, line width and other factors affecting line width. Chemical Shift: Standards employed in NMR, factors influencing chemical shift: electronegativity, shielding and deshielding, vander Waals deshielding magnetic anisotropy, H-bonding, diamagnetic and paramagnetic anisotropies, spin-spin coupling, chemical shift values and correlation for protons bonded to carbon and other nuclei, Instrumentation. Chemical shift equivalence and

magnetic equivalence, effects of chiral centre, Karplus curve-variation of coupling constants with dihedral angle. Complex NMR Spectra: Simplification of complex spectra-isotopic substitution, increased magnetic field strength, double resonance and lanthanide shift reagents;, Nuclear Overhauser Effect (NOE), variable temperature probe, FT-NMR Spectroscopy and advantages. ^{13}C -NMR Spectroscopy: Comparison of ^1H -NMR and ^{13}C -NMR, multiplicity-Proton decoupling-Noise decoupling-Off resonance decoupling-Selective proton decoupling- Chemical shift, application of CMR. NMR of ^{19}F , ^{31}P , ^{11}B and ^{15}N Applications of NMR: Structural diagnosis, conformational analysis, keto-enol tautomerism, Hbonding. Two dimensional NMR Spectroscopy: COSY, NOESY, MRI. [16 Hrs]

UNIT – II

Electron Spin Resonance Spectroscopy: Basic principles, hyperfine couplings, the 'g' values, factors affecting 'g' values, isotropic and anisotropic hyperfine coupling constants, Zero Field splitting and Kramer's degeneracy. Measurement techniques and Applications to simple inorganic and organic free radicals and to inorganic complexes.

NQR Spectroscopy: Quadrupolar nuclei, electric field gradient, nuclear quadrupole coupling constants, energies of quadrupolar transitions, effect of magnetic field. Applications.

Mössbauer spectroscopy: The Mössbauer effect, chemical isomer shifts, quadrupole interactions, measurement techniques and spectrum display, application to the study of Fe^{2+} and Fe^{3+} compounds, Sn^{2+} and Sn^{4+} compounds(nature of M-L bond, coordination number and structure), detection of oxidation states and inequivalent Mössbauer atoms.

[16 Hrs]

UNIT – III

Mass Spectrometry: Basic principles, Instrumentation -Mass spectrometer, interpretation of mass spectra, resolution, exact masses of nucleides, molecular ions, meta-stable ions and isotope ions. Different methods of ionization (chemical ionization, electron impact, field ionization, maldi etc). Fragmentation processes-representation of fragmentation, basic fragmentation types and rules. Factors influencing fragmentations and reaction pathways. McLafferty rearrangement. Fragmentations (fragmentation of organic compounds with respect to their structure determination) associated with functional groups- alkanes, alkenes, cycloalkanes, aromatic hydrocarbons, halides, alcohols, phenols, ethers, acetals, ketals, aldehydes, ketones, quinines, carboxylic acids, esters, amides, acid chlorides, nitro

compounds, amines & nitrogen heterocycles. Fragmentation patterns of glucose, myrcene, nicotine, retro Diels-Alder fragmentation. Application in structure elucidation and evaluation of heats of sublimation & ionization potential. Nitrogen rule. LC-MS and GC-MS, High resolution mass spectroscopy. Composite problems involving the applications of UV, IR, ^1H and ^{13}C -NMR and mass spectroscopic techniques. Structural elucidation of organic molecules. [16 Hrs]

REFERENCES:

1. Organic Spectroscopy-3rd Ed.-W.Kemp(Paggrave Publishers, New York), 1991.
2. Spectrometric Identification of Organic Compounds - Silverstein,Bassler & Monnill (Wiley) 1981.
3. Spectroscopy of Organic Compounds-3rd Ed.-P.S.Kalsi (New Age, New Delhi) 2000.
4. E.A.V.Ebsworth, D.W.H.Ranklin and S.Cradock: Structural Methods in Inorganic Chemistry, Blackwell Scientific, 1991.
5. J. A. Iggo: NMR Spectroscopy in Inorganic Chemistry, Oxford University Press, 1999.
6. C. N. R .Rao and J. R. Ferraro: Spectroscopy in Inorganic Chemistry, Vol I & II (Academic) 1970
7. Spectroscopy, B. P. Straughan and S. Salker, John Wiley and Sons Inc., New Yourk, Vol.2, 1976.
8. Application of Absorption Spectroscopy of Organic Compounds, John R. Dyer, Prentice/Hall of India Private Limited, New Delhi, 1974.
9. Organic Spectroscopy, V. R. Dani, Tata McGraw-Hall Publishing Company Limited, New Delhi. 1995.
10. Interpretation of Carbon-13 NMR Spectra, F.W. Wehrli and T. Wirthin, Heyden, London, 1976.
11. NMR spectroscopy-Powai

OCI SCT 2.51: SEPARATION TECHNIQUES

UNIT – I

Fundamentals of chromatography: General description, definition, terms and parameters used in chromatography, classification of chromatographic methods, criteria for selection of

stationary and mobile phase-nature of adsorbents, factors influencing the adsorbents, nature and types of mobile phases and stationary phases.

Column chromatography: Theories – plate theory, rate theory, band broadening-eddy diffusion, longitudinal diffusion and resistance to mass transfer, column efficiency, Van Deemter's equation and its modern version, optimization column performance, interrelationships-capacity factor, selectivity factor, column resolution, distribution constant and applications of conventional column chromatography, advantages and limitations.

Thin layer chromatography (TLC): Definition, mechanism, efficiency of TLC plates, methodology –selection of stationary and mobile phases, preparation of micro and macro plates, development, spray reagents, identification and detection, reproducibility of R_f values, qualitative and quantitative analysis.

Paper chromatography (PC): Definitions, theory and principle, techniques; one, two-dimensional and circular PC, mechanism of separation, types of paper, methodology-preparation of sample, choice of solvents, location of spots and measurement of R_f value, factors affecting R_f values, advantages and applications

High performance liquid chromatography (HPLC): Instrumentation, pumps, column packing, characteristics of liquid chromatographic detectors-UV, IR, refractometer and fluorescence detectors, advantages and applications. [16 Hrs]

UNIT – II

Gas chromatography (GC): Principle, instrumentation, columns, study of detectors – thermal conductivity, flame ionization, electron capture and mass spectrometry, factors affecting separation, retention volume, retention time, applications.

Ion exchange chromatography (IEC): Definitions, principle, requirements for ion-exchange resin and its synthesis, types of ion-exchange resins, basic features of ion-exchange reactions, resin properties-ion-exchange capacity, resin selectivity and factors affecting the selectivity, applications of IEC in preparative, purification and recovery processes.

Solvent extraction: definition, types, principle and efficiency of extraction, sequence of extraction process, factors affecting extraction-pH and oxidation state, masking and salting out agents, techniques-batch and continuous extraction, applications.

Size-exclusion chromatography: Theory and principle of size-exclusion chromatography, experimental techniques of gel-filtration chromatography (GFC) and gel-permeation chromatography (GPC), materials for packing - factors governing column efficiency, methodology and applications. [16 Hrs]

References:

1. Fundamental of Analytical Chemistry, D.A. Skoog, D.M. West, Holler and Crouch 8th edition, 2005, Saunders College Publishing, New York.
2. Analytical Chemistry, G.D. Christian, 5th edition, 2001 John Wiley & Sons, Inc. India.
3. Quantitative Analysis, R.A. Day and A.L. Underwood, 6th edition, 1993 Prentice Hall, Inc. New Delhi.
4. Vogel's Textbook of Quantitative Chemical Analysis, J. Mendham, R.C. Denney, J.D. Barnes and M.J.K. Thomas, 6th edition, Third Indian Reprint, 2003 Pearson Education Pvt. Ltd., New Delhi.
5. Analytical Chemistry Principles, John H. Kennedy, 2nd edition, Saunders College Publishing, California, 1990.
6. Introduction to Instrumental Analysis, Robert. D. Braun, Pharm. Med. Prem. India, 1987.
7. Instrumental Method of Analysis, W.M. Dean and Settle, 7th edition, 1986, CBS Publishers, New Delhi.
8. Instant Notes of Analytical Chemistry, Kealey and Haines, Viva Books Pvt. Ltd., 2002.
9. Modern Analytical Chemistry, David Harvey, McGraw Hill, New Delhi, 2000.
10. Principles and Practice of Analytical Chemistry, F. W. Fifield and Kealey, 5th edition, 2000, Blackwell Sci., Ltd. Malden, USA.

ANALYTICAL CHEMISTRY PRACTICALS

[64 Hrs]

1. Determination of percentage of chloride in a sample by precipitation titration - Mohr, Volhard and Fajan's methods.
2. Determination of silver in an alloy and Na₂CO₃ in soda ash by Volhard method.
3. Mercurimetric determination of blood or urinary chloride.

4. Determination of calcium in calcium gluconate/calcium carbonate tablets/injections and of calcium in milk powder by EDTA titration.
5. Analysis of commercial hypochlorite and peroxide solution by iodometric titration.
6. Determination of ascorbic acid in vitamin C tablets by titrations with KBrO_3 and of vitamin C in citrus fruit juice by iodimetric titration.
7. Determination of iron in pharmaceuticals by visual and potentiometric titration using cerium(IV) sulphate.
8. Determination of total cation concentration of tap water by ion-exchange chromatography.
9. Determination of magnesium in milk of magnesium tablets by ion-exchange chromatography.
10. Cation exchange chromatographic separation of cadmium and zinc and their estimation by EDTA titration.
11. Gas chromatographic determination of ethanol in beverages.
12. Determination of aspirin, phenacetin and caffeine in a mixture by HPLC.
13. Anion exchange chromatographic separation of zinc and magnesium followed by EDTA titration of the metals.
14. Separation and determination of chloride and bromide on an anion exchanger.
15. Thin layer chromatographic separation of amino acids.

References:

1. Fundamental of Analytical Chemistry, D.A. Skoog, D.M. West, Holler and Crouch 8th edition, 2005, Saunders College Publishing, New York.
2. Analytical Chemistry, G.D. Christian, 5th edition, 2001 John Wiley & Sons, Inc, India.
3. Quantitative Analysis, R.A. Day and A.L. Underwood, 6th edition, 1993, Prentice Hall, Inc. New Delhi.
4. Vogel's Textbook of Quantitative Chemical Analysis, J. Mendham, R.C. Denney, J.D. Barnes and M.J.K. Thomas, 6th edition, Third Indian Reprint, 2003, Pearson Education Pvt. Ltd., New Delhi.

5. Analytical Chemistry Principles, John H. Kennedy, 2nd edition, Saunders College Publishing, California, 1990.
6. Practical Clinical biochemistry methods and interpretations, R. Chawla, J.P. Bothers Medical Publishers (P) Ltd., 1995.
7. Laboratory manual in biochemistry, J. Jayaraman, New Age International Publishers, New Delhi, 1981.
8. Practical Clinical Biochemistry by Harold Varley and Arnold Heinmann, 4th edition.

OCI SCT 2.52: INDUSTRIAL INORGANIC CHEMISTRY

UNIT – I

Metal Carbides: salt like, covalent and industrial carbides. Intercalation compounds of graphite, alkali metals. Industrially important reactions of oxides with carbon.

Silicone polymers: Introduction, nature of chemical bonds containing silicon, general methods of preparation (fluids and resins) and properties of silicones. Applications. Industrial uses of silicon, silicon carbide and silicon dioxide.

Chemical reactivity and group trends of germanium, tin and lead: Applications, metallic tin and alloys, lead alloys and oxides of lead.

Compounds of arsenic, antimony and bismuth: Intermetallic compounds and alloys and their uses.

Ceramics: Raw materials used in ceramics and ceramic insulators.

[16 Hrs]

UNIT – II

Inorganic fibers: Introduction, properties, classification, asbestos fibers, optical fibers, carbon fibers, Applications.

Zeolites: Introduction, types of zeolites, manufacture of synthetic zeolites and applications.

Mineral fertilizers: Phosphorous containing fertilizers - Economic importance, importance of superphosphate, ammonium phosphates and their synthesis.

Nitrogen containing fertilizers - Importance and synthesis of ammonium sulfate, ammonium nitrate and urea.

Potassium containing fertilizers - Economic importance and manufacture of potassium sulfate.

Inorganic pigments: General information and economic importance.

White pigments – titanium dioxide pigments, zinc oxide pigments.

Colored pigments – Iron oxide, chromium oxide, mixed-metal oxide pigments and ceramic colorants.

Corrosion protection pigments, luster pigments, luminescent pigments, magnetic pigments.

[16 Hrs]

References:

1. Inorganic Chemistry Principles of Structure and Reactivity: James E. Huheey, Ellen A. Keiter, Richard L. Keiter, Okhil K. Medhi, Delhi University, New Delhi (2006)
2. Chemistry of the Elements – N.N. Greenwood and A. Earnshaw, Pergamon Press (1985).
3. Industrial Inorganic Chemistry – 2nd edition. K.H. Buchel, H.H. Moretto and P. Woditsh, Wiley - VCH (2000).

OCO SCT 2.53: Dyes & Insecticides

Unit I

Dyes: Introduction, modern theories of colour and chemical constitution. A general study of the following: Direct azo dyes (congo red, rosanthrene O, procion dyes), acid azo dyes (ponceau 2R, Naphthol blue black 6B), basic azo dyes (chrysoidin G, bismark brown), developed dyes, mordant dyes, vat dyes, disperse dyes, fibre reactive dyes, sulphur dyes and solvent dyes. Fluorescent brightening agents (tinopal B.V), cyanine dyes (classification, application in photography, quinoline blue and sensitol), chemistry of colour developer, and instant colour processes.

Synthesis and applications of malachite green, rhodamine-B, phenolphthalein and methyl orange.

Triphenylmethane dyes: crystal violet, pararosaniline, aurin, chrome violet.

Application of dyes: i. photography and ii. Biological studies.

[16 Hrs]

Insecticides: Introduction, classification, mode of action and synthesis of chlorinated insecticides (DDT, chlordane, heptachlor and hexachlorocyclohexane), Naturally occurring insecticides-pyrethroids-natural pyrethrins-isolation and structures, synthetic pyrethroids, allethrin, cypermethrin, phenvalerate.

Organophosphorous insecticides: Malathion, parathion, DDVP, diazenon.

Carbamate insecticides: Sevin, carbofluron, aldicab, beygon.

Insect Pheromones: Introduction, classification, use in insect pest control. Synthesis of disparlure, faranol, grandisol, brevicomin and bombykol.

Fungicides: Introduction, Inorganic & organic fungicides, Systemic fungicides-types & examples.

Herbicides: Introduction, study of sulfonyl ureas, heterocyclic sulfonamides, heterocyclic amines, dihydropyrano[2,3-*b*]pyridylimidazolinones, pyrrolopyridylimidazolinones, 1,2,4-triazine- 3,5-diones, hydroxyoxazolidinones & hydroxypyrrolidinones, pyridine herbicides & 1,3,4-oxadiazoles. Mechanism of action and toxicities of insecticides, fungicides and herbicides. [16 Hrs]

References

1. A Text Book of Fertilizers, Ranjan Kumar Basak.
2. Agronomy - Theory & Digest, Bidhan Chandra, Krishi Vishwavidyalaya, Mohanpur.
3. Fundamentals of Agronomy, S.S.Cheema, K.Dhaliwal, T.S. Shota, Punjab Agricultural University.
4. Principles and Practices of Agronomy, Shri.S.S.Singh, Allahabad Agricultural Institute.
5. Fertilizers, Organic Manures & Biofertilizers—A Product Quality Guide for Major & Micronutrients, HLS Tandon, Fertilizer Development and Consultation Organisation, New Delhi.
6. Handbook on Fertilizer Technology, Bham Swaminathan & Manish Goswami, The Fertilizer Association of India, New Delhi.
7. Outlines of Chemical Technology, Charles E. Dryden, Affiliated East-West Press, New Delhi.

8. Synthetic Organic Chemistry, G. R. Chatwal, Himalaya Publishing House.
9. Synthesis and Chemistry of Agrochemicals, Vol I & II, ACS, Wahington.
10. Chemistry of Pesticides, K H Buchel.
11. Advances in Pesticide Formulation Technology, ACS.
12. Chemicals for Crop Protection and Pest Managements, M B Green, G.S. Hartley West, Pergamon.
13. Chemistry of Insecticides and Fungicides, Sree Ramulu, Oxford & IBH, 1985.

OCP SCT: 2.54. NANOMATERIALS, SEMICONDUCTORS AND SUPERCONDUCTORS

UNIT – I

Chemistry of Nanomaterials: Introduction, nanoparticles, nanotubes (carbon nanotubes, SWNT and MWNT), nano wires, nano fibers and nano gel. Fullerenes and other bulk balls. Graphene and its applications. Quantum dots.

Synthesis: Chemical vapour deposition (CVD), sol-gel, silica-gel, solvothermal, hydrothermal methods, microwave, electrochemical, laser ablation, biological and bacterial methods. Characterization (X-ray, IR, UV and SEM).

Applications of Nanomaterials in: Renewable energy (nano solar cells), coloured glasses (gold and silver ruby glasses), chemical sensors, biosensors, SAM, electrical and electronics (RAM). Chemical and photocatalytic applications. Lithography, drug delivery targeting and medical applications, micro-electrochemical machines (MEMS). Inorganic and organic nanoporous gel.

[16 Hrs]

UNIT – II

Semiconductors: Band theory, energy bands, intrinsic and extrinsic semiconductors. Conductivity: electrons and holes, temperature dependence on conductivity, Optical properties: absorption spectrum, photoconductivity, photovoltaic effect and luminescence. Junction properties: metal-metal junctions, metal-semiconductor junctions, p-n junctions, transistors, industrial applications of semiconductors: Mixed oxides, spinels and other magnetic materials.

Superconductors: Meissner effect, type I and II superconductors, isotope effect, basic concepts of BCS theory, manifestations of the energy gap, Josephson devices. **[16 Hrs]**

Reference text books

1. Hand Book of Nanotechnology, Bharat Bhushan, Springer Publisher.
2. Nanotechnology, Richard Booker and Earl Boysen, Wiley.
3. Nanomaterials, A.K. Bandopadhyay, New Age International, 2nd edition.
4. Nanotechnology - Importance and Applications, M. H. Fulekar, Ink International publishing.
5. Solid State Chemistry – N.B. Hannay.
6. Introduction to Solids – Azaroff.
7. Solid State Chemistry and its applications – A.R. West.
8. Principles of the Solid State – H.V. Keer.
9. Basic Solid State Chemistry, 2nd edition, Anthony R. West.
10. Solid State Chemistry: An Introduction, 3rd edition, Lesley E. Smart and Elaine A. Moore.
11. Introduction to Solid state Physics—C. Kittel, 5th edition, Wiley Eastern, Limited.
12. C.N.R. Rao and J. Gopalakrishna “New Directions in solid state chemistry” Cambridge University Press, Cambridge (1999).

THIRD SEMESTER

OCO-HCT 3.1 : REAGENTS IN ORGANIC SYNTHESIS

UNIT – I:

OXIDATION AND REDUCTION Oxidation: Oxidation with chromium and manganese reagents (CrO₃, K₂Cr₂O₇, PCC, PDC, Sarret reagent, Jones reagent, MnO₂, KMnO₄), oxygen (singlet and triplet), ozone, peroxides and peracids, lead tetraacetate, periodic acid, OsO₄, SeO₂, NBS, chloramine-T, Sommelet oxidation, Oppenauer oxidation, Fenton's reagent, Sharpless epoxidation. Reductions: Catalytic hydrogenation (homogeneous and heterogeneous) – catalysts (Pt, Pd, Ra-C, Ni, Ru, Rh), solvents and reduction of functional groups, catalytic hydrogen transfer reactions. Wilkinson catalyst, LiAlH₄, NaBH₄, DIBAL-H, Sodium cyanoborohydride, dissolving metal reactions (Birch reduction). Leukart reaction (reductive amination), diborane as reducing agent, Meerwein-Ponndorf-Verley reduction, Wolff-Kishner reduction, Clemensen reduction, tributyl tinhydride, stannous chloride, Bakers yeast, Organoboron compounds: Introduction and preparations. Hydroboration and its applications. Reactions of organoboranes: isomerization reactions, oxidation, protonolysis, carbonylation, cyanidation. Reaction of nonallylic boron stabilized carbanions: alkylation

reactions, acylation reaction, Reactions with aldehydes or ketones (E and Z-alkenes).
Palladium reagents: Suzuki coupling, Heck reaction, Negishi reaction. [16 hrs]

UNIT – II:

REAGENTS AND REACTIONS IN ORGANIC SYNTHESIS

Use of following reagents in organic synthesis and functional group transformations: Lithium diisopropylamide (LDA), Gilman reagent, dicyclohexyl carbodimide (DCC), dichlorodicyanoquinone (DDQ), Silane reagents- trialkylsilyl halides, trimethylsilyl cyanide, trimethyl silane, TBDMS, phase transfer catalyst, crown ethers, cyclodextrins, Ziegler-Natta catalyst, diazomethane, Woodward and Prevost hydroxylation, Stark enamine reaction, phosphorous ylides - Wittig and related reactions, sulphur ylides – reactions with aldehydes and ketones, 1,3-dithiane anions - Umpolung reaction, Peterson reaction. Functional group transformations: Nitro to keto group (Neff reaction), alcohol to aldehyde. [16 hrs]

References:

1. H. Pine, Hendrickson, Cram and Hammond, Organic Chemistry, Mc Graw Hill, New York, 1987.
2. I.L. Finar, Organic Chemistry, ELBS Longmann, Vol. I & II, 1984.
3. R.K. Bansal, Organic Reaction Mechanism, Wiley Eastern Limited, New Delhi, 1993.
4. J. March, Advanced Organic Chemistry, Wiley Interscience, 1994.
5. F.A. Carey and Sundberg, Advanced Organic Chemistry – Part A & B, 3rd edition, Plenum Press, New York, 1990.
6. S.K. Ghosh, Advanced General Organic Chemistry, Book and Allied (P) Ltd, 1998.

Organic chemistry Practicals [64 hrs]

Multi step synthesis

1. Preparation of benzyl alcohol and benzoic acid via Cannizzaro reaction.
2. Oxidation of cyclohexanol to adipic acid via cyclohexanone
3. Esterification: Preparation of benzocaine from p-nitrotoluene
4. Diazotization (Sandmeyer's reaction): Preparation of p-chlorobenzoic acid from p-toluidine

5. Molecular rearrangement: Preparation of o-chlorobenzoic acid from phthalic anhydride
6. Preparation benzilic acid from benzaldehyde
7. Preparation of o-hydroxy benzophenone from phenyl benzoate via Fries rearrangement
8. Preparation of benzanilide from benzophenone oxime via Beckmann rearrangement.
9. Synthesis of m-chloriodobenzene from m-dinitrobenzene.
10. Preparation of benzyl alcohol and benzoic acid via Cannizzaro's reaction.

References:

1. Manual of Organic Chemistry - Dey and Seetharaman.
2. Modern Experimental Organic Chemistry by John H. Miller and E.F. Neugil, p 289.
3. An Introduction to Practical Organic Chemistry - Robert, Wingrove etc.
4. A Text Book of Practical Organic Chemistry – A.I. Vogel, Vol.III
5. Practical Organic Chemistry - Mann & Saunders

OCO HCT 3.2: Synthetic organic chemistry

Unit I

Addition reactions: Addition to C-C multiple bonds involving electrophiles, nucleophiles and free radicals. Markownikoff's rule and antiMarkownikoff's rule, Hydroboration.

Typical additions to carbonyl compounds: Addition of hydride, water, alcohol, thioalcohol, bisulphite, HCN, Grignard reagents and amino compounds to carbonyl compounds.

Aldol and related reactions: Keto-enol tautomerism, mechanism and synthetic applications of aldol condensations, Claisen reaction, Schmidt reaction, Perkin reaction, Knoevenogel, benzoin, Stobbe and Darzen's glysidic ester condensation, Cannizaro reaction, Tishchenko reaction, Michael addition, Robinson's annulation reactions.

Mechanism of ester formation and their hydrolysis, formation and hydrolysis of amides, decarboxylation mechanisms.

Elimination reactions: Mechanism and stereochemistry of eliminations—E1, E2, E1cb mechanism, *cis*-elimination, Hofmann and Saytzeff eliminations, competition between elimination and substitution, Chugaev reaction.

UNIT II:**Asymmetric synthesis:**

Definition, importance, mechanism, energy consideration, advantages and limitations, methods of determination of enantiomeric excess.

i. **Topocity - Prochirality**- Substrate selectivity - Diastereoselectivity and enantioselectivity-Substrate controlled methods-use of chiral substrates - examples

ii. Auxiliary controlled methods- **Use of chiral auxiliaries-Chiral enolates-alkylation of chiral imines - Asymmetric Diels - Alder reaction**

Reagent controlled methods- Use of chiral reagents - Asymmetric oxidation –Sharpless epoxidation - Asymmetric reduction - Use of lithium aluminium hydride and borate reagents. Synthesis and applications of oxazaborolidines, IPC-BBN, IPC₂BH, (S)-BINAP-DIAMINE and (R)-BINAL-H. Use of (R,R)-DIPAMP, (S,S)-CHIRAPHOS, (R,R)-DIOP, SAMP, RAMP, S-Proline, S-PBMgCl, (-)-BOAlCl₂, (+) and (-)-DET.

References:

1. H. Pine, Hendrickson, Cram and Hammond, Organic Chemistry, Mac Grow Hill, New York, 1987.
2. Organic Chemistry - Morrison and Boyd
3. I.L. Finar, Organic Chemistry, ELBS Longmann, Vol. 1 & II, 1984.
4. J. March, Advanced Organic Chemistry, Wiley Interscience, 1994.
5. E.S. Gould, Mechanism and Structure in Organic Chemistry, Halt, Rinhart & Winston, New York, 1964.
6. F.A. Carey and Sundberg. Advanced Organic Chemistry – Part A & B, 3rd edition, Plenum Press, New York. 1990.
7. Principles of Organic Synthesis - ROC Norman and Coxon.
8. S.K. Ghosh, Advanced General Organic Chemistry, Book and Allied (P) Ltd. 1998.

Organic Chemistry Practical – Isolation of natural products

[48 hrs]

1. Fractional crystallization: separation of mixture of naphthalene and biphenyl
2. Fractional distillation: Separation of mixture of hexane and toluene.

3. Thin layer chromatography: Separation of plant pigments
4. Column chromatography: Separation of mixture of o & p-nitro anilines
5. Paper chromatography: Separation of amino acids
6. Isolation of piperine from pepper
7. Isolation of caffeine from tea
8. Isolation of cysteine from hair
9. Isolation of hesperidene from orange peel
10. Isolation of azeleic acid from castor oil
11. Isolation and spectroscopic characterization of Lycopene
12. Isolation of lipids from egg yolks
13. Extraction of nicotine from Tobacco Leaves

References

1. Manual of Organic Chemistry – Dey and Seetharaman
2. Natural Products Chemistry by Raphael Ikhan
3. Modern experimental organic chemistry by John H. Miller and E. F. Neugil, p 289.

OCO HCT 3.3: Photochemistry, Pericyclic reactions and heterocyclic chemistry

Unit I

Photochemistry: General consideration: Activation in thermal and photochemical reactions. Light absorption and excitation. Singlet and triplet states. Morse curve, Franck-Condon principle.

Physical process, Jablonski diagram. Photosensitization (donor acceptor concept, resonance and collision transfer). Chemical process, quantum efficiency, quantum and chemical yields.

Photochemistry of functional groups:

- i) *Olefins*: *Cis-trans* isomerism, [2+2] cycloaddition, rearrangements. Reaction of conjugated olefins; di- π -methane rearrangement.
- ii) *Ketones*: Excited state of C=O. Norrish type-I and type-II cleavages. Paterno-Buchi reaction. α,β -unsaturated ketones. [2+2] addition, *cis-trans* isomerisation. Rearrangements of cyclohexadienones.
- iii) *Aromatic compounds*: Photorearrangement of benzene and its derivatives, cycloaddition of benzene.

iv) *Photochemical oxidations and reductions*: Cycloaddition of singlet molecular oxygen. Oxidative coupling of aromatic compounds, photoreduction by hydrogen absorptions. Photodegradation: Photocatalyst –ZnO, TiO₂, principle, application of ZnO/TiO₂ in the photodegradation of dyes (IC), pesticides (DDT, HCCHO and in industrial effluents. Effect of photodegradation on COD values. [16 Hrs]

Unit II

Pericyclic reactions: Classification of pericyclic reactions. Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene and allyl system.

Electrocyclic reactions: Woodward-Hofmann rules for electrocyclic reactions, FMO theory of electrocyclic reactions, correlation diagram for cyclobutadiene and cyclohexadiene systems.

Cycloaddition reactions: [2+2], [3+2] and [4+2] cycloadditions, analysis by FMO and correlation diagram method. Cycloadditions - antarafacial and suprafacial additions, [2+2] additions of ketenes.

1,3-dipolar cycloadditions: involving nitrile oxide, nitrile imine, nitrile ylide cycloaddition. Intra and intermolecular 3+2 cycloaddition and their application in organic synthesis.

[4+2] cycloaddition reactions: Diel's-Alder reaction, hetero Diel's-Alder reaction and their applications.

Sigmatropic rearrangements - Classification, stereochemistry and mechanisms. suprafacial and antarafacial shifts of H, sigmatropic shifts involving carbon moieties. [3,3]- and [5,5]-sigmatropic rearrangement, Claisen, Cope and aza-Cope rearrangements.

Chelotropic reactions: [16 Hrs]

Unit III

Chemistry of heterocyclic compounds II: Synthesis and synthetic applications of azirines & aziridines, azetidines, oxazolines, isoxazolines, isoxazole, triazole and azepines and benzodiazepines.

(16Hrs)

References:

1. J. March, *Advanced Organic Chemistry*, Willey Interscience, 1994.
2. F. A. Carey and Sundberg, *Advanced Organic Chemistry – Part A & B*, 3rd edition, Plenum Press, New York, 1990.
3. *Comprehensive Organic Chemistry*, Pergamon Press, New York, Vol 1, 1996,
4. H. Pine, Hendrickson, Cram and Hammond, *Organic Chemistry*, Mac Grow Hill, New York, 1987.

5. I. I. Finar, Organic Chemistry, ELBS Longmann, Vol. I & II, 1984
6. Comprehensive Organic Synthesis – B. M. Trost and I. Fleming series, Pergamon Press, New York, 1991.
8. S. K. Ghosh, Advanced General Organic Chemistry, Book and Allied (P) Ltd, 1998
9. *Heterocyclic Chemistry –Joule & Smith*
10. *Heterocyclic chemistry – Achaeson*
11. *Basic Principles of heterocyclic chemistry – L. A. Pacquette*
12. *Comprehensive heterocyclic chemistry –Kartritzky series, Pergamon Press, New York, 1984.*

OCO SCT 3.41: Carbohydrates, proteins and nucleic acids

UNIT – I:

CARBOHYDRATES: Introduction, Ring size determination of monosaccharides, configuration and conformations of monosaccharides, anomeric effect, Hudson's rules, epimerization and mutarotation. Synthesis, industrial and biological importance of glycosides, amino sugars, sucrose, maltose and lactose. Polysaccharides: General methods of structure elucidation. Industrial importance and biological importance of cellulose, starch, glycogen, dextran, hemicellulose, pectin, agar- agar. Photosynthesis and biosynthesis of carbohydrates. [16 Hrs]

UNIT – II:

AMINO ACIDS, PEPTIDES and PROTEINS

Amino Acids: General structure, physiological properties Peptides: Structure and conformation of peptide bond, peptide synthesis: Solution phase and Merrifield's solid phase synthesis, Racemization and use of HOBT, Synthesis of oxytocin and vasopressin, biological importance of insulin, selective cleavage of polypeptide bonds (chemical and enzymatic). Proteins: Structure determination: C and N terminal residue determination, primary, secondary, tertiary and quaternary structure determination, denaturing and renaturing of proteins. 16 Hrs

UNIT - III

Nucleic acids: Introduction, structure and synthesis of nucleosides and nucleotides, protecting groups for hydroxy group in sugar, amino group in the base and phosphate

functions. Methods of formation of internucleotide bonds: DCC, phosphodiester approach and phosphoramidite methods. Solid phase synthesis of oligonucleotides. Structure of RNA and DNA, Crick-Watson model, role of nucleic acids in the biosynthesis of proteins. Protecting groups: Protection of hydroxyl, carboxyl, carbonyl, thiol and amino groups. Illustration of protection and deprotection in synthesis. [16 Hrs]

References:

1. L. Finar, Organic Chemistry, ELBS Longmann, Vol. I & II, 1984.
2. K. Albert, L. Lehninger, D.L. Nelson, M.M. Cox, Principles of Biochemistry, CBZ publishers, 1st edition, New Delhi, 1993.
3. Harper's Biochemistry, Ed. R. Harper, 22nd edition, Prentice Hall Press, New York, 1990.

OCO SCT 3.42: Metals in Organic chemistry and Food Analysis

UNIT –I

Biochemistry of Calcium: Binding, transport and accumulation of Ca^{2+} , calcium and muscle contraction, calcium in blood clotting mechanisms.

Biochemistry of Cobalt: Vitamin B₁₂ and B₁₂ coenzymes, Coenzyme A, enzyme co-factor, NAD, FMN and FAD.

Bioenergetics: Energy in biology, energy transfer, the energy of ATP, Kinetic stability of ATP, standard free energy change entropy. High energy compounds, mitochondrial flow of electrons from NADH to O₂.

Bioinorganic Chemistry of Phosphorous: Phosphates, oxidative phosphorylation-substrate level phosphorylation, respiratory chain phosphorylation, mechanism of oxidative phosphorylation.

Transport and Storage of Iron: Ferritin, transferrin, hemosiderin and apoferritin.

Iron Transport in Microbes: Siderophores, *in vivo* microbial transport of iron.

[16 HOURS]

UNIT –II

Dioxygen metal complexes in biological system: Reactions of molecular oxygen, activation of dioxygen molecule in transition metal complexes.

Oxygen Carrying Proteins: Introduction to porphyrin system, substituent effects on porphyrin rings, hemoglobin and myoglobin, model compounds for oxygen carriers (cobalt, iridium, iron and nickel). Hemerythrin and hemocyanin.

Electron Transport Proteins: Iron-sulphur proteins (rubredoxins and ferredoxins) and cytochromes including cytochrome P450.

Iron and Copper Containing redox enzymes: Catalase and peroxidase. Superoxide dismutase.

Zinc containing enzymes: Alcohol dehydrogenase, carboxypeptidase A.

Molybdenum containing enzymes: Aspects of molybdenum chemistry, xanthine oxidase, aldehyde oxidase, sulphite oxidase, nitrogenase and nitrate reductase.

[16 HOURS]

Unit III

Food Analysis: Historical perspectives, objectives of food analysis. Sampling procedures. Detection and determination of sugars and starch. Methods for protein determination. Oils and fats and their analysis-iodine value, saponification value and acid value. Rancidity-detection and determination (peroxide number). Tests for common edible oils. Analysis of foods for minerals-phosphorus, sodium, potassium and calcium. General methods for the determination of moisture, crude fibre and ash contents of foods. Analysis of milk for fat and added water. Non-alcoholic beverages. Determination of chicory and caffeine in coffee; caffeine and tannin in tea. Alcoholic beverages-methanol in alcoholic drinks and chloral hydrate in toddy. Food additives. Chemical preservatives-inorganic preservatives-sulphur dioxide and sulphites, their detection and determination. Organic preservatives-benzoic acid and benzoates, their detection and determination. Artificial sweeteners-saccharin, cyclamate and dulcin-detection and determination. Flavouring agents-detection and determination of vanilla and vanillin. Coloring matters in foods-classification, certified colours, detection of water soluble dyes, colour in citrus fruits, beet dye in tomato products, mineral colour. Pesticide residues in foods. Determination of chlorinated organic pesticides.

[16 HOURS]

REFERENCES

1. Pharmaceutical Analysis, T. Higuchi and E.B. Hanssen, John Wiley and Sons, New York.

2. Pharmaceutical Analysis, Modern methods-Part A and B, Edited by James W. Munson.
3. Hawk's physiological chemistry-edited by B.L. Oser, 14th edn, Tata Mc Graw Hill.(1976).
4. The Essentials of Forensic Medicine and Toxicology-Dr.K.S. Narayana Reddy.
5. Practical clinical Biochemistry-Harold Varley and Arnold.Hein mann, 4th edn.
6. Chemical Analysis of Foods-H.E.Cox and pearson.
7. The Inorganic Chemistry of Biological Processes – 2nd edition, M.N. Hughes
8. Bioinorganic Chemistry –M. Satake and Y. Mido.
9. Bioinorganic Chemistry – G.R. Chatwal and Ajaykumar Bhagi.
10. Biological aspects of Inorganic Chemistry – A.W. Addison, W.R. Cullen, D. Dolphin and B.R. James.
11. Organometallic Chemistry – R.C. Mehrothra and A. Singh.
12. Fundamental Transition metal Organometallic Chemistry – Charles M. Lukehart.
13. Modern Aspects of Inorganic Chemistry –Emeleus and Sharpe.

OCO SCT 3.43 **Enzymes functions and their kinetics**

UNIT-I

Enzymes: Introduction, nomenclature, classification with examples and their functions.

The mechanistic role of the following co-enzymes in the living systems:- i. Thiamine pyrophosphate (TPP) in oxidative and non-oxidative decarboxylation of α -keto acids and formation of ketols; ii. Pyridoxal phosphate:- transamination, decarboxylation, dealdolization and elimination reactions of amino acids; iii. Lipoic acid in the transfer of acyl group and oxidation reactions; iv. Co-enzyme A: generation and transfer of acyl groups; v. biotin – in the addition of carboxyl groups to saturated carbon atoms and in transcarboxylation reactions; tetrahydrofolic acid – in one carbon transfer reactions at all oxidation levels except that of CO₂; Nicotinamide and flavin coenzymes – in biological oxidation-reduction reactions.

Biogenesis of fatty acids, terpenoids (mono and sesquiterpenoids), steroids, aminoacids, alkaloids.

(16 HOURS)

Unit II

ENZYME KINETICS: Effect of substrate concentration, Effect of pH, effect of catalysts and inhibitors (substrate, zeolite, Cr^{3+} , Fe^{2+} ZnO, U.V light) and effect of temperature. A brief kinetic and mechanistic applications of glucose oxidase and L-amino oxidase in the oxidation of glucose and L-amino acids.

Biological significance of Donnan membrane phenomenon. Micelles and involvement during digestion and absorption of dietary lipids. Diffusion of solutes across bio-membranes and its application in the mechanism of respiratory Exchange. "Salting In" and "Salting out" of proteins. Osmotic behaviour of cells and osmo-regulation and its application in the evolution of excretory systems of organisms. Significance of viscosity in biological systems- mechanism of muscle contraction, detection of intramolecular disulfide bonds in proteins, polymerization of DNA and nature of blood flow through different vessels. Effect of temperature solute concentration (amino acids) in surface tension. Biological significance of surface tension, stability of Alveoli in lungs, interfacial tension in living cells (Danielle and Davson model).

In metabolism studies; Radio immuno assay (labeling of antigens) Immune radiometry.

(16 Hours)

UNIT-III

PHARMACOKINETICS: Plasma concentration time curve, drug dissolution rate, physico-chemical factors effecting bioavailability. Pharmacokinetics applied to one component open model. Calculation of elimination rate constant and metabolism constant apparent volume of drug distribution and kinetics of drug clearance. Protein binding of drugs, Bioavailability and bio equivalence. Factors affecting bioavailability route of drug administration and kinetics of protein binding.

Chemical biology: What is life? Its chemical definition in the perspective of modern scientific progress. **Origin of life:** spontaneous generation of life and its failure; abiotic origin of life: Urey-Miller's experiment, Oparin-Haldane concept of origin of life, panspermic origin of life and genetic code (life material has come from extra- terrestrial source through meteorites. What is the first important polymer in the evolution of life? RNA based origin of life.

Water – the major constituent of life, its physical and chemical nature that makes it versatile as a solvent. Is life possible without water?

(16 HOURS)

References

1. Thermodynamics for chemists by S. Glasstone, Affiliated East-west press, New Delhi, (1965).
2. Chemical Thrmodynamics by I.M. Klotz, W.A. Benzamin Inc. New York, Amsterdam, (1964).
3. Basic Physical Chemistry by W.J. Moore, Prentice Hall of India Pvt. Ltd., New Delhi, (1986).
4. Text book of Physical Chemistry by Samuel Glasstone, MacMillan Indian Ltd., (II edition), (1974).
5. Theoretical chemistry by S. Glasstone.
6. Statistical themodynamics by B.C. Meclelland, Chapman and Hall, London (1973).
7. Elementary statistical thermodynamics by N.D. Smith Plenum Press, NY (1982).
8. Elements of classical and statistical thermodynamics by L.K. Nash, Addison-Wesley (1970).
9. Statistical thermodynamics by I.M. Klotz.
10. Introduction to Statistical Thermodynamics by M. Dole, Prantice-Hall, (1962).

FORTH SEMESTER

OCO HCT 4.1: Lipids, Porphyrins, anthocyanins and flavonoids

Unit I

Lipids: Nomenclature, classification, purification, structure and synthesis of fatty acids, phospholipids, sphingolipids. Biological importance of lipids (Lecithin, sphingolipids, oils and fats).

Prostaglandins: Introduction, classification and biological importance of PG's. Constitution of PGE₁. Synthesis of PGE & F series.

Terpenoids: Introduction, classification and general methods of structural elucidation. Biological importance of terpenoids. Chemistry of pinene, camphor, caryophyllene, santonin, abietic acid and vetivone.

[16 Hrs]

Unit II

Porphyrins: Introduction, structure and biological functions of haemin. Vitamin B₁₂ : structure and as coenzyme in molecular rearrangement reactions; Chlorophyll: structure and biological importance.

Flavonoids and Isoflavonoids: Occurrence, nomenclature and general methods of structure determination. Isolation and synthesis of Apigenin, Luteolin, Kaempferol, Quercetin, wedelolactone, Butein, Daidzein.

Biosynthesis of flavonoids and isoflavonoids: Acetate Pathway and Shikimic acid Pathway.
Biological importance of flavonoids and isoflavonoids

Carotenoids: Methods of isolation. Structure elucidation and synthesis of β -carotene. Structural relationship of α -, β - and γ -carotenes. [16 Hrs]

References

1. I. L. Finar, Organic Chemistry, ELBS Longmann, Vol. I & II, 1984.
2. K. Albert, L. Lehninger, D. L. Nelson, M. M. Cox, Principles of Biochemistry, CBZ publishers, 1st edition, New Delhi, 1993.
3. Harper's Biochemistry, Ed. R. Harper, 22nd edition, Prentice Hall Press, New York, 1990.
4. Encyclopedia of Chemical technology – Kirck-Othmer series
5. Harper's review of biochemistry – P. W. Martin, P. A. Mayer & V. W. Rodfwell, 5th edition, Maurzen Asian Edition, California, 1981.

ORGANIC CHEMISTRY PRACTICALS-III [64 hrs]

1. Determination of equivalent weight of acids by silver salt method
2. Determination of iodine value of n oil and fats by chloramine-T
3. Saponification value of an oil or fats
4. Estimation of sugars by Fehlings method
5. Determination of enol content by Meyer's method
6. Estimation of hydroxyl groups
7. Estimation of vicinal hydroxyl groups
8. Estimation of ketones by haloform reaction
9. Estimation of sugars by Bertrand's method
10. Estimation of nitro groups
11. Estimation of amino acids

12. Estimation of ketones by oxime method

References:

1. Manual of Organic Chemistry - Dey and Seetharaman.
2. A Text Book of Practical Organic Chemistry – A.I. Vogel, Vol.III
3. Practical Organic Chemistry - Mann & Saunders

OCO HCT 4.2: MOLECULAR REARRANGEMENTS, RETROSYNTHESIS, AND ORGANOMETALLIC COMPOUNDS

UNIT – 1

Molecular rearrangements: Introduction Carbon to carbon migration: Pinacol-pinacolone, Wagner-Meerwein, Demjanov, Benzidine, benzilic acid, Favorskii, Arndt-Eistert synthesis, Fries rearrangement, dienophine rearrangement. Carbon to nitrogen migration: Hofmann, Curtius, Lossen, Schmidt and Beckmann rearrangements. Miscellaneous rearrangements: Wittig, Smiles, Baeyer-Villiger rearrangement, Stevens, Sometlet-Hauser, Neber, Japp-Klingeman, allylic rearrangement.

Retrosynthesis: Introduction to disconnection approach: Basic principles and terminologies used in disconnection approach. One group C-X and two group C-X disconnections. Synthons and synthetic equivalents. Retrosynthesis and synthesis of benzofurans, p-methoxy acetophenone, saccharine, α - bisabolene, nuciferal, tetralone, ibuprofen. [16 hrs]

Unit II

Chemistry of organometallic compounds: Synthesis and reactions of organolithium (n-BuLi, PhLi), organocadmium, organomagnesium (Grignard reagent), organomanganese, organoselenium and organotellurium.

Organoaluminium reagents: Preparation, site selective and stereoselective additions of nucleophiles mediated by organoaluminum reagents, reaction with acid chlorides, allyl vinyl ethers, 1,2-addition to imines and application in the synthesis of natural products.

Organocopper reagents: Gilman reagent, preparation, reactions with aldehydes, ketones and imines. Application in the synthesis of brevicomin,

Organopalladium compounds: Suzuki coupling, Heck reaction.

Organozinc reagents: Preparation - oxidative addition and transmetallation, addition reactions of alkyl, aryl, allylic and propargylic zinc reagents, diastereoselective and enantioselective addition reaction with aldehydes, Reformatsky reaction.

Organosamarium reagents: Reactions promoted by samarium diiodide and dicyclopentadienyl samarium – Barbier type reaction, Reformatsky type reactions, ketyl-alkene coupling reactions, pinacolic coupling reactions, acyl anion reactions.

Organotin reagents: tributyltin hydride, Barton decarboxylation reaction, Barton deoxygenation reaction, Stille coupling, Stille-Kelley coupling reactions, Barton McCombie reaction, Keck stereoselective allylation and other applications.

(16 HOURS)

Unit III

Organoboron compounds: Introduction and preparations. Hydroboration and its applications. *Reactions of organoboranes:* isomerization reactions, oxidation, protonolysis, carbonylation, cyanidation. *Reaction of nonallylic boron stabilized carbanions:* Alkylation reactions, Acylation reaction, Reactions with aldehydes or ketones (E and Z-alkenes).

Organosulphur compounds: Introduction. Preparations, reactions, mechanism and synthetic applications of important sulphur containing reagents like dithiane, sulphur ylides etc.

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

Organophosphorous compounds: Nomenclature, synthesis and reactions of trialkyl phosphine, triarylphosphine, trialkyl phosphite, triaryl phosphite, trialkyl phosphate, triaryl phosphates. Wittig reaction and Wittig-Horner reactions: - mechanisms and synthetic uses. Arbasov reaction, transesterification.

Organofluorine compounds

(16 HOURS)

References:

1. J. March, *Advanced Organic Chemistry*, Willey Interscience, 1994.
2. F. A. Carey and Sundberg, *Advanced Organic Chemistry – Part A & B*, 3rd edition, Plenum Press, New York, 1990.
3. *Comprehensive Organic Chemistry*, Pergamon Press, New York, Vol 1, 1996,
4. H. Pine, Hendrickson, Cram and Hammond, *Organic Chemistry*, Mac Grow Hill, New York, 1987.

5. I. I. Finar, Organic Chemistry, ELBS Longmann, Vol. I & II, 1984
6. Comprehensive Organic Synthesis – B. M. Trost and I. Fleming series, Pergamon Press, New York, 1991.
8. S. K. Ghosh, Advanced General Organic Chemistry, Book and Allied (P) Ltd, 1998
9. *Heterocyclic Chemistry –Joule & Smith*
10. *Heterocyclic chemistry – Achaeson*
11. *Basic Principles of heterocyclic chemistry – L. A. Pacquette*
12. *Comprehensive heterocyclic chemistry –Kartritzky series, Pergamon Press, New York, 1984.*

OCO HCT 4.3 **DISSERTATION**

OCO SCT 4.41 : Advanced Medicinal chemistry

Unit I

Synthetic drugs: Introduction, pharmadynamics, pharmakinetics, pharmatherapeutics, chemotherapy, metabolites antimetabolites, agonists and antiagonists. Routes of drug administration, factors affecting choice of routes.

A general study of following class of drugs:

Sulpha drugs: Sulphonamides - Mechanism of action, resistance to sulphonamides, sulfametaoxazole.

Antipyretics: aspirin, paracetamol, phenacetin, novalgin and their mechanism of action.

Antimalarials: structure , synthesis and mechanism of action of quinine and chloroquine.

Hypnotics, analgesics and sedatives: phenosorbitol, chlordiazepoxide, mebrobamide.

Antihistamines: structure and its pharmacological action, adverse effects and precautions of chlorpheniramine.

Stimulants: structure and action of caffiene

Antineoplastics: structure, pharmacological action and adverse effects of 5-flurouracil, chlorambucil and phodophyllotoxin. **[16 Hrs]**

Unit II

Antineoplastic Agents: Introduction, cancer chemotherapy, role of alkylating agents and antimetabolites in treatment of cancer. Mention of carcinolytic antibiotics and mitotic

inhibitors. Synthesis of mechlorethamine, cyclophosphamide, melphalan, mustards and mercaptopurine. Recent development in cancer chemotherapy – podophyllotoxin and its derivatives, taxol.

Cardiovascular drugs: Introduction, cardiovascular diseases, drug inhibitors of peripheral sympathetic function, central intervention of cardiovascular output direct acting arteriolar dilators, synthesis of diltiazem, verapamil, methyldopa, atenolol, oxprenolol, antihypertensive drugs, lipid lowering agents (atorvastatin, statin derivatives).

Local antiinfective drugs: Introduction and general mode of action, structure of sulphonamides, forazolidone, nalidixic acid, ciprofloxacin, norfloxacin, dapsone, aminosalicic acid, isoniazid, ethionamide, ethambutal, fluconazole, griseofulvin, chloroquine and primaquine.

[16 Hrs]

Unit III

Antibiotics: Introduction, cell wall biosynthesis, inhibitors, β -lactam group of antibiotics - Penicillin, Ampicillin and Amoxicillin, amoxicillin, chloramphenicol, cephalosporin analogs, tetracycline, streptomycin, Erythromycin analogs and Ciprofloxacin.

ANTIPROTOZOAL DRUGS – Metronidazole

ANTIHELMINTHICS – Mebendazole/albendazole

ANTIVIRALS - Azothymidine(AZT), Acyclovir

ANTITUBERCULAR DRUGS - Ethambutol

ANTIFUNGALS - Griseofulvin

AUTACOIDS: Definition, Occurrence, Isolation, Classification, Stereochemical Studies, Synthesis, Biological and Therapeutic functions

Histamines : Histamine antagonists, -H1 blockers - Chlorpheniramine, -H2 blockers - Ranitidine

5-HT Serotonin, 5-HT receptor antagonist – Metaclopramide

Computational chemistry and combinatorial chemistry.

[16 Hrs]

References;

1. Introduction to medicinal chemistry, A Gringuage, Wiley-VCH.
2. Wilson and Gisvold's Text Book of organic medicinal and pharmaceutical chemistry, Ed Robert F. Dorge.
3. An introduction to drug design, S.S. Pandey and J.R. Dimmock, New Age International.
4. Burger's medicinal chemistry and drug discovery, Vol-1 (Chapter-9 and Ch-14), Ed. M.E. Wolff, John Wiley.
5. Goodman and Gilman's pharmacological basis of therapeutics, McGraw-Hill.
6. The organic chemistry of drug design and drug action, R. B. Silverman, Academic Press.
7. Strategies for organic drug synthesis and design, D. Lednicer, John Wiley.
8. Medicinal Chemistry, A Kar, Wiley, 2000.
9. Synthetic drugs, G. R. Chatwal, Himalaya, New Delhi, 1995.
10. Comprehensive organic chemistry, Vol. 5 (Antibiotics), D.H.R. Barton, W. D. Ollis, Pergamon Press, NY, 1979.
11. Instant Notes Medicinal Chemistry, P Graham, Viva, New Delhi, 2002.

OCO SCT 4.42 : Steroids, Alkaloids and Polymer chemistry

Unit I

Steroids: Introduction, structural elucidation of cholesterol, bile acids, ergosterol and its irradiation products. Sex hormones and corticosteroids: Synthesis of estrone, progesterone, androsterone, testosterone. Barton reaction for the synthesis of aldosterone. Brief discussion of homosteroids, norsteroids and oral contraceptives. Biological significance of anabolic steroids

[16 Hrs]

Unit II

Alkaloids: Introduction, classification, isolation and general methods of structural elucidation. Biological importance of alkaloids. Structure and synthesis of nicotine, papavarine, quinine, morphine, LSD and reserpine.

UNIT - III

Polymers

Importance of polymers. Basic concepts: Monomers, repeat units, degree of polymerization, linear, branched and network polymers. Classification and nomenclature of polymers.

Properties of polymers (brief explanation of molecular weight, glass transition temperature - T_g , solubility and visco-elasticity).

Methods of polymerization-addition and condensation polymerization, ionic and free-radical polymerization processes, polymerization with complex catalysts (Ziegler-Natta catalysis), co-polymerization and their mechanisms. Techniques of polymerization - bulk, emulsion etc.,

Stereospecific Polymers - Preparation and significance- classification of polymers based on physical properties - Thermoplastics - Thermosetting plastics - Fibers and elastomers - General applications.

Preparation of Polymers - Preparation of Polymers based on different types of monomers - Industrial applications-olefin polymers - Diene polymers- nylons - Glyptal resins - Urea-formaldehyde, phenol - formaldehyde and melamine resins - Epoxy resins - Ion exchange resins, polycarbonates and its applications. **[16 Hrs]**

References

1. I. L. Finar, Organic Chemistry, ELBS Longmann, Vol. I & II, 1984.
2. K. Albert, L. Lehninger, D. L. Nelson, M. M. Cox, Principles of Biochemistry, CBZ publishers, 1st edition, New Delhi, 1993.
3. Harper's Biochemistry, Ed. R. Harper, 22nd edition, Prentice Hall Press, New York, 1990.
4. Encyclopedia of Chemical technology – Kirck-Othmer series
5. Introduction to alkaloids – G. A. Swan.
6. The alkaloids- K. W. Bentley.
7. Steroids – L. Fischer & M. Fisher.
8. Steroids –Shoppe

OCO SCT 4.43. **Industrial Chemicals**

UNIT I

Perfumery: Introduction, Compounds used in perfumery and their classification, methods of preparation and importance of phenyl ethanol, Yara yara, Ionone musk ketone, musk ambrette, musk xylene, phenyl acetic acid and its esters, benzyl acetate, synthetic musks and jasmine.

Flavours: Introduction, classification, Chemical basis for flavour, flavours in diary products, flavours formed by heating or cooking-caramelisation & Maillard reaction, flavour degradation by oxidation-rancidity, molecular structure & odour/taste, sweetness, acidity & sourness, saltiness, bitterness, synthetic chemicals, Natural flavouring materials & classification. Flavouring materials-Acidulants, sweeteners, potentiators, enhancers & sodium-restricted food flavourings. Organic chemicals used in flavorings & food colorants. Essential oils: Source, constituents, isolation & uses.

Cosmetics: Detailed study of formulations and manufacturing of cream and lotions, lipstick and nail polish, shampoos, hair dyes and tooth pastes. A formulary of cosmetic preparation-Godwin.

[16 hrs]

UNIT II

Oils, soaps and Detergents: Refining of edible oils, manufacturing of soaps, detergents-classification-anionic, cationic, non-ionic and amphoteric detergents, comparison of soaps and detergents, detergent builders and additives, liquid soaps. Manufacturing of fatty acids and glycerol, greases from fatty acids, turkey red oil. Paints, varnishes and inks-constitutions, examples of preparation and applications.

Food Analysis: Moisture, ash, crude protein, crude fiber, fat, carbohydrate, calcium, potassium, sodium and phosphates, food adulteration-common adulteration in food, contamination of food stuffs, microscopic examination of food for adulterants, pesticide analysis in food products.

UNIT – III

Rubber: Natural and synthetic rubbers, structure elucidation of natural rubber.

Polymer degradation reactions: Thermal, oxidative and radiative processes.

Synthesis and properties of Buna-S and butyl rubbers.

Conducting Polymers: Polyanilines

Polymer Characterizations: Isolation and purification of polymers-Fractional precipitation, partial dissolution, gradient elution and Gel permeation chromatography. Principles of determination of molecular weights-End group analysis, viscosity, light scattering, osmometry, cryoscopy, ebulliometry and ultracentrifugation method. Thermal characterization- Isothermal gravimetric analysis, Thermogravimetry , Differential Thermal Analysis and Differential Scanning Calorimetry. Mechanical properties-Tensile, Impact and Flexural strengths. Flammability and Limiting Oxygen Index. Characterization and structural analysis of polymers - IR, NMR, ESR, X-Ray Diffraction and Scanning Electron Microscopic Methods.

[16 Hrs]

REFERENCES

1. Text book of polymer Science. F.W. Billmeyer, Jr., John Wiley. London (1994).
 2. Polymer Science. V. R. Gowrikar, N. V. Vishwanathan and J. Srreedhar, Wiley Eastern, New Delhi (1990).
 3. Fundamentals of Polymer Science and Engineering. A. Kumar and S.K. Gupta. Tata –McGraw Hill New Delhi (1978).
 4. Polymer Characterization, D. Campbell and J. R. White, Chapman and Hall, New York.
 5. Fundamental Principles of Polymer materials, R. L. Rosen, John Wiley and Sons, New York.
 6. Infrared spectroscopy by R. T. Conley, Allyn and Bacon, Inc.
 7. Functional monomers and polymers by K. Takemoto, Y. Inaki and P. M. Ottenbrite, Marcel dekker, Inc., New York, 1987.
 8. Progress in Inorganic Chemistry, by Stephen J. Lippard, John Wiley and Sons, Inc., New York, vol. 20, 1976.
1. Synthetic organic chemistry, G R Chatwal, Himalaya publishing house.
 2. A formulary of paints and other coatings, M Ash & I Ash
 3. Encyclopedia of Chemical Technology, Kiik & others.
 4. Perfumary Technology, B. Billot and F. V. Wells
 5. Lehninger principles of Biochemistry, David .L Nelson and Michael M Cox
 6. Dairy chemistry and animal nutrition, V.K. Chhozllani
 7. Principles of Animal nutrition and Feed technology Part I and II, D.V Reddy
 8. Feeds and Principles of animal nutrition, G.C.Banerjee.

9. Source book of flavors, Heath.

OPEN ELECTIVE:

OCO OET 3.61 APPLICATIONS OF SYNTHETIC PRODUCTS

Unit I

Acids and bases, electrophiles and nucleophiles, hybridization in carbon compounds, inductive effect, resonance effect, hydrogen bonding {types of hydrogen bonding, hydrogen bonding in HF, water, alcohols, acids, nitrophenols) bond angle and bond length.

Purification:- Crystallization, sublimation, fractional crystallization, distillation techniques (simple distillation, steam distillation, distillation under reduced pressure, fractional distillation).

Separation techniques:- Solvent extraction, continuous extraction, chromatography (principles of TLC, PC, column, GC, ion exchange chromatography) and electrophoresis

Characterization: Detection of elements, estimation of carbon, hydrogen, halogens, sulphur, nitrogen and phosphorous. Detection of functional groups (hydroxyl, carboxyl, keto, ester, amino, nitro, amide, thiol, ether etc) in the unknown samples. Basic principles for the determination of hydroxyl, carboxyl, keto, ester, amino, nitro groups. Estimation of sugars, aminoacids and proteins.

[16 Hrs]

Unit II

Basics of organic reactions:- Meaning and importance of reaction mechanism, classification and examples for each classes.

Structural determination of organic compounds by: UV spectroscopy –absorption maxima for simple organic molecules; **IR spectroscopy** –absorption frequencies for functional groups in simple organic molecules; **NMR-spectroscopy** – Chemical shift (δ -scale), spin-spin coupling, coupling constants, applications to simple molecules. [For all spectroscopic methods, simple molecules like ethyl alcohol, methyl cyanide, ethane, propane, ethylene, benzene, methyl amine, aniline, acetone, acetophenone and other simple molecules are considered].

[16 Hrs]

UNIT – III

Dyes: Colour and constitution, classification, dyeing method and their industrial importance.

Drugs: Basic concepts, classification, sources, the requirement of an ideal drug

Synthetic drugs: Structure and medicinal properties:

Sulphanilamide – an example of sulpha drug-paracetamol, aspirin, oil of wintergreen; Mephensin – a muscle relaxant; Ibuprofen – an anti-inflammatory drug; L-dopa – cures Parkinson's disease; Chloroquine – an antimalarial drug; Chlorpromazine – an antipsychotic agent; Phenobarbital – a barbiturate; Omeprazole – an drug; Ciprofloxacin – an antibacterial drug; Formulation of drugs – introduction and classification.

Polymers: Introduction, biodegradable and non-biodegradable polymers and their industrial importance, plastics (uses and effects on environment), natural and synthetic rubbers, polyamides and poly esters like nylon, decron, terelyne. Thermoplastics - poly carbonates, poly acrylates in lens applications, polyurethanes and conducting polymers. **[16 Hrs]**

References:

1. I.L. Finar, Organic Chemistry, ELBS Longmann, Vol. I & II, 1984.
2. K. Albert, L. Lehninger, D. L. Nelson, M. M. Cox, Principles of Biochemistry, CBZ publishers, 1st edition, New Delhi, 1993.
3. Harper's Biochemistry, Ed. R. Harper, 22nd edition, Prentice Hall Press, New York, 1990.

OCO OET 3.62: Natural and synthetic products

Unit I

Fats and oils: Isolation, purification, structure and biological importance.

Essential oils: Source, constituents, isolation & uses.

Phospholipids: Isolation, structure and biological significance of lecithin and cephalin

Sphingolipids: Examples with structure and biological importance.

Prostaglandins: Classification, source, structure, nomenclature and its significance.

Terpenoids: Introduction, classification, source, structure of biologically important terpenoids (antihelmentic, anticancer terpenoids, etc)

Steroids: Structure and biological significance of cholesterol, bile acids, androgen, estrone, progesterone and anabolic steroids. **[16 Hrs]**

Unit II

Flavonoids and Isoflavonoids: Occurrence, nomenclature, structure and their biological importance.

Porphyrins: Introduction, structure and biological functions of haemin. Vitamin B₁₂ : structure and as coenzyme in molecular rearrangement reactions; Chlorophyll: structure and biological importance.

Carotenoids: Methods of isolation, structure and their biological importance..

Alkaloids: Introduction, source, structure and biological significance of vinca alkaloids, chincona alkaloids, LSD, reserpine, morphine, codeine, strychnine, brucine, nicotine, yohimbine,

Vitamins: structure and biological functions of vitamin A, C, D, E, K, biotin, pyridoxine, thiamine. **[16 Hrs]**

UNIT III

Soaps and detergents: Production and their cleansing action.

Liquid crystals and their applications.

Surfactants

Cosmetics: Detailed study of formulations and manufacturing of cream and lotions, lipstick and nail polish, shampoos, hair dyes and tooth pastes.

Flavours: Natural flavouring materials and classification

Sweeteners: Natural and synthetic sweeteners.

Insecticides: Introduction, classification, applications and their effect on environment.

Pheromones: Introduction, Sources, biological importance.

Explosives: Introduction, RDX, Gun powder, TNT. **[16 Hrs]**

References

1. I. L. Finar, Organic Chemistry, ELBS Longmann, Vol. I & II, 1984.
2. Essentials of physiological chemistry – Anderson, John Wiley & Sons, New York, 1953.
3. K. Albert, L. Lehninger, D. L. Nelson, M. M. Cox, Principles of Biochemistry, CBZ publishers, 1st edition, New Delhi, 1993.
4. Harper's Biochemistry, Ed. R. Harper, 22nd edition, Prentice Hall Press, New York, 1990.

- 5 Encyclopedia of Chemical technology – Kirck-Othmer series
- 6 Harper's review of biochemistry – P. W. Martin, P. A. Mayer & V. W. Rodfwel, 15th edition, Maurzen Asian Edition, California, 1981.