M.Sc. CHEMISTRY

SEMESTER –I
THEORY: Marks - 80M

Paper-I: CHE 401T (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: 15 hrs

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), Td, Oh, 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: 15 hrs

Crystal Field Theory: Salient features of CFT. d-orbital splitting patterns in regular Octahedral, tetragonally distorted octahedral, Jahn-Tellar theorem , trigonal bipyramidal, trigonal planar, Pentagonal bipyramidal, and linear geometries. 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. Spin crossover: High spin, low spin cross over phenomenon in [Fe(Ophen)2(NCS)2] and [Fe(R2NCS2)3]. Spinels

IC-03: Coordination Equilibria: 15 hrs

Solvation of metal ions- Metal complex formation in solution-Binary metal complexes. Stability constants (types and relationships between them). – Factors influencing the stability constants: (i) Metal ion effects (charge/size, IP, crystal field effect, John-Teller effect, Pearson theory of hard and soft acids and bases (HSAB), elecronegativity and hardness and softness, symbiosis. (ii) Ligand effects (Basicity , Substituent effect , Steric , Chelate(size and number of chelate rings), Macrocyclic and Cryptate effects- crown ethers , crypton, size match selectivity or concept of hole size, limitations, Macrocycles with pendent groups– Methods used for the determination of

Stability constants (Basic Principles only): pH metric, Spectrophotometric and Polarographic methods. 3 3 Ternary Metal Complexes – definition – Formation of ternary metal complexes – Step-wise and simultaneous equilibria with simple examples

IC – 04: Ligational Aspects of Diatomic molecules 15 hrs

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(PPh3)2(CO)(NO)]+ and [RuCl(PPh3)2(NO)2] + . Stereo chemical control of valence in [Co(diars)2(NO)]2+ and [Co(diars)2(NO)(SCN)]+ . Metal Dinitrogen complexes: - N2 as aligand – Molecular orbitals of N2; Bonding modes – Terminal and Bridging; Stretching frequencies; Structures of Ru (II) and Os(II) dinitrogen complexes; Chemical fixation of dinitrogen.

Suggested References:

1. Symmetry and Group theory in Chemistry, Mark Ladd, Marwood Publishers, London

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).

Paper-II: CHE 402 T (Organic Chemistry) 80Marks

OC-01: Stereochemistry

OC-02: Reaction mechanism-

OC-03: Conformational analysis (Acyclic systems)

OC-04: Heterocyclic compounds & Natural products

OC-01: Stereochemistry 15 hrs

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: Axially chiral allenes,spiranes,alkylidene cycloalkanes, chiral biaryls, atropisomerism, planar chiral ansa compounds and trans- cyclooctene, helically chiral compounds and their configurational nomenclature Relative and absolute configuration: Determination of configuration by chemical correlation methods. 4 4 Racemisation and resolution techniques: Racemisation, 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 15 hrs

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 E2, E1, E1CB mechanisms. Orientation and stereoselectivity in E2 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 and crossover experiments. Use of IR and NMR in the investigation of reaction mechanism.

OC-03: Conformational analysis (acyclic systems) 15 hrs

Conformational isomerism: Introduction to the concept of dynamic stereochemistry. Conformational diastereoisomers and conformational enantiomers .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. 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-4: Heterocyclic compounds &Natural products 15 hrs

Heterocyclic compounds: Introduction, Nomenclature Synthesis and reactivity of indole, quinoline, isoquinoline, carbazole and acridine Natural products: Importance of natural products as drugs. Terpenoids: General methods in the structure determination of terpenes. Isoprene rule. Structure determination and synthesis of β-carotene, α-terpeniol and camphor. Alkaloids: General methods of structure determination of alkaloids. Structure determination and synthesis of papaverine

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 UK 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

Paper CH 403 (PHYSICAL CHEMISTRY)

PC-01: Thermodynamics-I

PC-02: Electrochemistry-I

PC-03: Quantum Chemistry-I

PC-04: Chemical Kinetics-1

PC-01: Thermodynamics-I **15 hrs**

Concept of Entropy, 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. Thermodynamic relations. Gibbs equations. Maxwell relations. Gibbs equations for non-equilibrium systems. Material equilibrium. Phase equilibium. 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. Solutions: Specifiying the Solution composition. Partial molar poperties-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.

PC-02: Electrochemistry- I **15 hrs**

Electrochemical Cells: Derivation of Nernst equation – problems. Chemical and concentration cells (with and without transference). Liquid junction potential (LJP) – derivation of the expression for LJP – its determination and elimination. Types of electrodes. Applications of EMF measurements: Solubility product, potentiometric titrations, determination of pH using glass electrode, equilibrium constant measurements. Decomposition potential and its significance. Electrode polarization – its causes and elimination. Concentration over-potential. 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 **15 hr**

s A brief review of Black body radiation-Planck's concept of quantization-Planck's equation, average energy of an oscillator (derivation not required), Wave particle duality and uncertain principle-significance of these for microscopic entities. Emergence of quantum mechanics. Wave mechanics and Schrödinger wave equation. Operators- Operator algebra. Commutation of operators, linear operators. Complex functions. 2∇ and ∇Hermitian operators. Operators . 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. 2ψ and ψParticle in a box- one dimensional and three dimensional. Plots of -discussion. Degeneracy of energy levels. Calculations using wave functions of the particle in a boxorthoganality, measurability of energy, position and momentum, average values and probabilities. Application to the spectra of conjugated molecules

PC-04: Chemical Kinetics- I **15 hr**

Theories of reaction rates: Collision theory, steric factor. Transition state theory. Thermodynamic formulation of transition state theory. Potential energy surface diagram, Reaction coordinate, Activated complex. Activation 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- H2-Br2 reaction. Derivation of rate law. Effect of structure on reactivity- Linear free energy relationships. Hammett and Taft *σ and σequations-substituent ( ) and reaction constant (ρ and ρ*) 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. Reactions in solutions: Primary and secondary salt effects. The reactivity-selectivity principle – Isokinetic temperature -Isoselectivty rule, Intrinsic barrier and Hammond's postulate.

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

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. Chemical Kinetics, K.J. Laidler, McGraw Hill 7 7

8. Kinetics and Mechanism of Chemical Transformations,J. Rajaraman and J. Kuriacose,

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

Paper-IV:CHE 404 (ANALYTICAL TECHNIQUES and SPECTROSCOPY- I)

ASP 01: Techniques of Chromatography

ASP 02: NMR spectroscopy-I (1 H NMR)

ASP 03: Rotational and Vibrational spectroscopy

ASP 04: Electronic spectroscopy

ASP-01: Techniques of Chromatography 15 hrs

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) 15 hrs

^{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 1 H 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(OPEt3)4] + , [HRh(CN)5] (Rh I=1/2), [Pt(acac)2]

ASP 03: Rotational, Vibrational and Raman spectroscopy 15 hrs

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 bond lengths from rotational spectra of diatomic molecules. Isotope effect on rotational spectra. Calculation of atomic mass from rotational spectra. Brief description of microwave spectrometer. b) 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. Vibrationrotation 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 NO3 - , SO4 2- and CO3 2- ions. c) Raman Spectroscopy- Classical and Quantum theories 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 15 hrs

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, mono substituted derivative (Ph-R), di substituted derivative (R-C6H4-R) and substituted benzene derivatives (R-C6H4-COR), Woodward-Fieser rules. Polynuclear aromatic compounds (Biphenyl, stilbene, naphthalene, anthracene, phenanthrene and pyrene). Heterocyclic systems. Absorption spectra of charge transfer complexes. 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. **References:**

1. Fundamentals of Molecular Spectroscopy, Banwell and McCash.

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.

11. Organic Spectroscopy, LDS Yadav

12. Organic Spectroscopy, Y.R. Sharma

13. Molecular Spectroscopy – Arhuldas

14. Vibrational spectroscopy – D.N. Satyanarayana

SEMISTER II

Paper CHE 451 T INORGANIC CHEMISTRY 80M

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: 15 hrs

Ligand substitution reactions: Energy profile of a reaction – Transition state or Activated Complex. Types of substitution reactions (SE, SN, SN1 , SN2). Langford and Grey classification – A mechanism, DMechanism, Ia, Id, and Intimate mechanism. Ligand substitution reactions in octahedral complexes: Aquation or Acid hydrolysis reactions, Factors effecting Acid Hydrolysis , Base Hydrolysis, Conjugate Base Mechanism, Evidences in favour of SN1 CB Mechanism. Substitution reactions with out Breaking Metal-Ligand bond. Anation reaction Ligand Substitution reactions in Square-Planar complexes: Mechanism of Substitution in Square-Planar complexes- Trans-effect, Trans-influence, Grienberg's Polarization theory and II -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. Factrors affecting direct electron transfer reactions, Cross reactions and Marcus-Hush theory.

IC-06: Bonding in Metal Complexes – II: 15 hrs

Free ion terms and Energy levels: Configurations, Terms, States and Microstates – Formula for the calculation of Microstates pn and dn configurations – L-S (Russel-Saunders) coupling scheme – j-j coupling scheme – Determination of terms for various pn and dn configurations of metal ions. 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.

IC-07: Metal Clusters: 15 hrs

Carbonyl clusters: Factors favouring Metal-Metal bonding – Classification of Clusters – Low Nuclearity Clusters : M3 and M4 clusters , structural patterns in M3(CO)12 (M=Fe,Ru,Os) and

M4(CO)12 (M=Co,Rh,Ir) Clusters. Metal carbonyl scrambling – High Nuclearity clusters M5, M6, M7, M8 and M10 Clusters-, Polyhedral skeletal electron pair theory and Total Electron Count theory – Capping rule – Structural patterns in [Os6(CO)18] 2- , [Rh6(CO)16], {Os7(CO)21] , {Rh7(CO)16] 3-, [Os8(CO)22] 2-, [Os10C(CO)24] 2- and [Ni5(CO)12] 2-. 12 12 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 [Re2Cl8] 2- and Octahedral halides of [Mo6(Cl)8] 4+ and [Nb6(Cl)12] 2+. Trinuclear halides of Re(III). Hoffman's Isolobal analogy and its Structural implications. Boranes, carboranes, STYX Rule. Stereo chemical non-rigidity in [Rh4(CO)12] and [Fe2(Cp)2(CO)4].

IC-08: Bio coordination chemistry: 15 hrs

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 (Hb) and Myoglobin (Mb) primary, secondary, tertiary and quarternary structures and non-covalent bonds present in them. Oxygenation equilibria for Mb and Hb. Factor effecting oxygenation equilibria. Cooperativity and its mechanism. Spin state of iron. Spatial and electronic aspects of dioxygen binding. Allosteric models (T and R states). Role of globin. Transport of NO and CO2. Hemocynin (Hc) and Hemerythrin (Hr): Introduction-structure of active sites with oxygen and without oxygen. Comparison of Hemerythrin and Hemocyanin with hemoglobin. Photosynthesis: Structural aspects of Chlorophyll. Photo system I and Photo system II. Vitamin B6 model systems: Forms of vitamin B6 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

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

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 LowPriced Student Edition, New Delhi (1998).

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Paper-II: CHE 482 T (Organic Chemistry)

OC-05: Reaction mechanism-II

OC-06: Pericyclic reactions-I

OC-07: Photochemistry

OC-08: Reactive intermediates and molecular rearrangements

OC-05: Reaction mechanism-II **15 hrs**

Nucleophilic Aromatic substitution: Aromatic Nucleophilic substitution: SN1(Ar), SN2 (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, Cycloalky l groups, σ and π- bonds. Introduction to nonclassical carbocations. Electrophilic substitution at saturated carbon and single electron transfer reactions. Mechanism of aliphatic electrophilic sustitution. SE1, SE2, and SEi. SET mechanism.

OC-06 Pericyclic reactions **15 hrs.**

Introduction, Classification of pericyclic reactions, Electrocyclic reactions: con rotation and dis rotation. Electrocyclic closure and opening in 4n and 4n+2 systems. Cycloaddition reactions: suprafacial and antara facial additions in 4n and4n+2 cycloadditions. Sigmatropic reactions: [i, j] shifts- suprafacial and antarafacial shifts, Cope and Claisen rearrangement reactions. 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. Molecular orbitals: ethylene, 1, 3-butadiene, 1, 3, 5-hexatriene, allyl cation, allyl radical, pentadienyl cation, pentadienyl radical. Frontier Molecular Orbital (HOMO-LUMO) approach-concept: Framing WoodwardHofmann 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- for electrocylic and cycloadditions & cycloreversions.

OC-07 Photochemistry 15hrs

Photochemistry: Photochemistry of π-π* transitions: Excited states of alkenes, cis-trans isomerisation, and photo stationary state. Photochemistry of 1,3-butadiene Electrocyclisation and sigmatropic rearrangements, di-π methane rearrangement. Intermolecular reactions, photocycloadditions, photodimeriastion of simple and conjugated olefins. Addition of olefins to α, β-unsaturated carbonyl compounds. Excited states of aromatic compounds, Photoisimerisation of benzene. 14 14 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 cycloalkane diones. 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-08: Reactive intermediates and Molecular rearrangements 15 hrs

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

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

Paper CHE- 453 T PHYSICAL CHEMISTRY

PC-05: Thermodynamics-II & Statistical Thermodynamics

PC-06: Photochemistry-I

PC-07: Quantum Chemistry-II

PC-08: Solid state chemistry PC-05:

Thermodynamics-II & Statistical Thermodynamics 15 hrs

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 15 Statistical Thermodynamics: Partition Functions: Concepts of distribution and probability, Boltzmann distribution law. Interpretation of partition functions- translational, rotational, vibrational and electronic partition functions. Relationship between partition functions and thermodynamic functions (only S & G).

PC-06: Photochemistry –I 15 hrs

Electronic transitions in molecules. The Franck Condon principle. Electronically excited molecules- singlet and triplet states. Radiative life times of excited states-theoretical treatment. Measured life times. Quantum yield and its determination. Experimental set up of a photochemical reaction. Actinometry-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. Introduction to fast reactions- Principle of flash photolysis.

PC-07: Quantum chemistry-II 15 hrs

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 pots 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, H2 + ion. The variationan integral for H2 + 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 wave function and the energy of H2 molecule MO by LCAO method and Valence bond method (detailed calculations not required)-comparison of MO and VB models.

PC-08: Solid state chemistry **15 Hrs**

Electronic properties of metals, insulators and semi-conductors: Electronic structure of solids, Band theory, band structure of metals, insulators and semi-conductors. 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 – Meissner effect. Types of superconductors. Theories of super conductivity – BCS theory. 16 16 High temperature superconductors: Structure of defect perovskites. High Tc superconductivity in cuprates. Phase diagram of Y-Ba-Cu-O system. Crystal structure of YBa2Cu3O7-x. Prepartion of 1-2-3 materials. Origin of high Tc superconductivity. Nanoparticles and their applications: Introduction to nanoparticles. Reduced dimensionality in solids – zero dimensional systems, fullerenes, quantum dots. One dimensional systems, carbon nano tubes, preparation of nano particles –top down and bottom up methods. Preparation of nanomaterials- – sol gel methods, and chemical vapour deposition method; thermolysis. Characterization of nanoparticles – experimental methods – powder X-ray diffraction, transmission electron microscopy (TEM), and atomic force microscopy (AFM) (detailed theory and instrumentation are not required). Optical properties of nanoparticles, Applications of nanoparticles.

References:

1. Atkin's Physical Chemistry, Peter Atkins and Julio de Paula, Oxford University press
2. Physical Chemistry, Ira N. Levine, McGraw Hill
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
10. Fundamentals of Photochemistry, K.K.Rohtagi-Mukherji, Wiley-Eastern
11. Molecular Photochemistry, N.J. Turro, Benjamin
14. Organic Photochemistry by J.M.Coxon and B.Halton, Cambridge University press.
15. Introductory Photochemistry by A.Cox and T.J.Kemp. McGraw-Hill, London.
16. Principles of the Solid State, H. V. Keer, New Age International
17. Elements of Physical Chemistry by Peter Atkins and Julio de Paula, Oxford University
20. Statistical Thermodynamics, M. C. Gupta, New Age International
21. Quantum Chemistry, D.A. McQuarrie, Prentice Hall
22. Elementary Quantum Chemistry, F. L. Pilar, McGraw Hill.
23. Nanostructured Materials and Nanotechnology, edited by Hari Singh Nalwa, Academic
26. The physics and chemistry of solids by Stephen Elliott, Wiley Publishers.
27. Introductory Photochemistry by A.Cox and T.J.Kemp. McGraw-Hill, London.

Paper-IV: CHE- 454 (ANALYTICAL TECHNIQUES and SPECTROSCOPY - II)

GC-05: Electro and thermal analytical Techniques.

GC -06: NMR- II

GC -07: Mass Spectroscopy

GC -08: Photoelectron & ESR spectroscopy

GC -05: Electro and thermal Analytical Techniques 15 hrs

Types and Classification of Electro analytical Methods: a) D.C Polarography:. Instrumentation - Dropping mercury electrode- -polarogram. Types of Currents: Residual, Migration, Limiting. Two and Three electrode assemblies. Ilkovic equation (derivation not necessary) and its consequences. Applications of polarography in qualitative and quantitative analysis. Analysis of mixtures. Application to inorganic and organic compounds. Determination of stability constants of complexes. b) 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 c) Amperometric titrations: Principle, Instrumentation. Types and applications of amperometric titrations. Determination of SO4 2-, metal ions viz., Mg2+, Zn2+, Cu2+ and other substances. d) Cyclic Voltammetry: Principle, instrumentation, Applications. Cyclic voltammetric study of insecticide parathion. II: Thermal Analysis: Thermal techniques-Introduction, types of thermo analytical methods. Thermogravimetry principle and applications of thermogravimetry, differential thermal analysis- principle and applications of DTA. Differential scanning calorimetry. DSC: Principle, and application of DSC.

GC 06: NMR spectroscopy-II (1 H, 19F and 31P NMR) 15 hrs

1 H, 19F, 31P and solid state NMR spectroscopy: First order and non first order spectra e.g., AX, AX2, AX3, A2X3, 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 moleculesbullvalene, [η5-C5H5M], [η5-(C5H5)2 Ti η1-(C5H5)2] and [η4C8H8Ru(CO)3]. 19F NMR spectroscopy: 19F chemical shifts, coupling constants. Applications of 19F NMR involving coupling with 19F, 1 H and 31P: 1,2 dichloro-1,1 difluoro ethane, BrF5, SF4, PF5, ClF3, IF5, CF3CH2OH 31P NMR spectroscopy: 31P chemical shifts, coupling constants. Applications of 31P NMR involving coupling with 31P, 19F, 1 H and 13C: ATP, Ph3PSe, P4S3,

H3PO4, H3PO3, H3PO2, HPF2, PF6 - , PH3, [Rh (PPh3)Cl3] (Rh I=1/2) Introduction to solid state NMR: Magic angle spinning (MAS).Applications of solid state NMR.

GC 07: Mass spectrometry 15 hrs

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 18 18 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.

GC 08: Photoelectron & ESR sprectroscopy 15 hrs

Photoelectron Spectroscopy Principle and Instrumentation, Types of Photoelectron Spectroscopy – UPS & XPS. Binding Energies, Koopman's Theorem, Chemical Shifts. Photoelectron Spectra of Simple Molecules: N2, O2, F2 - 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 and 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

M.Sc. ORGANIC CHEMISTRY SPECIALISATION

III SEMESTER SYLLABUS
(For the batch admitted during the academic year 2018-2019)

M.Sc. CHEMISTRY (ORGANIC CHEMISTRY)
III SEMESTER SYLLABUS
(For the batch admitted during the academic year 2018 -2019 under the CBCS pattern)

Paper-1-CHE (OC) 501T: Synthetic Reagents, Advanced NMR, Conformational Analysis and ORD

OC-09: Synthetic Reagents-I
OC-10: Synthetic Reagents-II
OC-11: ^{13}C NMR spectroscopy and 2D NMR techniques
OC-12: Conformational analysis (Cyclic systems) & ORD

OC-09: Synthetic Reagents I **15 Hrs**

1. **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 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) Organometallic Reagents:** Preparation and application of the following in organic synthesis: 1) Organo lithium 2) Organo copper reagents 3) Organo boranes in C-C bond formation 4) Organo silicon reagents: reactions involving β-carbocations and α-carbanions, utility of trimethyl silyl halides, cyanides and triflates. **iii) Carbonyl methylenation:** a) Phosphorous ylide mediated olefination 1) Witting reaction, 2) Horner-Wordsworth-Emmons reaction. b) Titanium- Carbene mediated olefination 1) Tebbe reagent,2)Petasisreagent3)Nystedreagent. **iv) Carbene insertions:** Rh based carbene complexes, cycloprpanations. **v) C-H Activation:** Introduction, Rh catalysed C-H activation.

OC-10:SyntheticReagentsII **15 Hrs**

ii) Oxidations: a) Oxidation of active C-H functions: DDQ and SeO_2. b) Alkenes to diols: Prevost and Woodward oxidation c) Alcohol to carbonyls: Cr^{VI} oxidants (Jones reagent, PCC, PDC) IBX, DMP, CAN, TEMPO, TPAP, Swern oxidation d) 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) Use of tri-n-butyl tin hydride: Radical reductions.

OC-11: ^{13}C NMR spectroscopy and 2D NMR techniques **15 Hrs**

i) ^{13}C NMR spectroscopy: Introduction**,** Types of ^{13}C nmr spectra: undecoupled, proton-decoupled and off-resonance 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, ^{2}H 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.

ii) 2D-NMR techniques: Principles of 2D NMR, Classification of 2D-experiments. Correlation spectroscopy (COSY) HOMO COSY (^{1}H-^{1}H COSY) , TOCSY (Total Correlation Spectroscopy), Hetero COSY (^{1}H,^{13}C COSY,HMQC), long range ^{1}H,^{13}C COSY (HMBC), Homonuclear and Heteronuclear 2D-J-resolved spectro-scopy, NOESY and 2D-INADEQUATE experiments and their applications. **OC-12:**

Conformational analysis (Cyclic systems) & ORD **15 Hrs** Study of conformations of cyclohexane, mono, di and tri substituted cyclohexanes, (1,3,5-trimethyl cyclo -hexanes and Menthols), cyclohexanone (2-alkyl and 3 -alkyl ketone effect), 2-halocyclohexanones, cyclo- heptane . Stereo chemistry of bicyclo [3,3,0] octanes, hydrindanes, decalins and perhydroanthracenes. Confor-mational structures of piperidine, N-Methylpiperidine, tropane, tropine, pseudotropine, decahydroquinoline and quinolizidine. Factors governing the reactivity of axial and equatorial substituents in cyclohexanes. (Oxidation, S_N2 reaction, rearrangements, Ester hydrolysis) Stereochemistry of addition to the carbonyl group of a rigid cyclohexanone ring.

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

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. Organic chemistry by Jonathan Clayden, Nick Greeves and Stuart Warren
9. Organic Reactions and their mechanisms by P.S.Kalsi
10. Organic reaction mechanisms by V.K.Ahulwalia and Rakesh Kumar Parashar
11. Spectroscopic identification of organic compounds by RM Silverstein, G C Bassler
12. Organic Spectroscopy by William Kemp
13. Spectroscopic methods in Organic chemistry by DH Williams and I Fleming
14. Modern NMR techniques for chemistry research by Andrew B Derome
15. NMR in chemistry - A multinuclear introduction by William Kemp
16. Spectroscopic identification of organic compounds by P S Kalsi
17. Introduction to organic spectroscopy by Pavia
18. Carbon-13 NMR for organic chemists by GC Levy and O L Nelson
19. Nuclear Magnetic Resonance Basic principles by Atta-ur-Rahman
20. Basic one and two-dimensional NMR spectroscopy by Horst Friebolin
21. NMR spectroscopy by H.Gunther

Paper II– CHE (OC) 502T: Modern Organic Synthesis

OC-13: Asymmetric synthesis
OC-14: Synthetic strategies
OC-15- New Synthetic reactions
OC-16: New techniques and concepts in organic synthesis

OC- l3:- Asymmetric synthesis 15 Hrs

Introduction: Brief revision of classification of stereo selective reactions

Prostereoisomerism: Topicity in molecules Homotopic, stereoheterotopic (enantiotopic and diastereotopic) groups and faces- symmetry criteria.

Prochiral nomenclature: Pro chiraility and Pro-R, Pro-S, Re and Si.

Conditions for stereoselectivity: Symmetry and transition state criteria, kinetic and thermodynamic control. Methods of inducing enantioselectivityy.

Analytical methods: % Enantiomeric excess and diastereomeric excess. Determination of enantiomeric excess: specific rotation, Chiral NMR; Chiral derivatizing agents, Chiral solvent, Chiral shift reagents and Chiral HPLC.

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

Chiral auxiliary controlled asymmetric synthesis: α-Alkylation of chiral enolates, Evan's oxazolidinone, 1, 4-Asymmetric induction and Prelog's rule..

Chiral reagent controlled asymmetric synthesis: Asymmetric reductions using BINAL-H. Asymmetric hydroboration using IPC_2 BH and $IPCBH_2$.

Chiral catalyst controlled asymmetric synthesis: Sharpless epoxidation. Asymmetric hydrogenations using chiral Wilkinson biphosphin catalyst.

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

OC-14: Synthetic Strategies 15 Hrs

Introduction: Terminology, Target, synthon, synthetic equivalent, functional group interconversion (FGI), functional group addition. Criteria for selection of target. Linear and convergent synthesis. Retrosynthetic analysis and synthesis involving chemoselectivity, regioselectivity, reversal of polarity and cyclizations. .

Order of events : S-Salbutamol, Propoxycaine..

One group C-C and C-X disconnections: Introduction .One group C-C disconnections in alcohols and carbonyl compounds. One group C-X disconnections in Carbonyl compounds, alcohols, ethers and sulphides.

Two group C-C and C-X disconnections : Introduction .Two group C-X disconnections in 1,1-difunc-tionalised, 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: oxanamide and mevalonic acid.

Strategic bond: definition, 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. Retrosynthesis of Retronecene, longifoline.

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, Bergman and Mannich reactions.

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

5. Click Chemistry: Click reaction, 1,3-dipolar 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: Phospho triester, phosphite triester and phosphoramidite pathway

3. Oligosaccharide synthesis: Glycosidation**:** 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, polymerization-cyclisation, 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 method.

Recommended Books:

1. Asymmetric synthesis by Nogradi
2. Asymmetric organic reactions by J D Morrison and H S Moschcr
3. Principles in Asymmetric synthesis by Robert E. Gawley & Jeffrey aube
4. Stereo differentiating reactions by Izumi
5. Some modern methods of organic synthesis by W Carruthers
6. Guidebook to organic synthesis, by R K Meckie, D M Smith & R A Atken
7. Organic synthesis by Michael B Smith
8. Organic Synthesis-The disconnection approach by S Warren
9. Organic Synthesis by C Willis and M Willis
10. Problems on organic synthesis by Stuart Warren
11. Organic chemistry Jonathan Clayden, Nick Greeves and Stuart Warren
12.The logic of chemical synthesis by Elias James Corey and Xue-Min Cheng

Elective-3A
Paper-III CHE (OC)503T (CB1): Bioorganic Chemistry
OC(CB1)-17: Carbohydrates
OC(CB1)-18: Nucleic acids and Lipids
OC(CB1)-19: Proteins and Enzymes
OC(CB1)-20: Coenzymes and Vitamins

OC(CB1)-17: Carbohydrates 15 Hrs

Introduction to the importance of Carbohydrates. Types of naturally occuring sugars. Deoxy sugars, aminosugars, branched chain sugars methyl ethers and acid derivatives of sugars. Determination of configuration and determination of ring size of D-glucose and D-Fructose. Conformational analysis of monosaccharides. $^4C_1$ and $^1C_4$ conformations of D-glucose. Reactions of six carbon sugars: Ferrier, Hanesian reaction and Ferrier rearrangement. Synthesis of amino, halo and thio sugars. Structure, ring size determination of sucrose and maltose. Conformational structures of sucrose, lactose, maltose, cellobiose and gentobiose. Structure and biological functions of starch, cellulose, glycogen and chitin. Role of sugars in cell to cell recognition, blood groups.

OC(CB1)-18: Nucleic acids & lipids 15 Hrs

Nucleic acids: Retro synthetic analysis of nucleic acids - Nucleotides, Nucleosides, Nucleotide bases and Sugars. Structure and synthesis of nucleosides and nucleotides. Primary, secondary and tertiary structure of DNA. Types of mRNA, tRNA and rRNA. Replication, transcription and translation. Genetic code. Protein biosynthesis. DNA finger printing.

Lipids: Introduction and classification of lipids. Stereochemical notation in lipids. Chemical synthesis and biosynthesis of phospholipids and glycolipids. Properties of lipid aggregates, micelles, bilayers, liposomes and biological membranes.

OC(CB1)-19: Proteins and Enzymes 15 Hrs

Proteins: Introduction. Peptide bond, classification and nomenclatue of peptides. Amino acid sequence of polypeptides and proteins: terminal residue analysis and partial hydrolysis. Peptide synthesis by solution phase and solid phase synthesis methods. Proteins - Biological importance and classification - Primary, secondary and tertiary structure of proteins. **Enzymes:** Definition. Classification based on mode of action. Mechanism of enzyme catalysis - Lock and Key, Induced- Fit and three point contact models. Enzyme selectivity –chemo, regio, diastereo and enantio selectivity – illustration with suitable examples. Factors affecting enzyme catalysis. Enzyme inhibition - reversible and irreversible inhibition. Enzymes in organic synthesis. Immobilised enzymes

OC(CB1)-20: Coenzymes and Vitamins 15Hrs

Coenzymes: 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, $FADH_2$ and iii) Flavin mononucleotide (FMN, $FMNH_2$) 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.

Vitamins: Introduction, classification and biological importance of vitamins. Structure determination and synthesis of vitamins A, B_1, and B_2. Synthesis of vitamins - B_6, C, E and K. Structure of vitamin B_{12}.

Reference Books:

1. Organic Chemistry Vol.I and Vol.II by I.L.Finar
2. Carbohydrate Chemistry by Barton Volumes
3. Carbohydrate chemistry by G.J.Boons
4. The chemistry of natural products:vol.V - carbohydrates by S.F.Dyke
5. Organic Chemistry by McMurry
6. Nucleic acids in Chemistry and Biology by G M Blackbum MI Gait
7. Lehninger Principles of Biochemistry by D L Nelson and M M Coxon
8. Outlines of Biochemistry by Conn and Stumpf
9. Enzyme structure and mechanism by Fersht and Freeman
10. Enzymes for green organic synthesis by V.K.Ahluwalia
11. Biotransformations in Organic Chemistry by K Faber.
12. Principles of biochemistry by Horton & others.
13. Bioorganic chemistry - A chemical approach to enzyme action by Herman Dugas and Christopher Penney.
14. Concepts in Biotechnology by D.Balasubramanian & others
15. Chemistry and physiology of the vitamins by H.R.Rosenberg.

Elective-4A

Paper-IV CHE (OC) 504T (CB3): Green chemistry and Organic materials

OC (CB3) - 21: Principles of Green chemistry
OC (CB3) -22: Green Synthesis
OC (CB3) -23: Organic nanomaterials
OC (CB3) -24: Supramolecular chemistry

OC (CB3) -21: Principles of Green Chemistry 15 Hrs

Green chemistry: Introduction

Principles of Green Chemistry: Designing a Green Synthesis using these principles; Prevention of Waste/by-products; maximum incorporation of the starting materials used in the synthesis into the final products (Atom Economy); prevention/minimization of hazardous/toxic products; designing safer chemicals ; selection of appropriate auxiliary substances - green solvents, ionic liquids and solvent-free synthesis: energy requirements for reactions -use of microwaves, ultrasonic energy in organic synthesis; prevention of unnecessary derivatization – careful use of protecting groups; use of catalytic reagents in preference to stoichiometric reagents; designing of biodegradable products; prevention of chemical accidents; strengthening/development of analytical techniques to prevent and minimize the generation of hazardous substances in chemical processes.

OC (CB3) -22: Green Synthesis 15Hrs

i) Microwave Assisted Organic Synthesis (MAOS): introduction, benefits and limitations

a) Microwave assisted reactions in organic solvents: Esterification, Fries rearrangement, Claisen rearrangement and Diels- Alder reaction.

b)Microwave assisted Solvent-free reactions: Deacetylation, saponification of esters, alkylation of reactive methylene compounds and synthesis of nitriles from aldehydes.

ii)Ultrasound Assisted Organic Synthesis: introduction, applications of ultrasound-Cannizaro reaction, Reformatsky reaction and Strecker synthesis.

iii)Organic Synthesis in Green Solvents: introduction

a) Aqueous Phase Reactions: Diels-Alder Reaction, Heck reaction, Hoffmann elimination, Claisen-Schmidt condensation hydrolysis and diydroxylation reactions.

b)Organic Synthesis using Ionic liquids: Introduction, applications-Beckmann rearrangement Suzuki Cross-Coupling Reaction and Diels- Alder reaction.

iv) Green Catalysts in organic synthesis: introduction

a) Phase Transfer Catalysts in Organic Synthesis: Introduction, Williamson ether synthesis and Wittig reaction.

b) Biocatalysts in Organic Synthesis: Biochemical (microbial) oxidations and reductions.

OC (CB3) -23: Organic Nanomaterials 15Hrs

Introduction: The 'top-down' approach, the 'bottom-up' approach and Nanomanipulation.

Molecular Devices: Photochemical devices, Liquid crystals, Molecular wires, Rectifiers, Molecular switches and Molecular Muscles.

New Carbon family: Types of Fullerenes, Types of Carbon nanotubes (Zig-Zag, Armchair and Chiral), Graphenes. Growth, Chemical Synthesis and optoelectronic properties of Fullerenes, CNTs (Zig Zag, Armchair and Chiral), singlewalled CNTs (SWCNTs) and multi walled MWCNTs)and Graphenes.

Structures of aromatics belts, nano car and molecular machines.

Optoelectronic molecules: OLEDs, Organic Solar Cells (Basic OLED mechanism and structures)

Natural Benz heterazoles and their synthetic modifications as optoelectronic molecules.

OC (CB3) -24: Supramolecular Chemistry 15Hrs

I**ntroduction**: Supramolecular interactions (ion-ion, ion-dipole, H-bonding, cation-π, anion-π, π-π and Van der Walls interactions),Ionophore and molecular receptors.

Host-Guest Chemistry: Lock and key anology, Structures and applications of Cryptands,Spherands, Calixerenes, Cyclodextrins, Cyclophanes, Carcerands and hemicarcirands.

Self-assembly: Ladder, polygons, helices, rotaxanes, catanenes, Molecular necklace, dendrimers, self-assembly capsules their synthesis, properties and applications.

Enantioselective molecular recognition: Cyclodextrins, Crown ethers with chiral frame work, Chiral receptor from Kemp's triacid. Chiral receptors for tartaric acid.

Recommended books:

1. P.T. Anastes & J.K. Warmer: Oxford Green Chemistry- Theory and Practical, University Press (1998).
2. A.S. Matlack: Introduction to Green Chemistry, Marcel Deckkar, (2001).
3. M.C. Cann & M.E. Connely: Real-World cases in Green Chemistry, A. C. S., Washington (2000).
4. M.A. Ryan & M. Tinnesand, Introduction to Green Chemistry, A. C. S., Washington
5. V.K. Ahluwalia & M.R. Kidwai: New Trends in Green Chemistry, Anamalaya Publishers
6. Enantioselective organocatalysis, Peter I Dallco, Willey-VCH
7. Core Concepts in Supramolecular Chemistry and Nanochemistry by Jonathan W. Steed, David R. Turner and Karl J. Wallace; John-Wiley and Sons Publications
9. Supramolecular Chemistry by Jonathan W. Steed and Jerry L. Atwood, John-Wiley and Sons Publications
10. Supramolecular Chemistry-Concepts and Perspectives by J M. Lehn; Wiley-VCH (1995) Publications
11. Supramolecular Chemistry by P. D. Beer, P. A. Gale and D. K. Smith; Oxford University Press (1999)
12. Stereochemistry of organic compounds - Principles & Applications by D Nasipuri
13. Nanochemistry by G.B. Sergeev; Elsevier
14. Nanochemistry: A chemical approach to nano materials , G.A. Ozin & A.C. Arsenault; RSC publishers

M.Sc. CHEMISTRY (ORGANIC CHEMISTRY)
IV SEMESTER SYLLABUS
(For the batch admitted during the academic year 2018 -2019 under the CBCS pattern)

Paper-1 CHE (OC) 551T: 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 and computer aided drug design
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: QSAR studies and computer aided drug design 15Hrs

QSAR: 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 Lipophilicity Substituent constants. Lipinski rule of five. Hansch analysis, Craig's plot,Topliss scheme, Free Wilson approach, cluster significant analysis. Three case studies (QSAR study on pyranenamine, design of Oxaminquine and Crizotinib).

Computer aided drug design: Introduction, active site, allosteric binding site, use of grids in docking program - Autodock, Dock-X; rigid docking of flexible ligands. Basic principles and

difference between structure and ligand based drug design, denovo drug design and utility to optimize the lead structure.

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 deconvolution-recursive 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.

Paper-II CHE (OC) 552T: 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 15 Hrs

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:
b) 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 15 Hrs

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 ofloxacin 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 agent-structural formula of Cyclosporin. Immunoenhancers-use of vaccines and strucrural formula of levamisol.

OC-31: Drugs acting on receptors and ion channel 15 Hrs

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 Ca^{2+}, Na^{+} and Cl^{-} channels and their mode of action. Structural formulae of Tetracaine and synthesis and of Nifedipine, Diltiazem, Tetracine and 4-Aminopyridine.

OC-32: Chiral drugs **15 Hrs**

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

Elective-3A
Paper-III CHE (OC)-553T (CB1): Advanced Heterocyclic Chemistry

OC (CB1) 33: Non aromatic heterocyclics & aromaticity
OC (CB1) 34: Five and six membered heterocyclics with two hetero atoms
OC (CB1) 35: Heterocyclics with more than two hetero atoms
OC (CB1) 36: Larger ring and other heterocycles

OC (CB1) 33: Nonaromatic heterocyclics & Aromaticity 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 andthietanes
Aromaticity: Introduction, 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 (CB1) 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 (CB1) 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 (CB1) 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
7. The aromaticity III level, units 17-19 British open university volumes
8. Aromatic character and aromaticity by G.M.Badger
9. Non-benzenoid aromatic compounds by D.Ginsberg
10. Nonbenzenoid compounds by Lloy

Elective-4A

Paper-IV CHE (OC) 554(CB3)T: Advanced Natural Products

Elective-4A Paper-IV CHE (OC) 554(CB3)T: Advanced Natural Products

OC(CB3)-37: Biosynthesis of natural products
OC(CB3)-38: Structure determination of natural products by chemical methods.
OC(CB3)-39: Structure determination and stereochemistry of natural products by spectral methods.
OC(CB3)-40: Total stereo selective synthesis of natural products.

OC(CB3)-37: 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(CB3)-38: Structure determination of natural products by chemical methods 15Hrs
Determination of structure and stereochemistry of morphine, reserpine, abietic acid, cholesterol and rotenone.

OC(CB3)-39: 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 **appericine**, Heteronuclear 2D-J resolved spectrum of **stricticine**, NOESY of **buxaquamarine**, HETEROCOSY of **strictanol**, 2D-INADEQUATE of **α-picoline** and **β-methyl tetrahydran furan**.
OC(CB3)-40: Total stereoselective synthesis of natural products. 15 Hrs
Nicalou's synthesis of Dynemicin A , 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 Spectrometric identification of organic compounds by Silverstein and Webster
3. Classics in total synthesis K C Nicolaou and E J Sorenson
4. Terpenoids by Mayo
5. Alkaloids by Pelletier
6. Total synthesis of Natural Products by Apsimon Vol 1-5
7. Principles of organic synthesis 3rd Ed.R O C Norman and J M Coxen
8. One and two dimensional nmr spectroscopy by Atta Ur Rahman