**DEPARTMENT OF CHEMISTRY**
**OSMANIA UNIVERSITY**
**(Effective from academic year 2023-2024 for Campus, Constituent and Affiliated colleges)**

## Semester I

| | Hrs. /week | internal assessment | Semester exam | Total | Credits |
|---|---|---|---|---|---|
| CH101T (*) | 3 | 30 marks | 70 marks | 100 marks | 3 |
| CH102T (*) | 3 | 30 marks | 70 marks | 100 marks | 3 |
| CH103T (*) | 3 | 30 marks | 70 marks | 100 marks | 3 |
| CH104T (*) | 3 | 30 marks | 70 marks | 100 marks | 3 |
| CH151P (IC LAB*) | 4 | | | 50 marks | 2 |
| CH152P (OC LAB*) | 4 | | | 50 marks | 2 |
| CH153P (PC LAB*) | 4 | | | 50 marks | 2 |
| CH154P (AC LAB*) | 4 | | | 50 marks | 2 |
| **Total** | | | | **600 marks** | **20** |

## Semester II

| | Hrs. /week | internal assessment | Semester exam | Total | Credits |
|---|---|---|---|---|---|
| CH201T (*) | 3 | 30 marks | 70 marks | 100 marks | 3 |
| CH202T (*) | 3 | 30 marks | 70 marks | 100 marks | 3 |
| CH203T (*) | 3 | 30 marks | 70 marks | 100 marks | 3 |
| CH204T (*) | 3 | 30 marks | 70 marks | 100 marks | 3 |
| CH251P (IC LAB*) | 4 | | | 50 marks | 2 |
| CH252P (OC LAB*) | 4 | | | 50 marks | 2 |
| CH253P (PC LAB*) | 4 | | | 50 marks | 2 |
| CH254P (ACS LAB*) | 4 | | | 50 marks | 2 |
| **Total** | | | | **600 marks** | **20** |

## M.Sc. CHEMISTRY SYLLABUS

**(Effective from academic year 2023-2024 for Campus, Constituent and Affiliated colleges)**

## SEMESTER –I

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

**Paper 1: CH 101 (Inorganic Chemistry)**

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

**IC-01: Symmetry of Molecules:** **15 hrs**

Symmetry Operations and 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. Molecular Point Groups: Definition and notation of point groups. Classification of molecules based on molecular point groups. Systematic assignment of point groups to molecules (flow chart). Exercises in molecular point groups: $C_1$, $C_s$, $C_i$, $C_n$, $C_{nv}$, $C_{nh}$, $C_{\infty v}$, $D_n$, $D_{nh}$, $D_{nd}$, $D_{\infty h}$, $S_n$ (n=even), $T_d$ ($CH_4$, $SiH_4$), $O_h$ ($SF_6$), $I_h$ $B_{12}H_{12}^{2-}$), $K_h$. Descent and ascent in symmetry with substitution (eg.$NH_3$, $CH_4$, $PCl_5$, $ML_6$). Symmetry restrictions on 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, tetrahedral, square planar, tetragonally distorted octahedral, Jahn-Tellar theorem, trigonal bipyramidal, trigonal planar, pentagonal bipyramidal, and linear geometries. Factors influencing magnitude of $\Delta_o$. Concept of weak field and strong fields. Calculation of crystal field stabilization energies (CFSE's) in six and four coordinate complexes. Applications of CFSE-normal and inverse spinels.

**Magnetic properties of transition metal complexes:** Types of magnetic behavior. 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.

**IC-03: Coordination Equilibria:** **15 hrs**

Solvation of metal ions. Metal complex formation in solution. Binary metal complexes. Stability constants: Types (concentration, Thermodynamic and Conditional), stepwise and overall stability constants and relationships between them. Factors influencing the stability constants - (i) Metal ion effects: charge, size, charge/size IP, crystal field effect (Irving-William's order of stability), Jahn-

Teller effect. (ii) Ligand effects: Basicity, substituent effect, steric, chelate (size and number of chelate rings), macrocyclic and cryptate effects (crown ethers, cryptands, size match selectivity or concept of hole size and its limitations), macrocycles with pendent groups. Pearson's theory of hard and soft acids and bases (HSAB): Principle and applications. Methods used for the determination of stability constants: pH metric, spectrophotometric and polarographic methods. Ternary metal complexes: Definition, formation of ternary metal complexes, step-wise and simultaneous equilibria with simple examples.

**References**


1. Chemical applications of group theory, F Albert Cotton, 3rd Edition, Wiley India (2009).
2. Symmetry and Spectroscopy of Molecules, K.Veera Reddy, New Age Int. (P) Ltd. (2002)
3. Symmetry in chemistry, Hans H Jaffe, Milton Archin, Dover publications Inc (2002)
4. Molecular symmetry and group theory, Allen Vincent, 2nd Edition, John Wiley & sons Ltd. (2010)
5. Advanced Inorganic Chemistry, F.A.Cotton & G.Wilkinson, 3rd Edition, Wiley Interscience Publications (1972).
6. Advanced Inorganic Chemistry. F.A.Cotton, G.Wilkinson, C.A.Murillo & M.Bochmann, 6th Edition, Wiley Interscience Publications N.Y (1999).
7. Inorganic Chemistry, J.E. Huheey, K.A.Keiter and R.L.Keiter, 4th Edition, Harper Cottens College Publications (1993).
8. Inorganic Chemistry, Keith F.Purcell and John C.Kotz, Holt-Saunders Int. Edn.London (1977).
9. Principles of Inorganic Chemistry, Puri, Sharma, Kalia, 33rd Edition, Vishal Publications (2022).
10. Metal complexes in Aqueous Solutions, A.E Martell and Robert Hancock, Springer Science (1996)






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**Paper-II: CH 102 (Organic Chemistry)**

OC-01: Stereochemistry

OC-02: Reaction mechanism-1

OC-03: Conformational analysis (Acyclic systems)

**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, buttressing effect, planar chiral ansa compounds and trans-cycloalkenes(upto cyclodecene and their methyl analogues), helically chiral compounds and their configurational nomenclature

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

**Racemisation and resolution techniques**: Racemisation; mechanism Via carbocation, carbanion and free radical. Resolution by direct crystallization, diastereoisomer salt formation chiral chromatography and asymmetrictransformation.

**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**

**Determination of reaction mechanism**: Introduction: product isolation, isolation, detection and trapping of intermediates, addition of suspected intermediate-von Richter rearrangement. Use of isotopes, isotope effects, and crossover experimentds. Use of IR and NMR in the investigation of reaction mechanism

**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 : $OsO_4$ 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.

**Nucleophilic Aromatic substitution:** Aromatic Nucleophilic substitution: $S_N1(Ar)$, $S_N2$ (Ar),and benzyne mechanisms and evidence.

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

**Conformational isomerism**: Introduction to the concept of dynamic stereochemistry. Conformational diastereoisomers and conformational enantiomers. Conformational nomenclature: Conventional method, limitations, Klyne-Prelog terminology. Study of conformations in, dihaloethanes, halohydrin, ethylene glycol, 2,3-dihalobutanes, butane-2, 3-diol, amino alcohols





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and 1,1,2,2-tetrahalobutanes.

**Conformations of unsaturated acyclic compounds**: Propylene, Acetaldehyde and Butanone

**Physical methods for conformational Analysis:** Use of dipole moment, UV, IR and NMR, spectral methods in conformationalanalysis.

**Conformational affects on the stability and reactivity of acyclic diastereoisomers**: Steric and stereoelectronic factors-examples. Conformation and reactivity (E2 eliminations, NGP, Stereochemistry-Rearrangements). The Curtin – Hammett principle.

**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. Advanced Organic Chemistry by Jerry March
4. Mechanism and Structure in Organic Chemistry S. Mukerjee
5. Organic chemistry by Jonathan Clayden, Nick Greeves and Stuart Warren
6. Organic Reactions and their mechanisms by P.S.Kalsi
7. Stereochemistry: Conformation & Mechanism by P S Kalsi






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**Paper-III: CH 103 (Physical Chemistry)**

PC-01: Thermodynamics

PC-02: Electrochemistry

PC-03: Quantum Chemistry-I

**PC-01: Thermodynamics** **(15 hrs)**

**Third law of thermodynamics**. Evaluation of absolute entropies from heat capacity data for solids, liquids and gases. Standard entropies.

Gibbs equations for non-equilibrium systems. Material equilibrium. Phase equilibium. Clausius-Clapeyron equation. Conditions for equilibrium in a closed system. The chemical potential. Chemical potential of ideal gases. Ideal-gas reaction equilibrium-derivation of equilibrium constant. Temperature dependence of equilibrium constant-the van't Hoff equation.

**Solutions:** Partial molar properties-significance. 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 coefficient. Determination of fugacity. Non ideal solutions. Activities and activity coefficients. Standard-state conventions for non-ideal solutions.

**Multicomponent phase equilibrium**: Vapour pressure lowering, freezing point depression and boiling point elevation

**PC-02: Electrochemistry** **(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-Gas electrodes, Metal-metal ion electrodes, reference electrodes, indicator electrode, Ion selective electrodes, Metal-insoluble salt-anion electrodes, Redox 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's law. Theory of electrolytic conductance. Derivation of Debye-Huckel-Onsager equation – its validity and limitations.

**PC-03: Quantum Chemistry- I** **(15 hrs)**

**Wave mechanics and Schrödinger wave equation**: Operators- Operator algebra. Commutation of operators, linear operators. Complex functions. Hermitian operators. Operators $\nabla$ and $\nabla^2$. Eigenfunctions and eigenvalues. Degeneracy. Linear combination of eigenfunctions of an operator. Well behaved functions. Normalized and orthogonal functions.

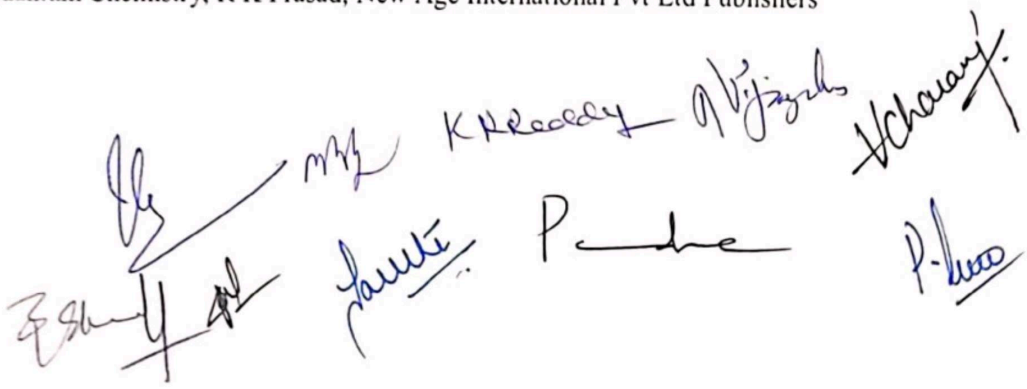
**Postulates of quantum mechanics**: Physical interpretation of wave function. Observables and Operators. Measurability of operators. Average values of observables. The time dependent Schrodinger equation. Separation of variables and the time-independent Schrodinger equation.

**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.

**Particle in a box- one dimensional and three dimensional:** Plots of $\psi$ and $\psi^2$ -discussion. Degeneracy of energy levels. 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.

**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. Introduction to Electrochemistry, S. Glasstone; East-West Press (Pvt.) Ltd.
6. Modern Electrochemistry, J. O. M. Bockris & A. K. N. Reddy, Plenum
7. Principles of physical chemistry, Samuel H. Maron and Carl F. Prutton, Oxford & IBH
8. Physical Organic Chemistry, N. S. Isaacs, ELBS
09. Elementary Quantum Chemistry, F. L. Pilar, McGraw Hill.
10. Quantum Chemistry – D.A. McQuarrie, Viva Publication
11. Quantum Chemistry, Ira N. Levine, Prentice Hall
12. Introduction to Quantum Chemistry, A.K. Chandra, Tata McGraw Hill
13. Quantum Chemistry, R K Prasad, New Age International Pvt Ltd Publishers

**Paper-IV: CH 104 (Analytical Techniques and Spectroscopy – I)**

ASP 01: Techniques of Chromatography & Electronic spectroscopy

ASP 02: NMR spectroscopy-I

ASP 03: Vibrational spectroscopy

**ASP-01: Techniques of Chromatography and UV Visible Spectroscopy** **15 hrs**

**Techniques of Chromatography:** 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.

**GC**: Principle, instrumentation, detectors - TCD, FID, ECD. Derivatization techniques. Programmed temperature gas chromatography. GC analysis of hydrocarbons in a mixture.

**HPLC**: Principle, instrumentation, detectors- UV detectors, Photodiode array detector, fluorescence detector. HPLC analysis of paracetamol tablets.

**UV Visible Spectroscopy:** Principle, selection rules, Woodward-Fieser rules. Congugated dienes, trienes and polyenes, Unsaturated carbonyl compounds, Benzene, mono substituted derivative (Ph-R), di-substituted derivative (R-$C_6H_4$-R′) and substituted benzene derivatives (R-$C_6H_4$-COR′).

**ASP 02: NMR spectroscopy-I** **15 hrs**

**$^1$H NMR spectroscopy:** Magnetic properties of nuclei, principles of NMR spectroscopy. Instrumentation: CW and pulsed FT instrumentation. Equivalent and non-equivalent protons. Homotopic, 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, factors affecting coupling constants. Chemically and magnetically equivalent protons.

**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, $[HNi(OPEt_3)_4]^+$, $[HRh(CN)_5]$ (Rh I= ½).

**ASP 03: Vibrational Spectroscopy** **15 hrs**

**Interaction of electromagnetic radiation with matter.** Factors affecting width and intensity of spectral lines.

**IR Spectroscopy**: Vibrational energy levels of diatomic molecules, selection rules (derivation not required). Calculation of force constant from vibrational frequency. Anharmonic oscillator. Morse potential energy diagram. Fundamental bands, overtones and hot bands, Fermi Resonance.

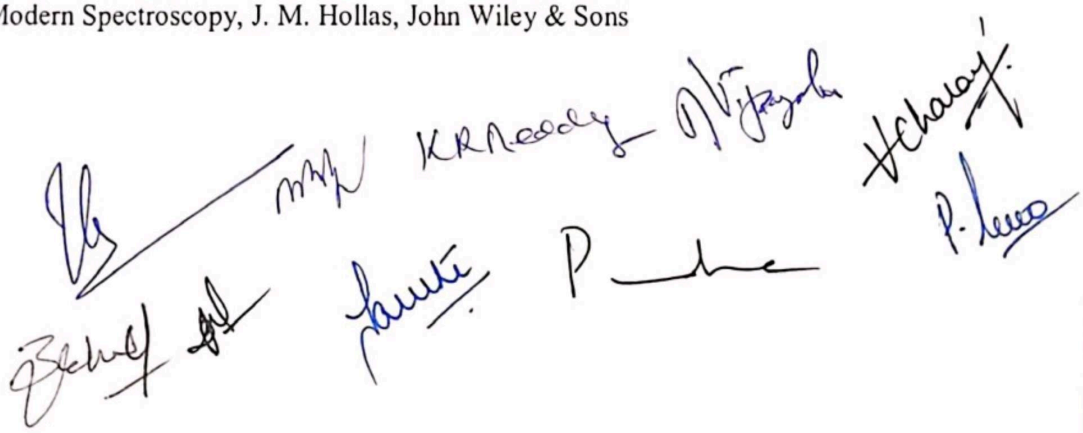
**Vibration rotation spectra of diatomic and poly atomic molecules:** Vibration – rotation spectroscopy, P, Q, R branches. Vibration – rotation spectra of polyatomic molecules – linear, symmetric top and asymmetric top molecules. Principles of FTIR.

**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.

**Raman spectroscopy:** Classical and quantum theories of Raman effect, Stokes and anti- Stokes lines. Complementary nature of IR and Raman spectra. Pure rotational, vibrational and vibrational – rotational Raman spectra. Selection rules. Depolarization factors of Raman lines and their relevance. Instrumentation and applications of Raman spectroscopy.

**References**


1. Fundamentals of Molecular Spectroscopy, Banwell and McCash McGraw Hill
2. Introduction to Molecular Spectroscopy, G.M. Barrow, McGrawHill
3. Absorption Spectroscopy of Organic Compounds, J.R. Dyer Prentice-Hall of India Pvt.Ltd
4. Introduction to Spectroscopy, Pavia Lampman Kriz. Cengage learning
5. Pharmaceutical analysis, Watson Elsevier
6. NMR in Chemistry- A multinuclear introduction, William Kemp, Springer
7. Organic Spectroscopy, William Kemp, Palgrave Macmillan
8. Spectroscopy of organic compounds, P.S. Kalsi, New Age International Publishers
9. Structural methods n Inorganic chemistry, E.A.V Ebsworth, John Wiley & Sons.
10. Organic Spectroscopy, LDS Yadav , Springer
11. Elementary Organic Spectroscopy, Y.R. Sharma S. Chand Limited
12. Molecular Spectroscopy by G Arhuldas, PHI Learning Private Ltd. New Delhi.
13. Vibrational Spectroscopy: Theory and Applications, D. N. Sathyanarayana, New Age International
14. Modern Spectroscopy, J. M. Hollas, John Wiley & Sons

**Practicals**

**Paper CH 151: Inorganic chemistry Lab course** **4 hrs/week**

**I. Preparation of complexes**

1. Hexaammine nickel (II) chloride.
2. Tris (acetylacetanato) manganese(III).
3. Tris(ethylenediamine) nickel(II) thiosulphate.

**II. Calibrations**

4. Calibration of weights.
5. Calibration of pipettes.
6. Calibration of standard flasks.
7. Calibration of burette.

**III. Titrimetric Analysis**

8. Estimation of $Fe^{2+}$ by cerimetry
9. Estimation of $Ni^{2+}$ by complexometry (direct titration method)
10. Estimation of $Cu^{2+}$ by complexometry (direct titration method)
11. Estimation of $Ca^{2+}$ by complexometry (substitution titration method)
12. Estimation of $Ni^{2+}$ by complexometry (back titration method)
13. Estimation of $Al^{3+}$ by complexometry (back titration method)

**IV. One component Gravimetric Analysis**

14. Estimation of $Zn^{2+}$
15. Estimation of $Ba^{2+}$

**References**


1. Text book of Quantitative Inorganic Analysis, 3rd edition, A.I.Vogel, ELBS (1969)
2. Vogel's text book of Quantitative Inorganic analysis, 4th edition, Jeffery etal, ELBS (1988).
3. Vogel's text book of Quantitative Inorganic Analysis, 6th edition, J.Mendham etal, Pearson education ltd (2002).
4. Practical Inorganic chemistry, G.Marr and B.W.Rockett, Van Nostrand Reinhold (1972).
5. Experimental Inorganic/Physical Chemistry – An Investigative integrated approach to Practical Project work, Mounir A.Malati, Woodhead publishing ltd (1999).
6. Advanced experimental Inorganic chemistry, Ayodhya Singh, Campus books international (2006)
7. Practical Inorganic Chemistry, G. Pass & H. Sutcliffe, University science books (1999)


**Paper CH 152: Organic Chemistry Lab course** **4 hours/ week**

**Synthesis of the following compounds:**

1 p-Bromoacetanilide
2 p-Bromoaniline,
3 2,4,6- tribromoaniline

4 1,3,5-Tribromobenzene
5 Tetrahydrocarbazole
6 7-Hydroxy-4-methyl coumarin
7 m-Dinitrobenzene
8 m-Nitroaniline
9 Hippuric acid
10 Azlactone
11 Anthracene-maleicanhydride adduct
12 2,4-Dihydroxyacetophenone
13 Phthalimide
14 Anthranilic acid
15 Methyl-4-nitrobenzoate

**References**

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

**Paper CH 153 Physical Chemistry Lab course** 4 hrs / week

**I. Data analysis I: Significant figures, Precision and accuracy**

**II. Chemical kinetics:**

1. Acid-catalyzed hydrolysis of methyl acetate both with 1N HCl
2. Acid-catalyzed hydrolysis of methyl acetate both with 2N HCl
3. Peroxydisulphate-$I^-$ reaction (overall order)
4. Oxidation of iodide ion by hydrogen peroxide-Iodine clock reaction.

**III. Conductometry:**

5. Determination of cell constant
6. Titration of strong acid vs strong base
7. Titration of weak acid vs strong base
8. Determination of dissociation constant of a weak acid

**IV. Potentiometry:**

9. Titration of strong acid vs strong base
10. Titration of weak acid vs strong base and determination of dissociation constant of a weak acid.
11. Determination of single electrode potential

**V. Polarimetry:**

12. Determination of specific rotation of sucrose
13. Determination of specific rotation of glucose
14. Determination of specific rotation of fructose

**VI. Adsorption:**

15. Adsorption of acetic acid on animal charcoal or silica gel

**References**


1. Senior Practical Physical Chemistry B.D. Khosla, V.C. Garg and A. Khosla; R Chand & Co.
2. Experimental Physical Chemistry: V. Athawale and P. Mathur, New Age, International.
3. Practical Physical Chemistry: B. Vishwanathan and P.S. Raghavan, Viva Books.
4. Practical in Physical Chemistry: P.S. Sindhu, Laxmi Publications.
5. Advanced Practical Physical chemistry: J.B.Yadav, Krishna Prakashan Media


**Paper CH 154: Analytical Chemistry -I Lab course** **4 hrs/week**

**I. Applied analysis:**

1. Estimation of acetic acid in commercial vinegar by acid base titration method
2. Estimation of iron in cement by dichrometry
3. Estimation of available chlorine in bleaching powder by iodometry
4. Estimation of calcium in calcium tablets by complexometry
5. Estimation of magnesium in talcum powder by complexometry

**II. Thin layer chromatography**

6. Determination of purity of the compounds prepared in CH 152]
7. Monitoring the progress of chemical reactions for any of the two preparations in CH 152

**III. Assay of drugs:**

8. Aspirin by acid base back-titration method
9. Ibuprofen by acid base titration method
10. Calcium in calcium gluconate by complexometry

**IV. Determination of Physical Properties of Solutions:**

11. Determination of molecular weight of a polymer by viscometry
12. Determination of critical solution temperature of phenol-water system
13. Effect of added electrolyte on the CST of phenol-water system

**V. Colorimetry**

14. Verification of Beer's law and calculation of molar extinction coefficient using $CuSO_4$ solution.
15. Verification of Beer's law and calculation of molar extinction coefficient using $KMnO_4$ solution

**References**


1. Advanced practical chemistry, R.Mukhopadhyay & P. Chatterjee, NCBA books (2016)
2. Advanced practical inorganic chemistry, Gurdeep Raj, GOEL publishing house (2015)
3. Advanced experimental Inorganic chemistry, Ayodhya Singh, Campus books Int. (2006)
4. Senior Practical Physical Chemistry: B.D. Khosla, V.C. Garg and A. Khosla
5. Advanced Practical Physical Chemistry: J.B.Yadav

# M.Sc. CHEMISTRY SYLLABUS

**(Effective from academic year 2023-2024 for Campus, Constituent and Affiliated colleges)**

## SEMESTER –II

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

**Paper-I: CH 201 (Inorganic chemistry)**

IC 04: Reaction mechanisms of transition metal complexes

IC 05: Bonding in metal complexes-II

IC 06: Metal clusters ligational aspects of diatomic molecules

**IC-04: 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, $SN^1$, $SN^2$). Langford-Gray classification: A mechanism, D-Mechanism, I-Mechanism $I_a$, $I_d$, and Intimate mechanism.

**Ligand substitution reactions in octahedral complexes:** Aquation or acid hydrolysis reactions, factors affecting acid hydrolysis. base Hydrolysis, conjugate base mechanism, evidences in favour of $SN^1CB$ Mechanism. Substitution reactions without breaking metal-ligand bond. Anation reactions.

**Ligand Substitution reactions in square-planar complexes:** Mechanism of substitution in square-planar complexes, trans-effect, trans-influence, Grienberg's polarization theory and $\pi$ - 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, Factors affecting direct electron transfer reactions, Cross reactions and Marcus-Hush theory.

**IC-05: Bonding in Metal Complexes – II:** **15 hrs**

**Free ion terms and Energy levels**: Configurations, terms, states and microstates. Calculation of the number of microstates for $p^n$ and $d^n$ configurations. Vector coupling of orbital angular momenta, spin angular momentum. Spin orbit coupling: L-S (Russel-Saunders) coupling scheme, j-j coupling scheme. Determination of terms for $p^1$,$p^2$,$d^1$ and $d^2$ 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 for (i) $d^1$, $d^4$,$d^6$, $d^9$ (ii) $d^2$,$d^3$,$d^7$,$d^8$ (iii) $d^5$ octahedral and tetrahedral complexes.

**IC-06: Metal Clusters and Ligational Aspects of Diatomic molecules** **15 hrs**

**Metal Clusters:** Definition, Factors favouring metal-metal bonding.

**Metal carbonyl clusters**: Bonding modes of CO: Terminal and bridging. 18 Valence electron rule and its applications. Classification of carbonyl clusters. Low nuclearity carbonyl 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. High nuclearity carbonyl clusters: $M_5$, $M_6$, $M_7$, $M_8$ and $M_{10}$ clusters. Polyhedral skeletal electron pair theory

and Total electron count theory. Capping rule. Structural patterns in $[Ni_5(CO)_{12}]^{2-}$, $[Os_6(CO)_{18}]^{2-}$, $[Os_7(CO)_{21}]$, $[Os_8(CO)_{22}]^{2-}$ and $[Os_{10}C(CO)_{24}]^{2-}$. Metal carbonyl scrambling, stereo chemical non-rigidity in $[Rh_4(CO)_{12}]$ and $[Fe_2(Cp)_2(CO)_4]$.

**Boranes and carboranes**: Wade's rules, STYX rule.

**Metal Nitrosyls**: Bonding modes of NO: Terminal (linear, bent) and bridging. Structural aspects of $[IrCl(PPh_3)_2(CO)(NO)]^+$ and $[RuCl(PPh_3)_2(NO)_2]^+$. Stereo chemical control of valence in $[Co(diars)_2(NO)_2]^{2+}$ and $[Co(diars)_2(NO)(SCN)]^+$.

**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 $[Nb_6(Cl)_{12}]^{2+}$.

**References**


1. Inorganic reaction mechanisms, M.L.Tobe & John Burgess, Wesley Longman (1999)
2. Reaction mechanisms in metal complexes, K.Veera Reddy, New age publishers (2020)
3. Mechanisms of Reactions at Transition Metal Sites, Richard A Henderson, Oxford Science Primers, London (1993).
4. Mechanisms of inorganic reactions, F.Basalo & R.G.Pearson, 2nd Edition, John Wiley and sons, New York (1967)
5. Inorganic reaction mechanisms, R.K.Sharma, Discovery publishing house (2007)
6. Advanced Inorganic Chemistry. F.A.Cotton, G.Wilkinson, C.A.Murillo and M.Bochmann, 6th Edition, Wiley Interscience, N.Y (1999)
7. Principles of Inorganic Chemistry, Puri,Sharma, Kalia, 33rd Edition, Vishal Publications (2022).
8. Concise coordination chemistry, R Gopalan & V Ramalingam, Vikas publishing house Pvt Ltd (2008)
9. Selected topics in inorganic chemistry, Wahid U. Malik, G.D. Tuli & R.D. Madan, S.Chand & Co Ltd (1998)
10. Concise Inorganic Chemistry, J.D.Lee, 5th Edition, Chapman & Hall (2016).
    Symmetry and Spectroscopy of Molecules. K.Veera Reddy, New Age International (P) Ltd. 2022.
11. Inorganic Chemistry, J.E. Huheey, K.A.Keiter and R.L.Keiter 4 th Edition Harper Cottens College Publications (1993).
12. The Chemistry of Metal Cluster Complexes. D.F.Shriver, H.D.Kaerz and R.D.Adams (Eds), VCH, NY (1990).



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**Paper-II: CH 202 (Organic Chemistry)**

OC-04: Reaction mechanism-II and Molecular Rearrangements,

OC-05: Pericyclic reactions-I

OC-06: Photochemistry

**OC-04: Reaction mechanism-II and Molecular Rearrangements** **15 hrs**

**Neighbouring group participation (NGP)** : Criteria for determining the participation of neighbouring group. Enhanced reaction rates, retention of configuration, isotopic labeling and cyclic intermediates. NGP involving Halogens, Oxygen, Sulphur, Nitrogen, Aryl. Introduction to nonclassical carbocations; NGP Cycloalkyl groups , σ and π- bonds. ( Stereospecific examples of NGP to be covered in conformational analysis)

**Reactive Intermediates:** Generation, detection, structure, stability and reactions of carbenes and nitrenes.

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

**OC-05 Pericyclic reactions** **15 hrs.**

**Pericyclic reactions**: Introduction, Classification of pericyclic reactions into Electrocyclic, cycloadditions, sigmatropic, ene and chelotropic 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] 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 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- for electrocylic and cycloadditions & cycloreversions.

**OC-06 Organic Photochemistry** **15hrs**

**Photochemistry:** Introduction, p hotochemistry of π-π* transitions: Excited states of alkenes, cis-trans isomerisation, and photo stationary state. Photochemistry of 1,3-butadiene, di-π methane





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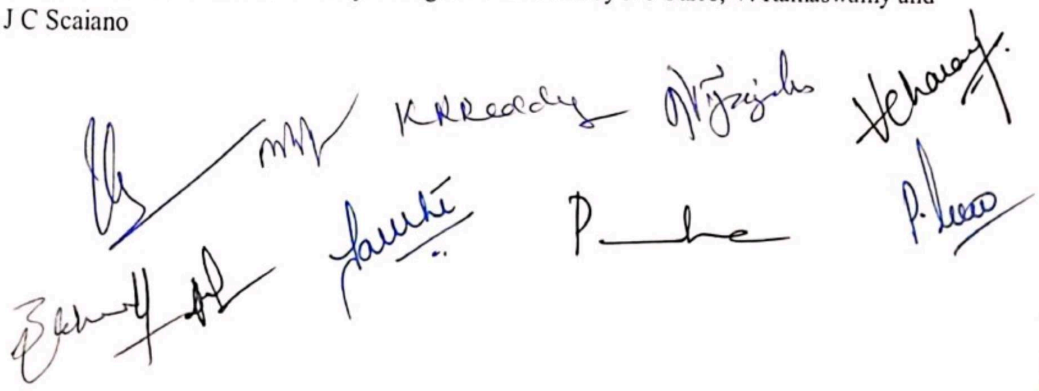
rearrangement. Intermolecular reactions, photocycloadditions, photodimeriastion of simple and conjugated olefins. Addition of olefins to α, β-unsaturated carbonyl compounds. Excited states of aromatic compounds, Photoisimerisation of benzene.

**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 strainedcycloalkane diones. Intermolecular abstraction of hydrogen: photoreduction-influence of solvent, nature of hydrogen donor and structure of the substrate.Intramolecular abstraction of hydrogen: Norrish type II reactions in ketones, esters and 1,2diketones, Addition to carbon-carbon multiple bonds, Paterno-Buchi reaction,Photochemistry of nitrites: Barton reaction.

## 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. Maya Shankar Singh, Reactive Intermediates in Organic Chemistry-Structure, mechanism and reactions, Wiley-VCH, 2012.
9. Organic chemistry Vol.I and II by I.L.Finar
10. Comprehensive organic chemistry Vol.5 D.H.R.Barton and W.D..Ollis
11. Pericyclic Reactions - A Textbook: Reactions, Applications and Theory by S. Sankararaman
12. Pericyclic reactions by Ian Flemming.
13. Organic photochemistry by J. M. Coxon and B, Halton
14. Introduction to organic Photochemistry by J. D. Coyle
15. Modern Molecular Photochemistry of Organic Molecules by N J Turro, V. Ramaswamy and J C Scaiano

**Paper-III: CH 203 (Physical Chemistry)**

PC-04: Chemical Kinetics and Photochemistry

PC-05: Quantum Chemistry-II

PC-06: Solid State Chemistry:

**PC-04: Chemical Kinetics & Photochemistry** **(15 hrs)**

**Chemical Kinetics:** Theories of reaction rates: Collision theory, steric factor. Transition state theory. Hammond's postulate. Thermodynamic formulation of transition state theory. 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-$H_2$-$Br_2$ reaction. Derivation of rate law.

Effect of structure on reactivity-Linear free energy relationships. Hammett and Taft equations-substituent ($\sigma$ and $\sigma^*$) and reaction constant ($\rho$ and $\rho^*$) with examples. Deviations from Hammett correlations, reasons- Change of mechanism, resonance interaction. Taft four parameter equation.

**Photochemistry:** The Franck Condon principle. Electronically excited molecules- singlet and triplet states. Radiative life times of excited states-theoretical treatment. Measured life times. Quantum yield. Derivation of fluorescence and phosphorescence quantum yields.

**Photophysical processes-** photophysical kinetics of unimolecular reactions. Calculation of rate constants of various photophysical processes-problems. Photosensitization. Quenching-Stern-Volmer equation. Introduction to fast reactions- Principle of flash photolysis.

**PC-05: 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. Particle 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 variation 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 wave function and the energy of $H_2$ molecule MO by LCAO method and Valence bond method (detailed calculations not required)-comparison of MO and VB models.

**PC-06: Solid state chemistry** **(15 Hrs)**

**Electronic properties of metals, insulators and semi-conductors:** Electronic structure of solids, Band theory, Fermi level, K space and Brillouin Zones, 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.





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**Superconductivity:** Occurrence of superconductivity. Destruction of superconductivity by magnetic fields – Meissner 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 YBa2Cu3O7-x. Preparation of 1-2-3 materials. Origin of high Tc superconductivity.

**Nanoparticles and their applications**: Introduction to nanoparticles. Reduced dimensionality in solids: systems with various dimensions -examples.

Preparation of nano particles – top down and bottom up methods. Preparation of nanomaterials- – sol gel methods, chemical vapour deposition method and thermolysis. Characterization of nanoparticles – experimental methods – Powder X-ray Diffraction, Scanning electron microscope (SEM), Transmission Electron Microscopy (TEM), and Atomic Force Microscopy (AFM) (Instrumentation not required). Optical properties of nanoparticles, Applications of nanoparticles.

**References**


1. Physical Chemistry-A Molecular approach, D.A. McQuarrie and J.D. Simon, Viva Books Pvt Ltd
2. Elements of Physical Chemistry by Peter Atkins and Julio de Paula, Oxford University Press
3. Chemical Kinetics and Reaction Mechanisms, J. H. Espenson, McGraw Hill
4. Chemical Kinetics, K.J. Laidler, McGraw Hill
5. The Physical Basis of Org. Chemistry by Howard Maskill, Oxford Univ. Press (New York)
6. Fundamentals of Photochemistry, K.K.Rohtagi-Mukherji, Wiley-Eastern
7. Molecular Reactions and Photo chemistry by Depuy and Chapman
8. Molecular Photochemistry, N.J. Turro, Benjamin
9. Photochemistry, R.P.Kundall and A. Gilbert, Thomson Nelson
10. Essentials of Molecular Photochemistry by A. Gilbert and J. Baggott, Blackwell Scientific Publications.
11. Organic Photochemistry by J.M.Coxon and B.Halton, Cambridge University press.
12. Introductory Photochemistry by A.Cox and T.J.Kemp. McGraw-Hill, London.
13. Quantum Chemistry, D.A. McQuarrie, Prentice Hall
14. Quantum Chemistry, Ira N. Levine, Prentice Hall
15. Introduction to Quantum Chemistry, A.K. Chandra, Tata McGraw Hill
16. Quantum Chemistry, R K Prasad, New Age International Pvt Ltd Publishers
17. Elementary Quantum Chemistry, F. L. Pilar, McGraw Hill.
18. Introduction to Solids, Leonid V. Azaroff, Tata McGraw Hill
19. Solid state Chemistry, D.K. Chakrabarthy, New Age International
20. Solid state Chemistry and its aplications, A.R. West, Plenum.
21. Principles of the Solid State, H. V. Keer, New Age International
22. The physics and chemistry of solids by Stephen Elliott, Wiley Publishers.
23. Nanostructured Materials and Nanotechnology, edited by Hari Singh Nalwa, Acad. Press
24. Self-Assembled Nanostructures, Jin Zhang, Zhong-lin Wang, Jun Liu, Shaowei Chen & Gan-Yu-Liu, Kluwer Academic/Plenum
25. Introduction to Nanotechnology, Charles P. Poole Jr, F. J. Owens, Wiley India Pvt. Ltd.

**Paper-IV: CH 204 (Analytical Techniques and Spectroscopy – II)** 15 hrs

ASP 04: Electro and Thermal Analytical Techniques

ASP 05: NMR-II and ESR Spectroscopy

ASP 06: Mass spectrometry

**ASP- 04: Electro and Thermal Analytical Techniques**

**Electro analytical techniques:** Types and Classification of Electro analytical Methods.

**Polarography:** Types of polarography: A.C Polarography and D.C Polarography. D.C Polarography: Instrumentation - Dropping mercury electrode, polarogram. Types of Currents: Residual, Migration and Limiting currents. 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.

**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.

**Cyclic Voltammetry**: Principle, instrumentation, Applications. Cyclic voltammetric study of insecticide parathion. HOMO-LUMO calculations of ferrocene using cyclic voltammetry.

**Thermal Analysis**:

Introduction, types of thermo analytical methods.

**Thermogravimetry**: Principle and applications of thermogravimetry- Study of calcium oxalate, calcium sulphate and silver nitrate, Differential thermal analysis: Principle and applications of DTA- Differential thermogram of sulphur,

Differential scanning calorimetry DSC: Principle and application of DSC- determination of glass transition temperatures and heat capacities of PVC and Bakelite.

**ASP- 05: NMR-II and ESR Spectroscopy** 15 hrs

**Multinuclear NMR ($^1H$, $^{19}F$ and $^{31}P$ NMR) 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, $[\eta^1\text{-}C_5H_5M]$, $[\eta^5\text{-}(C_5H_5)_2Ti\eta^1\text{-}(C_5H_5)_2]$ and $[\eta^4\text{-}C_8H_8Ru(CO)_3]$.

**$^{19}F$ NMR spectroscopy**: $^{19}F$ chemical shifts, coupling constants. Applications of $^{19}F$ NMR involving coupling with $^{19}F$, $^1H$ and $^{31}P$: 1,2-dichloro-1,1-difluoro ethane, $BrF_5$, $SF_4$, $PF_5$, $ClF_3$, $IF_5$, $CF_3CH_2OH$.

**$^{31}P$ NMR spectroscopy**: $^{31}P$ chemical shifts, coupling constants. Applications of $^{31}P$ NMR involving coupling with $^{31}P$, $^{19}F$, $^1H$ and $^{13}C$: ATP, $Ph_3PSe$, $P_4S_3$, $H_3PO_4$, $H_3PO_3$, $H_3PO_2$, $HPF_2$, $PF_6^-$, $PH_3$, $[Rh(PPh_3)_3Cl]$ (Rh: I= ½).

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

**Electron Spin Resonance Spectroscopy**: Introduction, principle, instrumentation, selection rules, calculation of 'g'. Study of free radicals.

**ASP - 06: Mass spectrometry** **15 hrs**

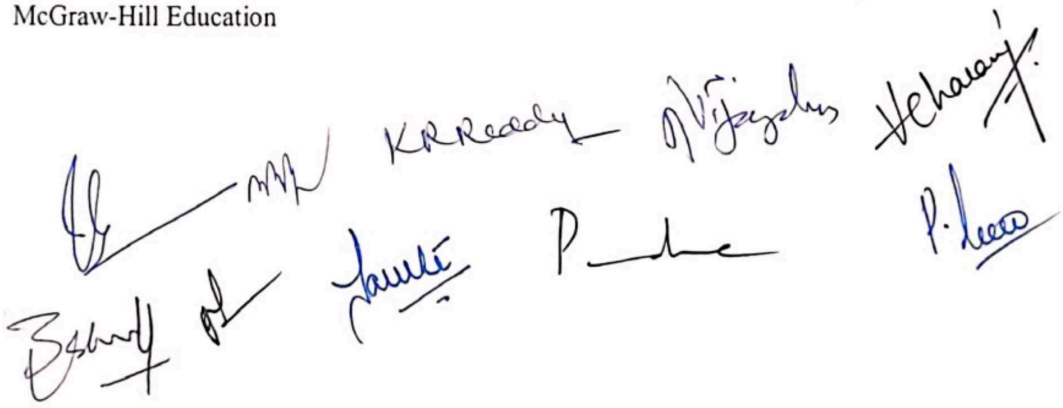
**Origin of mass spectrum**, principle of EI mass spectrometer. Types of fragments: Odd electron and even electron containing neutral and charged species (even electron rule), Nitrogen rule, isotopic peaks, determination of molecular formula, metastable ion peaks. High resolution mass spectrometry. Salient features of fragmentation pattern of organic compounds including β-cleavage, Mclafferty rearrangement, retro Diels – Alder fragmentation and ortho effect.

Principle of EI, CI, Atmospheric Pressure Ionisation (API), Secondary Ion Mass Spectrometry (SIMS), Electrospray ionization (ESI) and Matrix Assisted Laser Desorption Ionization (MALDI) methods.

Introduction, principle and applications of Gas Chromatography-Mass Spectrometry (GC-MS) and Liquid chromatography-Mass Spectrometry (LC-MS) techniques.

**References:**


1. Principles of Polarography, Heyrovsky, Elsevier Inc.
2. Principles of Polarography, Kapoor, John Wiley & Sons.
3. Modern Electroanalytical methods, edited by C.C harlot, Elsevier Company.
4. Principles of Instrumental analysis, Skoog, Holler and Nieman, Harcourt Asia PTE Ltd.
5. Analytical Chemistry-An Introduction, Skoog, West, Holler and Crouch, Saunders College Publishing.
6. Principles of Instrumental Analysis, Skoog and Leary, Saunders College Publishing.
7. Spectroscopic identification of organic compounds by R.M. Silverstein and F.X. Webster, John Wiley & Sons
8. Instrumental Methods of Chemical Analysis by B K Sharma, Krishna Prakashan Pvt. Ltd.
9. Instrumental Methods of Analysis by Willard, New York, Van Nostrand
10. Organic spectroscopy by William Kemp, Palgrave Macmillan.
11. NMR-A multinuclear introduction by William Kemp, Springer
12. Spectroscopic methods in organic chemistry by D.H. Williams and I. Fleming McGraw-Hill Education





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**Practicals**

**Paper CH 251: Inorganic chemistry Lab course** **4 hours/ week**

**I. Preparation of complexes:**

1. Mercury tetrathiocyanatocobaltate(II).
2. Chloropentamminecobalt(III) chloride
3. Tetramminecopper(II) sulphate

**II. Titrimetric Analysis of two ions in a mixture**

4. Estimation of $Pb^{2+}$ and $Ca^{2+}$
5. Estimation of $Zn^{2+}$ and $Mg^{2+}$
6. Estimation of $Mg^{2+}$ and $Mn^{2+}$

**III. Analysis of Two component mixtures**

7, 8. Separation of $Ag^{+}$ and $Ca^{2+}$ in a mixture and estimation of $Ag^{2+}$ (gravimetric) and $Ca^{2+}$(volumetric).

9, 10. Separation of $Cu^{2+}$ and $Ni^{2+}$ in a mixture and estimation of $Ni^{2+}$ (gravimetric) and $Cu^{2+}$ (volumetric)

11, 12. Separation of $Fe^{3+}$ and $Al^{3+}$ in a mixture and estimation of $Fe^{3+}$ (volumetric) and $Al^{3+}$(gravimetric).

**IV. Analysis of three component mixtures:**

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

**V. Ion exchange methods of analysis:**

14. Determination of capacity of an ion exchange resin.
15. Separation of $Mg^{2+}$ and $Zn^{2+}$ on an anion exchange resin and estimation of $Mg^{2+}$ and $Zn^{2+}$

**References**


1. Text book of Quantitative Inorganic Analysis, 3rd edition, A.I.Vogel, ELBS (1969)
2. Vogel's text book of Quantitative Inorganic analysis, 4th edition, Jeffery etal, ELBS (1988).
3. Vogel's text book of Quantitative Inorganic Analysis, 6th edition, J.Mendham etal, Pearson education ltd (2002).
4. Practical Inorganic chemistry, G.Marr and B.W.Rockett, Van Nostrand Reinhold (1972).
5. Experimental Inorganic/Physical Chemistry – An Investigative integrated approach to Practical Project work, Mounir A.Malati, Woodhead publishing ltd (1999).
6. Advanced experimental Inorganic chemistry, Ayodhya Singh, Campus books international (2006)
7. Practical Inorganic Chemistry, G. Pass & H. Sutcliffe, University science books (1999)


**Paper CH 252: Organic Chemistry Lab course** **4 hours/ week**

**Identification of organic compounds systematic qualitative analysis:**

1. BP / MP, Ignition test, solubility classification
2. Extra elements-N,S & Halogens,(Lassagnine sodium fusion test)
3. p-Nitrobenzoic acid/2-Chloro benzoic Acid



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4. Anisole
5. p- Chlorophenol
6. p-Chloroanilines
7. N-Methyl aniline/N-Ethylaniline
8. N,N-Dimethylaniline
9. Benzamide
10. p-Chloro benzadehyde
11. Acetophenone/ P-Chloro acetophenone,
12. Benzophenone
13. Nitrobenzene
14. Ethylbenzoate
15. Chlorobenzene/ Bromobenzene

**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

**Paper CH 253: Physical Chemistry Lab** **4hrs /week**

**I. Data analysis II:** Mean and standard deviation; absolute and relative errors; linear regression; covariance and correlation coefficient.

**II.Distribution**:

1. Distribution of I2 between cyclohexane and water
2. Distribution of I2 between cyclohexane and aq.KI solution - calculation of equilibrium constant.

**III. Chemical Kinetics:**

3. Stoichiometry of Peroxydisulphate - Iodide reaction
4,5. Peroxydisulphate - Iodide reaction: Comparison of strengths of KI solutions by isolation method

**IV. Conductometry:**

6. Titration of a mixture of strong and weak acids vs strong base
7. Determination of the hydrolysis constant of aniline hydrochloride
8. Determination of solubility product

**V. Potentiometry:**

9. Titration of $Cl^-$ vs $Ag^+$ (precipitation titration)
10. Determination of solubility product of sparingly soluble salt

**VI. Polarimetry:**

11. Inversion of cane sugar catalyzed by 1N HCl
12. Inversion of cane sugar catalyzed by 2N HCl

**V. pH metry:**

13. Calibration of a pH meter and preparation of phosphate buffers
14. Titration of strong acid vs strong base
15. Titration of weak acid vs strong base and determination of dissociation constant of weak acid





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**References**


1. Senior Practical Physical Chemistry B.D. Khosla, V.C. Garg and A. Khosla; R Chand & Co.
2. Experimental Physical Chemistry: V. Athawale and P. Mathur, New Age, International.
3. Practical Physical Chemistry: B. Vishwanathan and P.S. Raghavan, Viva Books.
4. Practical in Physical Chemistry: P.S. Sindhu, Laxmi Publications.
5. Advanced Practical Physical chemistry: J.B.Yadav, Krishna Prakashan Media


**Paper CH 254: Analytical Chemistry -II & Spectrscopy Lab course** **4 hours/ week**

**I. Applied analysis:**

1. Estimation of alkali content in antacid by acid base titration method
2. Estimation of ascorbic acid in vitamin C by iodometry
3. Estimation of available oxygen in hydrogen peroxide by permanganometry
4. Estimation of calcium in milk by complexometry
5. Determination of hardness of water by complexometry.

**II. Spectral analysis: Interpretation of IR, UV, $^1$H NMR and MS of the following representative compounds**

6. An aldehyde
7. An alcohol
8. A carboxylic acid
9. An amine
10. A Ketone

**III. Instrumental Analysis:**

**Conductometry:**

11. Titration of a mixture of strong and weak acids vs weak base

**Potentiometry:**

12. Titration of $Fe^{+2}$ vs $Cr_2O_7^{2-}$ (redox titration)
13. $Fe^{2+}$ vs $Ce^{4+}$ and calculation of formal redox potential of Fe(II)/Fe(III)
14. $Fe^{2+}$ vs $MnO_4^-$ and calculation of formal redox potential of Fe(II)/Fe(III)

**pH metry:**

15. Titration of a mixture of strong and weak acids vs strong base

**References:**


1. Vogel's text book of Quantitative Inorganic Analysis, 6th edition, J.Mendham etal, Pearson education ltd (2002)
2. Advanced practical chemistry, R.Mukhopadhyay & P. Chatterjee, NCBA books (2016)
3. Advanced practical inorganic chemistry, Gurdeep Raj, GOEL publishing house (2015)
4. Advanced experimental Inorganic chemistry, Ayodhya Singh, Campus Books International (2006)
5. Senior Practical Physical Chemistry: B.D. Khosla, V.C. Garg and A. Khosla
6. Advanced Practical Physical Chemistry: J.B.Yadav
7. Organic structures from spectra: L. D. Field, S. Sternhell, J. R. Kalman.






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# M.Sc. CHEMISTRY

## ORGANIC CHEMISTRY SPECIALISATION
## SYLLABUS OF III & IV SEMESTERS
## *REVISED AS PER NEW (CB) SYLLABUS*

## FOR STUDENTS ADMITTED FROM THE YEAR 2016 ONWARDS

# M.Sc. CHEMISTRY (ORGANIC CHEMISTRY SPECIALISATION)

## Syllabus for III and IV Semesters

**(for the batches admitted in academic year 2016 & later under CBCS pattern)**

***[Under Restructured CBCS Scheme]***

***Grand total marks and credits (all 4 semesters) 2400 marks – 96 credits***

**(Approved in the P.G.BOS meeting held on 01-07-2017)**

### SEMESTER-III

| Paper | Instruction Hrs/Week | Internal assessment marks* | Semester marks | Total marks | Total credits |
|---|---|---|---|---|---|
| CH(OC)301T | 4 | 20 | 80 | 100 | 4 |
| CH(OC)302T | 4 | 20 | 80 | 100 | 4 |
| CH(OC)303T | 4 | 20 | 80 | 100 | 4 |
| CH(OC)304T | 4 | 20 | 80 | 100 | 4 |
| CH(OC)351P | 9 | - | 100 | 100 | 4 |
| CH(OC)352P | 9 | - | 100 | 100 | 4 |
| **Total** | | | | **600** | **24** |

### SEMESTER - IV

| Paper | Instruction Hrs/Week | Internal assessment marks* | Semester marks | Total marks | Total credits |
|---|---|---|---|---|---|
| CH(OC)401T | 4 | 20 | 80 | 100 | 4 |
| CH(OC)402T | 4 | 20 | 80 | 100 | 4 |
| CH(OC)403T | 4 | 20 | 80 | 100 | 4 |
| CH(OC)404T | 4 | 20 | 80 | 100 | 4 |
| CH(OC)451P | 9 | - | 100 | 100 | 4 |
| CH(OC)452P | 9 | - | 100 | 100 | 4 |
| **Total** | | | | **600** | **24** |

** 15 marks for the written test and 5 marks for the assignment*

**Grand total all 4 semesters: 2400 marks and 96 credits**

**PAPER TITLES , M.Sc. ORGANIC CHEMISTRY SPECIALISATION**
**(For the batch admitted during the academic year 2016 onwards under the CBCS pattern)**

*[Under Restructured CBCS Scheme]*

| III SEMESTER SYLLABUS | IV SEMESTER SYLLABUS |
|---|---|
| **Paper-1CH (OC) 301T: Synthetic Reagents, Advanced NMR, Conformational Analysis and ORD**<br>OC-09: Synthetic Reagents-I<br>OC-10: Synthetic Reagents-II<br>OC-11: $^{13}$C NMR and 2D NMR spectroscopy<br>OC-12: Conformational analysis (Cyclic systems ) and ORD | **Paper-1 CH (OC) 401T: Drug Design and Drug Discovery**<br>OC-17: Principles of Drug design and drug discovery<br>OC-18: Lead modification and SAR Studies<br>OC 19: QSAR studies and computer aided drug design<br>OC 20: Combinatorial Synthesis |
| **Paper II– CH (OC) 302T: Modern Organic Synthesis**<br>OC-13: Asymmetric synthesis<br>OC-14: Synthetic strategies<br>OC-15: New Synthetic reactions<br>OC-16:New techniques and concepts in organic synthesis | **Paper-II CH (OC) 402T:Drug synthesis and mechanism of action**<br>OC-21: Drugs acting on metabolic process, cell wall and specific enzymes<br>OC-22: Drugs acting on genetic material and immune system<br>OC-23: Drugs acting on receptors and ion channels<br>OC-24: Chiral drugs |
| **Elective-3A**<br>**Paper-IIICH (OC)303T (CB1): Bioorganic Chemistry**<br>OC(CB1)-1: Carbohydrates<br>OC(CB1)-2: Nucleic acids and Lipids<br>OC(CB1)-3: Proteins and Enzymes<br>OC(CB1)-4: Coenzymes and Vitamins | **Elective-3A**<br>**Paper-III CH (OC)-403T (CB1): Advanced Heterocyclic Chemistry**<br>OC (CB1) 17: Non aromatic heterocyclics& aromaticity<br>OC (CB1)18: Five and six membered heterocyclics with two hetero atoms<br>OC (CB1) 19: Heterocyclics with more than two hetero atoms<br>OC (CB1) 20: Larger ring and other heterocycles |
| **Elective-3B:**<br>**Paper-III CH (OC) 303T (CB2): Forensic Chemistry and Toxicology**<br>OC(CB2)-5: Forensic chemistry- I<br>OC(CB2)-6: Forensic chemistry- II<br>OC(CB2)-7: Forensic Toxicology-I<br>OC(CB2)-8: Forensic Toxicology-II | **Elective-3B**<br>**Paper-III CH (OC)-403T (CB2): Polymers , dyes and Pigments**<br>OC (CB2) 21: Polymers- I<br>OC (CB2) 22: Polymers- II<br>OC (CB2) 23: Dyes-I<br>OC (CB2) 24: Dyes-II and pigments |
| **Elective-4A**<br>**Paper-IV CH (OC) 304T (CB3): Green chemistry and Organic materials**<br>OC (CB3) - 9: Principles of Green chemistry<br>OC (CB3) -10: Green Synthesis<br>OC (CB3) -11: Organic nanomaterials<br>OC (CB3) -12: Supramolecular chemistry | **Elective-4A (ID Paper)**<br>**Paper-IV CH (OC) 404(CB3)T: Advanced Natural Products**<br>OC(CB3)-25: Biosynthesis of natural products<br>OC(CB3)-26: Structure determination of natural products -I<br>OC(CB3)--27: Structure determination ofnatural products-II<br>OC(CB3)--28: Total stereo selective synthesis of natural products. |
| **Elective-4B**<br>**Paper-IV CH (OC) 304T (CB4): Pesticides**<br>OC (CB4) - 13: Introduction to pesticides<br>OC (CB4) - 14: Synthetic insecticides<br>OC (CB4) - 15: Natural insecticides & herbicides<br>OC (CB4) - 16: Fungicides, and Rodenticides | .**Elective-4B (ID Paper)**<br>**Paper-IVCH (OC) 404 (CB4) T: Biopharmaceutics and Pharmacodynamics**<br>OC(CB4)-29 : Pharmacokinetics<br>OC(CB4)-30 : Pharmacodynamics<br>OC(CB4)-31 : Principles of Therapeutics<br>OC(CB4)-32: Drug Interactions |
| **LABORATORY COURSES**<br>**Paper-V CH (OC) 351P**: Synthesis of organic molecules, isolation of natural products & TLC.<br>**Paper-VI CH (OC) 352P**: Separation and identification of organic compounds & Column chromatography | **LABORATORY COURSES**<br>**Paper-V CH (OC) 451P**: Spectroscopic identification of organic compounds & practice of chemistry software prgrammes<br>**Paper- VI CH (OC) 452P**: Synthesis and analysis of drugs |

## M.Sc. ORGANIC CHEMISTRY SPECIALISATION
## III SEMESTER SYLLABUS

**(For the batch admitted during the academic year 2016-2017)**

**Paper-1CH (OC) 301T: Synthetic Reagents, Advanced NMR,Conformational Analysis and ORD**

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

**Paper II– CH (OC) 302T: 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

**Elective-3A Paper-III CH (OC)303T (CB1): Bioorganic Chemistry**

OC(CB1)-1: Carbohydrates
OC(CB1)-2: Nucleic acids and Lipids
OC(CB1)-3: Proteins and Enzymes
OC(CB1)-4: Coenzymes and Vitamins

**Elective-3B: Paper-III CH (OC) 303T (CB2): Forensic Chemistry andToxicology**

OC(CB2)-5: Forensic chemistry- I
OC(CB2)-6: Forensic chemistry- II
OC(CB2)-7: Forensic Toxicology-I
OC(CB2)-8: Forensic Toxicology-II

**Elective-4A Paper-IV CH (OC) 304T (CB3): Green chemistry and Organic materials**

OC (CB3) - 9: Principles of Green chemistry
OC (CB3) -10: Green Synthesis
OC (CB3) -11: Organic nanomaterials
OC (CB3) -12: Supramolecular chemistry

**Elective-4B Paper-IV CH (OC) 304T (CB4): Pesticides**

OC (CB4) - 13: Introduction to pesticides
OC (CB4) - 14: Synthetic insecticides
OC (CB4) - 15: Natural insecticides & herbicides
OC (CB4) - 16: Fungicides, and Rodenticides

## Laboratory courses:

**Paper-V CH (OC) 351P**: Synthesis of organic molecules, isolation of natural products and TLC.

**Paper-VI CH (OC) 352P**: Separation and identification of organic compounds & Column chromatography.

**M.Sc. CHEMISTRY (ORGANIC CHEMISTRY)**
**III SEMESTER SYLLABUS**

**(For the batch admitted during the academic year 2016 -2017 under the CBCS pattern)**

## Paper-1CH (OC) 301T: Synthetic Reagents, Advanced NMR, Conformational Analysis and ORD

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

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

**i)Protecting groups:** a) Protection of alcoholsby ether, silyl ether and esterformation 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) Organolithium 2) Organo copper reagents3) Organoboranes 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) Phosphorousylide mediated olefination 1) Witting reaction, 2) Horner-Wordsworth-Emmons reaction.b) Titanium- Carbene mediated olefination 1) Tebbe reagent, 2) Petasis reagent 3) Nysted reagent.

**iv) Carbene insertions:** Rh based carbene complexes, cyclopropanations.

**v) C-H Activation:** Introduction, Rh catalysed C-H activation.

### OC-10:Synthetic Reagents II 15 Hrs

**i)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.

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

**OC-12: Conformational analysis (Cyclic systems) & ORD15 Hrs**

**Conformational analysis (Cyclic systems)**

Study of conformations of cyclohexane, mono, di and tri substituted cyclohexanes, (1,3,5-trimethyl cyclohexanes and Menthols), cyclohexanone (2-alkyl and 3 -alkyl ketone effect), 2-halocyclohexanones, cycloheptane . Stereo chemistry of bicyclo[3,3,0]octanes,hydrindanes, decalins and perhydroanthracenes. Conformational structures of piperidine, N-Methylpiperidine, tropane, tropine, pseudotropine, decahydroquinolineand 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 semiempiricalrules-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 and T B Morrill
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
22. Stereochemistry of organic compounds — Principles & Applications by D Nasipuri
23. Stereochemistry of Carbon compounds by Ernest L Eliel & Samuel H. wilen
24. Stereochemistry: Conformation & Mechanism by P S Kalsi
25. The third dimension in organic chemistry, by Alan Bassendale
26. Stereo selectivity in organic synthesis by R S Ward.
27. Advanced organic chemistry. Part A Structure & Mechanism by Francis A. Corey and Richard J. Sundberg
28. Optical rotatory dispersion by C Djerassi
29. Optical rotatory dispersion and circular dichroism by P Crabbe
30. Mechanism and Structure in Organic chemistry by S Mukherjee

## Paper II– CH (OC) 302T: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 synthesis15 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 forstereoselectivity: Symmetry and transition state criteria, kinetic and thermodynamic control. Methods of inducing enantioselectivityy.

**Analytical methods:** % Enantiomeric excess and diastereomeric ratio. Determination of enantiomeric excess: specific rotation, Chiral NMR; Chiralderivatizing 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:**Sharplessepoxidation. Asymmetric hydrogenations using chiral Wilkinson biphosphincatalyst.

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

**OC-14: SyntheticStrategies15 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 involvingchemoselectivity, 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-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**: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 ofRetronecene, longifoline.

**OC-15: New Synthetic reactions** **15 Hrs**

**1. Metal mediated C-C and C-X coupling reactions:**Suzuki, Heck, Stille,Sonogishira crosscoupling,Buchwald-Hartwigand Negishi-Kumadacoupling reactions.

**2. C=C Formation Reactions:**Shapiro, Bamford-Stevens, McMurreyreactions,Julia-Lythgoeolefinationand Peterson's stereoselective olefination.

**3. Multicomponent Reactions:**Ugi,Passerini, Biginelli, Bergman and Mannichreactions.

**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:**Phosphotriester, phosphitetriester and phosphoramidite pathway

**3. Oligosaccharide synthesis:**Glycosidation:cylicoxocarbeniumion, glycosyl donors and glycosyl acceptors, Kahneglycosidation, 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 disfavouredcyclisations.

**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
13. Name reactions by JieJacj Li


## Elective-3A

## Paper-III CH (OC)303T (CB1): Bioorganic Chemistry

**OC(CB1)-1: Carbohydrates**
**OC(CB1)-2: Nucleic acids and Lipids**
**OC(CB1)-3: Proteins and Enzymes**
**OC(CB1)-4: Coenzymes and Vitamins**

**OC(CB1)-1: Carbohydrates** **15 Hrs**

Introduction to the importance of Carbohydrates. Types of naturally occuring sugars. Deoxy sugars, aminosugars, branched chain sugars mrthyl 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, glycogenand chitin. Role of sugars in cell to cell recognition, blood groups.

**OC(CB1)-2: 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)-3: Proteinsand Enzymes15 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)-4: Coenzymes and Vitamins** **15 Hrs**

**Coenzymes:** Introduction. Co-factors -cosubstrates -prosthetic groups.

Classification — Vitamin derived coenzymes and metabolite coenzymes.Structure and biological functionsof 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 diphosphosugars (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. LehningerPrinciples of Biochemistry by D L Nelson and M MCoxon
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 Dugasand Christopher Penney.
14. Concepts in Biotechnology by D.Balasubramanian& others
15. Chemistry and physiology of the vitamins by H.R.Rosenberg.


## Elective-3B

## Paper-III CH (OC)303T (CB2): Forensic Chemistry & Toxicology

OC(CB2)-5: Forensic chemistry- I
OC(CB2)-6: Forensic chemistry- II
OC(CB2)-7: Forensic Toxicology-I
OC(CB2)-8: Forensic Toxicology-II

**OC(CB2)-5: Forensic chemistry-I 15 Hrs**

Forensic Chemistry - Introduction - Types of cases / exhibits - Preliminary screening - presumptive tests (colour and spot tests) - Examinations procedures involving standard methodsand instrumental techniques

Qualitative and quantitative forensic analysis of inorganic and organic material - Chemical fertilizers (N,P,K) _ Insecticides (Endosulfan, Malathion, Carbaryl) - Metallurgical analysis (Fe, Cu, Zn, Au, Ag) – Natural products (tobacco, tea, sugars, rubber) – Industrial chemicals - Sulphuric, Nitric and Hydrochloric acids, Sodium, Potassium hydroxide, Ammonium nitrate, Potassium chlorate, Organic solvents like Methanol, Ethanol, Acetone, Chloroform and Ether Organic chemicals like Acetanilide, P- Aminophenol, and Nitrobenzene etc. with reference to forensic work.

**OC(CB2)-6: Forensic chemistry-II 15 Hrs**

Examination of petroleum products - Distillation and fractionation - various fractions and theircommercial uses - Standard method of analysis of petroleum products – Analysis of petroleumproducts for adulteration and arson residues. Chemistry of fire - Investigation and evaluation of fires – Causes of fire - Analysis of arsonresidues by conventional and instrumental methods. Analysis of trace evidence - Cosmetics, Dyes, Trap related evidence materials, Paints, Pigments,Fibres, Oils fats, Greases, Industrial dusts, Chemicals and Plant materials.

**OC(CB2)-7: Forensic Toxicology-I15 Hrs**

Toxicology- Introduction- History- Scope- Areas of Toxicology- Role of forensic toxicologist- Poisons- Classification of poisons- Types of poisoning- Sample collection and preservation oftoxicological exhibits in fatal and survival cases- Storage of samples- Signs and symptoms ofpoisoning- Toxicological investigation/examination of poisoned death- Interpretationoftoxicologicaldata- Courtroom testimony in toxicological cases.Case Histories.

**OC(CB2)-8: Forensic Toxicology-II 15 Hrs**

Principles of Toxicology- Introduction – Pharmacokinetics - Methods of transportation oftoxicant- Absorption- Distribution- Storage of toxicants- Redistribution - Metabolism- Oxidation

– Reduction – Hydrolysis – Conjugation - Excretion- Other routes of elimination-Toxicokinetics- one and two compartmental model – Toxicodynamics- Spectrum of undesired(toxic) effects- Interaction of chemicals- Tolerance- Dose response relationship- Developmentaland reproductive toxicity- Mutagenicity- Toxicity testing.

**Recommended books:**


1. James, S. H. and Nordby, J. J.: Forensic Science: An Introduction to Scientific and Investigative Techniques, 2003.
2. Saferstein, R: Criminalistics - An Introduction to Forensic Science, Prentice Hall, 1995.
3. Sarkar, S: Fuels and Combustion, Orient Longman, 1990
4. Verma, R. M: Analytical Chemistry – Theory and Practice, CBS Pub., 1994
5. Svehla, G. Ed.: Vogel's Qualitative Inorganic Analysis, Longman, 1998.
6. Bassett: Vogel's Text Book of Quantitative Inorganic Analysis, Longman, 1978
7. Vogel, A. I: Text Book of Practical Organic Chemistry including Qualitative OrganicAnalysis, ELBS, 1971.
8. Narayanan, T. V: Modern Techniques of Bomb Detection and Disposal, R. A. Security System, 1995.
9. Almirall, J. R. and Furton, K. G: Analysis and Interpretation of Fire Scene Evidence, CRC Press, 2004.
10. Bogusz, M. J: Handbook of Analytical Separations : Vol. 2 ,Forensic Science, Elsevier, 2000.
11. Bureau of Indian Standards: Specifications and Methods of Analysis for Petroleum Products.
12. Wilson and Wilson's Comprehensive Analytical Chemistry Volumes
13. Standard Methods of Chemical Analysiss
14. AOAC: Official Methods of Analysis
15. Daeid, N.N.: Fire Investigation: Theory and Practice, Taylor and Francis, 2003
16. Klaassen, C. D.,:Casarett and Doull's Toxicology: The Basic Science of Poisons, 5thed, McGraw-Hill, 1995.
17. Moffat, A.C. : Osselton, D. M. Widdop, B. : Clarke's Analysis of Drugs and Poisons in Pharmaceuticals, body fluids and postmortem material, 3rd ed., Pharmaceutical Press2004.
18. Bogusz, M. J.,: Hand Book of Analytical Separations, Vol. 2: Forensic Science, 1st ed., Elsevier Science ,2000.
19. Siegel, J.A., Saukko, P. J., Knupfer, G.,: Encyclopedia of Forensic Sciences (Vol3), Academic Press, 2000.
20. Paranjape, H.M., Bothara, G.K., Jain, M.M.: Fundamentals of Pharmacology, 1st ed.,Nirali Prakashan,1990.
21. Budhiraja, R.D.: Elementary Pharmacology and Toxicology, Popular Prakashan, 2nd ed., 1999.
22. Laboratory procedure Manual, Forensic Toxicology: DFS, 2005
23. Cravey, R.H; Baselt, R.C.: Introduction to Forensic Toxicology , Biochemical Publications, Davis, C.A. (1981)
24. Stolmen, A.; Progress in Chemical Toxicology: Academic Press, New York (1963)
25. Modi, Jaisingh, P.; Textbook of Medical Jurisprudence& Toxicology, M.M. TripathiPublication (2001)
26. Eckert; An Introduction to Forensic Science, CRC Press

## Elective-4A

## Paper-IV CH (OC) 304T (CB3): Green chemistry and Organic materials

OC (CB3) -9: Principles of Green chemistry
OC (CB3) -10: Green Synthesis
OC (CB3) -11: Organic nanomaterials
OC (CB3) -12: Supramolecular chemistry

**OC (CB3)-9: 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) -10: 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 diydroxylationreactions.

**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) -11: 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 Benzheterazoles and their synthetic modifications as optoelectronic molecules.

**OC (CB3) -12: Supramolecular Chemistry** **15Hrs**

**Introduction**: 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, American Chemical Society, Washington (2000).

4. M.A. Ryan & M. Tinnesand, Introduction to Green Chemistry, American Chemical Society, Washington (2002).

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.

## Elective-4B
## Paper-IV CH (OC) 304T (CB4): Pesticides

OC(CB4)- 13:Introduction to pesticides
OC(CB4)- 14: Synthetic insecticides
OC(CB4)- 15:Natural insecticides& herbicides
OC(CB4)- 16:Fungicides, and Rodenticides

**OC (CB4)-13: Introduction to pesticides** **15 Hrs**

**i) Defination** ,Classification and importance of pesticides

**ii) Pest control**: Different methods –chemical – insecticides, fungicides, herbicides, rodenticides, fumigants, chitin synthesis inhibitors and insect repellents.

**a) Biological**–pheremones: Definition and classification, synthesis of Disparlure, Exobrevicomin, Endobrevicomin, frontalin and grandiso pheromones, synthetic sex attractants.

b) Insect juvenile hormones: JH-A, JH-B,Synthesis of juvabione. Structural formula and importance of methopren.

c) Moultingharmones-structural formulae and mode of action of ecdysones

d) Antibiotics and secondary metabolites of microbial origin as insecticides and fungicides in agricultiure. Structural formula and importance of Blasticidin-S, Kasugamycin, Avermectin-B, Invermectin, piercidins and phytoalexins.

**iii) Environmental pollution from pesticides**.iv) Integrated pest management.

v) Pesticide formulations: Dusts, Granules, Wettable powders, Emmulsions and Aerosols.

**OC (CB4)- 14: Synthetic insecticides** **15 Hrs**

i)**Organochlorine insecticides-** synthesis and mode of action of methoxychlor, perthan, Dicofol, Heptachlor, Dieldrin and Endosulfan.

ii) **Organophosphorous insecticides** –synthesis and mode action of Phosphoric acid derivatives, phosdrin, Dichlorophos, parathion, Zolone, Aninphomethyl, TEPP and Sachradan.

iii) **Carbamate insecticides-** synthesis and mode of action of carbamyl, Furadan, Baygon, Aldicarb and Zectron.

iv) Formulation and residue analysis of organochlorine, organophophorous and carbamate insecticides.

**OC (CB4)- 15: Natural insecticidesand herbicides15 Hrs**

i**) Insecticides of palnt origin** –synthesis and importance of pyrethrins (I and II), Rotenone and Nicotine. Main constituents Neem-structural formula of Azadirachtin. Synthesis of polygodial and warbunganol(Antifeedants).

ii)Synthesis of pyrethroids: synthesis of Allethrin, Bioallethrin, Cypermethrin, Fenvalerate, Decemethrin and pyrithrelone.

**iii) Concept of Bioinsecticides** – Bacillus thiuringiensis.

**iv) Concept of pro-insecticides-**structure and mode of action of pro-pheremones and pre-pro-insecticides.

**v) Herbicides** – synthesis,applications and mode of action of the following

a)Aryloxyalkyl carboxylic acid derivative:2,4-D, MCPA,2,4,5-T and 2,4,5-TP.b) Carbamates-propham and chloropham, c)Urea derivatives –Monouron and diuron, d) Aliphatic acids-Dalapon,TCA, e)Aromatic acids -2,3,6-TBA,Dicomba and Amiben, f)Nitrogen heterocyclic dericvatives –Simazine,Atrazine,Amitrole,Maleic hydrazide Diquat and paraquat, g) Phenols-PCP and Dinoseb, h) Benzonitrile compounds

**OC (CB4)-16: Fungicides, and Rodenticides 15 Hrs**

**i) Fungicides** –classification ,synthesis application and mode of action of the following classes: **a**)Carbamatesb)Quinones-chloranil,Dichloneand Benquinoxc)perchloromethylmercaptan derivative –captan,folpet,Difolatan and Mesulfan d) Benzimidazoles-carbendazim, Benomyl and Thiabandazole

**ii) Rodenticides**, a) Anticoagulents-synthesis and application of warfarin, Coumachlor, Vacor, Coumatetrallyl, Dicoumarol and Bromodiolen.b) Acute poisons- application of pindone,Ratindan,SodiumFluoroacetate ,Barium fluoroacetate,Antu,Tetramine,pindone and castrix.

**Referencebooks:**


1) Naturally occurring insecticides: M.Jacobson and D.G.Crosby.
2) Insecticides for future:Jacobson
3) Insect juvenile harmone chemistry and action : J.J Mann and M.Beroza
4) Polygodial and warburganal.Terpenoidantifeedants part-II rec,Tran,chin 106
5) Insect antifeedants :S.V.ley&P.L Toogood,chemistry in Britain ,Jan 1990 P.31
6) Synthesis of Insecticides :Metcalf
7) Fungicides-Frear
8) Fungicides-Nene
9) Residue reviews vol.36 : Melnikov
10) Safer insecticides :E.Hodgson
11) Crop protection agents from Nature: leonard G Copping
12) Biofertilizers and Bioinsecticides : A.M.Deshmukh
13) Insecticides and Fungicides :U Sriramulu.
14) Organo chlorine insecticides : persistent organic pollutants :F.Moriary
15) Herbicides :P.C.Kearney&D.D.Kaufnan
16) Analytical Method for pesticides :Z.Weig (Vol III)
17) Pesticide formulations :Van Valkenburg
18) Insecticides :A.S.Tahori
19) Herbicides,fungicides,formulation chemistry-A.S.Tahori
20) Environmental pollution by pesticides :C.A.Edwards
21) Pespticides managements and insecticide resistance :Watson and brown
22) Organo phosphorous pesticides M.eto

## Laboratory courses:

**Paper CH (O) 351P: Synthesis of organic molecules, isolation of natural products & TLC**

**(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.

**(C)Thin layer chromatography :**Thin layer chromatography: Determination of purity( All the above preparations) , monitoring the progress of chemical reactions (any of the four above preparations), identification of unknown organic compounds by comparing the $R_f$ values of known standards.

**Paper CH (O) 352P: Separation and identification of organic compounds & Column chromatography**

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 **09** mixtures should be separated and analyzed by these procedures.

**Cannizzaro reaction:** 4-Chloro benzaldehyde as substrate and separation of the resulting two component mixture

Separation of three component mixtures by chemical methods. A minimum of two mixtures should be separated and analyzed.

**Column chromatography**: Separation of a mixture of *ortho* and *para*-nitroanilinesand any one of the two component mixture using silica gel as adsorbent and chloroform as the eluent. The column chromatography should be monitored by TLC.

**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

**M.Sc. ORGANIC CHEMISTRY SPECIALISATION**
**IV SEMESTER SYLLABUS**
**(For the batch admitted during the academic year 2016-2017)**

**Paper-1 CH (OC) 401T: Drug Design and Drug Discovery**
OC-17: Principles of Drug design and drug discovery
OC-18: Lead modification and SAR Studies
OC 19: QSAR studies and computer aided drug design
OC-20: Combinatorial Synthesis

**Paper-II CH (OC) 402T: Drug synthesis and mechanism of action**
OC-21: Drugs acting on metabolic process, cell wall and specific enzymes
OC-22: Drugs acting on genetic material and immune system
OC-23: Drugs acting on receptors and ion channels
OC-24: Chiral drugs

**Elective-3A Paper-III CH (OC)-403T (CB1): Advanced Heterocyclic Chemistry**
OC (CB1) 17: Non aromatic heterocyclics& aromaticity
OC (CB1) 18: Five and six membered heterocyclics with two hetero atoms
OC (CB1) 19: Heterocyclics with more than two hetero atoms
OC (CB1) 20: Larger ring and other heterocycles

**Elective-3B Paper-III CH (OC)-403T (CB2): Polymers , dyes and Pigments**
OC (CB2) 21: Polymers- I
OC (CB2) 22: Polymers- II
OC (CB2) 23: Dyes-I
OC (CB2) 24:Dyes-II and pigments

**Elective-4A Paper-IV CH (OC) 404(CB3)T: Advanced Natural Products**
OC(CB3)-25: Biosynthesis of natural products
OC(CB3)-26: Structure determination of natural products -I
OC(CB3)-27: Structure determination of natural products-II
OC(CB3)--28: Total stereo selective synthesis of natural products.

**Elective-4B Paper-IV CH (OC) 404(CB4)T: Biopharmaceutics and Pharmacodynamics**
OC(CB4)-29 : Pharmacokinetics
OC(CB4)-30 : Pharmacodynamics
OC(CB4)-31 : Principles of Therapeutics
OC(CB4)-32: Drug Interactions

## Laboratory courses
**Paper-VCH (OC) 451P**: Spectroscopic identification of organic compounds & practice of chemistry software prgrammes
**Paper-VI CH (OC) 452P**: Synthesis and analysis of drugs

**M.Sc. CHEMISTRY (ORGANIC CHEMISTRY)**
**IV SEMESTER SYLLABUS**
**(For the batch admitted during the academic year 2016 -2017 under the CBCS pattern)**

## Paper-1 CH(OC) 401T: Drug Design and Drug Discovery

OC-17: Principles of Drug design and drug discovery
OC-18: Lead modification and SAR Studies
OC 19: QSAR studies and computer aided drug design
OC 20: Combinatorial Synthesis

**OC- 17: 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-18: 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-19: QSAR studies and computer aided drug design** **15Hrs**

**QSAR:**Introduction, physicochemical properties - pKa, electronic effects and Hammett constants($\sigma$), lipophilicity constant($\pi$), steric effects and Taft's constant, linear and nonlinear relationship between biological activityLipophilicity Substituent constants. Lipinski rule of five. Hansch analysis, Craig's plot,Topliss scheme, Free Wilson approach, cluster significant analysis. Two case studies (QSAR study on pyranenamine and design of Crizotinib).

**Computer aided drug design:** Introduction, active site, allosteric binding site,use of grids in docking , rigid docking , flexible docking and induced fit docking of ligands. Basic principles and difference between structure and ligand based drug design, denovo drug design and utility to optimize the lead structure.

**OC-20: 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.

**Reference 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 Harikishansingh
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 PovlKrogsgaard – 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.

http://www.pfizer.com/news/featured_stories/featured_stories_martin_edwards.jsp

## Paper-II CH (OC) 402T: Drug synthesis and mechanism of action

OC-21: Drugs acting on metabolic process, cell wall and specific enzymes
OC-22: Drugs acting on genetic material and immune system
OC-23: Drugs acting on receptors and ion channels
OC-24: Chiral drugs

**OC-21: 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-22: 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 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-23: 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- receptoragonists and antagonists- Biosynthesis of Dopamine. Synthesis of L-Dopa and Chlorpromazine.
d)Serotonin receptors: Introduction and classification.Serotonin receptoragonists 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-24: 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.

**Reference 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. Foyeetal.
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 Harikishansingh.
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

## Elective-3A

## Paper-III CH (OC)-403T (CB1): Advanced Heterocyclic Chemistry

OC (CB1) 17: Non aromatic heterocyclics& aromaticity
OC (CB1) 18: Five and six membered heterocyclics with two hetero atoms
OC (CB1) 19: Heterocyclics with more than two hetero atoms
OC (CB1) 20: Larger ring and other heterocycles

**OC (CB1) 17: Nonaromatic heterocyclics& Aromaticity15 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, Oxetanesandthietanes

**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) 18: 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) 19: 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) 20: Larger ring and other Heterocycles 15 Hrs**

Synthesis, structure, stability and reactivity ofAzepines, Oxepines and Thiepines. Synthesis of Diazepines rearrangements of 1,2 - diazepines. Synthesis of Benzoazepines, Benzodiazepines, Benzooxepines, Benzothiepines, Azocines and Azonines. Synthesis of selenophenes, Tellerophenes,Phospholesand 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-3B

## Paper-III CH (OC)-403T (CB2): Organic Polymers, Dyesand Pigments

OC (CB2) 21: Polymers- I
OC (CB2) 22: Polymers- II
OC (CB2) 23: Dyes-I
OC (CB2) 24:Dyes-II and pigments

**OC (CB2) 21:Organic Polymers - I15 Hrs**

Introduction, Classification of Polymers – according to origin, structure, intermolecular interactions. Types of polymerization – addition, condensation, radical, ionic and coplymerization with mechanism, Ziegler-Natta polymerization with mechanism. Stereochemistry of polymers, Plasticity – types of plastics. Molecular mass of polymers. Resins and plastics – Polystyrene and styrene copolymers, poly(vinyl chloride/vinyl acetate)and related polymers, acrylic polymers, polyesters, phenol-formaldehyde polymers, polyurethanes and epoxide polymers with examples. Natural and synthetic rubbers.

**OC (CB2) 22: Organic Polymers - II 15 Hrs**

a) Functional polymers :

i) Electrically conducting polymers: Introduction, basic principles. Brief description of polyanilines, polypyrroles, polyacetylenes, polythiophenes and their applications.

ii) Photoconductive polymers: Liquid crystal polymers, smectoc, nematicamd cholesteric structures, ion-exchange polymers – cationic, anionic exchange polymers and their uses.

iii) Smart materials: Uses in sensing device and communication networks.

iv)Biodegradable polymers: Definition, classification. Brief description polyhydroxyalkanoates, polycaprolactones, polyactic, polyvinyl alcohol and their applications.

b) Membranes: Filtration, micro, ultra, nano filtration. Separation of gases-Permeselectivity and gas permeability representative polymers. Liquid separation-dialysis, electroosmosis and reverse osmosis.

c) Fire retarding polymers and photonic polymers.

Polymers in biomedical application, artificial organs and controlled drug delivery.

**OC (CB2) 23: Dyes – I 15 Hrs**

**Synthetic and Natural dyes**

Introduction, nomenclature and classification of synthetic dyes. Color and constitution - chromospheres and auxochromes with suitable examples, Witt's theory, Armstrong's theory, Baeyer's theory, Nietzki's theory, Waston's theory, Modern theories, Valence Bond Theory and Molecular orbital theory. Chemistry and synthesis of triphenyl methane dyes[malachite green, rosaniline, para aniline blue, crystal violet methyl violet, hydroxytriphenyl methane dyes, Aurin, chrome violet], Azo dyes - types of azo dyes, synthesis of acidic and basic azo dyes, mono azo, di azo, tri azo and poly azo dyes. Chemistry and synthesis of cyanine dyes. Natural dyes – structure determination and synthesis of alizarine, Quinazarin and Indigo.

**OC (CB2) 24:Dyes–II and Pigments 15 Hrs**

a)**Introduction to Fluorescence dyes**

Interaction of organic molecules with electromagnetic radiation. Energy diagram. Activation and deactivation of organic molecules by light. Fluorescence and delayed fluorescence. Effect of molecular structure on fluorescence. General properties of fluorescent dyes and their requirements. Triplet-triplet absorption of organic molecules. Fluorescent quantum

yields and factors affecting them. Synthesis of Fluorescent aromatic hydrocarbons. and Fluorescent heteroaromatic compounds.

b)**Introduction to laser dyes**. Synthesis of Oligophenylenes. Oxazoles and benzoxzoles. Stilbenoid compoundsCoumarin laser dyes, Rhodamine laser dyes.

c) **Pigments:** Introduction, Structures of Porphyrins , Bile pigments. Synthesis of Haemin and Chlorophyll. Synthetic pigments – preparation of phthalocyanines.

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**ReferenceBooks**


1.Organic polymer chemistry by K.J.Sanders
2. Polymer syntheses, Vol.I by S.R.Sandler and W.Karo
3. The elements of Polymer Science and Engineering by A.Rudin
4. Principles of Polymer Chemistry by A.Ravve
5. Polymer Science by V.R.Gowariker , N.V.Viswanathan and J.Sreedhar
6. Polymer Chemistry by C.E.Carraher , Jr.
7. A text book of polymers, Vol. I,II,III, M.S. Bhatnagar , S. Chand
8. Polymer Chemistry, B. Vollmert
9. Textbook of Polymer Science, F. W. Billmeyer Jr, John Wiley & sons
10. Organic Chemistry , Vol.1,2 by I.L.Finar
11. Color and constitution of organic molecules by J.Griffiths
12. Functional Dyes, Elsevier BV 2006,,,,,,S H.KIM
13. Colorants for non-textile Applications, Elsevier BV 2000 …H S Freeman and A T Peters
14. Industrial Dyes-Chemistry, Properties, Applications. WILEY-VCH Verlag, 2003 Klaus Hunger
15. Introduction to Fluorescence Sensing, Springer 2009, by A P Demchenko
16. Natural Dyes and their Applications in Textiles by M. L. Gulrajani, IIT Delhi
17. Handbook on Natural Dyes for Industrial Applications by P. S. Vankar, National Institute of Industrial Research
18. Steroelectronic Effects in Organic Chemistry by Pierre Deslongchams, Pergamon Press
19. Chemistry and Biochemistry of plant pigments, Vol. 2, by T.W.Goodwin
20. Contemporary Polymer Chemistry, H. R. Alcock& F. W. Lambe, Prentice Hall
21. Materials scince and engineering an introduction by William D Callister, Jr. Wiley Publishers

## Elective-4A(ID Paper)
## Paper-IVCH (OC) 404(CB3)T: Advanced Natural Products

OC(CB3)-25: Biosynthesis of natural products
OC(CB3)-26: Structure determination of natural products-I
OC(CB3)--27: Structure determination of natural products-II
OC(CB3)--28: Total stereo selective synthesis of natural products.

**OC(CB3)-25: 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)-26:Structure determination of natural products-I15Hrs**

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

**OC(CB3)-27: Structure determination of natural products-II 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(CB3)-28: 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.

**Reference 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 3rdEd.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

**Elective-4B(ID Paper)**
**Paper-IV CH (OC) 404(CB4)T: Biopharmaceutics and Pharmacodynamics**

OC(CB4)-29 : Pharmacokinetics
OC(CB4)-30 : Pharmacodynamics
OC(CB4)-31 : Principles of Therapeutics
OC(CB4)-32: Drug Interactions

**OC(CB4)-29: Pharmacokinetics.**
Introduction and importance of ADME studies of drugs. Routes of administration . i)Absorption: Definition, absorption of drugs across the membranes. Physico chemical factors affecting the drug absorption (emphasis on pH partition hypothesis and Drug Dissolution). Methods of determination of drug absorption. Bioavailability. ii)Distribution: Apparent volume of drug distribution. Factors affecting distribution, plasma protein binding. iii) Metabolism: Sites of drug metabolism, metabolic rate constant, bioactivation and biotransformation of drugs ( phase I and phase II reactions) iv)Elimination: Types of elimination and overall apparent elimination rate constant and half-life, concept of clearance.

**OC(CB4)-29: Pharmacodynamics.**
Introduction, targets for drug action, receptor concept. Pharmacological binding terms. Two-statereceptor model, receptor families- structure and signal transduction mechanisms- channel linked proteins, gating mechanism, G-protein coupled receptors, G-protein and their role, Targets for G-proteins, Kinase linked receptors, receptors that regulate gene transcription. Theories of concentration -response relationship, dose-response curves.

**OC(CB4)-30: Principles of Therapeutics**
Plasma Drug concentration vs Time profile,Definition and explanation of various terms: MEC, MSC, MTC, AUC(graph). Peak plasma concentration, time of peak concentration. Therapeutic range. Steady state concentration, onset of action, onset of time, duration of action, intensity of action. LD50, ED50. Therapeutic objective. Dosage regimen, Design of dosage regimes: Dose size, dosing frequency, drug accumulation during multiple dosing, time to reach steady-state during multiple dosing, average concentration and body content on multiple dosing to steady state, loading dose, maintenance dose, maintenance of drug within the therapeutic range, design of dosage regimen from plama concentration. Kinetics of fixed dose, fixed time interval regimes. Modification to dosage regime: Dosing of drugs in obese patients, dosing of drugs in Neonates, infants & children, dosing of drugs in geriatrics (elderly), dosing of drugs in Hepatic disease, dosing of drugs in renal disease.

**OC(CB4)-31: Drug Interactions.**
Introduction, classification, Mechanisms of drug interactions.– pharmacokinetic interactions(alteration of gastrointestinal absorption, compexation and adsorption, alteration of distribution, alteration of metabolism and alteration of excretion) & pharmacodynamic interactions (antagonistic effects, synergistic effects, alteration of electrolyte levels, interactions involving adrenergic system, alteration of receptor site interaction and antibiotic combinations). Influence of alcohol( Anti biotics, Anti coagulants, Anti histamines, Anti psychotic drugs, sedatives and Hypnotics), smoking( Theophylline, Diazepam, a Tri cyclic antidepressants), food ( Bronchodaliators, Diuretics, ACE Inhibitors, Anti coagulants,Tetracyclines) on drug action.

**Reference books:**


1. Pharacokinetics. By Shobha Rani
2. Elements of Pharmacology. By Gandhi,Desani& Goyal.
3. Goodmann&Gilmann's " The pharmacological basis of therapeutics. By Gilman &Rali.
4. Pharmacology. By Rang.
5. Biopharmaceutics and pharmacokinetics By Brahmanikar
6. Pharmacology By Lippincot
7. Modern Pharmacology with Clinical Applications. By R.Craig.
8. Compehensive pharmacy review by Leon Shargel
9. Hospital and clinical pharmacy
10. Burger's medicinal chemistry and drug discovery. By Manfred E. Wolf.
11. Introduction to Medicinal chemistry. By Patrick.
12. Comprehensive medicinal chemistry. Vol 1-5 By Hanzsch.
13. Principles of medicinal chemistry. By William Foye
14. Biochemical approach to medicinal chemistry. By Thomas Nogrady.

## Laboratory courses

**Paper CH (OC) 451P: Spectroscopic identification of organic compounds & practice of chemistry software prgrammes**

1. Identification of unknown organic compounds by interpretation of IR, UV, $^{1}H$ -NMR, $^{13}C$ NMR, and mass spectral data( two examples with 2D-NMR). A minimum of 30 representative examples should be studied.

**2. Chemistry software programmes:** Chem Draw, analysis of IR and NMR using ACD/Id NMR processor. EXCEL: Drawing graphs, Molecular docking.

**Paper CH (OC) 452P: Synthesis and analysis of drugs**

**(A) Laboratory Synthesis of the following drugs:**

Paracetamol, Phenytoin, Benzocaine, 6-Methyluracil, Chloritone,FIuorescien, 4-Aminobenzene sulfonamide, antipyrineand phenothiazine

**(B) 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), Riboflavin (UV-Visible Spectrophotometer).

**Reference 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