DEPARTMENT OF ORGANIC CHEMISTRY

M.Sc. ORGANIC CHEMISTRY

SYLLABUS

TELANGANA UNIVERSITY

NIZAMABAD

M.Sc. COURSE STRUCTURE:

First Year (I-Semester)

Course No.	Subject	Periods/Week (1 hr)		Marks		Credits
		Theory	Practical	I.E.	U.E.	
CH-101T	Inorganic Chemistry	4	-	30	70	4
CH-102T	Organic Chemistry	4	-	30	70	4
CH-103T	Physical Chemistry	4	-	30	70	4
CH-104T	Analytical Techniques and Spectroscopy-I	4	-	30	70	4
CH-151P	Inorganic Chemistry Laboratory	-	6	-	75	3
CH-152P	Organic Chemistry Laboratory	-	6	-	75	3
CH-153P	Physical Chemistry Laboratory	-	6	-	75	3
CH-199	Seminar	2	-	-	-	-
	Periods/Marks	16	18	120	505	-
	Total Periods/Marks	34+2= 36		625		25

First Year (II-Semester)

Course No.	Subject	Periods/Week (1 hr)		Marks		Credits
		Theory	Practical	I.E.	U.E.	
CH-201T	Inorganic Chemistry	4	-	30	70	4
CH-202T	Organic Chemistry	4	-	30	70	4
CH-203T	Physical Chemistry	4	-	30	70	4
CH-204T	Analytical Techniques and Spectroscopy-II	4	-	30	70	4
CH-251P	Inorganic Chemistry Laboratory	-	6	--	75	3
CH-252P	Organic Chemistry Laboratory	-	6	--	75	3
CH-253P	Physical Chemistry Laboratory	-	6	--	75	3
CH-299	Seminar	2	-	-	-	-
	Periods/Marks	16	18	120	505	-
	Total Periods/Marks	34+2= 36		625		25

Semester-I and Semester-II syllabus is common for all specializations i.e., Inorganic, Analytical, Organic, Physical, Pharmacoinformatics and Physical-Organic.and Pharmaceutical chemistry.

Second Year (III-Semester)

Course No.	Subject	Periods/Week (1 hr)		Marks		Duration of Exam
		Theory	Practical	I.E.	U.E.	Hrs.
CH-301	Conformational Analysis, Asymmetric Synthesis and Biomolecules	4	--	30	70	3
CH-302	Modern Organic Synthesis	4	--	30	70	3
CH-303	Organic Spectroscopy and Pericyclic Reactions	4	--	30	70	3
CH-304	Photochemistry, Synthetic Strategies and Green Chemistry	4	--	30	70	3
CH-351	Separation and Identification of Organic Compounds	--	9	--	100	6
CH-352	Synthesis of Organic Molecules and Isolation of Natural Products	--	9	--	100	6
CH-399	Seminar	2	--	--	--	--
	Periods/Marks	16	18	120	480	-
	Total Periods/Marks	34+2= 36		600		-

Second Year (IV-Semester)

Course No.	Subject	Periods/Week (1 hr)		Marks		Duration of Exam
		Theory	Practical	I.E.	U.E.	Hrs.
CH-401	Drug Design and Drug Discovery	4	--	30	70	3
CH-402	Drug Synthesis and Mechanism of Action	4	--	30	70	3
CH-403	Advanced Heterocyclic Chemistry	4	--	30	70	3
CH-404	Advanced Natural Products	4	--	30	70	3
CH-451	Spectroscopic Identification of Organic Compounds and	--	9	--	100	6
CH-452	Synthesis and Analysis of Drugs	-	9	--	100	6
CH-499	Seminar	2	--	--	--	--
	Periods/Marks	16	18	120	480	-
	Total Periods/Marks	34+2= 36		600		-

M.Sc. CHEMISTRY SYLLABUS

(*effective from academic year 2011-12*)

SEMESTER - I

PAPER-I: CH 101T (INORGANIC CHEMISTRY)

IC 01: Symmetry of molecules
IC 02: Bonding in Metal Complexes - I
IC 03: Coordination equilibria
IC 04: Ligational aspects of diatomic molecules

IC-01: SYMMETRY OF MOLECULES:

Concept of Symmetry in Chemistry – Symmetry Operations – Symmetry Elements: Rotational Axis of Symmetry and Types of Rotational Axes, Plane of Symmetry and types of Planes, Improper Rotational Axis of Symmetry , Inversion Center and Identity Element – More about Symmetry Elements – Molecular Point Groups: Definition and Notation of Point Groups, Classification Molecules in to C1, Cs, Ci, Cn, Cnv, Cnh, C∞v, Dn, Dnh, Dnd, D∞h, Sn (n=even), T, Th, Td, O, Oh, I, Ih , Kh Groups. Descent in Symmetry with Substitution – Exercises in Molecular Point Groups – Symmetry and Dipole moment – Symmetry criteria for Optical activity.

IC-02: BONDING IN METAL COMPLEXES – I:

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

Types of magnetic behaviour – magnetic susceptibility – calculation of magnetic moment from magnetic susceptibility spin only formula, - Quenching of orbital angular momentum – Determination of magnetic moment from Guoy's method. Applications of magnetic moment data for the determination of oxidation states, bond type and stereochemistry.

IC-03: COORDINATION EQUILIBRIA:

Solvation of metal ions- Binary complexes: Formation of binary Metal Complexes and their stability – types of Stability Constants – relation between them- trends in Step-wise Stability Constants (Factors causing decrease and increase in Step-wise Stability) – Factors influencing the stability constants: (i) Ligand effects: Basicity, Substituent, Steric, Chelate (size and number of chelate rings), Macrocyclic and Cryptate effects- (ii) Metal ion effects: Ionic potential, Effective Nuclear charge and Atomic Number

(Irving-William's Order, geometry of Metal ion and Ligand) – Chelate effect and its Thermodynamic origin – Jahn-Tellar effect on Stability constants of Metal complexes – Pearson's Theory of Hard and Soft Acids and Bases (HSAB), Applications of HSAB, Electronegetivity Vs Hardness and Softness. Symbiosis – Methods used for the determination of Stability constants (Basic Principles only): pH metric, Spectro-photometric and Polarographic methods.

Ternary Metal Complexes – definition – Formation of ternary metal complexes – Stepwise and simultaneous equilibria with simple examples.

IC – 04: LIGATIONAL ASPECTS OF DIATOMIC MOLECULES:

Metal Carbonyls:- Carbon monoxide as a ligand–Molecular orbitals of CO-Donor and Acceptor molecular orbitals of CO; Bonding modes of CO-Terminal and Bridging; Evidence for multiple bonding from Bond lengths and Stretching frequencies; 18 Valence electron rule and its application.

Metal Nitrosyls: - NO as a ligand–Molecular orbitals of NO–Donor and Acceptor components; Bonding modes of NO Terminal (Linear, Bent) and Bridging; Structural aspects of $[IrCl(PPh_3)_2(CO)(NO)]^+$ and $[RuCl(PPh_3)_2(NO)_2]^+$. Stereochemical control of valence in $[Co(diars)_2(NO)]^{2+}$ and $[Co(diars)_2(NO)(SCN)]^+$.

Metal Dinitrogen complexes: - N_2 as aligand – Molecular orbitals of N_2; Bonding modes – Terminal and Bridging; Stretching frequencies; Structures of Ru(II) and Mo(0) dinitrogen complexes; Chemical fixation of dinitrogen.

SUGGESTED REFERENCES:

1. Symmetry and Group theory in Chemistry, Mark Ladd, Marwood Publishers, London (2000).
2. Molecular Symmetry and Group Theory, Robert L. Carter, John Wiley & Son (1998).
3. Symmetry and Spectroscopy of Molecules. K. Veera Reddy, New Age International (P) Limited (1999).
4. Advanced Inorganic Chemistry. F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann, 6th Edition, Wiley Interscience, N. Y. (1999).
5. Inorganic Chemistry, J. E. Huheey, K. A. Keiter and R. L. Keiter 4th Edition Harper Cottens College Publications (1993).
6. Homogeneous Catalysis by Metal complexes Vol. I, M. M. Taqui Khan and A. E. Martell, Academic Press NY (1974).
7. Inorganic Chemistry, Keith F. Purcell and John C. Kotz, Holt-Saunders International Editions, London (1977).

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PAPER-II: CH 102 T (ORGANIC CHEMISTRY)

OC-01: Stereochemistry
OC-02: Reaction mechanism-I
OC-03: Carbohydrates and Proteins
OC-04: Heterocyclic compounds

OC-01: STEREOCHEMISTRY:

Molecular representations: Wedge, Fischer, Newman and Saw-horse formulae, their description and interconversions.

Molecular Symmetry & Chirality: Symmetry operations and symmetry elements (Cn & Sn). Criteria for Chirality. Desymmetrization.

Axial, planar and helical chirality: Configurational nomenclature:Axially chiral allenes,spiranes,alkylidene cycloalkanes, chiral biaryls, atropisomerism.Planar chiral ansa compounds and trans- cyclooctene.Helically chiral compounds.

Relative and absolute configuration: Determination of absolute configuration by chemical correlation methods.

Racemisation, racemates and resolution techniques: Resolutions by direct crystallization, diastereoisomer salt formation chiral chromatography and asymmetric transformation.

Determination of configuration in E,Z-isomers: Spectral and Chemical methods of configuration determination of E,Z isomers. Determination of configuration in aldoximes and ketoximes.

OC-02: REACTION MECHANISM-I:

Electrophilic addition to carbon carbon double bond: Stereoselective addition to carbon carbon double bond ; *anti* addition- Bromination and epoxidation followed by ring opening. *Syn* addition of OsO_4 and $KMnO_4$.

Elimination reactions Elimination reactions E_2, E_1, E_1CB mechanisms. Orientation and stereoselectivity in E_2 eliminations. Pyrolytic *syn* elimination and α-elimination, elimination Vs substitution.

Determination of reaction mechanism: Determination of reaction mechanism: Energy profiles of addition and elimination reactions, transition states, product isolation and structure of intermediates, use of isotopes, chemical trapping, crossover experiments. Use of IR and NMR in the investigation of reaction mechanism.

OC-03: CARBOHYDRATES AND PROTEINS:

Carbohydrates: Determination of the relative and absolute configuration in D(+) glucose and D(-)fructose. Proof for the chair conformation of D(+)glucose. Occurence, importance and synthesis of monosaccharides containing functional groups such as amino, halo and sulphur. Structure elucidation and synthesis of sucrose.

Conformational structures of D(+)ribose, 2-deoxyD-ribose, sucrose, lactose maltose and cellobiose. Structural features of starch, cellulose and chitin.

Proteins: Acid and enzymatic hydrolysis of proteins. Determination of the amino acid sequence in polypeptides by end group analysis. Chemical synthesis of di and tripeptides. Merrifield's solid phase synthesis.

OC-4: HETEROCYCLIC COMPOUNDS:

Importance of heterocyclic compounds as drugs. Nomenclature of heterocyclic systems based on ring size,number and nature of hetero atoms.Synthesis and reactivity of indole, benzofuran, benzothiophene, quinoline, isoquinoline, coumarin, chromone, carbazole and acridine.

SUGGESTED REFERENCES:

1. Stereochemistry of carbon compounds by Ernest L. Eliel and Samuel H. Wilen
2. Stereochemistry of organic compounds-Principles and Applications by D. Nasipuri.
3. Heterocyclic Chemistry, T. L. Gilchrist, Longman U K Ltd, London (1985).
4. Benzofurans A. Mustafa, Wiley-Interscience, New York (1974).
5. Heterocyclic Chemistry, 3rd Edn J. A.Joule, K. Mills and G. F. Smith, Stanley Thornes Ltd, UK, (1998).
6. The Chemistry of Indole, R. J. Sunderberg, Academic Press, New York (1970).
7. An introduction to the chemistry of heterocyclic compounds, 2nd Edn. R. M. Acheson, Interscience Publishers, New York, 1967.
8. Advanced Organic Chemistry by Jerry March.
9. Mechanism and Structure in Organic Chemistry S. Mukerjee.
10. Guide Book to mechanism in Organic Chemistry, 6th Edition, Peter Sykes.
11. Organic Chemistry by Graham Solomous and Craig Fryhle.
12. Organic Chemistry by R. T. Morrison and R. N. Boyd.
13. Organic Chemistry, Vol. 2 by I. L. Finar.
14. Organic Chemistry: Structure and Reactivity by Seyhan Ege.

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PAPER-III: CH 103 T (PHYSICAL CHEMISTRY)

PC-01: Thermodynamics-I

PC-02: Electrochemistry-I

PC-03: Quantum Chemistry-I

PC-04: Chemical Kinetics-I

PC-01: THERMODYNAMICS-I:

Brief review of concepts of I and II laws of thermodynamics. Concept of entropy. Entropy as a state function. Calculation of entropy changes in various processes. Entropy changes in an ideal gas. Entropy changes on mixing of ideal gases. Entropy as a function of V and T. Entropy as a function of P and T. Entropy change in isolated systems- Clausius inequality. Entropy change as criterion for spontaneity and equilibrium.

Third law of thermodynamics. Evaluation of absolute entropies from heat capacity data for solids, liquids and gases. Standard entropies and entropy changes of chemical reactions. Helmholtz and Gibbs free energies (A and G). A and G as a criteria for equilibrium and spontaneity. Physical significance of A and G. Driving force for chemical reactions- relative signs of ΔH and ΔS.

Thermodynamic relations. Gibbs equations. Maxwell relations. Temperature dependence of G. Gibbs- Helmholtz equation. Pressure dependence of G.

Chemical potential: Gibbs equations for non-equilibrium systems. Material equilibrium. Phase equilibium. Clapeyron equation and Clausius-Clapeyron equation .

Conditions for equilibrium in a closed system. Chemical potential of ideal gases. Ideal-gas reaction equlibrium-derivation of equilibrium constant. Temperature dependence of equilibrium constant-the van't Hoff equation.

PC-02: ELECTROCHEMISTRY- I:

Electrochemical Cells : Derivation of Nernst equation – problems. Chemical and concentration cells (with and without transference). Liquid junction potential – derivation of the expression for LJP – its determination and elimination**.** Applications of EMF measurements : Solubility product, potentiometric titrations, determination of transport numbers, equilibrium constant measurements. Decomposition potential and its significance. Electrode polarization – its causes and elimination. Concentration overpotential. Concept of activity and activity coefficients in electrolytic solutions. The mean ionic activity coefficient. Debye-Huckel theory of electrolytic solutions. Debye-Huckel limiting law (derivation not required). Calculation of mean ionic activity coefficient. Limitations of Debye-Huckel theory. Extended Debye-Huckel law. Theory of electrolytic conductance. Derivation of Debye-Huckel-Onsager equation – its validity and limitations. Concept of ion association – Bjerrum theory of ion association (elementary treatment) - ion association constant – Debye-Huckel-Bjerrum equation.

PC-03: QUANTUM CHEMISTRY- I:

Black body radiation-Planck's concept of quantization-Planck's equation, average energy of an oscillator (derivation not required). Wave particle duality and uncertain

principlesignificance of these for microscopic entities. Emergence of quantum mechanics. Wave mechanics and Schroedinger wave equation.
Operators-operator algebra. Commutation of operators, linear operators.Complex functions. Hermitian operators. Operators Ñ and Ñ2 . Eigenfunctions and eigenvalues. Degeneracy. Linear combination of eigenfunctions of an operator. Well behaved functions. Normalized and orthogonal functions.
Postulates of quantum mechanics. Physical interpretation of wave function. Observables and operators. Measurability of operators. Average values of observables. The time dependent Schrodinger equation. Separation of variables and the time-independent Schrodinger equation.
Theorems of quantum mechanics. Real nature of the eigen values of a Hermitian operatorsignificance. Orthogonal nature of the eigen values of a Hermitian operator-significance of orthogonality. Expansion of a function in terms of eigenvalues. Eigen functions of commuting operators-significance. Simultaneous measurement of properties and the uncertainty principle.

PC-04: CHEMICAL KINETICS- I:

Theories of reaction rates : Collision theory, steric factor. Tranition state theory. Reaction coordinate, activated complex and the transition state. Thermodynamic formulation of transition state theory. Activtion parameters and their significance. The Eyring equation. Unimolecular reactions and Lindamann's theory.
Complex reactions-Opposing reactions, parallel reactions and consecutive reactions(all first order type). Chain reactions-general characteristics, steady state treatment. Example- H_2-Br_2 reaction. Derivation of rate law.
Effect of structure on reactivity- Linear free energy relationships. Hammett and Taft equations-substituent (s and s*) and reaction constant (r and r*) with examples. Deviations from Hammett correlations. reasons- Change of mechanism, resonance interaction. Taft four parameter equation. Correlations for nucleophillic reactions. The Swain – Scott equation and the Edward equation.
The reactivity-selectivity principle and the isoselectivty rule. The intrinsic barrier and Hammond's postulate.

SUGGESTED REFERENCES:

1. Atkin's Physical Chemistry, Peter Atkins and Julio de Paula, Oxford University press.
2. Physical Chemistry, Ira N. Levine, Mc Graw Hill.
3. Physical Chemistry-A Molecular approach, D. A. McQuarrie and J. D. Simon, Viva Books Pvt. Ltd.
4. Molecular Thermodynamics, D. A. Mc Quarrie and J. D. Simon, University Science Books.
5. Quantum Chemistry, Ira N. Levine, Prentice Hall.
6. Introduction to Quantum Chemistry, A. K. Chandra, Tata McGraw Hill.
7. Chemical Kinetics, K. J. Laidler, Mc Graw Hill.
8. Kinetics and Mechanism of Chemical Transformations, J. Rajaraman and J. Kuriacose, Mc Millan.
9. Introduction to Electrochemistry, S. Glasstone.
10. Modern Electrochemistry, J. O. M. Bockris & A. K. N. Reddy, Plenum.
11. Principles of physical chemistry, Samuel H. Maron and Carl F. Prutton, Oxford& IBH.
12. The Physical Basis of Organic Chemistry by Howard Maskill, Oxford University Press (New York).
13. Chemical Kinetics and Reaction Mechanisms, J. H. Espenson, McGraw Hill.
14. Physical Organic Chemistry, N. S. Isaacs, ELBS.

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PAPER-IV: CH 104 T (ANALYTICAL TECHNIQUES & SPECTROSCOPY- I)

ASP 01: Techniques of Chromatography
ASP 02: NMR spectroscopy-I (1H NMR)
ASP 03: Rotational and Vibrational spectroscopy
ASP 04: Electronic spectroscopy

ASP-01: TECHNIQUES OF CHROMATOGRAPHY:

i) Introduction, Classification of chromatographic techniques, differential migration rates, partition ratio, retention time, relation between partition ratio and retention time, capacity factor, selectivity factor. Efficiency of separation- resolution, diffusion, plate theory and rate theory.
ii) **GC:** Principle, instrumentation, detectors- TCD, FID, ECD. Derivatisation techniques, PTGC.
iii) **HPLC:** Principle, instrumentation, detectors- UV detectors, Photodiode array detector, fluorescence detector.
iv) Applications: Methods of quantitation for GC and HPLC: GC analysis of hydrocarbons in a mixture, GC assay of methyl testosterone in tablets, atropine in eye drops. HPLC assy of paracetamol and asprin in tablets.

ASP 02: NMR SPECTROSCOPY-I (^{1}H NMR):

^{1}H NMR spectroscopy: Magnetic properties of nuclei, Principles of NMR. Instrumentation, CW and pulsed FT instrumentation, equivalent and non equivalent protons, enantiotopic and diastereotopic protons, Chemical shifts, factors affecting the chemical shifts, electronegativity and anisotropy, shielding and deshielding effects,Signal integration, Spin-spin coupling: vicinal,germinal and long range, Coupling constants and factors affecting coupling constants. Applications of 1H NMR spectroscopy: Reaction mechanisms (cyclic bromonium ion,electrophilic and nucleophilic substitutions, carbocations and carbanions), E,Z isomers,conformation of cyclohexane and decalins, keto-enol tautomerism, hydrogen bonding, proton exchange processes (alcohols, amines and carboxylic acids), C-N rotation. Magnetic resonance imaging (MRI). ^{1}H NMR of organic molecules and metal complexes: ethyl acetate, 2-butanone, mesitylene, paracetamol, asprin, ethylbenzoate, benzyl acetate, 2-chloro propionic acid, $[HNi(OPEt_3)_4]^+$, $[HRh(CN)_5]$ Rh I=1/2, $[Pt(acac)_2]$.

ASP 03 :ROTATIONAL AND VIBRATIONAL SPECTROSCOPY:

i) Microwave Spectroscopy: Classification of molecules based on moment of inertia. Diatomic molecule as rigid rotator and its rotational energy levels. Selection rules (derivation not required). Calculation of bondlengths from rotational spectra of diatomic molecules. Isotope effect on rotational spectra. Calculation of atomic mass from rotational spectra. Brief description of microwave spectrometer.

ii) Vibrational Spectroscopy. Vibrational energy levels of diatomic molecules, selection rules (derivation not required). Calculation force constant from vibrational frequency. Anharmonic nature of vibrations. Fundamental bands, overtones and hot bands, Fermi Resonance. Vibration-rotation spectra diatomic molecules. Vibrations of poly atomic molecules. Normal modes of vibration, concept of group frequencies. Characteristics of vibrational frequencies of functional groups; Stereochemical effects on the absorption pattern in carbonyl group, cis-trans isomerism and hydrogen bonding. Isotopic effect on group frequency. IR spectra of metal coordinated NO_3 -, SO_4^{2-} and CO_3^{2-} ions.

Raman Spectroscopy- Quantum theory of Raman effect, Rotational raman and Vibrational Raman spectra, Stokes and anti- Stokes lines. Complementary nature of IR and Raman spectra.

ASP 04: ELECTRONIC SPECTROSCOPY:

Electronic spectroscopy: Electronic spectra: Elementary energy levels of molecules-selection rules for electronic spectra; types of electronic transitions in molecules. Chromophores: Congugated dienes, trienes and polyenes, unsaturated carbonyl compounds, benzene and its derivatives, Woodward-Fieser rules. Polynuclear aromatic hydrocarbons and diketones. Solvent and structural influences on absorption maxima, stereochemical factors. Cis-trans isomers and cross conjugation. Beer's law application to mixture analysis and dissociation constant of a weak acid.

SUGGESTED REFERENCES:

1. Fundamentals of Molecular Spectroscopy, Banwell and Mc Cash.
2. Introduction to Molecular Spectroscopy, G. M. Barrow.
3. Absorption Spectroscopy of Organic Compounds, J. R. Dyer.
4. Biochemistry: Hames and Hooper.
5. Introduction to Spectroscopy, Pavia Lampman Kriz.
6. Pharmaceutical analysis, Watson
7. NMR in Chemistry- A multinuclear introduction, William Kemp.
8. Organic Spectroscopy, William Kemp.
9. Spectroscopy of organic compounds, P. S. Kalsi.
10. Structural methods n Inorganic chemistry, E. A.V. Ebsworth.

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PAPER: CH 151P: INORGANIC CHEMISTRY PRACTICALS: (6 h/w)

I. CALIBRATIONS:

i) Calibration of weights.
ii) Calibration of pipettes.
iii) Calibration of standard flasks.
iv) Calibration of burette.

II. EDTA BACK-TITRATIONS:

i) Estimation of Ni^{2+}.
ii) Estimation of Al^{3+}.

III. EDTA SUBSTITUTION TITRATIONS:

Estimation of Ca^{2+}.

IV. PREPARATION OF COMPLEXES:

i) Hexaammine nickel (II) chloride.
ii) Tris (acetylacetanato) manganese.
iii) Tris (ethylenediamine) nickel (II) thiosulphate.
iv) Mercury tetrathiocyanato cobaltate (II).

V. PREPARATION OF COMPLEXES AND CALCULATION OF % PURITY:

i) Tetrammine copper (II) sulphate and estimation of NH_3 and calculation of % purity.
ii) Pentaammine (chloro) cobalt (III) chloride and estimation of Cl^- and calculation of % purity.
iii) Sodium trioxalato ferrate (III) and estimation of $C_2O_4^{2-}$ and Fe^{2+} and calculation of % purity.

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PAPER: CH 152P ORGANIC CHEMISTRY LAB COURSE: (6 h/w)

SYNTHESIS OF THE FOLLOWING COMPOUNDS:

i) *p*-Bromoacetanilide (using ceric ammonium nitrate and KBr)
ii) *p*- Bromoaniline
iii) 2,4,6-Tribromoaniline
iv) 1,3,5-Tribromobenzene
v) Tetrahydrocarbazole
vi) 7-Hydroxy-4-methylcoumarin
vii) m-Dinitrobenzene
viii) m-Nitroaniline
ix) Hippuricacid
x) Azlactone
xi) Anthracene-maleicanhydride adduct
xii) Phthalimide
xiii) 2,4-Dihydroxyacetophenone
xiv) Dihydropyrimidinone (using ethylacetoacetate , benzaldehyde and urea).

REFERENCES:

1. Text book of practical organic chemistry, Vogel.
2. Text book of practical organic chemistry, Mann and Saunders.

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PAPER: 153P PHYSICAL CHEMISTRY LAB COURSE: (6 h/w)

Physical properties: Determination of density, surface tension and viscosity of liquids

DISTRIBUTION:

i) Distribution of acetic acid between n-butanol and water
ii) Distribution of iodine between CCl4 and water

CHEMICAL KINETICS:

i) Acid-catalyzed hydrolysis of methyl acetate
ii) Peroxydisulphate- I- reaction (overall order)
iii) Oxidation of iodide ion by hydrogen peroxide- iodine clock reaction

CONDUCTOMETRY:

i) Titration of strong acid vs strong base
ii) Titration of weak acid vs strong base
iii) Determination of cell constant
iv) Determination of dissociation constant of a weak acid

POTENTIOMETRY:

i) Titration of strong acid vs strong base
ii) Titration of weak acid vs strong base
iii) Determination of dissociation constant of a weak acid
iv) Determination of single electrode potential

POLARIMETRY:

i) Determination of specific rotation of sucrose
ii) Acid-catalyzed hydrolysis of sucrose (inversion of sucrose)

ADSORPTION AND OTHERS:

i) Adsorption of acetic acid on animal charcoal or silica gel
ii) Determination of critical solution temperature of phenol-water system
iii) Effect of added electrolyte on the CST of phenol-water system

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M.Sc. CHEMISTRY SYLLABUS

(*effective from academic year 2011-12*)

SEMESTER - II

PAPER-I: CH 201T (INORGANIC CHEMISTRY)

IC 05: Reaction mechanisms of transition metalcomplexes
IC 06: Bonding in metal complexes-II
IC 07: Metal clusters
IC 08: Biocoordination chemistry

IC-05: REACTION MECHANISMS OF TRANSITION METAL COMPLEXES:

Ligand substitution reactions: Energy profile of a reaction – Transition state or Activated Complex. Types of substitution reactions (SE, SN, SN^1, SN^2).

Ligand substitution reactions in octahedral complexes: Aquation or Acid hydrolysis reactions, Factors effecting acid hydrolysis, base hydrolysis, conjugate Base Mechanism, Evidences in favour of SN^1CB Mechanism. Annation reactions. **Substitution reactions with out Breaking Metal-Ligand bond.**

Ligand Substitution reactions in Square-Planar complexes: Mechanism of Substitution in Square-Planar complexes- Trans-effect, Grienberg's Polarization theory and π–bonding theory–Applications of Trans-effect in synthesis of Pt (II) complexes.

Electron Transfer Reactions (or Oxidation-Reduction Reactions) in Coordination compounds: Mechanism of One-electron Transfer Reactions: Atom (or group) Transfer or Inner Sphere Mechanism, Direct electron Transfer or Outer Sphere Mechanism.Marcus –Hush theory.

IC-06: BONDING IN METAL COMPLEXES – II:

Free ion terms and Energy levels: Configurations, Terms, States and Microstates – Formula for the calculation of Microstates p^n and d^n configurations – L-S (Russel-Saunders) coupling scheme – j-j coupling scheme – Determination of terms for various p^n and d^n configurations of metal ins. Hole formalism – Energy ordering of terms (Hund's rules) Inter – electron repulsion Parameters (Racah parameters) – Spin-Orbital coupling parameters. Effect of weak cubic crystal fields on S, P, D and F terms- Orgel Diagrams. Jahn –Tellor theorem and its effects on terms.

IC-07: METAL CLUSTERS:

Carbonyl clusters: Factors favouring Metal-Metal bonding–Classification of Clusters – Low Nuclearity Clusters : M_3 and M_4 clusters , structural patterns in $M_3(CO)_{12}$ (M=Fe,Ru,Os) and $M_4(CO)^{12}$ (M=Co,Rh,Ir) Clusters-. Metal carbonyl scrambling – High Nuclearity clusters M_5, M_6, M_7, M_8 and M^{10} Clusters-, Polyhedral skeletal electron pair theory and Total Electron Count theory – Wades rules – Capping rule –

Structural patterns in $[Os_6(CO)_{18}]^{2-}$, $[Rh_6(CO)_{16}]$, $[Os_7(CO)_{21}]$, $[Rh_7(CO)_{16}]^{3-}$, $[Os_8(CO)_{22}]^{2-}$, $[Os_{10}C(CO)_{24}]^{2-}$ and $[Ni_5(CO)_{12}]^{2-}$.

Metal Halide clusters: Major structural types in Dinuclear Metal-Metal systems – Edge sharing Bioctahedra, Face sharing Bioctahedra, Tetragonal prismatic and Trigonal antiprismatic structures-. Structure and bonding in $[Re_2Cl_8]^{2-}$ and Octahedral halides of $[Mo_6(Cl)_8]^{4+}$ and $[Nb_6(Cl)_{12}]^{2+}$. Trinuclear halides of Re(III). Hoffman's Isolobal analogy and its Structural implications.

IC-08: BIO COORDINATION CHEMISTRY:

Metal ions in Biological systems: Brief survey of metal ions in biological systems. Effect of metal ion concentration and its physiological effects. Basic principles in the biological selection of elements.

Oxygen transport and storage: Hemoglobin and Myoglobin: Geometric, electronic and magnetic aspects of Dioxygen binding, oxygen adsorption isotherms and cooperativity in Hemoglobin and its physiological significance. Role of globin chain. Hemerythrin and Hemocyanin: Structure of deoxy forms, oxygen binding, Geometric, electronic and magnetic aspects. Comparison of Hemerythrin and Hemocyanin with hemoglobin.

Photosynthesis: Structural aspects of chlorophyll. Photo system I and Photo system II.

Vitamin B_6 model systems: Forms of vitamin B_6 with structures. Reaction mechanisms of (1) Transamination (2) Decarboxylation and (3) Dealdolation in presence of metal ions.

REFERENCES:

1. Inorganic Reaction Mechanisms. M. L. Tobe and John Burgess, Addison Wesley Longman (1999).
2. Metal ions in Reaction Mechanisms. K. Veera Reddy. Golgotia Publications (P) Ltd.
3. Mechanisms of Reactions in Transition Metal Sites. Richard A Henderson, Oxford Science Publications, London (1993).
4. Inorganic Reaction Mechanisms, F. Basolo and R. G. Pearson, New York (1967).
5. Advanced Inorganic Chemistry. F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann,
6 Th Edition, Wiley Interscience, N. Y. (1999).
6. Inorganic Chemistry, J. E. Huheey, K. A. Keiter and R. L. Keiter 4th Edition Harper Cottens College Publications (1993).
7. Inorganic Biochemistry Edited by G. L. Eichorn, Volume 1 Elsevier (1982).
8. The Chemistry of Metal Cluster Complexes. D. F. Shriver, H. D. Kaerz and R. D. Adams (Eds), VCH, NY (1990).
9. Inorganic Chemistry, Keith F. Purcell and John C. Kotz, Holt-Saunders International Editions, London (1977).
10. Bioinorganic Chemistry, I. Bertini, H. B.Gray, S. J. Lippard and S. J. Valentine, Viva Low-Priced Student Edition, New Delhi (1998).
11. Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life, W. Kain and B. Schwederski, John Wiley and Sons, NY (1999).
12. Bioorganic Chemistry – Dugas.

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PAPER-II: CH 202T (ORGANIC CHEMISTRY)

OC-05: Conformational analysis (acyclic systems)
OC-06: Reaction mechanism-II
OC-07: Reactive intermediates and Molecular rearrangements.
OC-08: Natural products (Terpenoids and Alkaloids).

OC-05: CONFORMATIONAL ANALYSIS (ACYCLIC SYSTEMS):

Introduction to conformational isomerism and the concept of dynamic stereochemistry. Study of conformations in ethane and 1,2-disubstituted ethane derivatives like butane, dihalobutanes, halohydrin, ethylene glycol, butane-2,3-diol amino alcohols and 1,1,2,2-tetrahalobutanes. Klyne-Prelog terminology for conformers and torsion angles Conformations of unsaturated acyclic compounds-Propylene, 1-Butene, Acetaldehyde, Propionaldehyde and Butanone. Conformational diastereoisomers and conformational enantiomers-. Factors affecting the conformational stability and conformational equilibrium–Attractive and repulsive interactions. Use of Physical and Spectral methods in conformational analysis.

Conformational affects on the stability and reactivity of acyclic diastereoisomers – steric and stereoelectronic factors-examples. Conformation and reactivity: The Winstein-Holness equation and the Curtin – Hammett principle.

OC-06: REACTION MECHANISM-II:

Nucleophilic Aromatic substitution: Aromatic Nucleophilic substitution: $SN^1(Ar)$, $SN^2(Ar)$, and benzyne mechanisms; evidence for the structure of benzyne. Von Richter rearrangement. Definition and types of ambident nucleophiles.

Neighbouring group participation : Criteria for determining the participation of neighbouring group. Enhanced reaction rates, retention of configuration, isotopic labeling and cyclic intermediates. Neighbouring group participation involving Halogens, Oxygen, Sulphur, Nitrogen, Aryl, Cycloalkyl groups, σ and π- bonds. Introduction to nonclassical carbocations.

Electrophilic substitution at saturated carbon and single electron transfer reactions.
Mechanism of aliphatic electrophilic sustitution. S_E1, S_E2, and S_Ei. SET mechanism.

OC-07: REACTIVE INTERMEDIATES AND MOLECULAR REARRANGEMENTS:

Reactive Intermediates: Generation, detection, structure, stability and reactions of carbocations, carbanions, carbenes, nitrenes and free radicals.

Molecular rearrangements: Definition and classification. Molecular rearrangements involving 1) electron deficient carbon: Wagner- Meerwein, Pinacol-Pinacolone, Allylic and Wolf rearrangement. 2) electron deficient Nitrogen: Hofmann, Lossen, Curtius, Schmidt and Beckmann rearrangements 3) electron deficient Oxygen: Baeyer-Villiger oxidation. 4) Base catalysed rearrangements: Benzilic acid, Favourski, Transannular, Sommlett-Hauser and Smiles rearrangement.

OC-08: NATURAL PRODUCTS-I (TERPENOIDS AND ALKALOIDS):

Importance of natural products as drugs. Isolation of natural products by steam distillation, solvent extraction and chemical methods. General methods in the structure determination of terpenes. Isoprene rule. Structure determination and synthesis of α-terpeniol and camphor. Biogenesis of monoterpenes. Structure determination and synthesis of β-carotene. General methods of structure determination of alkaloids. Structure determination and synthesis of papaverine and quinine.

SUGGESTED REFERENCES:

1. Stereochemistry of Carbon compounds by Ernest L. Eliel / Samuel H. Wilen.
2. Stereochemistry of organic compounds–Principles and applications by D Nasipuri.
3. The third dimension in organic chemistry, by Alan Bassindale.
4. Stereochemistry: Conformation and Mechanism by P. S. Kalsi.
5. Stereochemistry by V. M. Potapov.
6. Advanced Organic Chemistry by Jerry March.
7. Mechanism and Structure in Organic Chemistry S. Mukerjee.
8. Organic chemistry Vol. I and II by I. L. Finar.
9. Comprehensive organic chemistry Vol.5 D. H. R. Barton and W. D. Ollis.
10. Organic Chemistry, Vol. 2 by I. L. Finar.
11. Chemistry of Natural Products by Bhat, Nagasampagi and Siva Kumar.
12. Alkaloids by K.W. Bentley.
13. Steroids and Terpenoids by Bentle.

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PAPER-III: CH 203T (PHYSICAL CHEMISTRY)

PC-05: Thermodynamics-II

PC-06: Photochemistry-I

PC-07: Quantum Chemistry-II

PC-08: Solid state chemistry

PC-05: THERMODYNAMICS-II

Solutions: Specifying the Solution composition. Partial molar properties-significance. Relation between solution volume and partial molar volume. Measurement of partial molar volumes- slope and intercept methods. The chemical potential. Variation of chemical potential with T and P. Gibbs-Duhem equation-derivation and significance Ideal solutions. Thermodynamic properties of ideal solutions. Mixing quantities. Vapour pressure-Raoult's law. Thermodynamic properties of ideally dilute solutions. Vapour pressure- Henry's law. Nonideal systems. Concept of fugacity, fugacity coefficeient. Determination of fugacity. Non ideal solutions. Activities and activity coefficients. Standard-state conventions for non ideal solutions. Determination of activity coefficients from vapour pressure measurements. Activity coefficients of nonvolatile solutes using Gibbs-Duhem equation. Multicomponent phase equilibrium: Vapour pressure lowering, freezing point depression and boiling point elevation.

PC-06: PHOTOCHEMISTRY –I

Electronic transitions in molecules. The Franck Condon principle. Electronically excited molecules- singlet and triplet states. Radiative life times of excited states-theoretical treatment. Measured lifetimes. Quantum yield and its determination. Actinomety-ferrioxalate and uranyl oxalate actinometers-problems. Derivation of fluorescence and phosphorescence quantum yields. E-type delayed fluorescence-evaluation of triplet energy splitting(ΔEST). Photophysical processesphotophysical kinetics of unimolecular reactions. Calculation of rate constants of various photophysical processes-problems, State diagrams Photochemical primary processes. Types of photochemical reactions- electron transfer, photodissociation, addition, abstraction, oxidation and isomerization reactions with examples. Effect of light intensity on the rates of photochemical reactions. Photosensitization. Quenching-Stern Volmer equation. Experimental set up of a photochemical reaction. Introduction to fast reactions- Principle of flash photolysis.

PC-07: QUANTUM CHEMISTRY-II

Particle in a box-one dimensional and three dimensional. Plots of y and y2-discussion. Degeneracy of energy levels. Comparison of classical and quantum mechanical particles. Calculations using wave functions of the particle in a box-orthoganality, measurability of energy, position and momentum, average values and probabilities. Application to the spectra of conjugated molecules. Cartesian, Polar and spherical polar coordinates and their interrelations *Schrodinger equation for the hydrogen atom*-separation into three equations. Hydrogen like wave functions. Radial and angular functions. Quantum numbers n, l and m and their importance. The radial distribution functions. Hydrogen like orbitals and their representation. Polar plots, contour plots

and boundary diagrams. *Many electron systems*. Approximate methods. The variation method-variation theorem and its proof. Trial variation function and variation integral. Examples of variational calculations. Paricle in a box. Construction of trial function by the method of linear combinations. Variation parameters. Secular equations and secular determinant. *Bonding in molecules*. Molecular orbital theory-basic ideas. Construction of MOs by LCAO , H_2^+ ion. The variationan integral for H_2^+ ion. Detailed calculation of Wave functions and energies for the bonding and antibonding MOs. Physical picture of bonding and antibonding wave functions. Energy diagram. The MO and VB wave functions for H2 molecule and their comparision.

PC-08: SOLID STATE CHEMISTRY

Magnetic properties of solids- classification of magnetic materials, Magnetic susceptibility, Langevin diamagnetism, Weiss theory of para magnetism

Electronic properties of metals, insulators and semi conductors: Electronic structure of solids, Band theory, band structure of metals, insulators and semiconductors. Electrons, holes and Excitons. The temperature dependence of conductivity of extrinsic semi conductors. Photo conductivity and photovoltaic effect-p-n junctions.

Superconductivity. Occurrence of superconductivity. Destruction of superconductivity by magnetic fields-Meisner effect. Types of superconductors. Theories of super conductivity-BCS theory.

High temperature superconductors. Structure of defect perovskites. High Tc superconductivity in cuprates. Phase diagram of Y-Ba-Cu-O system. Crystal structure of $YBa_2Cu_3O_7^{-x}$. Preparation of 1-2-3 materials. Origin of high Tc superconductivity.

REFERENCES:

1. Atkin's Physical Chemistry, Peter Atkins and Julio de Paula, Oxford University press
2. Physical Chemistry, Ira N. Levine, McGraw Hill
3. Physical Chemistry-A Molecular approach, D.A. McQuarrie and J.D. Simon, Viva Books Pvt Ltd
4. Molecular Thermodynamics, D.A. McQuarrie and J.D. Simon, University Science Books
5. Quantum Chemistry, Ira N. Levine, Prentice Hall
6. Introduction to Quantum Chemistry, A.K. Chandra, Tata McGraw Hill
7. Introduction to Solids, Leonid V. Azaroff, Tata McGraw Hill
8. Solid state Chemistry, D.K. Chakrabarthy, New Age International
9. Solid state Chemistry and its aplications, A.R. West, Plenum.
10. Fundamentals of Photochemistry, K.K.Rohtagi-Mukherji, Wiley-Eastern
11. Molecular Photochemistry, N.J. Turro, Benjamin
12. Photochemistry, R.P.Kundall and A. Gilbert, Thomson Nelson
13. Essentials of Molecular Photochemistry by A. Gilbert and J. Baggott, Blackwell
14. Scientific Publications.
15. Organic Photochemistry by J.M.Coxon and B.Halton, Cambridge University press.
16. Introductory Photochemistry by A.Cox and T.J.Kemp. McGraw-Hill, London.
17. Principles of the Solid State, H. V. Keer, New Age International.

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PAPER-IV: CH 204 T (ANALYTICAL TECHNIQUES AND SPECTROSCOPY-II)

ASP-05: Electro analytical Techniques.

ASP-06: NMR- II

ASP-07: Mass Spectroscopy

ASP-08: Photoelectron & ESR spectroscopy

ASP-05: ELECTRO ANALYTICAL TECHNIQUES

a) Types and Classification of Electro analytical Methods.

i) Potentiometry- Types of electrodes, Hydrogen gas, Calomel, Quin hydrone and glass electrodes. Determination of pH. Potentiometric titrations.

ii) Conductometry – Definition of terms – conductivity, specific conductivity, cell constant. Mobility of ions, Conductometric titrations.

b) **D.C Polarography:** Dropping mercury electrode- Instrumentation-polarogram. Types of Currents: Residual, Migration, Limiting. Two and Three electrode assemblies. Ilkovic equation (derivation not necessary) and its consequences. Types of limiting Currents : Adsorption, Diffusion, Kinetic. Applications of polarography in qualitative and quantitative analysis. Analysis of mixtures. Application to inorganic and organic compounds. Determination of stability constants of complexes.

c) Brief account of following techniques and their advantages over conventional d.c.polargraphy.

(i) A.C.polarography (ii) Square-wave polarography (iii) Pulse polarography (iv) Differential pulse polarography

d) **Amperometric titrations**: Principle, Instrumentation. Types and applications of amperometric titrations. Determination of SO_4^{2-}, metal ions viz., Mg^{2+}, Zn^{2+}, Cu^{2+} and other substances.

e) **Cyclic Voltammetry**: Principle, instrumentation, reversible and irreversible cyclic voltammograms. Applications. Cyclic voltammetric study of insecticide parathion.

ASP 06: NMR SPECTROSCOPY-II (^{1}H, ^{19}F and ^{31}P NMR)

^{1}H, ^{19}F, ^{31}P and solid state NMR spectroscopy: First order and non first order spectra e.g., AX, AX_2, AX_3, A_2X_3, AMX and AB, ABC, Simplification of complex spectra: increased field strength, deuterium exchange, Lanthanide shift reagents and double resonance techniques. Discrimination of enantiomers by use of chiral NMR solvents (CSAs), chiral lanthanide shift reagents and Mosher's acid. Nuclear Overhauser enhancement (NOE). Fluxional molecules- bullvalene, [η^5-C_5H_5M], [η^5-$(C_5H_5)_2$ Ti η^1-$(C_5H_5)_2$] and [$\eta^4C_8H_8Ru(CO)_3$].

^{19}F NMR spectroscopy: ^{19}F chemical shifts, coupling constants. Applications of ^{19}F NMR involving coupling with ^{19}F,^{1}H and ^{31}P: 1,2 dichloro-1,1 difluoro ethane, BrF_5, SF_4, PF_5, ClF_3, IF_5, HF_2^-.

^{31}P NMR spectroscopy: ^{31}P chemical shifts, coupling constants. Applications of ^{31}P NMR involving coupling with ^{31}P, ^{19}F, ^{1}H and ^{13}C: ATP, Ph_3PSe, P_4S_3, $P(OCH_3)_3$, H_3PO_4, H_3PO_3, H_3PO_2, HPF_2, PF_6^-, PH_3, $[Rh(PPh_3)Cl_3]$ Rh I=1/2

Introduction to solid state NMR: Magic angle spinning (MAS).Applications of solid state NMR.

ASP 07: MASS SPECTROMETRY

Origin of mass spectrum, principles of EI mass spectrometer. Types of fragments: odd electron and even electron containing neutral and charged species (even electron rule), Nitrogen rule, isotopic peaks, determination of molecular formula, metastable ion peaks. High resolution mass spectrometry. Salient features of fragmentation pattern of organic compounds including β-cleavage, Mclafferty rearrangement, retro Diels – Alder fragmentation and ortho effect. Principle of EI, CI, Fast Atom Bombardment (FAB), Secondary Ion Mass Spectrometry (SIMS), Electrospray (ESI) ionization and Matrix Assisted Laser Desorption Ionization (MALDI) methods. Introduction to principle and applications of Gas Chromatography-Mass Spectrometry (GC-MS) and Liquid chromatography-Mass Spectrometry (LC-MS) techniques.

ASP-08: PHOTOELECTRON & ESR SPRECTROSCOPY

Photoelectron Spectroscopy: Principle and Instrumentation, Types of Photoelectron Spectroscopy – UPS & XPS Binding Energies, Koopman's Theorem, Chemical Shifts. Photoelectron Spectra of Simple Molecules: N_2, O_2, F_2, CO, HF, NH_3 and H_2O – Vibrational Structure of PES Bands, Potential energy curves, Interpretation of Vibrational spectral data for ionized (M^+) species, Prediction of Nature of Molecular Orbitals. ESCA in qualitative analysis, Principles of Auger electron spectroscopy.

Electron Spin Resonance: Introduction, principle, instrumentation, selection rules, interpretation of Lande's factor 'g'. Hyperfine and super hyperfine Coupling. Anisotropy in 'g' values and hyperfine coupling constants. Zero field splitting, Kramer's degeneracy, quadrupolar interactions. Study of free radicals and transition metal complexes. Evidence for covalency in complexes, ex. Cu(II) Bissalcylaldimine, Bis-acetylacetanatovanadyl(II) and hexachloroiridium(IV) complexes.

REFERENCES:

1. Spectroscopic identification of organic compounds by R.M. Silverstein and F.X. Webster.
2. Organic spectroscopy by William Kemp
3. Mass Spectrometry for Chemists and biochemists by M. Rose and R.A. W. Johnstone
4. Spectroscopic methods in organic chemistry by D.H. Williams and I. Fleming
5. Practical Pharmaceutical Chemistry by A. H. Beckett and J.B. Stenlake
6. Biological Mass Spectrometry by A.L. Burlingame
7. Principles and Practice of Biological Mass Spectrometry by Chhabil Das
8. Spectrscopic identification of organic compounds by R.M.Silverstein. G.C.Bassler and T.E.Morrill
9. NMR-A multinuclear introduction by William Kemp
10. Stereochemistry of Carbon compounds by Ernest L Eliel / Samuel H. Wilen
11. Principles of Polarography, Heyrovsky.
12. Principles of Polarography, Kapoor.
13. Modern Electroanalytical methods, edited by C.Charlot, Elsevier Company.
14. Principles of Instyrumental analysis, Skoog, Holler and Nieman, Harcourt Asia PTE Ltd.
15. Analytical Chemistry-An Introduction, Skoog, West, Holler and Crouch, Saunders College Publishing.
16. Prinicples of Instrumental Analysis, Skoog and Leary, Saunders College Publishing.
17. International series of Monographs, Vol. **53**: Photoelectron Spectroscopy, Edited by D. Beckerand D. Betteridge 1972.
18. Sructural methods in inorganic chemistry, E.A.V. Ebsworth.

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PAPER CH 251 P: INORGANIC CHEMISTRY PRACTICALS: 6 HRS/ WEEK

I. ONE COMPONENT GRAVIMETRIC ESTIMATIONS. (Use of sintered glass crucible)

i) Estimation of Zn^{2+}.

ii) Estimation of Ba^{2+}.

II. ANALYSIS OF TWO COMPONENT MIXTURES:

i) Separation of Ni^{2+} and Cu^{2+} in a mixture and estimation of Ni^{2+} (gravimetric) and Cu^{2+} (volumetric).

ii) Separation of Ag+ and Ca^{2+} in a mixture and estimation of Ag+ (gravimetric) and Ca^{2+} (volumetric).

iii) Separation of Al^{3+} and Fe^{3+} in a mixture and estimation of Al^{3+} (gravimetric) and Fe^{3+} (volumetric).

III. ANALYSIS OF THREE COMPONENT MIXTURES:

i) Separation of (Fe^{2+} and Ni^{2+}) from Zinc (Zn^{2+}) in the given mixture and estimation of Zinc (Gravimetric).

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

IV. ION EXCHANGE METHODS OF ANALYSIS:

i) Determination of capacity of an ion exchange resin.

ii) Separation of Zinc and Magnesium on an anion exchange resin and estimation of Mg^{2+} and Zn^{2+}.

SUGGESTED BOOKS :

1. Text book of Quantitative Inorganic Analysis by A.I.Vogel, 3rd edition, ELBS 1969.
2. Vogel's text book of Quantitative Inorganic analysis. Jeffery etal, 4th edition, ELBS 1988.
3. Vogel's text book of Quantitative Inorganic Analysis. 6 th edition, Pearson education Ltd. 2002.
4. Practical Inorganic chemistry By G.Marr and R.W.Rockett 1972.
5. Experimental Inorganic/Physical Chemistry – An Investigative integrated approach to Practical Project work By Mounir A.Malati, 1999.
6. Advanced experimental Inorganic chemistry by. Ayodhya Singh.
7. Practical Inorganic Chemistry by G.Pass & H. Sutchiffe, 2nd edn John Wiley &Sons.

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PAPER CH 252 P: ORGANIC CHEMISTRY LAB: 6 HRS/WEEK

Identification of organic compounds, systematic qualitative analysis: Physical data BP / MP, Ignition test, Lassaigne test – Nitrogen, Sulphur and halogens, solubility classification, Functional groups tests, Preparation of crystalline derivative and determination of their m.p.s and reference to literature to identify the compounds.

A minimum of **14** compounds covering different functional groups and solubility pattern. Glucose, benzoic acid, 2-chloro benzoic acid, anisic acid, p-nitrobenzoic acid; p-cresol, pchlorophenol, β-naphthol; aniline, o/m/p-chloroanilines; N-methylaniline/N-ethylaniline, N,N-dimethylaniline, benzamide, acetanilide, benzaldehyde, anisaldehyde, acetophenone, benzophenone, ethylbenzoate, methylbenzoate, nitrobenzene, chlorobenzene, bromobenzene, naphthalene, biphenyl and anthracene.

Identification of unknown organic compounds from their IR, UV, ^{1}H NMR and Mass Spectral data:

Analysis of recorded spectra of compounds belonging to i) alkynes, ii) alcohols and phenols iii) aldehydes and ketones iv) carboxylic acids, v) esters vi) acid amides and vii) primary and secondary amines.

REFERENCES

1. Text book of practical organic chemistry, Vogel
2. Text book of practical organic chemistry, Mann and Saunders.
3. Spectral identification of organic compounds Bassler, Silverstein 5th Edition.

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PAPER CH 253 P: PHYSICAL CHEMISTRY LAB: 6 HRS/WEEK

DISTRIBUTION:

i) Distribution of I_2 between CCl_4 and aq.KI solution- calculation of equilibrium constant.
ii) Study of complex formation between ammonia and metal ion

CHEMICAL KINETICS

i) Stoichiometry of peroxydisulphide-iodide reaction
ii) Peroxydisulphide- iodide reaction: order w.r.t [I^-] by isolation method.
iii) Peroxydisulphide-iodide reaction: order w.r.t [$S_2O_8^{2-}$] by initial rate method

CONDUTOMETRY:

i) Titration of a mixture of strong and weak acids vs strong base
ii) Determination of the hydrolysis constant of aniline hydrochloride
iii) Determination of solubility product

POTENTIOMETRY:

i) Titration of Fe^{+2} vs $Cr_2O_7^{-2}$ (redox titration)
ii) Titration of Cl^- vs Ag^+ (precipitation titration)
iii) Determination of solubility product

POLARIMETRY:

i) Determination of specific rotation of glucose and fructose
ii) Enzyme catalysed inversion of sucrose

COLORIMETRY:

i) Verification of Beer's law and calculation of molar absorption coefficient using $CuSO_4$ and $KMnO_4$ solutions

PH METRY:

i) Calibration of a pH meter and measurement of pH of different solutions
ii) Preparation of phosphate buffers

SOLUTIONS:

i) Determination of molecular weight of a non volatile substance by cryoscopic method
ii) Determination of degree of dissociation by cryoscopic method
iii) Study of surface tension-concentration relationship for solutions (Gibbs equation).

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M.Sc. CHEMISTRY (ORGANIC CHEMISTRY) SYLLABUS

(*effective from academic year 2011-12*)

SEMESTER – III

PAPER I: CH (OC) 301T: Conformational Analysis, Asymmetric Synthesis and Biomolecules

OC 09: Conformational Analysis (cyclic systems)
OC 10: Principles of Asymmetric synthesis
OC 11: Methodologies in asymmetric synthesis
OC 12: Biomolecules

OC 09: CONFORMATIONAL ANALYSIS (Cyclic systems) (15 Hrs)

Study of conformations of cyclohexane, mono, di and polysubstituted cyclohexanes, cyclohexene, cyclohexanone (2-alkyl and 3-alkyl ketone effect), 2-halocyclohexanones, cyclopentane, cyclobutane, cycloheptane and cyclooctane, Stereo chemistry of bicyclo[3,3,0]octanes, hydrindanes, decalins and perhydroanthracenes. Conformational structures of piperidine, *N*-Methylpiperidine, tropane, tropine, pseudotropine, decahydroquinoline and quinolizidine. Conformaijonal effects on the stability and reactivity of diastereomers in cyclic molecules - steric and stereo electronic factors – examples. Factors governing the reactivity of axial and equatorial substituents in cyclohexanes. Stereochemistry of addition to the carbonyl group of a rigid cyclohexanone ring.

OC 10: PRINCIPLES OF ASYMMETRIC SYNTHESIS (15 Hrs)

Introduction and terminology: Topicity in molecules Homotopic, stereoheterotopic (enantiotopic and diastereotopic) groups and faces- symmetry, substitution and addition criteria. Prochirality nomenclature: Pro-R, Pro-S, Re and Si. Stereoselective reactions: Substrate stereoselectivity, product stereoselectivity, enantioselectivity and diastereoselectivity. Conditions forstereoselectivity: Symmetry and transition state criteria, kinetic and thermodynamic control. Methods for inducing enantio and diastereoselectivity. Analytical methods: % Enantiomeric excess, enantiomeric ratio, optical purity, % diastereomeric excess and diastereomeric ratio. Techniques for determination of enantiomeric excess, specific rotation, Chiral NMR; Chiralderivatizing agents, Chiral solvent, Chiral shift reagents and Chiral HPLC.

OC 11: METHODOLOGIES IN ASYMMETRIC SYNTHESIS (15 Hrs)

Strategies in Asymmetric Synthesis: i) Chiral substrate controlled, ii) Chiral auxiliary controlled, iii) Chiral reagent controlled and iv) Chiral catalyst controlled.

i) Chiral Substrate controlled asymmetric synthesis: Nucleophilic additions to chiral carbonyl compounds. 1, 2- asymmetric induction, Cram's rule and Felkin-Anh model.

ii) Chiral auxiliary controlled asymmetric synthesis: α-Alkylation of chiral enolates, azaenolates, imines and hydrazones. 1, 4-Asymmetric induction and Prelog's rule. Use of chiral auxiliaries in Diels-Alder reaction.

iii) Chiral reagent controlled asymmetric synthesis: Asymmetric reductions using BINAL-H. Asymmetric hydroboration using IPC_2BH and $IPCBH_2$.

iv) Chiral catalyst controlled asymmetric synthesis: Sharpless and Jacobsen asymmetric epoxidations. Sharpless asymmetric dihydroxylation. Asymmetric hydrogenations using chiral Wilkinson biphosphine and Noyori catalys. Enzyme mediated enantioselective synthesis.

v) Asymmetric aldol reaction: Diastereoselective aldol reaction (chiral enolate & achiral aldehydes and achiral enolate & chiral aldehydes) its explanation by Zimmerman-Traxel model.

OC-12: BIOMOLECULES (15 Hrs)

i) Enzymes: Definition. Classification based on mode of action. Mechanism of enzyme catalysis. Lock and Key model and Induced- Fit model. Enantiomer discrimination by Three point Contact model. Factors affecting enzyme catalysis.Enzyme inhibition- reversible and irreversible inhibition. Enzymes in organic synthesis. Immobilised enzymes.

ii) Nucleic acids: Primary, secondary and tertiary structure of DNA. Types of mRNA, tRNA and rRNA. Replication, transcription and translation. Genetic code. Protein biosynthesis. Chemical Synthesis of nucleosides and nucleotides.

iii) Lipids: Lipid structure- acylglycerols, phosphoglycerides and sphingolipids. Biosynthesis of Lipids and chemical Synthesis of lipids.

Recommended Books:

1. Stereochemistry of organic compounds — Principles & Applications by D Nasipuri
2. Stereochemistry of Carbon compounds by Ernest L Eliel & Samuel H. wilen
3. Stereochemistry: Conformation & Mechanism by P S Kalsi
4. The third dimension in organic chemistry, by Alan Bassendale
5. Stereo selectivity in organic synthesis by R S Ward.
6. Asymmetric synthesis by Nogradi
7. Asymmetric organic reactions by J D Morrison and H S Moscher
8. Principles in Asymmetric synthesis by Robert E. Gawley & JEFFREY AUBE
9. Stereo differentiating reactions by Izumi
10. Some modern methods of organic synthesis by W Carruthers
11. Guidebook to organic synthesis, by R K Meckie, D M Smith & R A Atken
12. Organic synthesis by Michael B Smith
13. Enzyme structure and mechanism by Fersht and Freeman
14. Bio-Organic chemistry by Hennan Dugas
15. Nucleic acids in Chemistry and Biology by G M Blackburn MI Gait
16. Lehninger Principles of Biochemistry by D L Nelson and M M Cox
17. Outlines of Biochemistry by Conn and Stumpf
18. Biotransformations in Organic Chemistry by K Faber.
19. Principles of biochemistry by Horton & others.
20. Bioorganic chemistry - A chemical approach to enzyme action by Herman Dugas and Christopher Penney.

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PAPER II: CH (OC) 302T: MODERN ORGANIC SYNTHESIS

OC 13- Synthetic Reagents I
OC 14- Synthetic Reagents II
OC 15- New Synthetic reactions
OC 16- New techniques and concepts in organic synthesis

OC-13 SYNTHETIC REAGENTS I (15 Hrs)

i) Protecting groups: a) Protection of alcohols by ether, silyl ether and ester formation b) Protection of 1,2-diols by acetal, ketal and carbonate formation c) Protection of amines by acetylation, benzoylation, benzyloxycarbonyl, t-butyloxycarbonyl, fmoc and triphenyl methyl groups. d) Protection of carbonyls by acetal, ketal and thiol acetal (Umpolung) groups. e) Protection of carboxylic acids by ester and ortho ester (OBO) formation.

ii) Oxidations: 1) Oxidation of active C-H functions: DDQ and SeO_2. 2) Alkenes to diols: Prevost and Woodward oxidation 3) Alcohol to carbonyls; Cr(VI) oxidants (Jones reagent, PCC. PDC) IBX, DMP, CAN, TEMPO, TPAP, Swern oxidation 4). Oxidative cleavage of 1,2-diols: Periodic acid and Lead tetra acetate.

iii) Reductions: a) Catalytic hydrogenation: Homogenous (Wilkinsons's catalytic hydrogenation) and heterogeneous catalytic reduction. b) Non-metallic reductions: Diimide reduction c) Dissolving metal reductions: Birch reduction. d) Nucleophilic metal hydrides: $LiAlH_4$, $NaBH_4$, and their modifications. e) Electrophilic metal hydrides: BH_3, AlH_3 and DIBAL. f) Hydrogenolysis g) use of tri-*n*-butyl tin hydride; Radical reductions.

OC-14: SYNTHETIC REAGENTS II (15 Hrs)

i) Organometallic Reagents: a) Preparation and application of the following in organic synthesis: 1) Grignard, 2) Organo lithium and 3) Organo copper reagents b) Organo boranes in C-C bond formation c). Organo silicon reagents: reactions involving β-carbocations and α-carbanions, utility of trimethyl silyl halides, cyanides and triflates.

ii) Carbonyl methylenation: a) Phosphorous ylide mediated olefination: 1) Witting reaction, 2) Horner-Wordsworth-Emmons reaction b) Titanium- Carbene mediated olefination: 1) Tebbe reagent, 2) Petasis reagent c) Olefination by Nysted reagent.

OC-15: NEW SYNTHETIC REACTIONS (15 Hrs)

1. Metal mediated C-C and C-X coupling reactions: Suzuki, Heck, Stille, Sonogishira cross coupling, Buchwald-Hartwig and Negishi-Kumada coupling reactions.

2. C=C Formation Reactions: Shapiro, Bamford-Stevens, McMurrey reactions, Julia-Lythgoe olefination and Peterson's stereoselective olefination.

3. Multicomponent Reactions: Ugi, Passerini, Biginelli, Hantzsch and Mannich reactions.

4. Ring Formation Reactions: Pausan-Khand reaction, Bergman cyclisation, Nazerov cyclisation.

5. Click Chemistry: Criteria for Click reaction, Sharpless azides cycloadditions.

6. Metathesis: Grubb's 1st and 2nd generation catalyst, Olefin cross coupling metathesis (OCM), ring closing metathesis (RCM), ring opening metathesis (ROM), applications.

7. Other important synthetic reactions: Baylis-Hilman reaction, Eschenmoser-Tanabe fragmentation, Mitsunobu reaction, Stork-enamine reaction and Michael reactions.

OC-16: NEW TECHNIQUES AND CONCEPTS IN ORGANIC SYNTHESIS (15 Hrs)

1. Techniques in peptide synthesis: Solid phase peptide synthesis, commonly used resins (Rink resin, Wang resin and Ellman resin, synthesis of cross linked Merrifield resin and drawbacks of solid phase synthesis.

2) Solid phase oligodeoxynucleotide synthesis: Triester pathway and phosphoramidite pathway

3) Oligosaccharide synthesis: Protection of hydroxyl groups, cylic oxocarbenium ion, glycosyl donors and glycosyl acceptors, Kahne glycosidation, convergent and linear oligosaccharide synthesis.

4) Phase Transfer catalysis: Onium and crwon ethers as PTC.

5) Tandem synthesis: Tandem reactions; conjugate addition-aldol reaction, polymerizationcyclisation, elctrocylic-Diels Alder reaction.

6) Baldwin Rules: Exo and Endo cyclisation, tetrahedral, trigonal and diagonal systems, favoured and disfavoured cyclisations.

7) Chiron approach in organic synthesis: Nature's chiral pool, carbohydrates, amino acids, hydroxy acids, terpenes as chiral precursors. Synthesis of shikimic acid from D-arabinose, furanonycin from D-glucose, S-(-)-ipsenol from S-leucine. 8) Determination of absolute configuration: Mosher's methods.

RECOMMENDED BOOKS:

1) Some modern methods of organic synthesis by W. Carruthers
2) Guidebook to organic synthesis, by R K Meckie, D M Smith & R A Atken
3) Organic Synthesis by O House
4) Organic synthesis by Micheal B Smith
5) Reagents for organic synthesis, by Fieser & Fieser, Vol 1-11 (1984)
6) Organic synthesis by Robert E Ireland
7) Handbooks of reagents for organic synthesis by Reich and Rigby, Vol-I-IV
8) Total synthesis of natural products: the Chiron approach by S. Hanesian
9) Organic chemistry Jonathan Clayden, Nick Greeves and Stuart Warren

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PAPER III: CH (OC) 303T: ORGANIC SPECTROSCOPY AND PERICYCLIC REACTIONS

OC-17: ^{13}C NMR spectroscopy
OC-18: 2D NMR techniques and ORD
OC-19: Pericyclic reactions I
OC-20: Pericyclic reactions II

OC-17: ^{13}C NMR SPECTROSCOPY (15 Hrs)

CW and PFT techniques. Types of ^{13}C nmr spectra: undecoupled, proton- decoupled and offresonance decoupled (ORD) spectra. ^{13}C chemical shifts, factors affecting the chemical shifts, chemical shifts of organic compounds. Calculation of chemical shifts of alkanes, alkenes and alkynes. Homonuclear (^{13}C, ^{13}C J) and heteronuclear (^{13}C, ^{1}H J and ^{13}C- 2H J) coupling.

Applications of ^{13}C-NMR spectroscopy: Structure determination, stereochemistry, reaction mechanisms and dynamic processes in organic molecules. ^{13}C-NMR spectral editing techniques: principle and applications of APT, INEPT and DEPT methods.

OC-18 2D NMR TECHNIQUES AND ORD (15 Hrs)

1) 2D-NMR techniques: Principles of 2D NMR, Classification of 2D-experiments. Correlation spectroscopy (COSY) HOMO COSY (1H-1H COSY) , TOCSY (Total Correlation Spectroscopy), Hetero COSY (1H,13C COSY,HMQC), long range 1H,13C COSY (HMBC), Homonuclear and Heteronuclear 2D-J-resolved spectroscopy, NOESY and 2D-INADEQUATE experiments and their applications.

2) Optical Rotatory Dispersion (ORD) and CD Spectroscopy: Optical rotation, circular birefringence, circular dichroism and Cotton effect. Plain curves and anomalous curves. Empirical and semiempirical rules-The axial haloketone rule, the octant rule, Helicity rule, Exciton chirality method-Exciton coupling between identical chromophores. Benzene sector and chirality rule. Application of the rules to the study of absolute configuration and conformations of organic molecules.

OC-19 PERICYCLIC REACTIONS I (15 Hrs)

Introduction - Characteristics and classification of pericyclic reactions— Electrocyclic, cycloaddition & cycloreversions and sigmatropic reactions—4ne and 4n+2e type examples. Approaches for the interpretation of mechanism of pericyclic reactions-Aromatic Transition States (ATS)/Perturbation Molecular Orbitals (PMO) approach-Concept of Huckel –Mobius aromatic and antiaromatic transition states. Framing Woodward-Hofmann selection rules for all the pericyclic reactions by ATS approach. Solving problems based on ATS approach. Aromaticity: Aromatic and anti aromatic compounds. Criteria for aromaticity. Huckel's 4n+2 electron rule for benzene and non benzenoid aromatic compounds. Eg. Cyclopropenium ion, cyclopentadienyl ion, cycloheptatrienium ion, azulene and annulenes.

OC-20 PERICYCLIC REACTIONS II (15 Hrs)

Molecular orbitals-definition and their origin-Non-mathematical writing up of molecular orbitals and their symmetry properties for acyclic conjugated systems. Frontier Molecular Orbital (HOMO-LUMO) approach-concept-Framing Woodward-Hofmann selection rules for all the pericyclic reactions by Frontier Molecular Orbital

(FMO) approach. Solving problems based on FMO approach. Conservation of orbital symmetry (Correlation Diagrams) approach-concept- Framing Woodward-Hofmann selection rules for electrocylic and cycloadditions & cycloreversions by Conservation of orbital symmetry approach.

RECOMMENDED BOOKS:

1. Spectroscopic identification of organic compounds by RM Silverstein, G C Bassler and T B Morrill
2. Organic Spectroscopy by William Kemp
3. Spectroscopic methods in Organic chemistry by DH Williams and I Fleming
4. Modern NMR techniques for chemistry research by Andrew B Derome
5. NMR in chemistry - A multinuclear introduction by William Kemp
6. Spectroscopic identification of organic compounds by P S Kalsi
7. Introduction to organic spectroscopy by Pavia
8. Carbon-13 NMR for organic chemists by GC Levy and O L Nelson
9. Nuclear Magnetic Resonance Basic principles by Atta-ur-Rahman
10. Advanced organic chemistry. Part A Structure & Mechanism by Francis A. Corey and Richard J. Sundberg
11. Optical rotatory dispersion by C Djerassi
12. Optical rotatory dispersion and circular dichroism by P Crabbe
13. Mechanism and Structure in Organic chemistry by S Mukherjee
14. Advanced Organic Chemistry: Reactions, Mechanisms & Structure by Michael B Smith & Jerry March
15. Pericyclic Reactions by Mukherjee S M
16. Conservation of Orbital Symmetry by Woodward and Hoffmann
17. Organic Reactions and Orbital Symmetry, Gilchrist and Storr
18. Pericyclic Reactions — a problem solving approach, Lehr and Merchand
19. The Nature of Chemistry — Units 17-19 - Aromaticity — Open University, U K. Publications
20. The aromaticity III level, units 17-19 British open university volumes
21. Aromatic character and aromaticity by G.M. Badger
22. Non-benzenoid aromatic compounds by D.Ginsberg
23. Nonbenzenoid compounds by Lloyds

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PAPER IV CH (OC) 304T: PHOTOCHEMISTRY, SYNTHETIC STRATEGIES AND GREEN CHEMISTRY

OC-21 Photochemistry
OC-22 Synthetic strategies - I
OC-23 Synthetic strategies - II
OC-24 Green Chemistry

OC-21: PHOTOCHEMISTRY (15Hrs)

Photochemistry of (π, π^*) transitions: Excited states of alkenes, cis-trans isomerisation, photostationary state, electrocyclisation and sigmatropic rearrangements, di-π methane rearrangement. Intermolecular reactions, photocycloadditions, photodimerisation of simple and conjugated olefins, addition of olefins to α, β-unsaturated carbonyl compounds. Excited states of aromatic compounds, Photoisimerisation of benzene
Photochemistry of (n-π^*) transitions: Excited states of carbonyl compounds, homolytic cleavage of α- bond, Norrish type I reactions in acyclic and cyclic ketones and strained cycloalkanediones.Intermolecular abstraction of hydrogen: photoreduction - influence of temperature, solvent, nature of hydrogen donor and structure of the substrate. Intramolecular abstraction of hydrogen:Norrish type II reactions in ketones, Esters and 1, 2-diketones, Addition to carbon-carbon multiple bonds, Paterno-Buchi reaction, Photochemistry of nitrites-Barton reaction.

OC-22: SYNTHETIC STRATEGIES I (15 Hrs)

Synthetic Strategies; Introduction, Terminology: target, synthon, synthetic equivalent, functional group interconversion (FGI), functional group addition, functional group elimination. Criteria for selection of target. Linear and convergent synthesis. Retrosynthetic analysis and synthesis involving chemoselectivity, regioselectivity, reversal of polarity and cyclizations. Order of events in synthesis by retrosynthetic approach, explanation with examples Ssalbutamol, Propoxycaine and Dinocap. Introduction to one group C-C and C-X disconnections. One group C-C disconnections, Alcohols and carbonyl compounds. One group C-X disconnections ,Carbonyl compounds, alcohols, ethers and sulphides.

OC-23: SYNTHETIC STRATEGIES II (15 Hrs)

Introduction to two group C-C and C-X disconnections, Two group C-X disconnections; 1,1-difunctionalised, 1,2-difunctionalised and 1,3-difunctionalised compounds. Two group C-C disconnections; Diels-Alder reaction, 1,3-difunctionalised compounds, 1,5-difunctionalised compounds, Michael addition and Robinson annulation. Control in carbonyl condensations, explanation with examples oxanamide and mevalonic acid. Strategic bond: definition, choosing disconnection/ guidelines for disconnection; disconnection of C-X bonds, disconnect to greatest simplification, using symmetry in disconnection, disconnection corresponding to known reliable reaction, high yielding steps and recognizable starting materials. Other approaches to retro synthesis – biomimetic approach (Johnsons polyene cyclisation), and retro mass spectral fragmentation. Application of the strategies to the synthesis of (+) Disparlure, Retronecene, longifoline.

OC-24: GREEN CHEMISTRY **(15 Hrs)**

Introduction. Principles, atom economy and scope. Introduction to alternative approaches.

1. Solvent free reactions-principle, scope, utility of solvent free condition reactions. Organic Synthesis in solid state (without using any solvent): Michael addition, Beckmann rearrangement, Synthesis of aziridines; solid supported organic synthesis: Synthesis of aziridines, pyridines, chromenes and flavones.
2. Aqueous Phase Reactions: Diels-Alder Reaction, Heck reaction, epoxidation, Dihydroxylation (Syn- & Anti-)
3. Microwave Technology: Microwave equipment, activation-benefits, limitations, microwave effects.

a) Microwave Solvent free reactions (Solid state Reactions) - Deacetylation, deprotection, saponification of esters, alkylation of reactive methylene compounds, synthesis of nitriles from aldehydes, reductions.

b) Microwave assisted reactions in water - Hoffmann elimination, hydrolysis, oxidation, saponification reactions.

c) Microwave assisted reactions in organic solvents - Esterification reactions, Fries rearrangement, Orthoester Claisen rearrangement, Diels-Alder reaction, decarboxylation.

d) Microwave assisted reactions under PTC conditions:

4. Ultrasound assisted reactions: introduction, substitution reactions, addition, oxidation, reduction reactions.
5. Organocatalysis: Aldol reactions, Acyl transfer reactions, nucleophilic N-heterocyclic carbenes in asymmetric organocatalysis, setter reaction and Baker's Yeast.
6. Ionic liquids: Introduction and applications in organic synthesis (illustrate with two examples).

RECOMMENDED BOOKS

1. Green chemistry, Theory and Practical, Paul T.Anastas and John C.Warner.
2. New trends in green chemistry By V.K.Ahulwalia and M.Kidwai.
3. Organic Synthesis: Special techniques. V.K.Ahulwalia and Renu Aggarwal.
4. Enantioselective organocatalysis, Peter I Dallco, Willey-VCH.
5. Molecular Reactions and Photo chemistry by Depuy and Chapman
6. Photochemistry by C W J Wells
7. Organic Photochemistry by Turro
8. Molecular Photochemistry by Gilbert & Baggo
9. Organic Photochemistry by D Coyle
10. Organic Synthesis-The disconnection approach by S Warren
11. Organic Synthesis by C Willis and M Willis
12. Problems on organic synthesis by Stuart Warren

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III SEMESTER PRACTICALS

PAPER CH (O) 351P: SEPARATION AND IDENTIFICATION OF ORGANIC COMPOUNDS

Separation of two component mixtures by chemical methods and their identification by chemical reactions - separation by using solvent ether, 5 % aqueous sodium bicarbonate, 5% sodium hydroxide and dil hydrochloric acid, checking the purity of the two components by TLC, identification of the compounds by a systematic study of the physical characteristics (mp/bp), extra elements (nitrogen, halogens and sulfur), solubility, functional groups, preparation of crystalline derivatives and identification by referring to literature. A minimum of 10 mixtures should be separated and analyzed by these procedures. Separation of three component mixtures by chemical methods. A minimum of two mixtures should be separated and analyzed.

PAPER CH (O) 352P: SYNTHESIS OF ORGANIC MOLECULES & ISOLATION OF NATURAL PRODUCTS

A) Laboratory synthesis of the following compounds:

2-Phenyl indole (Fischer indole synthesis), 7-hydroxy-3-methyl flavone (Baker – Venkatraman reaction), 2,5-Dihydroxy acetophenone (Fries reaction), 4-Chlorotoluene from p-toluidine (Sandmeyer reaction), Benzilic acid from benzoin (Benzillic acid rearrangement), Benzpinacol (photochemical reaction), 7-hydroxy coumarin (Pechman synthesis), Photo-dimerization of maleic anhydride, benzophenone (Friedel-Crafts reaction), Benzanilide (Beckmann rearrangement), Vanillyl alcohol from vanillin ($NaBH_4$ reduction), 2- and 4-nitrophenols (nitration and separation by steam distillation), Acridone from Phthalic anhydride.

B) Isolation of the following natural products:

Caffeine from tea leaves (solvent extraction), Piperine from pepper (Soxhlet extraction), Eucalyptus oil from leaves (steam distillation), Lycopene from tomatoes.

RECOMMENDED BOOKS:

1. Practical organic chemistry by Mann & Saunders
2. Text book of practical organic chemistry by Vogel
3. The systematic identification of organic compounds by Ralph L. Shriner, Christine K. F. Hermann, Terence C. Morrill and David Y. Curtin

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M.Sc. CHEMISTRY (ORGANIC CHEMISTRY) SYLLABUS

(*effective from academic year 2011-12*)

SEMESTER – IV

PAPER I: CH (OC) 401T: DRUG DESIGN AND DRUG DISCOVERY

OC-25: Principles of Drug design and drug discovery
OC-26: Lead modification and SAR Studies
OC 27: QSAR studies
OC 28: Combinatorial Synthesis

OC- 25: PRINCIPLES OF DRUG DESIGN AND DRUG DISCOVERY (15 Hrs)

Introduction to drug discovery. Folklore drugs, stages involved in drug discovery-disease, drug targets, bioassay. Discovery of a lead- screening of natural products and synthetic compound libraries. Existing drugs as leads (me too drugs). Pharmacokinetics (ADME), pharmacodynamics. Nature of drug – receptor interactions and their theories – Occupancy theory, Induced – fit theory, Macromolecular purturbation theory and Two-state model of receptor activation. Natural products as lead structures in drug discovery – Pharmacophore - structure pruning technique e.g. morphine. Discovery of lead structure from natural hormones and neurotransmitters. Principles of design of agonists (e.g.Salbutamol), antagonists e.g. cimitidine) and enzyme inhibitors (e.g. captopril). Drug discovery without lead – serendipity-Penicillin and Librium as examples. Principles of prodrug design. Introduction to drug patents and Clinical trials.

OC-26: LEAD MODIFICATION AND SAR STUDIES (15 Hrs)

SAR*:* Lead modification strategies, Bioisosterism, variation of alkyl substituents,chain homologation and branching, variation of aromatic substituents,extension of structure, ring expansion and ring contraction, ring variation, variation and position of hetero atoms, ring fusion, simplification of the lead, rigidification of lead.Discovery of oxaminquine, salbutamol, cimitidine and captopril Structure-Activity Relationship studies in sulfa drugs,benzodiazepines, and taxol analogs.

OC-27: QUANTITATIVE STRUCTURE- ACTIVITY RELATIONSHIP (QSAR) STUDIES (15 Hrs)

Introduction, physicochemical properties - pKa, electronic effects and Hammett constants (σ), lipophilicity constant(π), steric effects and Taft's constant, linear and nonlinear relationship between biological activity and Hammett/ Lipophilicity Substituent constants. Lipenski rule of five. Hansch analysis, Craig's plot,Topliss scheme, Free Wilson approach, cluster significant analysis. Three case studies. Principles of molecular modeling in drug design.

OC-28: COMBINATORIAL SYNTHESIS (15Hrs)

Introduction. Combinatorial approach. Combinatorial libraries, technologies. Solid phase synthesis, types of resins. Linkers. Reactants for solid phased synthesis. Methods of Parallel synthesis: Haughton's tea bag procedure. Automated parallel synthesis. Methods in Mixed combinatorial synthesis: general principles. Furkas mix and split combinatorial synthesis, Structure determination of active compounds-Deconvolution, Methods in deconvolutionrecursive deconvolution, tagging and use of

decoded sheets. Examples of Combinatorial Chemistry. Planning and designing of combinatorial synthesis, Spider like scaffolds, drug molecules. Automation in Combinatorial chemistry. High throughput screening.

Recommended books

1. Burger's medicinal chemistry and drug discovery by Manfred E. Wolf.
2. Introduction to Medicinal chemistry by Patrick.
3. Introduction to drug design by R Silverman
4. Comprehensive medicinal chemistry. Vol 1-5 by Hanzsch.
5. Principles of medicinal chemistry. by William Foye
6. Biochemical approach to medicinal chemistry. by Thomas Nogrady.
7. Pharmaceutical Chemistry and Drug synthesis by Roth and Kleeman
8. Drug design by E.J.Arienes
9. Principles of Medicinal Chemistty Vol I & II by Kadam et al
10. Medicinal chemistry An introduction by Garreth Thomas
11.Organic and Pharmaceutical chemistry By Delgrado
12. Organic Pharmaceutical chemistry By Harikishan singh
13. Medicinal Chemistry By Ashtoshkar
14. Medicinal Chemistry By Chatwal
15. Organic Drug synthesis By Ledneicer Vol 1-6
1 6.Strategies for organic drug synthesis and design By Daniel Ledneicer.
1 7.Top Drugs: Top synthetic routes By John Saunders
I 8.Chirotechnoiogy By Roger A. Sheldon
19. Burger's Medicinal Chemistry and Drug Discovery: Principles and Practices. Vol. 1.
20. Medicinal Chemistry by G. Patricks.
21. Text book of Drug Design and Discovery, Edited by Povl Krogsgaard – Larsen Tommy Liljefors.
22. Structure Based Drug Design of Crizotinib (PF-02341066), a Potent and Selective Dual Inhibitor of Mesenchymal–Epithelial Transition Factor (c-MET) Kinase and Anaplastic Lymphoma Kinase (ALK) Martin P. Edwards, J. Med. Chem., 2011, 54 (18), pp 6342–6363.

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PAPER II: CH (OC) 402T: DRUG SYNTHESIS AND MECHANISM OF ACTION

OC-29: Drugs acting on metabolic process, cell wall and specific enzymes
OC-30: Drugs acting on genetic material and immune system
OC-31: Drugs acting on receptors and ion channels
OC-32: Chiral drugs

OC-29: DRUGS ACTING ON METABOLIC PROCESS, CELL WALL AND SPECIFIC ENZYMES

Basic concepts of mechanism of drug action: Introduction to macromolecular targets, carbohydrates, proteins, lipids and nucleic acids as possible drug targets. Classification of drugs. Enzyme inhibition and its types.

a) Drugs acting on metabolic process:

Antifolates –Discovery and mechanism of action of sulphonamides, Synthesis of sulfomethoxazole, sulfodoxine, sulfaguanidine and dapsone. Diaminopyrimidines - trimethoprim, bacterial resistance to sulfonamides and drug synergism.

b) Drugs acting on cell wall: Structure of bacterial cell wall, β-Lactam antibiotics – mechanism of action of penicillins and cephalosporins. Synthesis of pencillin-G and cephalosporin-C, cefalexin and cycloserine. Resistance to pencillins, broad spectrum penicillins – cloxacillin, methicillin, ampicillin, amoxicillin and carbenicillin. β-Lactamase inhibitors – Structural formulae and mode of action of clavulanic acid and sulbactum.

c) Drugs acting on specific enzymes: H+/K+ -ATPase inhibitors- synthesis of Omeprazole and Carbonic anhydrase inhibitors-synthesis of Acetazolamide.

OC-30: DRUGS ACTING ON GENETIC MATERIAL AND IMMUNE SYSTEM

Drugs acting on genetic material: Introduction, classification and mechanism of action.

a) DNA-intercalating agents-Anticancer and antimalarial agents. Structural formulae of Daunomycin, Adriamycin and Amsacrine. Synthesis of Amscarine, Nitracrine, Quinacrine and Chloroquine.

b) DNA-Binding and nicking agents: Antiprotozoal drugs. Synthesis of Metronidazole, Dimetridazole and Tinidazole.

c) DNA-Alkylators: Synthesis of Cyclophosphamide and Bisulphan.

d) DNA-Polymerase inhibitors: Antiviral agents- Synthesis of Acyclovir and AZT.

e) DNA-Topoisomerase inhibitors: Anti bacterial agents. Synthesis of Ciprofloxacin and Norfloxacin. Structural formulae of loxacin and Lomefloxacin.

f) Inhibitors of transcribing enzymes: Anti-TB and antileprosy agents-structural formulae of Rifamycins and partial synthesis of Rifampicin.

g) Drugs interfering with translation process: Antibacterial drugs- Structural formulae of Erythromycin, 5-Oxytetracycline and Streptomycin. Synthesis of Chloromycetin

Drugs acting on immune system: Introduction to immune system. Immunosupressing agentstructural formula of Cyclosporin. Immunoenhancers-use of vaccines and strucrural formula of levamisol.

OC-31: DRUGS ACTING ON RECEPTORS AND ION CHANNELS

Introduction to nervous system: structure of neuron, nerve transmission. Definition and examples of agonist, antagonist, neurotransmitters and receptors. Drugs acting on receptors:
a) Adrenergic receptors - Introduction and classification. α-Adrenergic-receptor agonists and antagonists- Synthesis and biological activity of Nor-adrenaline, Methyl L dopa and Tetrazosin. β-Adrenergic-receptor- agonists and antagonists – Synthesis and pharmacological activity of Salbutamol, Tetrabutalin, Propranolol and Atenolol.
b) Cholinergic-receptors: Introduction and classification. Cholinergic-receptor agonists and antagonists- Structural formulae of Nicotine, Atropine and Tubocurarine. Synthesis of Acetyl choline and Succinyl choline
c) Dopamine receptors: Introduction and classification. Dopamine- receptor agonists and antagonists- Biosynthesis of Dopamine. Synthesis of L-Dopa and Chlorpromazine.
d) Serotonin receptors: Introduction and classification. Serotonin receptor agonists and antagonists-synthesis and pharmacological activity of Serotonin and Metoclopramide.
e) Histamine receptors: Introduction and classification. Histamine receptor agonists and antagonists-synthesis and biological action of Histamine, Chloropheneramine, and Ranitidine.
f) Hormones and their receptors: Introduction to estrogen receptors, Structural formulae of Tamoxifen Drugs acting on ion channels: Introduction to ion channels, drugs acting on Ca2+, Na+ and Clchannels and their mode of action. Structural formulae of Tetracaine and synthesis and of Nifedipine, Diltiazem, Tetracine and 4-Aminopyridine.

OC-32: CHIRAL DRUGS

Introduction to chiral drugs. Three-point contact model, Eutomer, Distomer and eudesmic ratio. Pfeiffer's rule. Role of chirality on biological activity: Distomers – a) with no side effects b) with undesirable side effects c) both isomers having independent therapeutic value d) combination products having therapeutic advantages e) metabolic chirality inversion. Synthesis and pharmacological activity of S-Ibuprofen, S-Metaprolol, Ininavir sulfate, Levocetrazine, 2S-Verapamil, S,S-Ethambutol, (+)Lomefloxacin, Fluvastatin, Dextropropoxyphen, (+)Ephedrine, (+)Griseofulvin, Dexormaplatin, R-Indacrinone, Nateglinide, Oxybutynin hydrochloride, S,S- Captopril and S,S,S- Enalaprilate.

RECOMMENDED BOOKS:

1. Burger's medicinal chemistry and drug discovery. By Manfred B. Wolf.
2. Introduction to Medicinal chemistry. By Graham Patrick.
3. Introduction to drug design. By R.B.Silverman
4. Comprehensive medicinal chemistry. Vol 1-5 by Hanzsch.
5. Principles of medicinal chemistry. By William O. Foye etal.
6. Biochemical approach to medicinal chemistry. By Thomas Nogrady.
7. Pharmaceutical Chemistry and Drug synthesis By Roth and Kleeman
8. Drug design By E.J. Arienes
9. Principles of Medicinal Chemistry. Vols.1 & 2 By Kadam etal
10. Medicinal chemistry An introduction By Gareth Thomas
11. Wilson and Gisvold,s text book of Organic, Medicinal and Pharmaceutical chemistry By J.N. Delgado and W.A.Remers.
12. Organic Pharmaceutical chemistry By Harikishan singh.
13. Medicinal Chemistry By Ashutoshkar
14. Medicinal Chemistry By G.Chatwal
15. Organic Drug synthesis By Ledneiser Vol 1-6
16. Strategies for organic drug synthesis and design By Daniel Ledneiser
17. Top Drugs: Top synthetic routes By John Saunders
18. Chirotecchnology By Roger A. Sheldon

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PAPER III: CH (OC) 403T: ADVANCED HETEROCYCLIC CHEMISTRY

OC-33: Non aromatic heterocyclics
OC-34: Five and six membered heterocyclics with two hetero atoms
OC-35: Heterocyclics with more than two hetero atoms
OC-36: Larger ring and other heterocycles

OC-33: NONAROMATIC HETEROCYCLICS (15 Hrs)

Different types of strains, interactions and conformational aspects of nonaromatic heterocycles. Synthesis, reactivity and importance of the following ring systems. Azirines, Aziridines, Oxiranes, Thiiranes, Diazirenes, Diaziridines, Oxaziridines, Azetidines, Oxetanes and Thietanes.

OC-34: FIVE AND SIX MEMBERED HETEROCYCLICS WITH TWO HETERO ATOMS (15 Hrs)

Synthesis, reactivity, aromatic character and importance of the following heterocycles: Pyrazole, Imidazole, Oxazole, Thiazole, Isoxazole, Isothiazole, Pyridazine, Pyrimidine. Pyrazine, Oxazine, thiazine, benzimidazole, benzoxazole and benzthiazole.

OC-35: HETEROCYCLICS WITH MORE THAN TWO HETERO ATOMS (15 Hrs)

Synthesis, reactivity, aromatic character and importance of the following Heterocycles: 1,2,3-triazoies,1,2,4-triazoles, Tetrazoles, 1,2,4-oxadiazole, 1 ,3,4-oxadiazole, 1,2,5-oxadiazole, 1,2,3-thiadiazoles, 1,3,4-thiadiazoles, 1,2,5- thiadiazoles, 1,2,3-triazine, 1,2,4- triazine, 1,3,5-triazine, tetrazines. Synthesis and importance of purines and pteridines. Syntheis of Caffeine, theobromine and theophylline.

OC-36: LARGER RING AND OTHER HETEROCYCLES (15 Hrs)

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

RECOMMENDED BOOKS:

1. Heterocyclic Chemistry, T.Gilchrist
2. An introduction to the Chemistry of heterocyclic compounds, R.M.Acheson
3. Heterocyclic Chemistry, J.A.Joule & K.Mills
4. Principles of Modern Heterocyclie Chemistry, A.Paquette
5. Heterocyclic Chemistry, J,A.Joule & Smith
6. Handbook of Heterocyclic Chemistry, A.R.Katritzky.

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PAPER IV: CH (OC) 404T(CB1): ADVANCED NATURAL PRODUCTS

OC(CB1)-1: Biosynthesis of natural products
OC(CB1)-2-: Structure determination and stereochemistry of natural products by chemical methods.
OC(CB1)--3: Structure determination and stereochemistry of natural products by spectral methods.
OC(CB1)--4: Total stereo selective synthesis of natural products.

OC(CB1)-1: BIOSYNTHESIS OF NATURAL PRODUCTS (15 Hrs)

Biosynthesis of secondary metabolites: Introduction, Difference between Laboratory synthesis and biosynthesis. Methods for determination of biosynthetic mechanism. Isolation and identification of Biosynthetic precursors, Feeding experiments – use of radioisotopes Measurement of incorporation – absolute incorporation, specific incorporation. Identification of the position of labels in labeled natural products by chemical degradation and spectral methods. Major biosynthetic pathways: 1) Acetate-Malonate pathway: Biosynthesis of aromatic compounds, 2) Shikimic acid pathway ; Biosynthesis of essential amino acids – phenylalanine, tyrosine and tryptophan, carboxylic acid derivatives, flavonoids and morphine alkaloids. 3) Mevalonic acid pathway : Biosynthesis of terpenes – mono, sesqui, di, tri (β-amyrin) and carotenoids, steroids – cholesterol.

OC(CB1)-2: STRUCTURE DETERMINATION AND STEREOCHEMISTRY OF NATURAL PRODUCTS BY CHEMICAL METHODS (15 Hrs)

Determination of structure and stereochemistry of morphine, reserpine, abietic acid, cholesterol and rotenone.

OC(CB1)-3: STRUCTURE DETERMINATION AND STEREOCHEMISTRY OF NATURAL PRODUCTS BY SPECTRAL METHODS (15 Hrs)

Spectroscopic techniques IR, UV, ^{1}Hnmr, ^{13}Cnmr, COSY, HETEROCOSY, NOESY, 2D INADEQUATE and MS in the structure elucidations of natural products, Examples, flavones, biflavones, flavanones, isoflavones, coumarins, quinolines, isoquinolines.
Study of the following solved problems: Mass, IR, ^{1}H, ^{13}C NMR, HOMOCOSY, HECTOR, DEPT, 2D-INADEQUATE and NOE of Geraniol, INEPT of menthol, APT of apparicine, Heteronuclear 2D-J resolved spectrum of stricticine, NOESY of buxaquamarine, HETEROCOSY of strictanol, 2D-INADEQUATE of α-picoline and β-methyl tetrahydran furan.

OC (CB1)-4: TOTAL STEREOSELECTIVE SYNTHESIS OF NATURAL PRODUCTS (15 Hrs)

Woodward's synthesis of reserpine and cholesterol, Corey's synthesis of prostaglandins (E2, F2α) and paeoriflorin, Sharpless synthesis of L-hexoses, Nicolaous synthesis of taxol, Danishefsky synthesis of indolizomycin, Takasago synthesis of menthol, Hoffmann-LaRoche synthesis of Biotin.

RECOMMENDED BOOKS:

1. Textbook of organic chemistry, Vol II by I L Finar
2. Chemistry of natural products, Vol 12, by Atta-Ur-Rahman
3. An introduction to the chemistry of terpenoids and steroids, by William templeton
4. Systematic identification of flavonoid compounds by Mabry & Markham
5. Steroids by Fieser arid Fieser
6. Alkaloids by Manske
7. Alkaloids by Bentley
8. The chemistry of terpenes by A Pinder
9. The terpenes by Simenson
10. Terpenoids by Mayo
11. Alkaloids by Pelletier
12. Total synthesis of Natural Products by Apsimon Vol 1-5
13. Biosynthesis by Geismann
14. Principles of organic synthesis 3rd Ed.R O C Norman and J M Coxen
15. One and two dimensional nmr spectroscopy by Atta Ur Rahman
16. Classics in total synthesis K C Nicolaou and E J Sorenson
17. Spectrometric identification of organic compounds by Silverstein and Webster.

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PAPER-IV CH (OC) 404 T(CB2): BIOORGANIC CHEMISTRY

OC (CB2) -1: Enzymes and their action
OC (CB2) -2: Enzyme models and Enzymatic transformations
OC (CB2) -3: Recombinant DNA and Fermentation technology
OC (CB2) -4: Coenzymes

OC (CB2)-1: ENZYMES AND THEIR ACTION (15 Hrs)

Introduction to enzymes. Transition state theory. Acid-Base catalysis. Covalent catalysis-Binding modes of catalysis (i) Proximity effect (ii) Transition state stabilization (iii) Strain and Distortion. Examples of some typical enzyme mechanisms for (1) Triose phosphate isomerase, (ii) α-chymotrypsin and serine protease (iii) Lysozyme (iv) Carboxy peptidase-A (v) Ribonuclease.

OC (CB2)-2: ENZYME MODELS AND ENZYMATIC TRANSFORMATIONS (15 Hrs)

Introduction — Biomimetic chemical approach to biological systems-Enzyme models Advantage of enzyme models. Requirements necessary for the design of enzyme models. Host-Guest complexation chemistry. Examples of some host molecules-Crown ether cryptanes, cyclodextrins. Cyclodextrin based enzyme models-Valixarenes, ionophores, micelles and synzymes (synthetic enzymes)-chiral recognition and catalysis.Introduction to industrial enzymes. Enzymatic synthesis of α-amino acids and peptides. Transformations of lipases and esterases. Kinetic resolutions of catboxylic acids, esters and alcohols - Transesterification. Amine resolution-use of oxido-reductase. C-C bond formation using enzymes-asymmetric cyanohydrin formation and asymmetric aldol condensations.

OC (CB2) -3: RECOMBINANT DNA AND FERMENTATION TECHNOLOGY (15 Hrs)

Introduction to genetic engineering. Recombinant DNA technology-restriction endonuclease, cloning, linkers, adaptors. Application of recombinant DNA technology in production of pharmaceuticals, diagnosis of diseases, insect control, improved biological detergents, gene therapy-examples. Principles of finger printing technology- Site directed mutagenesis. Fermentation technology: Introduction to fermentation. Industrial fermentation. Advantages and limitations of fermentation. Production of drugs and drug intermediates from fermentationexamples. Chiral hydroxy acids, vitamins, amino acids, β-lactam antibiotics. Precursor fermentation and microbial oxidation and reductions.

OC (CB2) -4: COENZYMES (15 Hrs)

Introduction. Co factors — cosubstrates — prosthetic groups. Classification — Vitamin derived coenzymes and metabolite coenzymes.Structure and biological functions of coenzyme A, thiamine pyrophosphate (TPP), pyridoxal phosphate (PLP), oxidized and reduced forms of I) nicotinamide adenosine dinucleotide / their phosphates (NAD), NADH, NADP+ NADPH) ii) Flavin adenine nucleotide FAD, FADH2 and iii) Flavin mononucleotide (FMN, FMNH2) lipoic acid, biotin, tetrahydrofolate and ubiquinone. Adenosine triphosphate (ATP) and adenosine diphosphate (ADP), S-adenosyl methionine (SAM) and uridine diphospho sugars (UDP-sugars). Mechanism of reactions catalyzed by the above coenzymes.

RECOMMENDED BOOKS

1. Concepts in biotechnology by D. Balasubramananian & others
2. Principals of biochemistry by Horton & others.
3. Bioorganic chemistry-A chemical approach to enzyme action by Herman Dugas and P. Christopher.

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PAPER IV: CH (OC) 404 T(CB3): PHYSICAL- ORGANIC CHEMISTRY

OC (CB3) -1: MO and VB theory of reactivity
OC (CB3) -2: Kinetic, isotopic, structural, solvent, steric and conformational effects
OC (CB3) -3: Nucleophilic, electrophilic and free radical reactivity
OC (CB3) -4: Supramolecular chemistry

OC (CB3) -1 MOLECULAR ORBITAL (MO) AND VALENCE BOND (VB) THEORY OF REACTIVITY

Introduction to Huckel molecular orbital (MO) method as a means to explain modern theoretical methods. Advanced techniques in PMO and FMO theory. Molecular mechanics, semiemperical methods and ab inito and density functional methods. Scope and limitations of several computational programmes. Quantitative MO theory-Huckel molecular orbital (HMO) method as applied to ethane energy levels .Orbital symmetry, orbital interaction diagrams. MO of simple organic systems such as ethane, allyl, butadiene, methane and methyl group. Conjugation and hyperconjugation. Aromaticity. Valence bond (VB) configuration mixing diagrams. Relationship between VB configuration mixing and resonance theory. Reaction profiles. Potential energy diagrams. Curve crossing model nature of activation barrier in chemical reactions. Principle of reactivity Mechanistic significance of entropy, enthalpy and Gibbs free energy. Arrhenius equation, transition state theory. Uses of activation parameters, Hammonds postulate. Bell-Evans-Polanyi principle. Potential energy surface model. Marcus theory of electron transfer. Reactivity and Selectivity principles

OC (CB3) -2: KINETIC,ISOTOPIC, STRUCTURAL,SOLVENT, STERIC AND CONFORMATIONAL EFFECTS

Theory of isotope effects, Primary and secondary kinetic isotope effects. Heavy isotope effects. Tunneling effect Solvent effects. Structural effects on reactivity: Linear free energy relationship (LFER.). The Hammett equation, substituent constants, theories of substituent effects. interpretation of σ-values. Reaction constant ρ. Deviations from Hammett equation. Dual-parameter correlations, inductive substituent constant The Taft model, σ1,σR scales. Solvation and solvent effects: Qualitative understanding of solvent- solute effects on reactivity Thermodynamic measure of solvation. Effects of solvation on reaction and equilibrium. Various empirical indexes of solvation based on physical properties, solvent- sensitive reaction rates, spectroscopic properties and scales for specific solvation. Use of solvation scales in mechanistic studies. Solvent effects from the curve-crossing model. Various type of steric strain and their influence on reactivity. Steric acceleration. Molecular measurements of steric effects upon rates. Steric LFER. Conformational barrier to bond rotation-spectroscopic detection of individual conformers. Acyclic and monocyclic systems. Rotation around partial double bonds. Winstein-Holness and Curtin-Hammet principle.

OC (CB3) -3: NUCLEOPHILIC,ELECTROPHILIC AND FREE RADICAL REACTIVITY

Bases, nucleophiles, Electrophiles and Catalysts. Acid-base dissociation. Electronic and structural effects, acidity and basicity. Acidity functions and their applications. Hard and soft acids and bases. Nucleophilicity scales, Nucleofugacity. The α-effect.-Ambivalent nucleophiles. Acid-base catalysis. Specific and general catalysis. Bronstéd catalysis. .nucleophilic and electrophilic catalysis. Catalysis by non-covalent binding micellar catalysts. Nucleophilic and electrophilic Reactivity:Structural and electronic effects on SN1 and SN2 reactivity. Solvent effects,kinetic isotope effects. Intramolecular assistance. Electron transfer nature of SN^2 reaction. Nuclcophilicity and SN^2 reactivity based on curve-crossing model. Relationship between polar and electron transfer reactions. SRN^1 mechanism. Electrophilic reactivity, general mechanism. Kinetics of SE_2-Ar reaction, Structural effects on rates and selectivity. Curve crossing approach to electrophilic reactivity. Radical and pericyclic reactivity. (a)Radical stability, polar influences, solvent and steric effects. A curve crossing approach to radical addition, factors affecting barrier heights in additions, regioselectivity in radical reactions. Reactivity, specificity and periselectivity in pericyclic reactions.

OC (CB3) -4: SUPRAMOLECULAR CHEMISTRY

Properties of covalent bonds- bond length, inter-bond angles, force constant, bond and molecular dipole moments. Molecular and bond polarisability, bond dissociation enthalpy, entropy. Intermolecular forces, hydrophobic effects. Electrostatic, induction, dispersion and resonance energy, magnetic interactions, magnitude of interaction energy, forces between macroscopic bodies, medium effects, Hydrogen bond. Principles of molecular association and organization as exemplified in biological macromolecules like enzymes, nucleic acids, membranes and model systems like micelles and vesicles. Molecular receptors and design principles. Cryptands, cyclophanes, calixeranes, cyclodextxins. Supramolecular reactivity and catalysis. Molecular channels and transport processes. Molecular devices and nanotechnology.

Recommended books:

1. Molecular mechanics. By U. Bukert and N.L. Allinger, ACS Monograph 177,1982
2. Organic Chemistry book of Orbitals. L.Salem and W.L. Jorgenson
3. Mechanism and theory in Organic Chemistry, Lowry, K.C. Richardson, Harper and Row
4. Introduction to theoretical Organic Chemistry and molecular modeling by W. B. Smith,
5. VCH, Weinhein.
6. Physical Organic chemistry, N.S. Isaaçs
7. Suprarnolecular Chemistry - concepts and perspectives by J M .Lehn,
8. The Physical basis of Organic Chemistry by H.Maskill.
9. Physical Organic Chemistry by Jack Hine

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SEMESTER IV
LABORATORY COURSES

PAPER CH (OC) 451P: SPECTROSCOPIC IDENTIFICATION OF ORGANIC COMPOUNDS AND CHROMATOGRAPHY

1. Identification of unknown organic compounds by interpretation of IR, UV, ^{1}H - NMR, ^{13}C NMR and mass spectral data. A minimum of 30 representative examples should be studied.
2. Thin layer chromatography: Determination of purity of a given sample, monitoring the progress of chemical reactions, identification of unknown organic compounds by comparing the Rf values of known standards.
3. Separation by column chromatography: Separation of a mixture of *ortho* and *para*nitroanilines using silicagel as adsorbant and chloroform as the eluent. The column chromatography should be monitored by TLC.

PAPER CH (OC) 452P: SYNTHESIS AND ANALYSIS OF DRUGS

1. **Laboratory Synthesis of the following drugs:** Paracetamol, Phenytoin, Benzocaine, 6-Methyluracil, Chloritone, 4-Aminobenzene sulfonamide, FIuorescien and antipyrine.
2. **Estimation of the following drugs:** Aspirin (titrimetry), Ibuprofen (titrimetry), Analgin (titrimetry), Chloride in Ringer's lactate (argentometry), ascorbic acid {titrimetry, Iodometry and Cerimetry), colorimetry}, Isoniazid(Iodometry), Riboflavin(colorimetry),Zn ions in Bactracin Zinc, Ca^{+2} ions in Calcium gluconate injection(complexometry), Diazepam (UV-Visible Spectrophotometer).

RECOMMENDED BOOKS:

1. Practical organic chemistry by Mann & Saunders
2. Text book of practical organic chemistry by Vogel
3. The systematic identification of organic compounds by Shriner et.al
4. Analytical chemistry by G N David Krupadanam et.al
5. Advanced practical medicinal chemistry by Ashutoshkar
6. Pharmaceutical drug analysis by Ashutoshkar
7. Quantitative analysis of drugs in pharmaceutical formulations by P D Sethi
8. Practical pharmaceutical chemistry part-1 and part-2 by A H Beekett and J B Stenlake
9. Spectroscopic identification of organic compounds by R M Silverstein and F X Webster.

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