MANGALORE UNIVERSITY

M. Sc. Degree Programme in Organic Chemistry: CHOICE BASED CREDIT SYSTEM (CBCS) SEMESTER SCHEME COURSE PATTERN AND SCHEME OF EXAMINATION

Semester	Paper	Instruction hrs/week	Duration of Exam(hrs)	Marks			Credits		
				IA	Exam	Total	Situits		
I/II	4Theory Papers	4x4	4x3	4x30	4x70	4x100	4x4		
	3 Practicals and 1 theory paper 1 of 2 hours duration/ week	3x4 1x2	3x4 1x2	3x15 1x15	3x35 1x35	3x50 1x50	3x2 1x2		
	Semester Total 18	8T+12P	<u></u>	180	420	600	24		
III/IV	4Theory Papers	4x4	4x3	4x30	4x70	4x100	4x4		
	3 Practicals	3x6	3x5	3x25	3x50	3x75	3x3		
	Seminar	1		25	-	25	1		
Semester Total 16T+18P					430	650	26		
Grand Total									
In the III Semester, there will be a choice based course in lieu of one of the theory papers									
and in the IV Semester, there may be a project work/dissertation in lieu of 1 or 2 Practicals.									

(Year 2014-15 onwards)

M. Sc. DEGREE PROGRAMMES IN ORGANIC CHEMISTRY

The First, Second and Third Semesters of the course involve theory and practicals, while the IV Semester involves theory, practicals and project work. The project work shall be carried out for 6 to 8 weeks (at least 30 hrs per week), after the Second Semester of the course, either in the concerned Department or in an Approved Industry or in both, under the supervision of a teacher and submit a project report. Experts from the industries may also be involved in the project work as co-guides and in the evaluation of project reports.

BASIS FOR INTERNAL ASSESSMENT:

Internal assessment marks in theory papers shall be based on tests. The tests may be conducted 8 and 12 weeks after the start of a semester. Practical internal assessment marks shall be based on test and records. The practicals test may be conducted 10 weeks after the start of a semester. The Seminar shall be of at least 45 minutes duration. The project report shall be evaluated for 75 marks. The Seminar in IVSemester shall be related to the project.

THEORY QUESTION PAPERS PATTERN

The Syllabus of each paper shall be grouped into units of 14 teaching hours. All the papers, except, Environmental Chemistry (1st semester) and Diffraction & Electroanalytical Techniques (2nd Semester) shall contain four such units each. Question Papers in all the four semesters shall consist of Parts A and B. Part A shall contain twelve (12) very short answer objective type questions carrying 2 marks each drawn from all the four units of the syllabus (3 questions per unit). Ten (10) questions out of Tweleve (12) are to be answered. Part B shall contain eight (8) brief and/or long answer questions carrying 10 marks each drawn from all the four units of the syllabus (2 questions per unit). There may be a maximum of three sub-divisions per question, carrying 3 or more marks per sub-division. Five (5) out of eight (8) questions are to be answered.

The Syllabi of the papers, in AC 405/OC 405/CA 405 - Environmental Chemistry (1st semester) and in in AC 455/OC 455/CA 455 - Diffraction & Electroanalytical Techniques (2nd Semester) shall also be grouped into units of 14 teaching hours. They shall contain two such units each. Question Papers in AC 405/OC 405/CA 405 and AC 455/OC 455/CA 455 shall also consist of Parts A and B. Part A shall contain six (6) very short answer objective type questions carrying 2 marks each drawn from both the units of the syllabus (3 questions per unit). Four (4) questions are to be answered. Part B shall contain five (5) brief and/or long answer questions carrying 9 marks each drawn from both the units of the syllabus (2 questions per unit and a combined question from both the units). There may be a maximum of three sub-divisions per question, carrying 3 or more marks per sub-division. Three (3) out of five (5) questions are to be answered.

PRACTICALS EXAMINATION PATTERN

In the I& II semesters, the 35 marks shall be awarded based on the experiment. But in the III & IV semesters, out of 50 marks, 10 marks are for the viva to be conducted during the practical examinations and 40 marks for the experiment.



Description of Papers	Teaching	Hrs.of	Max Marks:	Credits for
	Hrs/week	Exam	Exam+IA	the Course
I Semester: i)Theory				
OC 401 : Inorganic Chemistry	4	3	70+30	4
OC 402 : Organic Chemistry	4	3	70+30	4
OC 403 : Physical Chemistry	4	3	70+30	4
OC 404 : Molecular Spectroscopy	4	3	70+30	4
OC 405: Environmental Chemistry	2	2	35+15	2
ii) Practicals				
OC 406 : Inorganic Chemistry Practicals-I	4	4	35+15	2
OC 407 : Organic Chemistry Practicals-I	4	4	35+15	2
OC 408 : Physical Chemistry Practicals-I	4	4	35+15	2
II Semester: i) Theory				
OC 451 : Advanced Inorganic Chemistry	4	3	70+30	4
OC 452 : Advanced Organic Chemistry	4	3	70+30	4
OC 453 : Advanced Physical Chemistry	4	3	70+30	4
OC 454 : Molecular Symmetry & Spectroscopy	4	3	70+30	4
OC 455: Diffraction and Electroanalytical Techniques	2	2	35+15	2

Organic Chemistry Course

ii) Practicals							
OC 456 : Inorganic Chemistry Practicals-II	4	4	35+15	2			
OC 457 : Organic Chemistry Practicals-II	4	4	35+15	2			
OC 458 : Physical Chemistry Practicals-II	4	4	35+15	2			
III Semester : i)Theory							
OC 501 : Choice Based Paper	4	3	70+30	4			
OC 502 : Reaction Mechanism & Photochemistry	4	3	70+30	4			
OC503:Synthetic Reagents & Spectroscopic	4	3	70+30	4			
Techniques	4	3	70+30	4			
OC 504 : Industrial and Heterocyclic Chemistry							
ii) Practicals	6	5	50+25	3			
OC 505 : Organic Chemistry Practicals -III	6	5	50+25	3			
OC 506 : Organic Chemistry Practicals -IV	6	5	50+25	3			
OC 506 : Organic Chemistry Practicals -V	2		25	1			
OC 507 Seminars							
IV Semester: i)Theory	4	3	70+30	4			
OC 551 : Organometalics& Analytical Techniques	4	3	70+30	4			
OC 552 : Organic Synthetic Methods	4	3	70+30	4			
OC 553 : Bio-organic & Medicinal Chemistry	4	3	70+30	4			
OC 554 : Chemistry of Natural Products							
ii) Practicals	6	5	50+25	3			
OC 555 : Organic Chemistry Practicals -VI	6	5	50+25	3			
OC 556 : Organic Chemistry Practicals -VII							
iii) Project Work (6 to 8 weeks)	30		75	3			
OC 557 : Project Report	2		25	1			
OC 588 : Seminars	7						
100 20 20 20 20 20 20 20 20 20 20 20 20 2							

FIRST SEMESTER M. Sc. Course in Organic Chemistry

OC 401: INORGANIC CHEMISTRY

UNIT-I:

Ionic bond: Properties of ionic substances, coordination number of an ion, structures of crystal lattices- NaCl, CsCl, ZnS and rutile. Lattice energy- Born Lande equation, Born-Haber cycle, Uses of Born-Haber type of calculations. Ionic radii, methods of determining ionic radii, factors affecting ionic radii, radius ratio rule, covalent character in ionic bonds, hydration energy and solubility of ionic solids.

Covalent bond: valence bond theory, resonance, hybridisation, Bent's rules and enregetics of hybridization, Deduction of molecular shapes – VSEPR theory.

M.O.theory, application to homo- and hetero-diatomic and -triatomic molecules. UNIT -II: [14 Hours]

Alkali and alkaline earth metal complexes of crown ethers, cryptands and calixarenes and their biological significance.

Halogens and Noble gas chemistry –interhalogens, psuedohalogens, polyhalide ions, oxyhalogen species, xenon oxides and fluorides. Oxy- and peroxy acids of N, P and S. Graphitic compounds, carbides, pure silicon, silica and silicates, zeolites.

UNIT-III:

Theories of acids and bases – Lux-Flood theory, Bronsted and Lewis acids and bases, gas phase vs. solution acidity, solvent leveling effects, hardness and softness, HSAB concept. super acids. Reactions in non-aqueous media: Liquid ammonia, anhydrous sulphuric acid, glacial acetic acid, anhydrous HF, bromine trifluoride, liquid sulphur dioxide and dinitrogen tetroxide. Reactions in molten salts.

UNIT-IV:

Sampling techniques, preparation of samples for analysis. Nature of errors, statistical treatment of errors, the t- and F-tests, significant figures, rejection of data.

Precipitation phenomena: precipitation from homogeneous solutions, organic precipitants in inorganic analysis. Solvent extraction of metal ions, nature of extractant, distribution law, partition coefficients, types of extractions and applications.

Theories of redox indicators, titration curves, feasibility of redox titrations.

Chelometric titrations- titration curves with EDTA, feasibility of EDTA titrations, indicators for chelometric titrations, selective masking and demasking techniques, industrial applications of masking.

References:

1. J.E Huheey, Keiter, Keiter and Medhi: Inorganic Chemistry (4th ed.), Pearson Education, 2006.

2.Shriver, Atkins and Langford : Inorganic Chemistry (3rdedn.) OUP, 1999.

3.J.D.Lee: Concise Inorganic Chemistry, (5thedn.) Blackwell Science, 2000.

4.B.E.Douglas, D.McDaniel& A Alexander: Concepts & Models of Inorganic Chemistry, Wiley 2001 5.W.W.Porterfield: Inorganic chemistry – A Unified Approach, Elsevier, 2005.

[14 Hours]

[14 Hours]

OC 402: ORGANIC CHEMISTRY

UNIT –I:

Nature of Bonding in Organic Molecules:Hybridization and Index of Hybridization, Localized and delocalized bonding: Conjugation crossconjugation, resonance, hyperconjugation and tautomerism. Huckel rule, Homo-aromatic, non-aromatic and anti-aromatic systems. Aromaticity in benzenoid and non-benzenoid molecules. Annulenes and heteroannulenes. Physical methods to study aromaticity-UV, IR &¹H NMR. 7 hrs

Bonds weaker than covalent: Addition compounds, crown ether complexes, cryptands, inclusion compounds, catenanes, fluxional molecules. 2 hrs

Acids and Bases: Introduction to acids and bases, Bronsted-Lowry and Lewis acid- bases concept, organic acids and bases, pKa and pH, effect of solvent on acid and base strength, effect of structure of organic compound on acid & base strength. Running scale of acidity, General & specific acid-base catalysis. 5hrs

UNIT-II:

Methods of Determining Reaction Mechanism: Kinetic and non-kinetic methods, Identification of products, detection of intermediates, isotopic labeling, stereochemical evidences, cross-over experiments, Limitation of reactions, kinetic evidences and kinetic isotopic effects. 4 hrs

Reaction Intermediates: Generation, structure, stability, reactivity and detection of classical and non-classical carbocations, carbanions, free radicals, carbenes, nitrenes and arynes. Singlet oxygen-generation and reactions with organic molecules. 4 hrs

Aliphatic Nucleophilic Substitution Reactions: Mechanism and scope of aliphatic nucleophilic substitution reactions- $S_N 1$, $S_N 2$ and $S_N i$. Stereochemistry of nucleophilic substitution reactions, allylic nucleophilic substitution reactions, Walden inversion, neighbouring group participation and anchimeric assistance. Factors influencing the rates of nucleophilic substitution reactions. 6 hrs

UNIT-III: Stereochemistry

Optical Isomerism: Conformation and configuration of molecules, projection formulae, Fischer, Saw-horse, Newman and Flying wedge representations. Interconversion of these Absolute configuration (D.L) and (\mathbf{R},\mathbf{S}) systems. Elements formulae. of symmetry, Psedoassymmetric centres, chirality, molecules with more than one chiral centre, threo and erythro isomers, methods of resolution, stereospecific and stereoselective synthesis, asymmetric synthesis, Cram's and Prelog's rules. Optical activity in the absence of chiral carbon-biphenyls, allenes and spiranes. Conformational analysis of cycloalkanes and decalins. Effect of conformation on reactivity. Acyclic & cyclic systems-Substituted cyclohexanes, cyclohexanones, cyclohexanols, Curtain-Hammet Principle. Stereochemistry of compounds containing nitrogen, sulphur and phosphorus. 11 hrs

Geometrical Isomerism: Cis-trans isomerism resulting from double bonds, monocyclic compounds & fused ring systems. E,Z-notations, determination of configuration of geometrical isomers, syn& anti isomers. 3 hrs

UNIT-IV: Carbohydrates & Heterocycles

Carbohydrates: Introduction, Configuration and conformation of monosaccharides, Chemistry of important derivatives of monosaccharides-ethers, esters, acetals, ketals,

[14 Hours]

[14 Hours]

[14 Hours]

deoxysugars, aminosugars, Structure of disaccharides-maltose, cellobiose and sucrose. General methods of structural degradation of polysaccharides-methylation, partial hydrolysis, periodate oxidation, Smith degradation and alkaline degradation techniques. Structures of cellulose, chitin, starch and glycogen. 8hrs

Heterocycles: Introduction, Biologically important heterocycles, Synthesis and reactions of five membered simple and fused heterocycles-furan, pyrrole, thiophene, pyridine, benzofuran, benzothiophene& indole. 6 hrs

References:

1. Organic Chemistry-P.Y.Bruice (Pearson Education Pvt. Ltd., New Delhi), 2002.

2. Stereochemistry, Conformation and Mechanism-P.S. Kalsi (Wiley Eastern, New Delhi) 1993.

3. Stereochemistry of Carbon Compounds-E.L. Eliel (Tata McGraw Hill, New. Delhi) 1994.

4.Advanced Organic Chemistry-Reactions, mechanisms & structure-J.March(Wiley, NY)2000.

5.Organic Chemistry-Vol. -1,2 &3-Mukherji, Singh and Kapoor. (Wiley Eastern,) 1994.

6.A guide book of mechanisms in Organic Chemistry-P.Sykes (Orient- Longman) 1985.

7.Organic Chemistry-R.T. Morrison and R.N. Boyd (Prentice Hall, New Delhi) 1994.

8.Organic Chemistry 4thEdn.–S.H. Pine et al (McGraw-Hill, London) 1987.

9. Advanced Organic Chemistry- R.A. Carey and R.J. Sundberg (Plenum, New York)1990.

10. Modern Concepts of Advanced Organic Chemistry-R.P. Narein (Vikas, Delhi) 1997.

11.A Text book of Organic Chemistry-Tewari, Vishnoi and Mehrotra (Vikas, New Delhi)1998.

12.A Text book of Organic Chemistry-3rdEdn.-R.K. Bansal, (New Age, New Delhi) 1997.

13.Organic Chemistry-3rdEdn- F.A. Carey (Tata McGraw Hill, New Delhi) 1996.

14.Stereochemistry by K.Mislow.



OC 403: PHYSICAL CHEMISTRY

UNIT – I : [14 hours]

Catalysis: Homogeneous catalysis-equilibrium and steady state treatments, activation energies of catalysed reactions. Acid-base catalysis (general and specific), protolytic and prototropic mechanisms, catalytic activity and acid strength measurements. Kinetics of enzyme catalysed reactions-Michaelis-Menten equation. Effect of pH, temperature & inhibitors 7 hrs.

Surface reaction kinetics: A review of adsorption isotherms, uni- and bi-molecular reactions. multilayer adsorption-BET equation- application in surface area determination. Harkin–Jura equation-application. Desorption & heterogeneous catalysis–catalytic activity at surfaces, semiconductor catalysis, n-&p-type. Mechanism of surface reactions. 7 hrs.

UNIT

II:

[14hours]

Chemical Kinetics: Complex reactions- parallel, consecutive and reversible reactions. Chainreactions(H2-halogen reactions). Branched chain reactions- general rate expression,explosionlimitsandOscillatoryreactions.4 hrs.Oscillatory

Reactions in solution: Ionic reactions - salt and solvent effects. Substituent effects on the rates of reactions - Hammett and Taft equations, linear free energy relationships. 4 hrs.

Fast reactions-Introduction, Study of fast reactions by-flow, relaxation, molecular beam and photolysis and line broadening methods. 4 hrs

Theories of Reaction Rates: Collision theory of reaction rates, limitations and an introduction to transition state theory.

UNIT-III : [14hours]

Electrochemistry of solutions: Ionic atmosphere-introduction, derivation and its effect on the theory of conductivity. Walden's rule. Debye-Huckel limiting law (DHL)- Concept of Ionic strength and activity coefficient, derivation of DHL equation, modifications to DHL equation- qualitative tests and verification of DHL equation. Bjerrum theory of ion association, triple ion formation and significance, abnormal conductance 5hrs.

Corrosion: Introduction, principles, loss due to corrosion, Forms of corrosion (Galvanic, Atmospheric, stress, microbial, and soil). Corrosion rate measurement, EMF series &Galvanic series and their limitations. Thermodynamics (Pourbaix diagram) and Kinetics (mixed potential theory) of corrosion. Kinetics of passivity. Protection against corrosion (Design improvement, Anodic and cathodic protection, inhibitors, coating).Corrosion failure and its treatment. 9hrs.

UNIT-IV : [14 hours]

Photochemistry: Introduction to photochemistry. Actinometry. Frank-Condon principle. Absorption and emission spectra- effect of solute solvent interactions on electronic spectraspectral shifts. Physicochemical properties of electronically excited molecules-excited state dipole moments, acidity constants. Flash photolysis technique.

Photophysical pathways- Jablonski diagram, Radiationless transitions and selection rules. Photochemical kinetics of unimolecular and bimolecular processes. Quenching-collisions in the gas phase, solution (Stern-Volmer equation). Photoisomerization, photo Fries rearrangement and Norrish type cleavage reactions with specific examples.

REFERENCES:

- 1. Physical Chemistry, 5th Ed., Atkins (ELBS) 1995.
- 2. Physical chemistry G. M. Barrow (McGraw Hill, Int. St. Ed) 1988.
- 3. Fundamentals of Physical Chemistry Maron and Lando (Collier, Macmillan) 1974.
- 4. Chemical Kinetics K. J. Laidler (Harper and Row) 1987.
- 5. Kinetics of Chemical Reactions, S K Jain (Vishal Publications, Delhi) 1982.
- 7. Principles and Applications of Electrochemistry-Crow (Chapman hall, New York) 2014.
- 8. Electrochemistry and Corrosion Science-NebtorFerez (Springer Pvt.Ltd.), Delhi, 2010.
- 9. Fundamentals of Photochemistry Rohatgi and Mukherje (New Age Bangalore), 2000.



OC 404: MOLECULAR SPECTROSCOPY

UNIT-I:

[14 hours]

[14

Unifying Principles -Electromagnetic radiation, dual nature, regions of the spectrum, interaction of electromagnetic radiation with matter - absorption, emission, transmission, reflection, refraction, dispersion, polarization and scattering. Natural line width and broadening, intensity of spectral lines. Rotational, vibrational and electronic energy levels, selection rules.

Microwave Spectroscopy- The rotation and classification of molecules, rotation spectra of diatomic and polyatomic molecules. Rigid and non-rigid rotator models. Determination of bond lengths, isotope effect on rotation spectra. Stark effect, nuclear and electron spin interaction. Microwave Spectrometer.

Vibrational Spectroscopy: Vibration spectra of diatomic molecules - linear harmonic oscillator, vibrational energies, zero point energy, force constants & bond strengths; anharmonicity of molecular vibrations- Morse PE diagram, selection rules, fundamental, overtones and hot bands. Vibrations of polyatomic molecules- normal modes of vibrations & nature of molecular vibrations (Ex-CO₂& H₂O).

UNIT-II :[14 hours]

Vibration-rotation spectra of diatomic and polyatomic molecules, selection rules, PQR branches. IR Spectrophotometer-Instrumentation, sample handling techniques, FTIR Spectroscopy. Far IR region.

Raman Spectroscopy: Classical and quantum theories of Raman effect, concept of polarizability and polarizability ellipsoid. Rotational and vibrational Raman spectra, selection rules, Raman activity of vibrations, vibrational - rotational Raman spectra, selection rules, mutual exclusion principle, polarization of Raman lines. An introduction to Laser Raman Spectroscopy. Raman Spectrometer – instrumentation. Applications of IR and Raman spectroscopy in elucidation of molecular structure (Ex - H₂O, N₂O & CO₂ molecules).

UNIT–III: [14 hours]

Application of infrared spectroscopy in the structural study-identity by finger printing and identification of functional groups. Characteristic vibrational frequencies of common functional groups (alkanes, alkenes, alkynes, aromatic compounds, alcohols, ethers, phenols and amines). Study of vibrational frequencies of carbonyl compounds (ketones, aldehydes, esters, amides and acids). Factors affecting band positions and intensities such as effect of hydrogen bonding, phase and solvent on vibrational frequencies, overtones, combination bands and Fermi resonance.

Polarimetry:Plane polarized light, instrumentation, acid-catalyzed muta rotation of glucose, inversing of cane sugar-relative strengths of acids. Optical rotatory dispersion & circular dichroism–introduction, selection rules, deduction of absolute configuration, octant rule for ketones and cotton effect.

UNIT-IV: Nuclear Magnetic Resonance Spectroscopy hours]

Magnetic properties of nuclei, theory and measurement techniques, NMR spectrometer, FT NMR and its advantages. Solvents used, chemical shift and its measurements, factors affecting chemical shift. Integration of NMR signals, spin-spin coupling, coupling constant. Shielding and deshielding. Chemical shift assignment of major functional groups, Classification (ABX, AMX, ABC, A₂B₂), spin decoupling; effects of chemical exchange, fluxional molecules, Hindered rotation through NMR spectrum, Karplus relationships (Karplus curve–variation of coupling constant with dihedral angle), double resonance techniques, NMR shift reagents, solvent effects and NulearOverhauser Effect. High resolution ¹H NMR. Applications of NMR spectroscopy in structure elucidation of simple

organic and inorganic molecules. ¹H NMR in the structural study of complex organic compounds. Pulse techniques in NMR, two dimensional and solid state NMR.Use of NMR in Medical diagnostics.

REFERENCES:

1.Fundamentals of Molecular Spectroscopy, Banwell&McCash (Tata McGraw Hill, New Delhi) 2007.

- 2. Spectroscopy, H. Kaur (PragathiPrakashana, Meerut), 2012.
- 3.Spectroscopy, Donald L.Pavia (Cengage learning India Pvt.Ltd., Delhi), 2007.
- 4. Spectroscopy, B.K. Sharma (Goelprakashan, Meerut), 2013.
- 5. Organic Spectroscopy-3rd ed.-W.Kemp (Pagrave Publishers, New York), 1991.
- 6.Spectrometric Identification of Organic Compounds-
- Silverstein, Bassler & Monnill (Wiley) 1981.



OC 405: ENVIRONMENTAL CHEMISTRY

UNIT-I:

Environmental segments, evolution of earth's atmosphere. Air pollution : Air pollutants, prevention and control, Green house gases and acid rain. Carbon monoxide, industrial sources and tranportation sources. SO_x - sources, ambient concentration, test methods, control techniques - scrubbing, , limestone injection process. Ozone hole and CFC's. Photochemical smog and PAN. NO_x - Sources, ambient concentration, test methods, NO_x , control techniques. Particulates : Size distribution, , particulate collection - settling chambers, centrifugal separators, wet scrubbers, electrostatic precipitators & fabric filters. Catalytic converters for mobile sources. Bhopal gas tragedy.

UNIT-II:

Hydrologic cycle, sources, chemistry of sea water, criteria and standards of water qualitysafe drinking water, maximum contamination levels of inorganic and organic chemicals, radiological contaminants, turbidity, microbial contaminants. Public health significance and measurement of colour, turbidity, total solids, acidity, alkalinity, hardness, chloride, residual chlorine, sulphate, fluoride, phosphate and different forms of nitrogen in natural and polluted water. Chemical sources of taste and odour, treatment for their removal, sampling and monitoring techniques. Determination and significance of DO, BOD ,COD and TOC. Water purification for drinking and industrial purposes, disinfection techniques, demineralization, desalination processes and reverse osmosis.

REFERENCES :

1. A.K. De : Environmental Chemistry, (Wiley Eastern).

- 2. S.K.Banerji : Environmental Chemistry, (Prentice Hall India), 1993.
- 3 S.D. Faust and O.M. Aly : Chemistry of Water Treatment, (Butterworths), 1983.
- 4. G.D. Christian : Analytical Chemistry, (4th Ed.), (John Wiley)
- 5. Sawyer and McCarty, Chemistry for Environmental Engineering(McGraw Hill) 1978
- 6. I.Williams, Environmental Chemistry, John Wiley, 2001

OC 406: INORGANIC CHEMISTRY PRACTICALS - I

1. Analysis of Hematite-insoluble residue by gravimetry and Iron by volumetry using Ce^{4+.}

2. Analysis of Dolomite - insoluble residue be gravimetry and Ca, Mg by complexometry.

- 3. Pyrolusite Insoluble residue by gravimetry and Manganese content by oxalate method.
- 4. Analysis of solder Pb and Sn by EDTA method.
- 5. Complexometric determination of Mn, Cu, Ni and Fe-Cr mixture
- 6. Hardness of water
- 7. Analysis of Halide Mixture Iodide by KIO₃ and total halide by gravimetrically.
- 8. Colorimetric Determination of Iron by thiocyanate and Cu by aqueous ammonia.
- 9. Gravimetric Determinations of Mn, Ni, Mo, Pb/Cr, sulphide, thiocyanate.
- 10. Statistical Analysis of Data.

Reference :

1. Vogel's Text Book of Quantitative Chemical Analysis(5th Ed), G.H.Jeffrey, J.Bassette, J.Mendham and R.C.Denny, Longman, 1999.

OC 407 : ORGANIC CHEMISTRY PRACTICALS - I

Single and two stage organic preparations

- 1. Electrophilic substitution reactions–Preparations of p-bromoaniline, p-nitroaniline, and picric acid
- 2. Alkylations-Preparations of nerolin and N-methyl anthranilic acid.
- 3. Acetylations–Preparations of β -D-glucose penta-acetate and 2-naphthyl acetate.

[14 hours]

[14 hours]

- 4. Reactions with ring formation–Preparations of 1,2,3,4–tetrahydrocarbazoleand 7–hydroxy-4-methyl-coumarin.
- 5. Diazotisation reactions-Preparations of iodo, chloro and azo compounds.
- 6. Dehydration reactions–Preparations of cyclohexene and succinic anhydride
- 7. Condensation reactions–Condensations involving diethylmalonate and ethyl acetoacetate. Aldol condensation and Perkin reactions.
- 8. Halogenation reactions-Preparation of n-butylbromide& α , β -dibromocinnamic acid.
- 9. Reduction reactions-Reductions of nitro compounds and carbonyl compounds.

10. Oxidation reactions-Preparation of p-nitrobenzoic acid, p-benzoquinone and adipic acid. **References :**

- 1. Laboratory Manual in Organic Chemistry–R. K. Bansal (New Age, New Delhi)1990.
- 2. Experimental Organic Chemistry-Vol. I & II-P. R. Singh et al (TMH New Delhi)1981
- 3. Laboratory Manual in Organic Chemistry–Dey&Sitaraman(Allied, New Delhi)1992.
- 4. Vogel's Text Book of Practical Organic Chemistry including Qualitative Organic Analysis-B. S. Furniss et al., (Longman ELBS, London), 1989.

OC 408 : PHYSICAL CHEMISTRY PRACTICALS - I

Any 12 experiments are to be carried out

- 1. Potentiometric titration of halides in mixtures (Cl⁻, Br⁻ and I⁻) with silver nitrate
- 2. Potentiometric determination of redox potentials (Fe⁺ Vs. I Mn^{+7} , Ce⁺⁴).
- 3. Potentiometric and conductometric acid –base titrations in partial, aqueous & non-aqueous media.
- 4. Conductometric titrations of displacement and precipitation reactions.
- 5. Determination of equivalent conductances and dissociation constants of weak acids.
- 6. Determination of solubility of lead iodide at different T & hence molar heat of solution
- 7. Determination of pH of buffer solutions with a pH meter & evaluation of pK_a of acids
- 8. Verification of Walden's rule (relation between viscosity of a solution and the electrical conductivity.
- 9. Study of variation of viscosity of a liquid with temperature
- 10. a)Determination of parachor value for CH₂ group by S.T method,
 - b) Determination of the composition of a solution by S.T measurement and
 - c) Determination of CMC of a soap solution by S.T measurement
- 11. Potentiometric determination of solubility of insoluble silver halide and the standard electrode potential using quinhydrone electrode
- 12. Determination of degree of hydrolysis of CH₃COONa and NH₄Cl.
- 13. Determination of hydrolysis constant of aniline hydrochloride.
- **14.** Verification of Nernst equation for Ag^+ , Cu^{2+} and Zn^{2+} species.

References:

- 1. Findlay's Practical Physical Chemistry- B. P. Levitt (Longman, London).
- 2. Experiments in Physical Chemistry-James and Prichard.
- 3. Experimental Physical Chemistry Daniels et al.
- 4. Experimental Physical Chemistry-Das & Behera (Tata McGraw Hill, New Delhi)1983.
- 5. Advanced Practical Physical Chemistry–Yadav (1989).
- 6. Experiments in Physical Chemistry-J. C. Ghosh (BharathiBhavan)1974.

SECOND SEMESTER M. Sc. Course in Organic Chemistry

OC 451: ADVANCED INORGANIC CHEMISTRY

Unit -I:

Chemistry of higher boranes, classification, structures and M.O. description of bonding, framework electron counting, Wade's rules, chemistry of B_5H_9 , $B_{10}H_{14}$ and $B_nH_n^{2^-}$. Carboranes and metallocarboranes. Cyclophosphazenes, phosphazene polymers, P-O and P-S cage compounds. S-N compunds : binary sulphur nitrides- S_4N_4 , S_2N_2 and $(SN)_x$. Borazines and boron nitride, Isopoly and heteropoly acids of transition metals.

Unit -II:

[14 Hours]

Coordination numbers 2-10 and their geometry, crystal field theory of coordination compounds, d-orbital splittings in octahedral, square planar and tetrahedral fields, spectrochemical series, and Jahn-Teller effect.

Structural evidences for ligand field splittings – hydration, ligation and lattice energies, site preference energies. MO theory of coordination compounds- MO energy level diagrams for octahedral and tetrahedral complexes.

Stepwise and overall formation constants, factors affecting stability of metal complexes, determination of binary formation constants by pH-metry and spectrophotometry.

Unit-III:

Metal Pi-acceptor complexes: metal carbonyls – preparative methods, structure and bonding, vibrational spectra of metal carbonyls for bonding and structural elucidation, magnetic and X-ray evidences of structures, M.O.representation of bi- and tri-nuclear carbonyls,. Reactions of metal carbonyls. Metal carbonylates and carbonyl halides – preparation and important reactions. Chemistry of metal nitrosyls – preparation, structure and bonding; dinitrogen and dioxygen complexes. Metal-metal bonding in carbonyls and halides evidences for M-M bonding, factors favouring M-M bond formation. Metal clusters- bi-, tri-, tetra-, penta- and hexanuclear metal clusters, bonding in metal clusters. Zintl ions and Chevrel phases.

Unit -IV:

Methods of reduction of oxide ores, Ellingham diagram, chemical and electrolytic reductions, reduction potentials, Latimer and Frost diagrams, effect of complexation on potential.

Trends in oxidations states, stereochemistry and ionic sizes of metals, comparison of 3d, 4d and 5d series by taking Ti subgroup as example. Lanthanides and actinides: electronic structure, oxidation states, extraction and separation of lanthanides, stereochemistry, spectral and magnetic properties of lanthanide and actinide complexes, lanthanide complexes as NMR shift reagents. Comparison with d-block ions.

References:

1. J.E Huheey, E.A..Keiter, R.L.Keiter& O K Medhi: Inorganic Chemistry (4thedn.), Pearson, 2006.

2. Shriver, Atkins and Langford : Inorganic Chemistry (3rdedn.) OUP, 1999.

3. J.D.Lee: Concise Inorganic Chemistry, (5thedn.) Blackwell Science, 2000.

4. B.E.Douglas, D.McDaniel&A Alexander: Concepts & Models of Inorganic Chemistry, Wiley 2001

5. W.W.Porterfield: Inorganic chemistry – A Unified Approach, Elsevier, 2005.

[14 Hours]

[14 Hours]

OC 452: ADVANCED ORGANIC CHEMISTRY

UNIT - I:

Aliphatic Electrophilic Substitution Reactions: Bimolecular mechanisms-S_E1, S_E2 and S_Ei mechanism. Electrophilic substitution reactions accompanied by double bond shifts. hrs

Aromatic Electrophilic and Nucleophilic Substitution Reactions: Mechanism of aromatic electrophilic substitution reactions, Arenium ion mechanism, orientation and reactivity, energy profile diagram. The ortho/para ratio, ipso attack, orientation in other ring systems. Mechanism of Vilsmeir-Haack reaction, Pechmann reaction and Fries rearrangement. Mechanisms of aromatic nucleophilic substitution reactions- S_NAr, S_N1 &aryne mechanism. Von-Richter rearrangement, Sommelet-Houser rearrangement, Smiles rearrangement.

11 hrs

UNIT-II:

Free Radical Reactions: Types, mechanisms of free radical substitution reactions &neighbouring group assistance. Reactivity for the aliphatic and aromatic substances at a bridgehead. Reactivity of attacking radical. Effect of solvent on reactivity. Auto-oxidation, coupling of alkynes. Arylation of aromatic compounds by diazonium salts. Sandmeyer, Ullmann & Hunsidiecker reactions.

5 hrs

Elimination Reactions: Discussions of E1, E2 and E1cB mechanisms. Orientation during elimination reactions. Saytzeff and Hofmann rules. Reactivity-effects of substrate structures, attacking base, leaving group and solvent medium. 5 hrs

Pyrolytic Eliminations: Mechanisms of pyrolysis of esters of carboxylic acids. Chugaev reactions, Hofmann degradation, Cope elimination and xanthate pyrolysis. Δ hrs

UNIT-III:

Formation and Hydrolysis of Esters: Plurality of mechanism. Mechanism of esterification reactions. Ester hydrolysis-A_{AC}2, B_{AC}2, A_{AC}1 & A_{AL}1 mechanism. Transesterification.4 hrs Addition to Carbon-Carbon Multiple Bonds: Addition reactions involving electrophiles, nucleophiles and free radicals. Cyclicmechanisms. Orientation and stereochemistry. Addition of halogens, hydrogen halides, carboxylic acids and amines. Addition to cyclopropanes, hydroboration, Michael addition. Addition of oxygen across double bonds. 6 hrs

Addition to Carbon-Hetero Multiple Bonds: Electrophilic, nucleophilic and free radical additions to C=O and C=N systems. Addition of Grignard reagents. Reformasky reaction, aldol condensation, Knoevenagel condensation, Perkin reaction and Wittig reactions. 4 hrs

UNIT- IV: Chemistry of Heterocyclic Compounds

Synthesis and reactions of three membered heterocycles-aziridines, oxiranes, episulfides, diaziridines, oxazirines and diazirines. Synthesis and reactions of four membered heterocycles-oxetanes, azetidines and thietanes. Synthesis & reactions of selenophenes, tellurophenes, oxazoles, imidazoles, thiazoles and oxazines..

References:

1.Organic Reactions and Their Mechanisms- P.S. Kalsi (New Age, New Delhi), 1996.

2. Advanced Organic Chemistry 4th Edn- J. March (Wiley, NY) 2000.

3. Organic Reaction Mechanisms- Bansal (Tata McGraw Hill, New Delhi) 1978.

4.Organic Chemistry-Vol.-I & II-Mukherji, Singh and Kapoor(Wiley Eastern, New Delhi) 1985.

[14 Hours]

[14 Hours]

[14 Hours]

5. Mechanism and Theory in Organic Chemoistry-Lowry and Richardson Harper and Row, 1987.

- 6.An Introduction to the Chemistry of Heterocyclic Compounds-Acheson (Wiley–Eastern) 1987.
- 7. Heterocyclic Chemistry-J. Joule & G. Smith, (Van-Nostrand, ELBS), 1978.
- 8. Reaction Mechanisms in Organic Chemistry-Mukherji, Singh and Kapoor (McMillan) 1978.
- 9. Organic Chemistry-P.Y. Bruice (Pearson Education, New Delhi) 2002.



OC 453: Advanced Physical Chemistry

UNIT - I:

[14 hours]

Chemical Thermodynamics : Entropy, dependence of entropy on variables of a system (S,T & V; S,T and P). Thermodynamic equations of state. Irreversible processes-Clausius inequality.

Free energy, Maxwell relations and significance, temperature dependence of free energy-Gibbs Helmholtz equation, applications of Gibbs Helmholtz equation.

Partial molar quantities, chemical potential and Gibbs-Duhem equations, determination of partial molar volume and enthalpy.

Fugacity, relation between fugacity and pressure, determination of fugacity of a real gas. Activity. variation of fugacity and activity with temperature and pressure.

Thermodynamics of mixing, Gibbs-Duhem-Margules equation, Henry's law.

Excess thermodynamic functions-free energy, enthalpy, entropy and volume, Determination of excess enthalpy and volume.

Chemical affinity and thermodynamic functions, effect of temperature and pressure on chemical equilibrium-vant Hoff reaction isochore and isotherm.

Third law of thermodynamics, Nernst heat theorem, determination of absolute entropies using third law, entropy changes in chemical reactions.

UNIT - II: Statistical and Irreversible thermodynamics [14 hours]

Statistical Thermodynamics : Basic terms: Probability, cell, phase space, micro and macro states, thermodynamic probability, statistical weight factor, statistical equilibrium, assembly, ensemble and its classification, Derivation of Boltzmann-Maxwell, Bose-Einstein and Fermi-Dirac statistics, partition function and derivations of translational, rotational, vibrational and electronic partition functions, thermodynamic functions such as internal energy, heat capacity,

entropy, work function, pressure, heat content, etc. Partition function and third law of thermodynamics, applications of partition function to mono atomic gases, diatomic molecules, equilibrium constant. Heat capacity of solids -the vibrational properties of solids, Einsteins theory and its limitations, Debye theory and its limitations. 9hrs.

Irreversible Thermodynamics-Thermodynamics of irreversible processes with simple examples. Uncompensated heat and its physical significance. Entropy production-rate of entropy production, entropy production in chemical reactions, the phenomenological relations. The principle of microscopic reversibility, Onsager reciprocal relations – validity (linear and non-linear rections) and application (Electrokinetic, Thermoelectric phenomena).

UNIT-III: Quantum Chemistry-1

Particle waves and Schrödinger wave equation, wave functions, properties of wave functions, Normalization and orthogonality of wave functions. Operators and their algebra, linear and hermitian operators, operators for the dynamic variables of a system such as, position, linear momentum, angular momentum, total energy, eigen functions, eigen values and eigen value equation. Quantum numbers and their characteristics.

Shrodinger wave equation- significance and derivation. Eigen values and eigen functions. Statistical interpretation of ψ . Solution of SWE for simple systems-particle in a box(1D & 3D), particle in a ring, harmonic oscillator, rigid rotor, the H atom (solution of r, θ , Φ equations), tunneling the harmonic oscillator, the rigid rotator, and the hydrogen atom. Quantum numbers and their characteristics.

UNIT-IV: Quantum Chemistry-II

Approximates methods of solving SWE- Principle of Variation and Perturbation methods. Application of variation method to H and He atoms. Secular equations and determinants.

[14 hours]

[14 hours]

Chemical Bonding: Covalent bond-Valence bond and molecular orbital approaches with comparison. Application of VBT to H₂.

MO theory applied to homonuclear and heteronuclear diatomic molecules -calculation of BO.

Hybridisation-construction of wave function of hybrid orbitals (sp, sp^2 and sp^3). Calculation of bond angle between hybrid orbitals.

Huckel molecular orbital theory of conjugated systems - secular equations and determinants. Applications to linear (ethane, allyl, 1-3 butadiene) and cyclic (benzene) systems.

Calculation of charge density, bond order, free valence and delocalisation energy.

References:

Physical Chemistry, 5th Ed., - Atkins, (ELBS) 1995
 Physical Chemistry, 4thed.,Ignacia Tinowa Jr, Kenneth Sauer etal., (Pearson), 2011.

3. Chemical Themodynamics, Rajaram and Kuriokose (East-West)Pearson, Chennai, 2013.

4. Thermodynamics, 3rd Ed., R.C. srivastava and Subit K Saha (Prentice-Hall of India, Delhi), 2007.

5. Statistical Thermodynamics, M. C. Gupta (Wiley eastern Ltd.) 1993.

6. Advanced Physical Chemistry- Gurdeep R Chatwal (Goel Publishes, Meerut), 1992.

7. Introductory Quantum Chemistry – A.K.Chandra (Tata McGraw Hill) 1994.

8. Quantum Chemistry, A.B. Sannigrahi (Book and Allied Pvt.Ltd., Kolkatt), 2013.

9. Quantum Chemistry, Donald A.P (Viva Books, Delhi), 2013.

10. Physical Chemistry, 4th Edn., K.J. Laidler, J.H. Meiser, B.C.Sanctuary(Houghton Mifflin), 2003



OC 454: MOLECULAR SYMMETRY AND SPECTROSCOPY

[14 Hours]

UNIT- I: Symmetry and Group Theory

Definitions of group, subgroup, relation between orders of a finite group and its subgroup. Conjugacy relation and classes, symmetry elements and symmetry operations, Schonflies symbols, Matrix representations of symmetry operations, products of symmetry operations, some properties of matrices and vectors, classification of molecules into point groups. Reducible and irreducible representations. The Great Orthogonality theorem (without proof), character tables. The direct product. Applications of group theory - Molecular vibrations, group theoretical selection rules for electronic transitions, for infra red and Raman spectra. Hybrid orbitals and Molecular orbitals, transformation properties of atomic orbitals. **UNIT- II:** [14 Hours]

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. 4 hrs

NQR Spectroscopy:Quadrupolar nuclei, electric field gradient, nuclear quadrupole coupling constants, energies of quadrupolar transitions, effect of magnetic field. Applications.3 hrs

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. 4 hrs

Photoelectron spectroscopy: Basic principles, valence &core binding energies, shifts in energies due to chemical forces, Photoelectron spectra of simple molecules, Auger transitions, measurement techniques. Applications. 3 hrs

UNIT- III:

UV/Electronic Spectroscopy: Basic principles, Beer-Lambert law, molar absorptivity, energy levels, types of electronic transitions. Franck - Condon principles, ground and excited electronic states of diatomic molecules. Chromophores, auxochromes, electronic spectra of polyatomic molecules. Emission spectra, spectra of transition metal complexes, charge transfer spectra. Instrumentation and application. Factors affecting the positions of UV bands. Electronic transitions and empirical correlations of predicting λ_{max} of organic compounds. Woodward–Fieser rules. UV absorption of aromatic compounds - effect of substituents and solvent effects. Emperical rules to calculate λ_{max} . Application of UV spectroscopy in the structural study of organic molecules.

7 hrs

NMR of nuclei other than proton:¹³C chemical shift & factors affecting it Coupling constants. Decoupling-Noise decoupling & broad band decoupling. Off-resonanceproton decoupling-some representative examples. ¹⁹F & ³¹P NMR- Predicting the spectra of simple inorganic compounds, NMR of paramagnetic complexes. 7 hrs

UNIT- IV:

[14 Hours]

Mass Spectrometry: Basic principles, Instrumentation -Mass spectrometer, interpretation of mass spectra, resolution, exact masses of nucleides, molecular ions, meta-stable ions and isotope ions. 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, nitrocompounds, amines & nitrogen heterocycles. Fragmentation patterns of carbohydrates, terpenoids, alkaloids, steroids, peptides & proteins-some representative examples, ion analysis, ion abundance, retro Diels-Alder fragmentation. Application in structure elucidiation and evaluation of heats of sublimation & ionization potential. Nitrogen rule. High resolution mass spectroscopy. 9 hrs

Composite problems involving the applications of UV, IR, ¹H and ¹³C NMR and mass spectroscopic techniques. Structural elucidation of organic molecules5 hrs REFERENCES:

- 1. Fundamentals of Molecular Spectroscopy, Banwell&McCash (Tata McGraw Hill)2001.
- 2. Organic Spectroscopy-3rd Ed.-W.Kemp(Pagrave Publishers, New York), 1991.
- 3. Spectrometric Identification of Organic Compounds Silverstein, Bassler&Monnill (Wiley)1981.
- 4. Applications of Absorption Spectroscopy of Organic Compounds-Dyer(Prentice Hall,NY) 1965.
- 5. Spectroscopy of Organic Compounds-3rd Ed.-P.S.Kalsi (New Age, New Delhi) 2000.
- 6. E.A.V.Ebsworth, D.W.H.Ranklin and S.Cradock: Structural Methods in Inorganic Chemistry, Blackwell Scientific, 1991.
- 7. R.S.Drago: Physical Methods for Chemists, Saunders College Publishing, 1992.
- 8. D.N.Satyanarayana: ElectronicAbsorption Spectroscopy and Related Techniques,
- 9. G.Aruldhas, Molecular Structure and Spectroscopy, Prentice Hall, 2001
- 10. J. A. Iggo: NMR Spectroscopy in Inorganic Chemistry, Oxford University Press, 1999.
- 11. C.N.R.Rao and J.R. Ferraro: Spectroscopy in Inorganic Chemistry, Vol I&II(Academic)1970
- 12. Analytical Chemistry-Open Learning : Mass spectrometry.
- 13. Spectroscopic Methods in Organic Chemistry Williams and Fleming, TMH.



OC 455: Diffraction and Electroanalytical Techniques

UNIT-I:

hours]

Diffraction Techniques: Introduction, production of X-ray, X-ray diffraction-Bragg`s law, Laue equations, Ewald`s diagram, X-Ray diffraction experiments-Powder method (Debye-Scherrer and photographic methods), Interpretation of power patterns. Single crystal technique- :Laue and Rotation photographic methods). Moving Film method (Weissenberg method). X-ray diffractometers. Systematic absences. Intensities of diffracted X-rays and structural analysis, X-ray scattering by atoms and molecules, Factors affecting X-ray intensities, Crystal structure analysis. 10 hrs

Electron Diffraction: Scattering intensity vs. scattering angle, qualitative aspects of Wierl equation, measurement technique, Elucidation of structure of simple gas molecules, Low Energy Electron Diffraction and structure of surfaces.

Basic theory and applications of Neutron diffraction.

4 hrs

UNIT- II:

[14 hours]

Electroanalytical Techniques: Theory of classical polarography, polarograhic measurements, polarograms, polarographic currents. Factors influencing diffusion currents, advantages and limitations of using dropping mercury electrode. half wave potential, oxygen interference, Applications of polarographic measurements. Modern Polarography : Necessity and development of new voltammetric techniques and their comparison with classical polarography. Fundamentals of DC polarography (Tast), oscilliography, differential and derivative voltammetry, cyclic, pulse, alternating current and square wave polarography.

Cyclic Voltammetry: Principle, Instrumentation, current-potential relation applicable for Linear Sweep Voltammetry (LSV) and Cyclic Voltammetry (CV), interpretation of cyclic voltammograms and parameters obtainable from voltammograms.

Principle, measurement technique and the applications of Coulometry, Amperometry and Electrogravimetry.

Chrono Methods: Basic concepts and applications of chronopotentiometry, chronoampermetry.

References:

1. A Basic Course in Crystallography, JAK Tareen and TRN Kutty, University Press, Hyderabad (2001).

2. Essentials of Crystallography, M.A. Waheb, Narosa Publishing House, New Delhi (2009),

3. Polarography and Allied Techniques, V. Suryanarayana Rao (University Press, Hyderabad), (2002).

- Principles of Instrumental Analysis, D.A. Skoog, F.J. Holler and T.A. Nieman, 5th Ed., (Saunders College Publishing, Harcourt Brace & Company, U.S.A.) 1998.
- 6. Electrochemical Methods: Fundamentals and Applications, A.J. Bard and L.R. Faulkner, 2nd Ed. (Wiley, New York), 2000.

[14

OC 456: INORGANIC CHEMISTRY PRACTICALS-II

Qualitative Analysis of mixtures of Inorganic Salts containing 4 metal ions and 2 anions (2 less common metal ions like Tl, W, Mo, V, Zr, Th, U, Ce, Ti and Li to be included among anions organic acid radicals, phosphate, borate and fluoride separation included).

References:

1. Vogel's Text Book of Quantitative Chemical Analysis (5th Ed), G. H. Jeffrey, J. Bassette, J.Mendham and R. C. Denny, Longman, 1999

2. Vogel's Qualitative Inorganic Analysis (7th Ed), G. Svehla, Longman (2001).

OC 457: ORGANIC CHEMISTRY PRACTICALS-II

SEPARATION AND SYSTEMATIC QUALITATIVE ANALYSIS OF BINARY MIXTURES OF ORGANIC COMPOUNDS CONTAINING BOTH MONO AND BIFUNCTIONAL GROUPS AND PREPARATION OF SUITABLE DERIVATIVES.

References:

1. Practical Organic Chemistry-F .G. Mann and B. C. Saunders (ELBS, England), 2001.

2. Practical Organic Chemistry - A. I. Vogel (Longman-ELBS, England), 1971.

3. Experimental Organic Chemistry–Vol.I&II Singh et al(TMH, New Delhi)1981.

4. Semimicro Qualitative Organic Analysis-Cheronisetal Wiley-Eastern, New Delhi) 1964.

5. Vogel's Text Book of Practical Organic Chemistry Including Qualitative Organic Analysis- B. S. European EL BS, England), 1978

Furniss et al (Longman-ELBS, England), 1978.

OC 458 : PHYSICAL CHEMISTRY PRACTICALS - II

At least 12 experiments are to be carried out

- 1. Determination of cryoscopic constants of solvents and molecular weight of non volatile substances by thermal method.
- 2. Determination of degree of dissociation &Vant Hoff factor of an electrolyte by cryoscopic method.
- 3. Heat of solution of substances by solubility method.
- 4. Phase diagram of two component systems by thermal analysis.
- 5. Kinetics of acid catalysed hydrolysis of methyl acetate and determination of (a) order and rate constant, (b) Relative strength of two acids and (c) Energy of activation.
- 6. First and second order kinetics of reaction between potassium persulphate and KI.

7. Kinetics of (a) inversion of cane sugar, (b) sodium formate-iodine reaction.

8. Determination of heat of neutralisation, integral and differential heat of solution calorimetrically.

- 9. Thermometric titration of an acid with a base.
- 10. Direct determination of the latent heat of evaporation of carbon tetrachloride.
- 11. Measurement of the vapour pressure and latent heat of vapouration of Benzene using tensemeter.

12. Detn.of association constants carboxylic acids in organic solvents by distribution method.

- 13. Preparation of colloidal solutions.
- 14. Verification of F & L adsorption isotherms for acetic acid on activated charcoal.
- 15. To study the adsorption of iodine on charcoal from alcoholic solution.
- 16. To study the effects of gelatin solution on the precipitation values.
- 17. To determine the surface and interfacial tension and the effect of detergents.

18. Thermodynamic prediction and measurement of the solubility of naphthalene in benzene. 19.

Study of association of benzoic acid in benzene/toluene. Any other relevant experiments of interest.

References:

- 1. Findlay's Practical Physical Chemistry- B. P. Levitt (Longman, London).
- 2. Experiments in Physical Chemistry-James and Prichard.
- 3. Experimental Physical Chemistry Daniels et al.
- 4. Experimental Physical Chemistry-Das & Behera (Tata McGraw Hill, New Delhi) 1983.
- 5. Advanced Practical Physical Chemistry–Yadav (1989).
- 6. Experiments in Physical Chemistry-J. C. Ghosh (BharathiBhavan) 1974.



THIRD SEMESTER M.Sc. Course in ORGANIC CHEMISTRY

OC 501: CHOICE BASED COURSE

OC 502: REACTION MECHANISM AND PHOTOCHEMISTRY

UNIT-I:

Organic Name Reactions: Reactions, Mechanisms and synthetic uses of the following: Stobbe condensation, Darzen condensation, Gattermann-Koch reaction. Cannizzaroreaction, Duff reaction Chichibabin reaction, Benzoin condensation, Claisen-Schmidt condensation, Claisen reaction, Simon-Smith reaction, Stork Enamine reactions, Sharpless asymmetric epoxidation, Hofmann-Loffler-Freytag reaction, Suzuki coupling, Heck reaction, Woodward and Prevost Hydroxylation, Bucherer reaction, Ullmann reaction. Wittig reaction-Mitsunobu reaction, Stephen reaction.

UNIT-II:

Molecular Rearrangements: Classification and general mechanistic treatment of nucleophilic, electrophilic and free radical rearrangements. Intermolecular and Intramolecular migration, nature of migration and migratory aptitudes. Mechanism of Wagner-Meerwein, Dienone-Phenol, Pinacol-Pinacolone, Demaynov, Benzil-Benzilic acid, Fries, Wolff, Favorskii, Neber, Benzidine, Baever-Villiger, Beckmann, Lossen, Curtius, Schmidt, Stevens, Shapiro, Baker-Venkatraman and Amadori rearrangement.

UNIT-III:

Organic Photochemistry: Bonding and antibonding orbital, σ and π orbitals, σ^* and π^* orbitals, singlet and triplet states, relative energies and excited states, Chemistry of excited states of organic molecules, Jablonski diagram and quantum yield, Photodissociation, Photoreduction, Photochemical isomerisation, Photocyclisation and related reactions. Norrish Type-I and Type-II reactions, Di-pi methane rearrangement, Optical pumping, Barton reaction and Photo Fries rearrangement, Paterno-Buchi reaction, Photochemistry of alkenes, benzenes, photochemistry of substituted cyclohexanes- Yang cyclisation. Photochemistry of vision, Introduction to Photochemical cells, energy conversion and storage.

UNIT-IV:

[14 Hours]

Pericyclic Reactions: Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3butadiene, 1,3,5-hexatriene and allyl systems. Classifications of Pericyclic reactions. Woodward-Hoffmann correlation diagram and FMO approach.

Electrocyclic Reactions: Introduction, Con-rotatory and dis-rotatory Process, 4n and 4n+2 systems. Reactions of cations and anions, formation and cyclisation of Dipolar molecules.

Cycloaddition reaction: Suprafacial and Antrafacial addition, 2+2 and 4+2 systems, 1,3dipolar cycloaddition reactions and their applications in the synthesis of five membered heterocycles, nitrile oxid and sydnones

Sigmatropic reactions: Suprafacial and Antrafacial shift of H, [1,3] [1,5] [1,7] and [3,3]sigmatropic shifts. Claisen, Cope, Oxy-Cope and Aza-Cope rearrangements.

References:

- 1. O. L. Chapman, Organic Photochemistry. Vol I & II. Marcel Decker.
- 2. Francis A Carey and R. J. Sundberg, Advanced Organic Chemistry- Part A & B (Plenum)
- 3. Mukherji Singh and Kapoor, Organic Chemistry, Vol 1-3, (Wiley Eastern, New Delhi)
- 4. Synthetic Organic Chemistry- G.R.Chatwal (Himalaya, Bombay), 1994.
- 5. Organic Reaction Mechanisms ,V.K.Ahluw alia &R.K.Parashar (Narovasa publishing house), 2006
- 6. Organic Chemistry, Vol I-II, I.L.Finar, (Longmann ELBS, London), 1973.
- 7. Advanced Organic Chemistry-Reaction Mechanisms, Reinhard Bruckner (Academic), 2005.
- 8. Pericyclic reactions, S. M. Mukherji(The McMillan Bangalore), 1979.

[14 Hours]

[14 Hours]

9. Organic Reactions and their mechanisms-P.S.Kalsi (New Age, New Delhi), 1996.



OC 503: SYNTHETIC REAGENTS AND SPECTROSCOPIC TECHNIQUES

UNIT –I:

[14Hours] IR,¹H NMR and ¹³C-

NMR: Characteristic vibrational frequencies of alkanes, alkenes, alkynes, aromatic compounds, alcohols, ethers, phenols and amines. Detailed study of vibrational frequencies of carbonyl compounds (Ketones, aldehydes, esters, amides, acids, anhydrides, lactones, lactams and conjugated carbonyl compounds). Effect of H-bonding & solvent effect on vibrational frequencies.

Chemical shift of different class of organic compounds. Spin-spin coupling - illustrate with different examples. AB, AX-Spin system. Chemical exchange, effct of deuteration, complex spin-spin interaction between two, three, four and five nuclei. Stereochemistry, hindered rotation;Karplus-Curve. Variation of coupling constant with dihedral angle.Pulsetechniques,Techniques simplication for of spectra,Heteronuclear coupling, INDOR, 2D-NMR, FT-NMR. Applications of NMR

Composite problems involving the application of UV, IR,¹H NMR and ¹³C-NMR and Mass spectroscopy technique in the structural elucidation of organic molecules.

Green Techniques:

Crown Ethers: Introduction, Nomenclature, Synthesis of Dibenzo[18]crown-6, Aza-crown, Cryptates, Synthetic applications like esterification, saponification, elimation reactions, superoxide anion, generation of carbenes.

Microwave induced reactions: Introduction, advantages, limitations, precautions, application like Deprotection, Hydrolysis, Condensation, ortho ester claisen rearrangement.

Ionic Liquids: Introduction, properties, types, preparation, applications like Epoxidation, Alkene Metathesis, Oxidation, Reduction and Enzyme catalysed synthesis.

UNIT-II:

[14Hours]

Assymmetric Synthesis: The Chiral pool; Alpha amino acids in the synthesis of Benzodiapines, Carbohydrates(Benzyl D-Mannose to Swainsonine) Preparation of tomolal from D-mannitol, Felion-Ahn model and Cram's chelation control.Enantiomeric excess and its determination.

Chiral Auxiliaries:Oxazolidinones, Chiral sulfoxides in controlling the reduction of ketones, Use of chiral Auxillaries in Diels-Alder and aldol reactions.

Chiral Reagents: BINOL, DIBAL, Tartarates, Lithium diamides.

Chiral Catalysts: Rhodium and Ruthenium catalysts with Chiral phosphine ligands like (R)-BINAP, (R,R)-DIOP. Enzymatic methods using enzymes.

UNIT- III: Reagents in Organic Synthesis-I [14 Hours]

Organometallic Reagents: Preparation and properties of Organolithium and organomagnesiumcompounds. Their uses in organic synthesis and in the preparation of Organometallic compounds. Methods of preparation, properties, reactivity and reactions of Organozinc, Organocadmium,Organomercury and Organoindium reagents.

Boron containing Reagents: Introduction, preparations, Hydroborations, reactions of Organoboranes- Isomerization, oxidation, protonolysis, carbonylation, cyanidation. Synthesis of esters, E and Z alkenes, conjugated dienes and alkynes.

Organotin Compounds: Synthesis of Organostannanes and their utility in C-C bond forming reactions. Barton decarboxylation reaction, Barton deoxygenation, Stelly-Kelly coupling reaction.

UNIT- IV: Reagents in Organic Synthesis-II

[14 Hours]

Use of the following reagents in Organic synthesis and functional group transformation: Gillman's reagent, Lithium dimethylcuprate, Lithium diisopropylamide (LDA), Dicyclohexylcarbodiimide (DCC), 1,3-dithiane (reactivity-umpolong), Trimethylsilyliodide, DDQ, Selenium dioxide, Wilkinsons catalyst, Phase transfer catalysts, Baker's yeast, polyphosphoric acid. Trimethyl silyl cyanide, trimethylsilane, Peterson reagent, Chloramine-T, Nickel chloride, cobalt chloride, metal carbonyls and its synthetic applications.

References:

1. J. March, Advanced Organic chemistry 5th edition, John Wiley and sons.

2. Nasipuri, Stereochemistry of Organic compounds, New Age International.

3. P.S. Kalsi, Stereochemistry of Organic compounds, Wiley Eastern.

4. J. Clayden, N. Greeves, S. Warren and P. wothers, Organic chemistry, Oxford University Press.

5. E. Eliel and S.H. Wilen, Stereochemistry of Organic compounds, John Wiley.

6.Organic Spectroscopy- William Kemp (Palgrave) 2005.'

7. Organic Synthesis, special Techniques by V.K. Ahluwalia and Renu Agrawal (Narosa Publications).



OC 504: INDUSTRIAL AND HETEROCYCLIC CHEMISTRY

UNIT I

Synthetic polymers: Classification and Nomenclature, Properties of polymers (molecular weight, Glass transition temperature, Solubility and Viscosity). Methods of polymerization, Mechanism and Stereochemistry, Addition polymerization (Anionic, Cationic and Free radical process), Condensation and Stepwise polymerization, Coordination polymerization, Study of polyesters, polyamides, Phenol-Formaldehyde resins, Urea-Formaldehyde resins, Epoxy resins, Polyurethanes, Polycarbonates, Synthetic rubber. Structural features and manufacture of natural rubber and Regenerated cellulose. Ziegler-Natta catalyst. Ring opening polymerization. Mechanism of co polymerization.

Properties, Structure and applications of Polythene, Polypropylene, PVC, Polystyrene & Acrylic polymers, Teflon, Phenol-formaldehyde, Urea-formaldehyde, Nylon (polyamides), polvesters(tervlines), caprolactum based polvmers.

UNIT -II:

[14Hours] Dves:Colour and constitution (electronic concept). Classification of dyes, methods of applying dyes to the fabrics. A general study of Azo dyes, Orange -II, Mordant brown, Congo red and methyl orange; Triphenylmethane dyes- Malachite green, Rosaniline, Crystal violet and Phenolphthalein; Cyanin dyes- Ethyl Red, Cyanin blue and Quinaldine; Reactive dyes and Optical brighteners-Tinapal and Blankophor. Pigments: Fast violet, Lake red and Orange R.

Pesticides and Insecticides: Introduction and classification. Natural insecticides-Nicotine, Pyrethrins, Rotenone and Allethrin; Organic insecticides-DDT, Methoxychlor, BHC, Aldrin, Malathion and Parathion. Fumigants and repellants.

UNIT -III: Heterocyclic Chemistry-I

Nomenclature of Heterocycles, Replacement and systematic nomenclature, Hantzsch-Widman system for monocyclic, fused and bridged heterocycles. Structure, synthesis and reactions of six membered heterocycles- α - and γ -Pyrones, Pyrazines, Pyridazines, Pyrimidines. Synthesis and reactions of seven membered heterocycles-Azepines, Oxepines and Thiepines. reactions of heterocycles-Ouinolines, Synthesis and fused Isoquinolines, Coumarins, Naphthyridines and Purines.

UNIT -IV: Heterocyclic Chemistry-II

Mesoionic compounds: Introduction, Synthesis and reactions of sydnones.

Anthocyanins and Anthocyanidins: Introduction and general methods of synthesis.

Flavones, Flavonols and Isoflavones: Introduction and synthesis of flavone, flavonal and quercetin. Structural elucidation and synthesis of Uric acid, Caffeine.

Heterocycles in functional group and ring transformations: Alkanes from thiophenes, dienes from pyrroles, alcohols from isooxazolines, conversion of coumarin to benzofuran, sydnone to pyrazole, chromones to pyrazoles, furans to pyridines, pyrrole to pyridines, pyrimidine to pyrazole, isatins to quinolines, indoles to quinoline.Dimroth and

References:

1 An Introduction To the Chemistry of Heterocyclic Compounds-Acheson (Wiley Eastern), 1997.

2. Heterocyclic Chemistry- J.Joule&G.Smith (Van Nostrand ELBS), 1978.

3. Polymer Science- V.R.Gowariker, N.V.Vishwanathan&T.Shridhar (Wiley Eastern)

- 4. Comprehensive Heterocyclic Chemistry Vol-I-VI Ed. Katritzky& Rees (Pergamon), 1984.
- 5. Synthetic Dyes Vol-I- Venkataraman, 1999.

[14Hours]

[14 Hours]

OC 505: ORGANIC CHEMISTRY PRACTICALS -III

Quantitative determination of sugars, amino acids, phenols, carboxylic acids, amides, esters, aldehydes, ketones, urea by various methods. Determinations of acid & ester and acid & amide in the mixtures.

Determination of functional groups like hydroxyl, vic-hydroxyl, enol, amino, amide, unsaturation and nitro groups by various methods. Semi-micro analysis of Nitrogen, Halogen, Alkoxy, C-methyl and active hydrogens.

OC 506: ORGANIC CHEMISTRY PRACTICALS -IV

Isolation and Charecterization of natural products like Caffeine, Recinoleic acid, Azelic acid, Piperine, Hespiridine, Cysteine, Casein, Lycopene and enzymes like Lipase and Sucrase. Extraction of Groundnut oil and Coconut oil. Determination of Saponification and Iodine values of oils and fats using chloramine-T. Isolation of Carotenes. Purification by paper, TLC andColumn. Charecterization of natural products by oxidation studies & derivatization of natural products.

OC 507: ORGANIC CHEMISTRY PRACTICALS -V

Seperation, purification, analysis and derivatization of ternary mixture of organic compounds, Identification, separation and qualitative analysis of the individual compounds and preparation of suitable derivative for each component, identification of derivative by m.p., TLC and spectral techniques.

References:

- 1. Elementary Practical Organic Chemistry-Vol. III quantitative Organic Analysis- A.I Vogel
- 2. Vogel's Text Book of Practical Organic Chemistry- Furniss et al.(ELBS, London)1978.
- 3. Experimental Organic Chemistry- Vol. I &II- P.R.Singh, Tata McGraw-Hill, 1981.
- 4. Practical Organic Chemistry- IV Ed- Dey&.Sitaraman(Allied)
- 5. Laboratory Experiments in Organic Chemistry-Adam, Johnson & Wicon(McMillan, London), 1979.
- 6. Experimental Organic Chemistry- H.D.Durst&G.E.Goke(McGraw-Hill)1980

FOURTH SEMESTER M.Sc. Course in ORGANIC CHEMISTRY

OC 551: ORGANOMETALICS AND ANALYTICAL TECHNIQUES

UNIT-I:

Transition metal-carbon pi complexes: Preparative methods, nature of bonding, structural features of olefinic, acetylenic, allylic, butadiene, cyclobutadiene, η^5 - cyclopentadienyl, η^6 -benzene and other arenes, cycloheptatriene and cyclooctatetraene complexes. Important reactions relating to nucleophilic and electrophilic attack on ligands. Fluxional isomerism in olefin, allyl, dienyl and cyclopentadienyl complexes. Isolobal concept.

UNIT- II:

[14 Hours]

Catalysis by organometallic compounds:16-and 18-electron rules, oxidative addition, insertion, deinsertion and reductive elimination reactions.

Homogeneous catalysis by organometallics: Hydrogenation, hydrosilation, hydrocyanation and isomerization of olefins, immobilisation of homogeneous hydrogenation catalysts, hydrocarbonylation of olefins (oxo reaction-cobalt and rhodium oxo catalysts), carbonylation of alcohols-Monsanto acetic acid process. Polymerization of olefins and acetylenes: Ziegler-Natta catalyst systems. Fischer-Tropsch reaction, Water Gas Shift reactions.

UNIT- III:

Paper Chromatography (PC): Definitions, theory and principle, techniques; one, twodimensional and circular PC, mechanism of separation, structure of cellulose and types of paper, methodology, preparation of sample, choice of solvents, location of spots and measurements of RF value, factors affecting RF values, advantages and applications.

Thin Layer Chromatography (TLC): Definition, mechanism, efficiency of TL plates, methodology selection of stationary and mobile phases, preparation of plates. Spotting, development, identification and detection, reproducibility of RF values, comparison of TLC with high performance thin-layer chromatography, paper chromatography and column chromatography. Qualitative and quantitative analysis.

UNIT-IV:

Gas chromatography (GC): Principle, comparison of GSC and GLC, instrumentation columns pack and tubular, study of detectors-thermal conductivity. Flame ionization, electron capture and mass spectrometry. Factors affecting the separation, applications.

High Pressure Liquid Chromatography (HPLC): Apparatus, pumps, column packing, charecteristics of liquid chromatographic detectors-UV, IR, refractometer and fluorescences detectors, advantages and applications.

Ion Exchange Chromatography (IEC): Definitions, requirements for ion-exchange resin, synthesis and types of ion-exchange resins, Principles, 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 process.

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

References:

1. J.P.Collman, L.S.hegedus, J.R.Norton and R.G.Finke: Principles and Applications of

2. Organotransition Metal Chemistry, University Science Books, 1987.

3. R.C.Mehrotra and A.Singh: Organometallic Chemistry, New Age International, 1999.

[14 Hours]

[14 Hours]

- 4. R.H.Crabtree:Organometallic Chemistry of Transition Metals, Wiley , 1999.

- K.H.Crabtree:Organometallic Chemistry of Transition Metals, wiley, 1999.
 F.A.Cotton and G.Wilkinson : Advanced Inorganic Chemistry, Wiley, 1991.
 Chromatography-E. Heftman (Ed), Part A and Part B, 5th ed. Elsevier, 1992.
 Chromatography Today- D. F. Poole and S.K. Poole, Elsevier , 1991.
 Principles of Instrumental Analysis-Skoog, Holler and Nieman, 5th ed. Saunders, 1998
 Quantitative Analysis-R. A. Day and A. L. Underwood, 5th ed. Prentice-Hall, 1998.
 Instrumental Methods of Chemical Analysis -B. K. Sharma, 19thed, Goel, 2000.



OC 552: ORGANIC SYNTHETIC METHODS

UNIT- I:

Reduction Reactions: Catalytic hydrogenation: Introduction, catalysts and solvents employed reduction of functional groups, mechanisms and stereochemistry of catalytic hydrogenations, Hydrogenolysis, and homogeneous catalytic hydrogenation.

Metal hydride reduction: Reduction with LiAlH₄ and NaBH₄, Stereo chemistry of reduction, Functional group transformation during reduction, Reduction with diborane and related reactions.Reduction in Biological systems-NADH,FAD.

Dissolving Metal Reductions: Mechanisms of reduction of conjugated system and carbonyl compounds, Bimolecular reductions of esters, Birch reduction, Wolf-Kishner reduction and related reactions, Reaction with diimide and related compounds.

UNIT-II:

Oxidation reactions: Introduction and different oxidative processes, Mechanism of oxidation reaction with chromium and manganese salts, peracids and peresters, periodic acid, Lead tetra acetate, Ozone, Osmium tetroxide and their synthetic importance in functional group transformation.

Halogenation: Halogenation of olefins, carbonyl compounds, Benzyllic and Allylic halogenation, Dehalogenation reactions. Dehydrogenation with S, Se, Pt, Pd, Ni.

UNIT-III:

Synthetic Design: Carbon skeleton frame work, Classification of carbon-carbon single bond and double bond forming reaction and their use in carbon skeleton ring formation. Ring forming and ring cleaving reactions, use of Thorpe condensation, Carbene insertion reaction, Friedel-Crafts reaction, 1,3-dipolar addition and Ene reaction in ring formation, Oxidative cleavage of rings and Retro Diel's-Alder reactions.

Planning of Organic Synthesis:Selection of starting materials and key intermediates during the synthesis. Synthesis of Cubane and Iswarane. Use of Robinson annulation, Dieckmann cyclisation, Arndt-Eistert synthesis, Diel's- Alder reaction in organic synthesis.

Functionality: Synthesis of 6- and 7- methoxytetralones, biotin and penicillin-V with special reference to the introduction of functional groups. Stereo chemical consideration and stereo selectivity during organic synthesis.

UNIT-IV:

General introduction to disconnection approach. Basic principles and technologies used in disconnection approach. Synthons and synthetic equivalents. Interconversion of functional groups. One group C-X and two group. C-X disconnections.

Protecting groups: Principle of protection of hydroxyl amino carboxylic and carbonyl groups.

Retrosynthetic analysis: Analysis of alcohols, carbonyl compounds cyclic and acyclic alkanes, benzocaine, p-methoxyacetophenone, acetonecyanohydrin, 2-methyl-6-methoxyindole-3-aceticacid, 6-methylquinoline & 1-phenyl-4-p-methoxyphenyl-1,3-butadiene, Limonene, Danishefsky'spentalenolactone, Benziodarone, nitrofurazone, Warfarin andJuvabione.

References :

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

[14 Hours]

[14 Hours]

[14 Hours]

OC 553: BIOORGANIC AND MEDICINAL CHEMISTRY

UNIT- I:

Drugs: Introduction, Classification and nomenclature of drugs. Theories of drug action such as Occupancy theory, Rate theory, Induced fit theory and Perturbation theory. Analogues and Prodrugs, Factors governing drug design. Rational approach to drug design, Variation method of drug designing, tailoring of drugs, Physico-Chemical factors and biological activities. Factors governing the ability of drugs, Isosterism and Bio-isosterism.

Antipyretic Analgesics: Classification, synthesis of Phenacetin, Aspirin, Cinchophen, Phenazone and Mefenamic acid, mode of action.

General Anesthetics: Introduction and classification, synthesis of anesthetic ethermethoxyfluorane, Thiopental sodium and Fentanyl citrate, Mode of action.

Local anesthetic: Introduction and classification, synthesis of benzocaine, α -Eucaine, Lignocaine hydrochloride and Dibucaine hydrochloride, Mode of action.

UNIT –II:

[14 Hours]

[14 Hours]

Cardiovascular drugs: Introduction, classification, Synthesis of Hydralazine, Methyldopa, Diazoxide, Procainamide, Propranolol, Bretyliumtosylate, Isoxsupurine, Prenylamine& their mode of action.

Antimalarials: Introduction and classification, Synthesis of Chloroquine phosphate, Pamaquine, Meparine hydrochloride, Proguanil hydrochloride, pyrimethanine and dapsone, mode of action.

Antineoplastic agents: Introduction and classification, Synthesis of Mechlorethamine hydrochloride, Busalfantriethylenemelamine, Methotrexate, Mercaptopurinum and Flurouracil, Mode of action.

Antiviral drugs: Introduction, classification, mechanism of action study of some representative drugs like Methisazone, Idoxuridine, Amantidine hydrochloride.

UNIT -III: Chemistry of Bio Molecules

Peptides & Proteins:Peptide bond formation and synthesis of polypeptides, Amino and carboxy protecting group in peptide synthesis, Solid phase peptide synthesis-Merrifield method, Peptide structure determination-Sequence and End group anaysis (N-Terminus and C-Terminus), Secondary, Tertiary and Quaternary structure of proteins.

Nucleic acids:Nucleosides and Nucleotides, Occurrence, Isolation and Classification of nuleosides and nucleotides. Chemical synthesis of nucleosides and nucleotides. Poly nucleotides- Structure and functions of DNA and RNA.Solid phase synthesis of oligonucleotides.

Non steroidal hormones: Study of the Oxytocin, Vasopressin and synthetic analogs, General study of ACTH, Growth hormones, Somotropin and Insulin.

UNIT -IV: Vitamins and Antibiotics

Vitamins: Introduction, Classification and Nomenclature-Source and Deficiency diseases-Biological, functions of Vitamins- Study of the following Vitamins: VitaminA₂, VitaminB₃, B₄, B₅ and B₁₂, Vitamin C, Vitamin K₁ and K₂.

Antibiotics: Introduction, Classification, Chemistry of Pencillin V, Cephalosporine C, Streptomycin, Chloramphenicol and Tetracyclin.

References:

1. Medicinal Chemistry- AshutoshKar (New Age.), 2005,

2. Medicinal Chemistry- G. R.Chatwal (Himalaya) 2002.

2. Natural Products Chemistry, Vol-I-II- G.R.Chatwal (Himalaya), 1990.

- 4. Principles of Drug Action- II Ed. A.Goldstein Lewis Arnold & SunerM.Kalman (Wiley Int.Ed.)
- 5.Organic Chemistry by I.L.Finar, Vol.1 & Vol.2

[14 Hours]

OC 554: CHEMISTRY OF NATURAL PRODUCTS

IT-I:

Alkaloids: Definition, Classification and isolation of alkaloids, general methods of structural determination of alkaloids, detailed study of structure elucidation, stereochemistry, rearrangement, Synthesis and biogenesis of Papaverine, Adrenaline, Ephedrine, Piperine, Cinchonine, Quinine, Morphine, Yohimbine, Reserpine and Lysergic acid.

UNIT-II:

Terpenoids: Introduction, classification, isoprene rules, methods of structure determination. Structural elucidation & synthesis of Geraniol, Menthol, α -Pinene, Camphor, Farnesol, Zingiberene and α -Santonin, Vetivones, Caryophylene.

Diterpenoids: Abieticand Gibberillic acid.

Triterpenoids: Squalene and Phytol.

Carotenoides: Introduction and geometrical isomerization of Carotenes. Structure and Synthesis of β -Carotene and Lycopene.

UNIT- III: [14 Hours]

Steroids: Introduction and Nomenclature of steroids, Blanc's rule, Barbier-Wieland degradation, Oppenauer oxidation, Diel's hydrocarbon, Chemistry of Cholestrol, Ergosterol, Vitamin-D & bile acids.

Steroidal hormones: Chemistry of Oestrone, esterdiol, estriol and their chemical relationship. Progesterone, androsterone and testosterone - Structure and Synthesis of Cortisone, Cortisol and Aldosterone. Transformations in steroids and hormones.

UNIT-IV:

Hours]

Chemistry Lipids: Introduction, Classification and biological functions, phospholipids, spingolipids.

Oils and fats: introduction and properties, synthesis of mono, di and mixed glycerides

Fatty acids: Introduction, classification, analysis of oils and fats, synthesis of oleic acid, recinoleic acid, linolenic acid, total synthesis of fatty acids,

Prostaglandins: Introduction, Nomenclature, Classification and Biological role of Prostaglandins, Structural elucidation and stereochemistry of PGE_1 , PGE_2 and PGE_3 . Total synthesis of PGE_1 (Corey's method & Up John's synthesis).

References:

1. Natural Products Chemistry Vol-I & II. G. R. Chatwal (Himalaya Bombay) 1990.

2. Chemistry of Natural Products – Vol-I & II – O. P. Agarwal(Goel Gorakhpur), 1985.

3. Organic Chemistry-Vol-I-II- I. L. Finar (Longmann ELBS London), 2000.

OC 555: ORGANIC CHEMISTRY PRACTICALS -VI

Preparation of Ethyl resorcinol from Resorcinol, 3-Bromo-4-methyl benzaldehyde from p-Toluedine, ε -Caprolactam from cyclohexanone, p-Aminobenzoic acid from p-Nitrotoluene, s-Tribromobenzene from aniline, o-hydroxyacetophenone from phenol, Benzanilide from Benzophenone, Benzylic acid from Benzoin, Benzopinacolone from Benzophenone, p-Chlorotoluene from p-Toludine, 2,5-Dihydroxyacetophenone from Hydroquinone, 2,4-Dinitrophenylhydrazine from Chlorobenzene, m-Nitrobenzoic acid from Benzoic acid, 2,4-Dinitrophenol from Chlorobenzene, o-Aminobenzoic acid from Phthalic acid, 2-Carbethoxycyclopentanone from Adipic acid, α -Acetylaminocinnamic acid from Glycine, p-Aminoazobenzene from Aniline.

[14 Hours]

[14

Synthesis of one derivative each of Furan, Indole, Pyrazole, Quinoline, Thiazole, Acridine, Coumarin and Triazole containing heterocycles. Synthesis of Picric acid, Para red, Methyl red, Methyl orange, Flourescein, Eosin, Indigo and dyeing of fabrics.

OC 556: ORGANIC CHEMISTRY PRACTICALS -VII

Separation of components from mixture of organic compounds by fractional crystallization, fractional distillation, adsorption, Paper, TLC and column chromatography. The purification and characterization of organic compounds.

Determination of pKa values, molar extinction coefficients, keto-enol equilibrium, order of reactions- S_N1 and S_N2 reactions, salt effect and effect of acidity on reaction rates.

Preparation and Estimation of aryloxyacetic acids,anilinoacetic acids,Carbohydrates,Proteins. Elucidation of structure of organic compounds using UV, IR, NMR and Mass spectra. Locating an organic compound by reference to literature (Chemical Abstract).

Applications of computers in the study of conformation and geometry of some simple organic molecules. Utility of Chem draw and Chem sketch.

References:

- 1. Elementary Practical Organic Chemistry-Vol. III quantitative Organic Analysis- A.I Vogel
- 2. Vogel's Text Book of Practical Organic Chemistry- Furniss et al.(ELBS, London)1978.
- 3. Experimetal Organic Chemistry- Vol. I &II- P.R.Singh, Tata McGraw-Hill, 1981.
- 4. Practical Organic Chemistry- IV Ed- Dey&.Sitaraman(Allied)
- 5. Laboratory Experiments in Organic Chemistry-Adam, Johnson & Wicon(McMillan, London), 1979.
- 6. Experimental Organic Chemistry- H.D.Durst&G.E.Goke(McGraw-Hill)1980
- 7. More Spectroscopic Problems in Organic Chemistry-A.J. Baker et al.(Heyden) 1975.
- 8. Spectral Problems in Organic Chemistry- Davis & Wells(Chapman & Hall)1984.

