

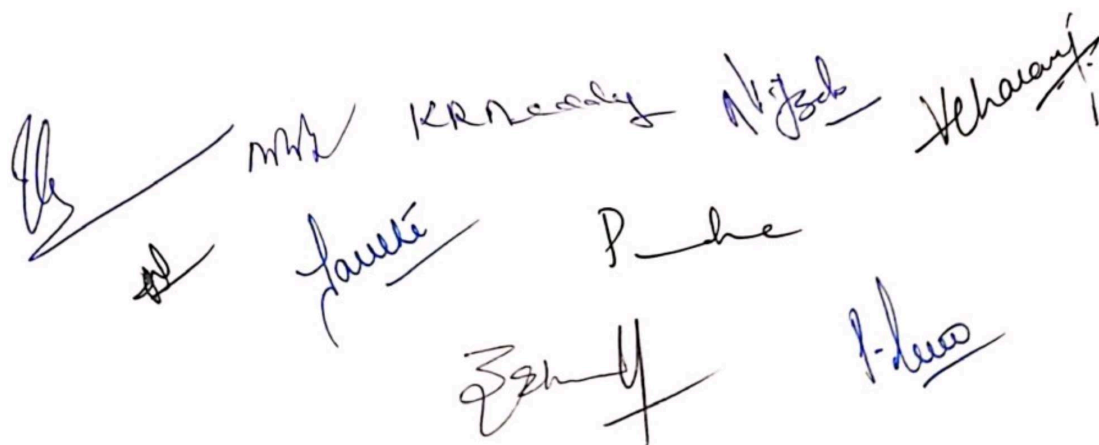
**DEPARTMENT OF CHEMISTRY**  
**OSMANIA UNIVERSITY**  
 (Effective from academic year 2023-2024 for Campus, Constituent and  
 Affiliated colleges)

**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
<b>Total</b>				<b>600 marks</b>	<b>20</b>

**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
<b>Total</b>				<b>600 marks</b>	<b>20</b>



## 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-Teller 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-

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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, 3<sup>rd</sup> 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, 2<sup>nd</sup> Edition, John Wiley & sons Ltd. (2010)
5. Advanced Inorganic Chemistry, F.A.Cotton & G.Wilkinson, 3<sup>rd</sup> Edition, Wiley Interscience Publications (1972).
6. Advanced Inorganic Chemistry. F.A.Cotton, G.Wilkinson, C.A.Murillo & M.Bochmann, 6<sup>th</sup> Edition, Wiley Interscience Publications N.Y (1999).
7. Inorganic Chemistry, J.E. Huheey, K.A.Keiter and R.L.Keiter, 4<sup>th</sup> 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, 33<sup>rd</sup> 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-I

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 ( $C_n$  &  $S_n$ ). 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 asymmetric transformation.

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

**OC-02: Reaction mechanism-I**

**15 hrs**

**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 experiments. 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  $\alpha$ -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 conformational analysis.

**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 equilibrium. 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.

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**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, orthogonality, 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

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**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. Conjugated dienes, trienes and polyenes. Unsaturated carbonyl compounds, Benzene, mono substituted derivative (Ph-R), di-substituted derivative (R-C<sub>6</sub>H<sub>4</sub>-R') and substituted benzene derivatives (R-C<sub>6</sub>H<sub>4</sub>-COR').

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

**<sup>1</sup>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 <sup>1</sup>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). <sup>1</sup>H-NMR of organic molecules and metal complexes: ethyl acetate, 2-butanone, mesitylene, paracetamol, aspirin, ethylbenzoate, benzyl acetate, 2-chloro propionic acid, [HNi(OPEt<sub>3</sub>)<sub>4</sub>]<sup>+</sup>, [HRh(CN)<sub>5</sub>] (Rh I= 1/2).

**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.

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**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 in 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

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## Practicals

### Paper CH 151: Inorganic chemistry Lab course

4 hrs/week

#### I. Preparation of complexes

1. Hexaammine nickel (II) chloride.
2. Tris (acetylacetonato) 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  $\text{Fe}^{2+}$  by cerimetry
9. Estimation of  $\text{Ni}^{2+}$  by complexometry (direct titration method)
10. Estimation of  $\text{Cu}^{2+}$  by complexometry (direct titration method)
11. Estimation of  $\text{Ca}^{2+}$  by complexometry (substitution titration method)
12. Estimation of  $\text{Ni}^{2+}$  by complexometry (back titration method)
13. Estimation of  $\text{Al}^{3+}$  by complexometry (back titration method)

#### IV. One component Gravimetric Analysis

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

#### References

1. Text book of Quantitative Inorganic Analysis, 3<sup>rd</sup> edition, A.I.Vogel, ELBS (1969)
2. Vogel's text book of Quantitative Inorganic analysis, 4<sup>th</sup> edition, Jeffery etal, ELBS (1988).
3. Vogel's text book of Quantitative Inorganic Analysis, 6<sup>th</sup> 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

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- 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<sup>-</sup> 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

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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 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  $\text{CuSO}_4$  solution.
15. Verification of Beer's law and calculation of molar extinction coefficient using  $\text{KMnO}_4$  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

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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<sup>1</sup>, SN<sup>2</sup>). Langford-Gray classification: A mechanism, D-Mechanism, I-Mechanism I<sub>a</sub>, I<sub>d</sub>, 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<sup>1</sup>CB 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<sup>n</sup> and d<sup>n</sup> 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<sup>1</sup>, p<sup>2</sup>, d<sup>1</sup> and d<sup>2</sup> 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<sup>1</sup>, d<sup>4</sup>, d<sup>6</sup>, d<sup>9</sup> (ii) d<sup>2</sup>, d<sup>3</sup>, d<sup>7</sup>, d<sup>8</sup> (iii) d<sup>5</sup> 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<sub>3</sub> and M<sub>4</sub> clusters, structural patterns in M<sub>3</sub>(CO)<sub>12</sub> (M=Fe, Ru, Os) and M<sub>4</sub>(CO)<sub>12</sub> (M=Co, Rh, Ir) clusters. High nuclearity carbonyl clusters: M<sub>5</sub>, M<sub>6</sub>, M<sub>7</sub>, M<sub>8</sub> and M<sub>10</sub> clusters. Polyhedral skeletal electron pair theory

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and Total electron count theory. Capping rule. Structural patterns in  $[\text{Ni}_5(\text{CO})_{12}]^{2-}$ ,  $[\text{Os}_6(\text{CO})_{18}]^{2-}$ ,  $[\text{Os}_7(\text{CO})_{21}]$ ,  $[\text{Os}_8(\text{CO})_{22}]^{2-}$  and  $[\text{Os}_{10}\text{C}(\text{CO})_{24}]^{2-}$ . Metal carbonyl scrambling, stereo chemical non-rigidity in  $[\text{Rh}_4(\text{CO})_{12}]$  and  $[\text{Fe}_2(\text{Cp})_2(\text{CO})_4]$ .

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

**Metal Nitrosyls:** Bonding modes of NO: Terminal (linear, bent) and bridging. Structural aspects of  $[\text{IrCl}(\text{PPh}_3)_2(\text{CO})(\text{NO})]^+$  and  $[\text{RuCl}(\text{PPh}_3)_2(\text{NO})_2]^+$ . Stereo chemical control of valence in  $[\text{Co}(\text{diars})_2(\text{NO})_2]^{2+}$  and  $[\text{Co}(\text{diars})_2(\text{NO})(\text{SCN})]^+$ .

**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  $[\text{Re}_2\text{Cl}_8]^{2-}$  and octahedral halides of  $[\text{Mo}_6(\text{Cl})_8]^{4+}$  and  $[\text{Nb}_6(\text{Cl})_{12}]^{2+}$ .

## 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, 2<sup>nd</sup> 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, 6<sup>th</sup> Edition, Wiley Interscience, N.Y (1999)
7. Principles of Inorganic Chemistry, Puri,Sharma, Kalia, 33<sup>rd</sup> 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, 5<sup>th</sup> 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,  $\sigma$  and  $\pi$ - 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, Sommelet-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 antarafacial additions in  $4n$  and  $4n+2$  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

-Möbius 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 electrocyclic and cycloadditions & cycloreversions.

**OC-06 Organic Photochemistry**

**15hrs**

**Photochemistry:** Introduction, photochemistry of  $\pi-\pi^*$  transitions: Excited states of alkenes, cis-trans isomerisation, and photo stationary state. Photochemistry of 1,3-butadiene, di- $\pi$  methane

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rearrangement. Intermolecular reactions, photocycloadditions, photodimerisation of simple and conjugated olefins. Addition of olefins to  $\alpha$ ,  $\beta$ -unsaturated carbonyl compounds. Excited states of aromatic compounds, Photoisomerisation of benzene.

**Photochemistry of ( $n-\pi^*$ ) transitions:** Excited states of carbonyl compounds, homolytic cleavage of  $\alpha$ - bond, Norrish type I reactions in acyclic and cyclic ketones and strained cycloalkane 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 1,2-diketones, 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 Fleming.
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

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**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 Lindemann'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 plots and boundary diagrams.

**Many electron systems:** Approximate methods. The variation method-variation theorem and its proof. Trial variation function and variation integral. Examples of variational calculations. 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  $T_c$  superconductivity in cuprates. Phase diagram of Y-Ba-Cu-O system. Crystal structure of  $YBa_2Cu_3O_{7-x}$ . Preparation of 1-2-3 materials. Origin of high  $T_c$  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 applications, 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.

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**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  $\text{SO}_4^{2-}$ , metal ions viz.,  $\text{Mg}^{2+}$ ,  $\text{Zn}^{2+}$ ,  $\text{Cu}^{2+}$  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 ( $^1\text{H}$ ,  $^{19}\text{F}$  and  $^{31}\text{P}$  NMR) and solid state NMR spectroscopy:**

First order and non-first order spectra e.g., AX, AX<sub>2</sub>, AX<sub>3</sub>, A<sub>2</sub>X<sub>3</sub>, 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,  $[\eta^1\text{-C}_5\text{H}_5\text{M}]$ ,  $[\eta^5\text{-(C}_5\text{H}_5)_2\text{Ti}\eta^1\text{-(C}_5\text{H}_5)_2]$  and  $[\eta^4\text{-C}_8\text{H}_8\text{Ru(CO)}_3]$ .

**$^{19}\text{F}$  NMR spectroscopy:**  $^{19}\text{F}$  chemical shifts, coupling constants. Applications of  $^{19}\text{F}$  NMR involving coupling with  $^{19}\text{F}$ ,  $^1\text{H}$  and  $^{31}\text{P}$ : 1,2-dichloro-1,1-difluoro ethane,  $\text{BrF}_5$ ,  $\text{SF}_4$ ,  $\text{PF}_5$ ,  $\text{ClF}_3$ ,  $\text{IF}_5$ ,  $\text{CF}_3\text{CH}_2\text{OH}$ .

**$^{31}\text{P}$  NMR spectroscopy:**  $^{31}\text{P}$  chemical shifts, coupling constants. Applications of  $^{31}\text{P}$  NMR involving coupling with  $^{31}\text{P}$ ,  $^{19}\text{F}$ ,  $^1\text{H}$  and  $^{13}\text{C}$ : ATP,  $\text{Ph}_3\text{PSe}$ ,  $\text{P}_4\text{S}_3$ ,  $\text{H}_3\text{PO}_4$ ,  $\text{H}_3\text{PO}_3$ ,  $\text{H}_3\text{PO}_2$ ,  $\text{HPF}_2$ ,  $\text{PF}_6^-$ ,  $\text{PH}_3$ ,  $[\text{Rh}(\text{PPh}_3)_3\text{Cl}]$  (Rh: I= 1/2).

**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.

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## 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  $\beta$ -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, 3<sup>rd</sup> edition, A.I.Vogel, ELBS (1969)
2. Vogel's text book of Quantitative Inorganic analysis, 4<sup>th</sup> edition, Jeffery etal, ELBS (1988).
3. Vogel's text book of Quantitative Inorganic Analysis, 6<sup>th</sup> 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,(Lassaigne 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 benzaldehyde
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 I<sub>2</sub> between cyclohexane and water
2. Distribution of I<sub>2</sub> 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<sup>-</sup> vs Ag<sup>+</sup> (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



## 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 & Spectroscopy 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, <sup>1</sup>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<sup>2+</sup> vs Cr<sub>2</sub>O<sub>7</sub><sup>2-</sup> (redox titration)
13. Fe<sup>2+</sup> vs Ce<sup>4+</sup> and calculation of formal redox potential of Fe(II)/Fe(III)
14. Fe<sup>2+</sup> vs MnO<sub>4</sub><sup>-</sup> 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, 6<sup>th</sup> 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**  
**PHARMACO INFORMATICS SPECIALISATION**  
**SYLLABUS (2017 – 18) ONWARDS**

**III and IV SEMESTERS**  
**(2017 - 2018)**

**FOR STUDENTS ADMITTED IN THE YEAR (2016 – 17)**  
**UNDER INNOVATIVE INTERDISCIPLINARY PROGRAM OF**  
**UGC REVISED AS PER NEW (CB) SYLLABUS**  
**APPROVED IN BOS ON \_\_\_\_\_**



## M. Sc. CHEMISTRY (PARMACOINFORMATICS)

### Syllabus for III and IV Semesters

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

*[Under Restructured CBCS Scheme]*

(Approved in the P.G. BOS meeting held on \_\_\_\_\_ )

#### Semester - III

	Instruction Hrs/week	Internal assessment marks	Semester marks*	Total	Total Credits
CH(CPI) 301T	4	20	80	100	4
CH(CPI) 302T	4	20	80	100	4
CH(CPI) 303T (CB)	4	20	80	100	4
CH(CPI) 304T (CB)	4	20	80	100	4
CH(CPI) 351P	9	--	100	100	4
CH(CPI) 352P	9	--	100	100	4
<b>Total</b>				<b>600</b>	<b>24</b>

\*Theory: 3 hours; Practical's: 6 hours

#### Semester - IV

	Instruction Hrs/week	Internal assessment marks	Semester marks*	Total	Total Credits
CH(CPI) 401T	4	20	80	100	4
CH(CPI) 402T	4	20	80	100	4
CH(CPI) 403T (CB)	4	20	80	100	4
CH(CPI) 404T (CB)	4	20	80	100	4
CH(CPI) 451P	9	--	100	100	4
PROJECT	9	--	100	100	4
<b>Total</b>				<b>600</b>	<b>24</b>
(Choice based paper (CB) = Paper offered by the same Department)					

\*Theory: 3 hours; Practical's: 6 hours

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

## SEMESTER – III

### **PAPER- I :CH(CPI)301 T : Database Management, Sources and Scripting Languages**

CPI - 09 : Chemical Information Sources and Searches  
CPI - 10 : Database Design and Management  
CPI - 11 : Data Sequencing and Mining  
CPI - 12 : Scripting Languages

### **PAPER-II: CH(CPI)302 T : Computational Chemistry ,Molecular Modeling & Its Applications.**

CPI – 13 : Computational Chemistry -I  
CPI – 14 : Computational Chemistry -II  
CPI – 15 : Drug Design Methods I - Ligand Based  
CPI – 16 : Drug Design Methods II - Structure Based

### **PAPER-III: CH(CPI)303 T: ELECTIVE 3A: Synthetic Reagents, Advanced NMR, Conformational Analysis and ORD**

CPI - 17 : Synthetic Reagents-I  
CPI - 18 : Synthetic Reagents-II  
CPI - 19 : <sup>13</sup>C NMR and 2D NMR spectroscopy  
CPI - 20 : Conformational analysis (Cyclic systems) & ORD

### **PAPER-III: CH(CPI)303 T:ELECTIVE 3B: Advanced Natural Products**

CPI-21: Biosynthesis of natural products  
CPI-22: Structure determination of natural products by chemical methods.  
CPI-23: Structure determination and stereochemistry of natural products by spectral methods.  
CPI-24: Total stereo selective synthesis of natural products.

### **PAPER-IV: CH(CPI)304 T:ELECTIVE 4A: Modern Organic Synthesis**

CPI - 25 : Asymmetric Synthesis  
CPI - 26 : Synthetic strategies  
CPI - 27 : New Synthetic reactions  
CPI - 28 : Chiral Drug

### **PAPER-IV : CH(CPI)304 T:ELECTIVE 4B: Intellectual Property Rights**

CPI - 29 : Introduction  
CPI - 30 : International Organizations & Treaties  
CPI - 31 : Patent Search  
CPI - 32 : IP Reports Generation

### **LABORATORY COURSES**

PAPER-V :CH(CPI)351 P : Molecular Modeling Lab

PAPER-VI :CH(CPI)352 P : Synthesis, Isolation and Mixture separation of Organic Compounds

## **SEMESTER – III**

### **PAPER - I**

#### **CH(CPI)301T: DATABASE MANAGEMENT, SOURCES AND SCRIPTING LANGUAGES**

CPI - 09: Chemical Information Sources and Searches

CPI - 10: Database Design and Management

CPI - 11: Data Sequencing and Mining

CPI - 12: Scripting Languages

#### **CPI – 09 : Chemical Information Sources and Searches**

Introduction to information sources and searching strategies, tactics for searches, Advantages and Limitations of computer searching, Keyword based general bibliographic searches, Chemical connectivity and structure searches (2D), Chemical structure, property and shape based searches (3D), Searching for the synthesis (or) reactions of specific compounds or classes of compounds, Searching of chemical abstracts.

Types of Publications: Journals, Technical reports, Patents, Conference Papers, Dissertations, Electronic Publications.

Types of databases: Public databases - NCBI, RCSB, CSD, Expasy, Swiss-Prot and Paid databases - CAT'STN and SciFinder.

Web-based cross platform solutions for Cheminformatics: BLAST, ClustalW, SAVES, ProSA.

#### **CPI – 10 : Database Design and Management**

Introduction to Computers and it's components, Operating System (Windows & Linux).

Introduction to DBMS, Database concepts, Database models and ER diagrams, Normalization.

Introduction to SQL, DDL, DML, DCL, and TCL; Creation of databases, Searching database using SQL, Built-in-functions, String manipulation, improving query performance (where, 'Group By', having Clause), cursors, stored procedures. Introduction to MySQL, configuring and running MySQL on Linux. Data Processing, Information systems and computing, Data presentation for computing, Distributed processing.

#### **CPI – 11: Data Sequencing and Mining**

Introduction to Data Mining, working principles of Data Mining, Architecture form of data Mining, Difference between Data Mining and Machine learning techniques, Supervised and unsupervised learning methods and its application to QSAR. Data Visualization: Visualizing Data mining models, Decision Tree. Data warehousing: Data mining and analytic technology, Comparing different Models using visualization.

#### **CPI – 12 : Scripting Languages**

Introduction to Shell scripting, Common Linux commands (Bash), Basic shell Programming: addition, subtraction, loops, conditional-loops, un-conditional loops, Linux text editors (Vi).

**Perl:** Introduction, basics, sequences, uses, implementation issues, changes from other languages, advantages, and disadvantages. Strings: operations, support with Perl, advantages, accessing MySQL database using Perl, getting id, Sequence from a Database Object, matching a sequence in a Database Object, Subroutines. Introduction to Bio-Perl, Perl for Cheminformatics / Bioinformatics.

#### **References**

1. MySQL (TM): The Complete Reference by Jeremy D. Zawodny and Derek J. Balling. O'Reilly & Associates, April 2004.
2. Data Mining: Concepts and Techniques by Jiawei Han and Micheline Kamber, Third Edition, 2012, Elsevier Inc.

3. Mastering UNIX Shell Scripting by Randal K. Micehal Wiley Publisher, Inc, Indianapolis, Indiana.
4. Upgrading and Repairing PC's by SCOTT MUELLER's.
5. Data Mining Techniques by Arun K. Pujari.
6. Perl Tutorial by Chan Bernard Ki Hong
7. Bio-Perl Course by Catherine Letondal and Katja Schuerer.
8. Quick, Painless Introduction to the Perl Scripting Language. Norman Matloff. University of California, Davis c 2002 - 2007.

## PAPER-II

### **PAPER-II: CH(CPI)302 T : Computational Chemistry ,Molecular Modeling &Its Applications.**

CPI – 13 : Computational Chemistry -I

CPI – 14 : Computational Chemistry -II

CPI – 15 : Drug Design Methods I - Ligand Based

CPI – 16 : Drug Design Methods II - Structure Based

#### **CPI – 13: Computational Chemistry – I**

Introduction to Molecular Modeling, Single molecule calculations, assemblies of molecules and reactions of molecules - Co-ordinate systems: Cartesian and Internal Co-ordinates, Z-matrix - Potential energy surface - Conformational search; Global minimum, Local minimum, Conformational analysis of ethane - Force field ; Features of Molecular Mechanics, Bonded and Non-bonded interactions, Bond Stretching, Angle Bending, Torsional Terms (Improper Torsions, out of Plane Bending Motions, Cross Terms), Non Bonded Interactions (Electrostatic Interactions, Van-der Waals interactions), Hydrogen Bonding Interactions.

#### **CPI – 14: Computational Chemistry - II**

Force Field Equation in Energy minimization (Energy as function of  $r$ ,  $\theta$ ,  $\omega$ ) - Introduction to Derivative Minimization Methods (First Order Minimization), Types of energy minimization Methods; Steepest Descent, Conjugate Gradient, Conformational Search procedures - Geometry optimization procedures - Molecular Dynamics: Introduction, description of Molecular Dynamics, basic elements of Monte-Carlo method, differences between Molecular Dynamics and Monte-Carlo method, Qualitative exposure to Molecular Dynamics Simulations.

#### **CPI – 15: Drug Design Methods I - Ligand Based**

Lead Molecule - Structure Activity Relationship (SAR), Quantitative Structure Activity Relationship (QSAR), Distinguish between SAR and QSAR - Physicochemical parameters ; Electronic effects, Hydrophobicity, Steric Factors Taft's Steric function, Molar Refractivity, Verloop Steric factor - Molecular Descriptor analysis: Craig plot, Topliss scheme, Bioisosteres - Hansch model, Free-Wilson model for QSAR equations - Regression analysis: Multi Linear Regression and Partial Least Square (terms:  $n$ , SD,  $r$ ,  $r^2$ ,  $r^2\%$ , F) - Examples for linear and non-linear equations - 3D QSAR: CoMFA and CoMSIA - Differences between 2D and 3D QSAR.

#### **CPI – 16: Drug Design Methods II - Structure Based.**

Database similarity searches - Pair-wise alignment: Global sequence analysis (Needleman-Wunsch), Local Sequence Alignment (Smith Waterman), Multiple Sequence Alignment -

Homology Modeling: Query sequence, Template selection, Alignment, Backbone Modeling, Loop Modeling, Side chain Modeling, Model optimization, Energy minimization - Model Evaluation: Ramachandran Plot, Verify 3D, Errata and ProSA - Active site Identification - Docking, Docking Algorithms: Genetic Algorithm, Incremental construction - Molecular Interactions, Scoring functions - Virtual Screening: Ligand Based and Structure Based. De novo ligand design and its limitations.

### **References:**

1. Molecular Modelling: Principles and Applications, by Andrew Leach, Longman Publications.
2. Computational Chemistry, Guy H. Grant & W. Graham Richards, Oxford University Press.
3. Computational Chemistry: Introduction to the theory and Applications of Molecular and Quantum Mechanics, Errol Lewars, Springer Publications.
4. Recent advances in Bioinformatics by I. A. Khan and A Khanum Ukaaz publications, 2003.
5. Molecular modelling – Basic Principles and Applications by Hans Dieter Holtje and Gerd Folkers, Wiley-VCH, 1996
6. Introduction to Computational Chemistry by Jensen, Wiley Publishers, second edition
7. Bioinformatics – A Primer by P. Narayanan, New Age International, (P) Ltd, 2005.
8. Introduction to Bioinformatics by Arthur M. Lesk, Oxford University Press (Indian. Edition), 2002
9. Principles of Medicinal Chemistry Vol. II by Dr. SS Kadam Pragati books Pvt. Ltd; 2007
10. Principles of Medicinal Chemistry, by Patrick.
11. Bioinformatics: Methods and Applications: Genomics, Proteomics and Drug Discovery. S.C. Rastog, Namita Mendiratta, Parag Rastogi, PHI Larning Pvt. Ltd; 2006
12. Pharmacy Practice Vol.I and II by Remington.
13. Burger's Medicinal Chemistry and Drug Discovery, 5th Edition.
14. Text book of Drug design and Vol.1 discovery 3rd Edition by POVL krogsgaard- larsen tommy liljefors and ULF madsen.

## PAPER-III : CH(CPI)303 T

### ELECTIVE 3A

#### **Synthetic Reagents, Advanced NMR, Conformational Analysis and ORD**

CPI-17: Synthetic Reagents-I

CPI-18: Synthetic Reagents-II

CPI-19:  $^{13}\text{C}$  NMR and 2D NMR spectroscopy

CPI-20: Conformational analysis (Cyclic systems) & ORD

#### **CPI-17: Synthetic Reagents I**

**15 Hrs**

- i) Protecting groups: a) Protection of alcohols by ether, silyl ether and ester formation b) Protection of 1,2-diols by acetal, ketal and carbonate formation c) Protection of amines by benzyloxycarbonyl, t-butyloxycarbonyl, fmoc and triphenyl methyl groups. d) Protection of carbonyls by acetal, ketal and thiol acetal (Umpolung) groups. e) Protection of carboxylic acids by ester and ortho ester (OBO) formation.
- ii) Organometallic Reagents: Preparation and application of the following in organic synthesis: 1) Organo lithium 2) Organo copper reagents 3) Organo boranes in C-C bond formation 4) Organo silicon reagents: reactions involving  $\beta$ -carbocations and  $\alpha$ -carbanions, utility of trimethyl silyl halides, cyanides and triflates.
- iii) Carbonyl methylenation: a) Phosphorous ylide mediated olefination 1) Wittig 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.

#### **CPI-18: Synthetic Reagents II**

**15 Hrs**

- ii) Oxidations: a) Oxidation of active C-H functions: DDQ and  $\text{SeO}_2$ . b) Alkenes to diols: Prevost and Woodward oxidation c) Alcohol to carbonyls: CrVI oxidants (Jones reagent, PCC, PDC) IBX, DMP, CAN, TEMPO, TPAP, Swern oxidation d) Oxidative cleavage of 1,2-diols: Periodic acid and Lead tetra acetate.
- iii) Reductions: a) Catalytic hydrogenation: Homogenous (Wilkinson's catalytic hydrogenation) and heterogeneous catalytic reduction. b) Non-metallic reductions: Diimide reduction c) Dissolving metal reductions: Birch reduction. d) Nucleophilic metal hydrides:  $\text{LiAlH}_4$ ,  $\text{NaBH}_4$ , and their modifications. e) Electrophilic metal hydrides:  $\text{BH}_3$ ,  $\text{AlH}_3$  and DIBAL. f) Use of tri-n-butyl tin hydride: Radical reductions.

#### **CPI-19: $^{13}\text{C}$ NMR and 2D NMR spectroscopy**

**15 Hrs**

- i)  $^{13}\text{C}$  NMR spectroscopy: Introduction, Types of  $^{13}\text{C}$  nmr spectra: uncoupled, proton-decoupled and off-resonance decoupled (ORD) spectra.  $^{13}\text{C}$  chemical shifts, factors affecting the chemical shifts, chemical shifts of organic compounds. Calculation of chemical shifts of alkanes, alkenes and alkynes. Homonuclear ( $^{13}\text{C}$ ,  $^{13}\text{C}$  J) and heteronuclear ( $^{13}\text{C}$ ,  $^1\text{H}$  J and  $^{13}\text{C}$ ,  $^2\text{H}$  J) coupling. Applications of  $^{13}\text{C}$ -NMR spectroscopy: Structure determination, stereochemistry, reaction mechanisms and dynamic processes in organic molecules.  $^{13}\text{C}$ -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) HOMO COSY ( $^1\text{H}$ - $^1\text{H}$  COSY), TOCSY (Total Correlation Spectroscopy), Hetero COSY ( $^1\text{H}$ ,  $^{13}\text{C}$  COSY, HMQC), long range  $^1\text{H}$ ,  $^{13}\text{C}$  COSY (HMBC), Homonuclear and Heteronuclear 2D-J-resolved spectroscopy, NOESY and 2D-INADEQUATE experiments and their applications.

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, tropine, tropane, pseudotropine, decahydroquinoline and quinolizidine. Factors governing the reactivity of axial and equatorial substituents in cyclohexanes.

(oxidation, SN<sub>2</sub> 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 semiempirical rules-The axial haloketone rule, the octant rule, Helicity rule, Exciton chirality method. Application of the rules to the study of absolute configuration and conformations of organic molecules.

**Recommended Books:**

1. Some modern methods of organic synthesis by W. Carruthers
2. Guidebook to organic synthesis, by R K Meckie, D M Smith & R A Atken
3. Organic Synthesis by O House
4. Organic synthesis by Micheal B Smith
5. Reagents for organic synthesis, by Fieser & Fieser, Vol 1-11 (1984)
6. Organic synthesis by Robert E Ireland
7. Handbooks of reagents for organic synthesis by Reich and Rigby, Vol-I-IV
8. Organic chemistry by Jonathan Clayden, Nick Greeves and Stuart Warren
9. Organic Reactions and their mechanisms by P.S.Kalsi
10. Organic reaction mechanisms by V.K.Ahulwalia and Rakesh Kumar Parashar
11. Spectroscopic identification of organic compounds by RM Silverstein, G C Bassler 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-III: CH(CPI)303 T

### ELECTIVE 3B

#### Advanced Natural Products

CPI - 21 : Biosynthesis of natural products

CPI - 22 : Structure determination and stereochemistry of natural products by chemical methods

CPI - 23 : Structure determination and stereochemistry of natural products by spectral methods

CPI - 24 : Total stereo selective synthesis of natural products

#### **CPI - 21 : Biosynthesis of natural products**

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 ( $\beta$ -amyrin) and carotenoids, steroids – cholesterol.

#### **CPI - 22 : Structure determination and stereochemistry of natural products by chemical methods**

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

#### **CPI - 23 : Structure determination and stereochemistry of natural products by spectral methods**

Spectroscopic techniques IR, UV,  $^1\text{Hnmr}$ ,  $^{13}\text{Cnmr}$ , 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,  $^1\text{H}$ ,  $^{13}\text{C}$  NMR, HOMOCOSY, HECTOR, DEPT, 2D-INADEQUATE and NOE of Geraniol, INEPT of menthol, APT of apparicine, Heteronuclear 2D-J resolved spectrum of striticine, NOESY of buxaquamarine, HETEROCOSY of strictanol, 2D-INADEQUATE of  $\alpha$ -picoline and  $\beta$ -methyl tetrahydran furan.

#### **CPI - 24 : Total stereo selective synthesis of natural products**

Nicalou's synthesis of Dynemicin A , Corey's synthesis of prostaglandins (E2, F2 $\alpha$ ) and paeoriflorin, Sharpless synthesis of L-hexoses, Nicolaous synthesis of taxol, Danishefsky synthesis of indolizomycin, Takasago synthesis of menthol, Hoffmann-LaRoche synthesis of Biotin.

#### **Recommended books:**

1. Textbook of organic chemistry, Vol II by I L Finar
2. Chemistry of natural products, Vol 12, by Atta-Ur-Rahman
3. An introduction to the chemistry of terpenoids and steroids, by William templeton
4. Systematic identification of flavonoid compounds by Mabry & Markham
5. Steroids by Fieser and 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 3<sup>rd</sup> Ed. R O C Norman and J M Coxen
15. One and two dimensional nmr spectroscopy by Atta Ur Rahman
16. Classics in total synthesis K C Nicolaou and E J Sorenson
17. Spectrometric identification of organic compounds by Silverstein and Webster

#### **PAPER-IV: CH(CPI)304 T**

#### **ELECTIVE-4A**

##### **Modern Organic Synthesis**

- CPI - 25 : Asymmetric Synthesis
- CPI - 26 : Synthetic strategies
- CPI - 27 : New Synthetic reactions
- CPI - 28 : Chiral Drugs

##### **CPI - 25 : Asymmetric Synthesis**

**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 chirality and Pro-R, Pro-S, Re and Si.

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

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

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

**Chiral auxiliary controlled asymmetric synthesis:**  $\alpha$ -Alkylation of chiral enolates, Evans's oxazolidinone, 1, 4-Asymmetric induction and Prelog's rule..

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

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

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

##### **CPI - 26 : Synthetic strategies**

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

**Order of events** : S-Salbutamol, Propoxycaïne..

**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 of Retronecene, longifoline.

### **CPI - 27 : New Synthetic reactions**

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

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

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

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

**5. Click Chemistry:** Click reaction, 1,3-dipolar cycloadditions.

**6. Metathesis:** Grubb's 1<sup>st</sup> and 2<sup>nd</sup> 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.

### **CPI - 28 : Chiral Drugs**

Introduction to chiral drugs. Eutomer, distomer and eudesmic ratio. Pfeiffer's rule, Three point contact model. Synthesis and pharmacological activity of Menthol, S-Naproxen, S-Ibuprofen (anti inflammatory), S-Timolol, oxazolidone, Captopril, Enalapril, Diltiazam (Calcium antagonist), Indinavir sulphate (HIV-1-protease inhibitor), Ethambutal (anti-tubercular). Cloxacillin, Cephalexin (Antibiotic), Oxybutynine hydrochloride (Antispasmodic Agent), Dexormaplatin (Antitumour Agent), indacrinone (Diuretic), Griseofulvin, (Antifungal) Levocitizine (Antihistamine) and Metoprolol ( $\beta$ 1- blocker).

### **Recommended Books:**

1. Asymmetric synthesis by Nogradi
2. Asymmetric organic reactions by J D Morrison and H S Moscher
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. Organic Drug synthesis By Ledneiser Vol 1-6
14. Strategies for organic drug synthesis and design By Daniel Ledneiser
15. Top Drugs: Top synthetic routes By John Saunders
16. Chirotechnology By Roger A. Sheldon

### **PAPER-IV : CH(CPI)304 T**

#### **ELECTIVE-4B**

#### **Intellectual Property Rights**

- CPI - 29 : Introduction
- CPI - 30 : International Organizations & Treaties
- CPI - 31 : Patent Search
- CPI - 32 : IP Reports Generation

#### **CPI - 29 : Introduction**

Introduction : Legal Rights and obligations, Concept of Property, Kinds of Property, General concept and Significance of Intellectual Property (IP), Intellectual Property Rights (IPR), Intellectual property, Introduction to IPR, contents of IPR and their protection, Recent Developments, IP Organisations. Introduction to Patents, Trademarks, Copyrights, Trade secrets, Industrial designs and Geographical indications.

#### **CPI - 30 : International Organizations & Treaties**

Paris Convention for the Protection of Industrial Property, Berne Convention for the Protection of Literary and Artistic Works, Patent Cooperation Treaty (PCT) which facilitates obtaining of patents in several countries by filing a single application, World Trade Organization (WTO), Trade Related Aspects of Intellectual Property (TRIPS), Madrid system for the international registration of marks, The Hague system for the international deposit of industrial designs, Budapest treaty on the international recognition of the deposit of microorganisms for the purpose of patent procedure, International convention for the protection of new varieties of plants.

#### **CPI - 31 : Patent Search**

What is a patent search. Who needs a patent search. Patent Search Types and Methodologies, Novelty Searches, Validity Searches, Infringement Searches, State-of-the-art searches. Searching in Patent Databases: Free search databases: USPTO, EPSPACE, WIPO, Free Patents Online, Fresh Patents and JSPTO, Paid search databases: Micropat, Delphion, DialogPro, Patent Optimiser, Aureka and PatentCafe, Structure based search: STN search, SciFinder.

#### **CPI - 32 : IP Reports Generation**

Novelty search reports, Infringement search reports, Prior-art search reports, Patent invalidation reports, Competitive search reports, and Business analysis reports, Patent Filing and Drafting, Patent filing procedures, Indian patent act, patent drafting, PCT applications, provisional and complete specifications.

#### **References**

1. Fundamentals of Jurisprudence by Dhyani, Allahabad Publication, Central Law.
2. Jurisprudence of Legal Theory by Dwivedi S.P. Allahabad Central Law Agency.
3. Text Book on Jurisprudence by Hilari WC Cobrey, Oxford Publications.

4. Treaties on Intellectual Property Rights by Blackstone
5. W.T.O. by Myneni, Asia Law House.
6. W.T.O. by Vasudeva, Minerva Publications, Delhi.
7. Law of Practice of Intellectual Property in India by Vikas Vashistha, Bharat Law Publications, Delhi.
8. Intellectual property rights by B L Wadhera, Universal Law Publications.
9. Trade Marks Act by Mittal, Eastern Book Company.
10. Patent Law by Narayana P, Eastern Book Company.

### SEMESTER -III

#### LABORATORY COURSES

#### **PAPER-V: CH(CPI) – 351P: (Molecular Modeling Lab)**

1. Dos and Linux commands
2. Shell Scripting : if, if else, for, do while
3. Perl Scripting : if, if else, for, while
4. Creating Database : Creation of tables and Insertion of rows using MySQL
5. Perl scripting for accessing MySQL database objects using DDL, DML, DCL.
6. Perl scripting for Sequence analysis :
  - a. Translate DNA sequence into RNA sequence
  - b. Finding common Ktup (k = 1, 2, 3) between two sequences
  - c. Local and global alignment of two sequences (DNA/RNA/Protein)
  - d. Multiple sequence alignment
7. Drawing and minimizing molecules in modeling software, calculating physicochemical parameters.
8. 2D QSAR Studies (COX 1 and 2, DHFR inhibitors).
9. 3D QSAR: Pharmacophore model generation and pharmacophore match searching in database.
10. Homology Modeling: Retrieving Query Sequence, Finding Template, Pair-wise alignment, 3D model generation, energy minimization and structure validation.
11. Molecular Docking of COX 1 and 2, DHFR inhibitors into respective receptors.

#### **PAPER-VI:CH(CPI) – 352P : Synthesis, Isolation and Mixture separation of Organic Compounds**

##### **1. Synthesis of Drugs**

Benzocaine (Anaesthetic), Antipyrine (Antipyretic), Sulphonamide (antibacterial), Clofibrate(Anti-lipidemic), 2-phenyl-Indole, Quinoxalinone, Isoniazid (Anti-Tubercular), Benzillic acid rearrangement, Beckmann rearrangement and stereo selective reduction of ethyl acetoacetate by bakers yeast.

##### **2. Isolation of Herbal Drugs:**

1.Piperine from black Pepper 2. Caffeine from tea leaves 3. Cineole from Eucalyptus leaves

##### **3. Mixture Separation – At least 6 mixtures**

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) Solid - Solid - 3 mixtures
- b) Solid - Liquid – 3 mixtures
- c) Liquid - Liquid – 3 mixtures

## SEMESTER – IV

### **PAPER– I :CH(CPI) 401 T: Pharmacokinetics**

- CPI - 33 : Biopharmaceutics
- CPI - 34 : Drug Absorption and Distribution
- CPI - 35 : Drug Metabolism and Excretion
- CPI - 36 : Pharmacokinetic Models

### **PAPER–II:CH(CPI) 402T : Principles of Drug Discovery, Drug Targets and chemistry of Pharmacology**

- CPI - 37 : Principles of Drug Discovery and SAR Studies
- CPI - 38 : General Principles of Pharmacology and drug Targets, drugs acting on ANS and CNS
- CPI - 39 : Drugs Acting on Cardio Vascular and Respiratory System
- CPI - 40 : Drugs acting on metabolic process, cell wall, genetic material and immune system

### **PAPER- III : ELECTIVE 3A: Pharmaceutical Analysis**

- CPI - 41: Spectral Methods in Pharmaceutical Analysis
- CPI - 42: Chromatography in Pharmaceutical Analysis-I
- CPI - 43:Chromatography in Pharmaceutical Analysis-II
- CPI - 44: Titrimetry, Chemical and Extraction methods in Pharmaceutical Analysis

### **PAPER-III: ELECTIVE 3B: Bio organic Chemistry**

- CPI - 45: Carbohydrates and Proteins
- CPI - 46: Nucleic Acids and Lipids
- CPI - 47: Enzymes
- CPI - 48: Coenzymes

### **PAPER-IV: ELECTIVE 4A: Advanced Heterocyclic Chemistry**

- CPI - 49: Non Aromatic Hetero cyclics & aromaticity
- CPI - 50: Five and Six membered hetero cyclics with two hetero atoms
- CPI - 51: Hetero cyclics with more than two hetero atoms
- CPI - 52: Larger ring and other hetero cyclics

### **PAPER- IV : ELECTIVE 4B: Green chemistry and Organic materials**

- CPI - 53: Principles of Green chemistry
- CPI - 54: Green Synthesis
- CPI - 55: Organic nanomaterials
- CPI - 56: Supramolecular chemistry

### **LABORATORY COURSES**

- PAPER – V :CH(CPI)451 P : Quantitative Analysis of Pharmaceuticals
- PAPER – VI :CH(CPI)452 P: Project Work

## PAPER – I

### **CH(CPI) 401 T: Pharmacokinetics**

CPI - 33 : Biopharmaceutics

CPI - 34 : Drug Absorption and Distribution

CPI - 35 : Drug Metabolism and Excretion

CPI - 36 : Pharmacokinetic Models

#### **CPI-33: Biopharmaceutics**

Introduction, definition of pharmacokinetics, pharmacodynamics, ADME processes. Rate, Rate Constants and order of reactions- zero order kinetics, first order kinetics, mixed order kinetics. Routes of administration: Enteral (oral, sublingual, buccal, rectal) perenteral (intravenous, intramuscular and subcutaneous), topical (dermal, trans dermal, ophthalmic, intranasal), advantages and disadvantages.

Plasma drug concentration vs time profile: pharmacokinetic parameters (Peak plasma concentration, time of peak concentration, AUC), pharmacodynamic parameters (MEC, MSC, Therapeutic range, onset of action, onset of time, duration of action, intensity of action).

Dissolution: Definition and theories of drug dissolution, Diffusion layer model, Danckwert's model & interfacial barrier model. Factors influencing dissolution, dissolution tests for tablets and capsules (basket apparatus, paddle apparatus, flow through cell apparatus). In vitro - in vivo correlation of dissolution.

#### **CPI-34: Drug Absorption and Distribution**

**Absorption:** Structure of cell membrane, Mechanism of drug absorption - Passive diffusion, Pore-transport, facilitated diffusion, active transport, ionic or electrochemical diffusion, ion-pair transport, endocytosis. **Factors influencing drug absorption:** Dosage form, pH (pH partition hypothesis), Lipophilicity, Gastric emptying. **Bioavailability:** Objectives of bioavailability studies, absolute versus relative bioavailability. Plasma level- time studies (single dose and multiple dose). Concept of steady state concentration. **Distribution:** Volume of distribution, Apparent volume of drug distribution and its determination. Factors affecting drug distribution, Plasma protein binding.

#### **CPI - 35: Drug Metabolism and Excretion**

Definition of biotransformation, drug metabolizing organs, drug metabolizing enzyme. Chemical pathways of drug biotransformation- Phase-I reactions and Phase-II reactions.

##### **Phase-I reactions:**

a) Oxidative reactions, Cytochrome-P450 Oxidation-reduction cycle i) Aromatic hydroxylation (Acetanilide), ii) Aliphatic hydroxylation (Ibuprofen), iii) N-Dealkylation (Diazepam), iv) Oxidative deamination (Amphetamine), v) N-Hydroxylation (Paracetamol), vi) S- oxidation (Phenothiazine). B) Reductive reactions- i) Reduction of carbonyls (Chioral hydrate) ii) N-Compounds (Nitrazepam). c) Hydrolytic reactions (Asprin).

**Phase-II reactions:** (Real detoxication pathways). i) Conjugation with D-Glucuronic acid ( Benzoic acid), ii) Conjugation with Sulfate moieties (Paracetamol), iii) Conjugation with  $\alpha$ -Amino acids (Salicylic acid). iv) Acetylation (p-Amino Salicylic acid), v) Methylation (Histamine).

Factors affecting biotransformation of drugs i) physiochemical properties of drugs, ii) chemical factors, iii) biological factors, Bioactivation and tissue toxicity.

Excretion of drugs. Definition of excretion, Types of excretion- (Renal and non-renal excretion). The process of Renal excretion of drugs-Glomerular filtration, Active tubular secretion and active or passive tubular reabsorption, concept of clearance, factors effecting renal excretion, nonrenal routes of excretion, biliary excretion, salivary excretion and pulmonary excretion.

### **CPI - 36 : Pharmacokinetic Models**

Definition, classification of models(mammillary and catenary). One Compartment open model (I.V bolous, IV infusion, Extravascular administration), Two Compartment open model (I.V bolous, IV infusion, Extravascular administration), Application of these models to determine the various pharmacokinetic parameters. Calculations and non- compartmental approaches to pharmacokinetics. Non-linear pharmacokinetics: causes of nonlinearity, Michaelis-Menten kinetics- characteristics, basic kinetic parameters. Calculations.

### **Text Books**

1. Biopharmaceutics and Pharmacokinetics – An Introduction by Robert E. Notary, 2nd edn. 1975, Marcel Dekkar Inc., New York
2. Applied BioPharmaceutics and Pharmacokinetics 5th Edition, McGrawhill Medical Publishing 2005 by Shargel, Wupong, Yu Andrew.
3. Pharmacokinetics. By Shobha Rani
4. Elements of Pharmacology. By Gandhi, Desani & Goyal.
5. Goodman & Gilman's " The pharmacological basis of therapeutics. By Gilman & Rali.
6. Pharmacology. By Rang.
7. Physical Pharmacy by Martin
8. Biopharmaceutics and pharmacokinetics By Brahmanikar
9. Pharmacology By Lippincot
10. Modern Pharmacology with Clinical Applications. By R.Craig.
11. Comprehensive pharmacy review by Leon Shargel
12. Hospital and clinical pharmacy
13. Advanced Pharmacokinetics - Venkateswarlu

## PAPER-II

### **CH(CPI) 402T : Principles of Drug Discovery, Drug Targets and chemistry of Pharmacology**

CPI - 37 : Principles of Drug Discovery and SAR Studies

CPI - 38 : General Principles of Pharmacology and drug Targets, drugs acting on ANS and CNS

CPI - 39 : Drugs Acting on Cardio Vascular and Respiratory System

CPI - 40 : Drugs acting on metabolic process, cell wall, genetic material and immune system

#### **CPI - 37 : Principles of Drug Discovery and SAR Studies**

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. Natural products as lead structures in drug discovery – Pharmacophore - structure pruning technique e.g. morphine. Discovery of lead structure from natural hormones and neurotransmitters(one example). Principles of design of agonists (Salbutamol), antagonists (cimetidine) and enzyme inhibitors (captopril). Drug discovery without lead – serendipity - Penicillin and Librium as examples. Principles of Prodrug design; Existing drugs as leads (me too drugs). Introduction to drug patents and Clinical trials.

SAR Introduction; 1. Binding role of hydroxy group, Amino group, aromatic ring, double bond, ketones and amides. 2. Variation of substituents- alkyl substituents, aromatic substituents, extension of structure, chain extension, ring expansion/contraction, ring variation, ring fusion. 3. Simplification of the structure, rigidification, conformational blockers, X-ray crystallographic studies. Ex: A case study of Oxaminquine (schistosomiasis), Sulpha drugs (antibacterial), and Benzodiazepines (Hypnotics).

#### **CPI - 38 : General Principles of Pharmacology and drug Targets, drugs acting on ANS and CNS**

Introduction - Nature and sources of drugs - Routes of administration of drugs - Concept of absorption – bioavailability - Drug distribution - Biotransformation and excretion drugs - Biological half-life and its significance/toxicity - Mechanism of action including drug receptor - Interactions and factors influencing them - Dose response relationship.

Introduction to molecular targets - lipids, carbohydrates, proteins (catalytic and non-catalytic) and nucleic acids. A brief introduction to the architecture of the Cells - Human Cell structure, Bacterial Cell wall, Cell membrane-membrane lipids, membrane proteins, membrane carbohydrates.

#### **Pharmacology of Drugs Acting on ANS and CNS**

Introduction - Transmission - Distribution and Functions of drugs acting on Autonomic Nervous System; Cholinergic agonists (Acetylcholine), Anti-cholinergic agents (Atropine), Anti Cholinesterase (Physostigmine), Local Anaesthetics (Procaine), Adrenergic stimulants (Dopamine), Adrenoreceptor antagonist (Doxazosin). Anti-Histamine agents (Cimetidine).

Distribution and Functions of Drugs acting on Central Nervous System: CNS Neurotransmitters; CNS Stimulants - Analeptics (Nikethamide), Psychomotor stimulants (Amphetamine), Anti-depressants (Imipramine), Hypnotics and Anxiolytics: Anti-psychotic Agents (Chlorpromazine), Anti-epileptic Agents (Phenytoin), General Anesthetics (Haloethanes (inhalation anesthetic)), Thiopentone (I.V. anesthetic). Neurodegenerative disorders: Alzheimers disease (Donepezil), Parkinson disease (Levodopa).



### **CPI - 39 : Drugs Acting on Cardio Vascular and Respiratory System**

General considerations - Pharmacology of drugs used in the treatment of congestive heart failure - Anti-arrhythmics - Classification with examples, Anti-hypertensives, ACE inhibitors (captopril), beta1-blockers (Propranolol), Drugs acting on Ion channels -  $\text{Ca}^{2+}$ ,  $\text{Na}^{+}$  and  $\text{Cl}^{-}$  channels and their mode of action. Structural formulae of Tetracaine and synthesis and of Amlodipine, Nifedipine, Diltiazem, Tetracaine and 4-Aminopyridine.  $\alpha$ -Adrenoreceptor stimulant (Clonidine),  $\alpha$ - Adrenoreceptor blocking agent (Prazocin), Anti-hyperlipidemic (Clofibrate).

Pharmacology of Drugs affecting Respiratory System: Drugs used in the treatment of disorders of Respiratory Function and Bronchial Asthma - Broncho dilators - i)  $\beta$ -adrenergic agents (Albuterol) ii) Phosphodiesterase inhibitors (Aminophylline), Anticholinergic agents (Atropine), Corticosteroids (Beclomethasone), Inhibitors of mediator release (Cromolyn Sodium), Anti-tussives (Codeine) and Expectorants (Guaifenesin).

Pharmacology of Drugs affecting Gastro intestinal System -  $\text{H}^{+}/\text{K}^{+}$ -ATPase inhibitors (omeprazole) Pharmacology of purgatives/laxatives (Dulcolax), Anti-diarrhoeals (Lopramide).

### **CPI - 40 : Drugs acting on metabolic process, cell wall, genetic material and immune system**

a) Drugs acting on metabolic process: Antifolates - Discovery and mechanism of action of sulphonamides, Structure of sulfamethoxazole, and dapsone. Diaminopyrimidines - trimethoprim, and drug synergism.

b) Drugs acting on cell wall:  $\beta$ -Lactam antibiotics - mechanism of action of penicillins and cephalosporins. Resistance to penicillins, broad spectrum penicillins - ampicillin and amoxicillin.  $\beta$ -Lactamase inhibitors - Structural formulae and mode of action of clavulanic acid and sulbactam.

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

a) DNA-intercalating agents - Anticancer and Antimalarial agents. Structural formulae of Daunomycin, Amsacrine and Chloroquine.

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

c) DNA-Polymerase inhibitors: Antiviral agents - AZT.

d) DNA-Topoisomerase inhibitors: Anti bacterial agents. Structural formulae of Ciprofloxacin and Norfloxacin

e) Inhibitors of transcribing enzymes: Anti-TB and antileprosy agents-structural formulae of Rifamycins.

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

Drugs acting on immune system: Introduction to immune system. Immunosuppressing agent-structural formula of Cyclosporin. Immunoenhancers-use of vaccines and structural formula of levamisole.

### **Recommended books**

1. Burger's medicinal chemistry and drug discovery. By Manfred E. Wolf.
2. Introduction to Medicinal chemistry. By Patrick.
3. Introduction to drug design. By 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. Pharmacology and Pharmacotherapeutics, R.S. Satoskar and S.D. Bhandarker, Popular Prakashan, Mumbai.
9. Pharmacology, H.P. Rang, M.M. Dale & J. M. Ritter : Churchill Livingstone, 4th edition.
10. Basic and Clinical Pharmacology, 9th edition – Bertram. G. Katzung.
11. Pharmacology and Pharmacotherapeutics, R.S. Satoskar and S.D. Bhandarker, Popular Prakashan, Mumbai.
12. Pharmacology, H.P. Rang, M.M. Dale & J. M. Ritter : Churchill Livingstone, 4th edition.
13. Basic and Clinical Pharmacology, 9th edition – Bertram. G. Katzung. Reference Books
14. Essentials of Medical Pharmacology, K.D. Tripathi, J. P. Brothers Medical Publishers.
15. Lewis's Pharmacology, by J. Crossland, Churchill Livingstone.
16. Pharmacological Principles of Medical Practice, by Krantz and Care, Williams and Wilkins co.
17. Goodman and Gilman's, The Pharmacological Basis of Therapeutics. J. G. Hardman and Lee E. Limbard, Mc. Graw Hill, Health professions Division.
18. Burger's medicinal chemistry and drug discovery. By Manfred B. Wolf.
19. Introduction to Medicinal chemistry. By Graham Patrick.
20. Introduction to drug design. By R.B.Silverman
21. Comprehensive medicinal chemistry. Vol 1-5 by Hanzsch.

## PAPER- III : CH(CPD)403 T

### ELECTIVE-3A

#### **Pharmaceutical Analysis**

CPI - 41: Spectral Methods in Pharmaceutical Analysis

CPI - 42: Chromatography in Pharmaceutical Analysis-I

CPI - 43: Potentiometry, polarography, thermal and radiopharmaceutical methods-Applications

CPI - 44: Titrimetry, Chemical and Extraction methods in Pharmaceutical Analysis

#### **CPI - 41: Spectral Methods in Pharmaceutical Analysis**

(A) **Ultraviolet and Visible Spectroscopy** - Introduction, UV spectra of some representative drug molecules : Steroid enones, Ephedrine [the benzoid chromophore], ketoprofen [extended benzene chromophore], Procaine [amino group auxochrome], Phenylephrine [hydroxyl group auxochrome]. Application of UV-Vis Spectrophotometry to Pharmaceutical quantitative Analysis : Assay of Frusemide in tablet, Assay of Penicillin by derivatization. Assay of Drugs by i) Direct UV method ii) Suitable Chromogens and iii) Charge transfer Complexes. Difference spectrophotometry, Derivative Spectra, Applications of UV-Visible Spectrophotometry in Pre - formulation and formulation.

(B) **Infrared Spectroscopy** - Introduction, Sample preparation, Application of IR Spectrophotometry in Structure Elucidation, interpretation of IR spectra of Paracetamol, aspirin, dexamethasone and phenoxymethyl penicillin potassium. Examples of IR Spectra of Drug molecules, IR Spectrophotometry as a fingerprint technique. **Near IR analysis (NIRA)** : Introduction, Examples of NIRA application

– determination of particle size in United states Pharmacopia grade Aspirin, determination of blend uniformity, determination of active ingredients in multi- component dosage forms, moisture determination.

(C) **Nuclear Magnetic Resonance Spectroscopy** - Introduction,  $^1\text{H}$  NMR : Application of NMR to Structure Confirmation in some drug molecules,  $^1\text{H}$  NMR spectral analysis of Benzocaine, Phenacetin, Clofibrate and phenylephrine.  $^{13}\text{C}$  NMR :  $^{13}\text{C}$  NMR spectrum of Salbutamol sulphate, Two Dimensional NMR Spectra – Proton-proton correlation spectrum of Tranexamic acid, Application of NMR to Quantitative analysis.

#### **CPI - 42: Chromatography in Pharmaceutical Analysis-I**

(A) **Thin Layer Chromatography** – Introduction, Instrumentation, TLC Chromatogram, Stationary Phases, Eluotropic series and Mobile phases, Modification of TLC, Adsorbents, detection of compounds on TLC plate following development, Applications of TLC analysis – qualitative identity tests, limit tests. High performance TLC (HPTLC), Applications of HPTLC – Assay for rifampicin (R), isoniazid (I) and pyrazinamide(P).

(B) **High performance Capillary Electrophoresis** – Introduction, Instrumentation, control of separation. Application of capillary electrophoresis in pharmaceutical analysis, Separation of Atenolol and related impurities. Analysis of Non-steroidal anti-inflammatory drugs. Micellar Electrokinetic Chromatography, Analysis of flavonoids by MECC.

(C) **Gas Chromatography** – Introduction, Instrumentation, Selectivity of Liquid Stationary Phases, Use of Derivatization in GC ,Application of GC in quantitative analysis, Determination of manufacturing and degradation residues by GC, Determination of pivalic acid in dipivefrin eye drops, Determination of residual solvents, Application of GC in Bioanalysis.

(D) **High Performance Liquid Chromatography** – Introduction, Instrumentation, Structural factors which govern rate of elution of drugs from HPLC columns, Application of

HPLC to the quantitative analysis of drugs in formulations, Assay of hydrocortisone cream with one point calibration against an internal standard, Assays involved in more specialized HPLC techniques, Assay of adrenaline injection by chromatography with an anionic ion-pairing agent.

#### **CPI - 43: Chromatography in Pharmaceutical Analysis-II**

(A) **Potentiometric Titrations:** assay of Aspirin, assay of Iron (II) succinate in ferromynS tablets, Determination of fluoride in tablets and solutions by Fluoride Ion Selective Electrode.

(B) **Radiopharmaceuticals:** Fundamentals of radioactivity, Measurement of radioactivity, Radiopharmaceuticals-requirements, radiochemical methods in analysis-Isotope dilution analysis IDA, Radioimmuno assay RIA-Thyroxin, and thyroid stimulating Hormone.

(C) **Thermal Method of Analysis:** Classification of thermoanalytical techniques, Applications of DSC/DTA/TGA in pharmaceutical analysis- Detection of polymorphism and pseudopolymorphism in pharmaceutical by DSC/DTA. Analysis of Drug Phenacetin by DSC.

(D) **Polarography:** Pharmaceutical applications of polarography in analysis of Antibiotics, Alkaloids, Trace metals and metal containing drugs, Blood serum and cancer diagnosis, insecticides, Vitamins, Hormones.

#### **CPI - 44: Titrimetry, Chemical and Extraction methods in Pharmaceutical Analysis**

(A) **Titrimetry and Chemical Methods** - Introduction, Direct Acid/Base titrations in the aqueous phase, Indirect Titrations in aqueous phase – estimation of alcohols and hydroxyl values by reaction with acetic anhydride. Non-aqueous titrations – analysis of phenylephrine, Argentimetric Titrations – assays of Sodium chloride, potassium chloride, thiamine hydrochloride, Complexometric Titrations – metal salts estimations, Redox Titrations - assays of ferrous salts, hydrogen peroxide, sodium perborate and benzoyl peroxide by titration with  $\text{KMnO}_4$ , Iodometric Titrations – Assay of phenolglycerol injection, Ion-pair Titrations, Diazotization Titrations – assay of sulphanilamide, Karl-Fischer Titrations

(B) **Extraction Methods** - Introduction, Commonly used excipients in formulations – (i) tablets and capsules (ii) suspensions and solutions (iii) creams and ointments. Solvent Extraction methods, (i) extraction of organic bases and acids utilizing their ionized and un-ionized forms. Partition between organic solvents, ion-pair extraction. Solid phase Extraction – Introduction, Methodology, types of adsorbents used in Solid phase Extraction – (i) Lipophilic silica gels. (ii) Polar surfaced modified silica gels.

#### **Recommended Text Books:**

1. Pharmaceutical Analysis by David G. Watson
2. Practical pharmaceutical chemistry Part I by Beckett & Stenlake
3. Pharmaceutical analysis by Ashtoshkar
4. Physical pharmacy by AN.Martin,J, Swarlbick etal
5. Biopharmaceutics and pharmacokinetics by Brahmanikar
6. Text book of physical pharmaceuticals by Subramaniyan
7. Inorganic pharmaceutical chemistry By Black
8. British Pharmacopoeia Vol I,II
9. Indian Pharmacopoeia Vol I,II
10. Bentley's Text book of pharmaceutics by Rowlinson
11. The science and practice of pharmacy by Remington
12. Thermal methods of Analysis-D.G Watson

## PAPER-III: CH(CPI) 403 T

### ELECTIVE-3B

#### **Bioorganic Chemistry**

CPI-45: Carbohydrates

CPI-46: Nucleic acids and Lipids

CPI-47: Proteins and Enzymes

CPI-48: Coenzymes and Vitamins

#### **CPI-45: Carbohydrates**

**15 Hrs**

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

#### **CPI-46: 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.

#### **CPI-47: Proteins and Enzymes**

**15 Hrs**

**Proteins:** Introduction. Peptide bond, classification and nomenclature 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

#### **CPI-48: Coenzymes and Vitamins**

**15 Hrs**

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

Classification — Vitamin derived coenzymes and metabolite coenzymes. Structure and biological functions of coenzyme A, thiamine pyrophosphate (TPP), pyridoxal phosphate (PLP), oxidized and reduced forms of I) nicotinamide adenosine dinucleotide / their phosphates (NAD), NADH, NADP<sup>+</sup> NADPH) ii) Flavin adenine nucleotide FAD, FADH<sub>2</sub> and iii) Flavin mononucleotide (FMN, FMNH<sub>2</sub>) lipoic acid, biotin, tetrahydrofolate and ubiquinone. Adenosine triphosphate (ATP) and adenosine diphosphate (ADP), S-adenosyl methionine (SAM) and

uridine diphospho sugars (UDP-sugars) Mechanism of reactions catalyzed by the above coenzymes.

**Vitamins:** Introduction, classification and biological importance of vitamins. Structure determination and synthesis of vitamins A, B<sub>1</sub>, and B<sub>2</sub>. Synthesis of vitamins - B<sub>6</sub>, C, E and K. Structure of vitamin B<sub>12</sub>.

**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 Blackburn MI Gait
7. Lehninger Principles of Biochemistry by D L Nelson and M M Coxon
8. Outlines of Biochemistry by Conn and Stumpf
9. Enzyme structure and mechanism by Fersht and Freeman
10. Enzymes for green organic synthesis by V.K.Ahluwalia
11. Biotransformations in Organic Chemistry by K Faber.
12. Principles of biochemistry by Horton & others.
13. Bioorganic chemistry - A chemical approach to enzyme action by Herman Dugas and Christopher Penney.
14. Concepts in Biotechnology by D.Balasubramanian & others
15. Chemistry and physiology of the vitamins by H.R.Rosenberg.

## PAPER-IV: CH(CPI)404 T

### ELECTIVE-4A

#### **Advanced Heterocyclic Chemistry**

CPI - 49: Non aromatic heterocyclics & aromaticity

CPI - 50: Five and six membered heterocyclics with two hetero atoms

CPI - 51: Heterocyclics with more than two hetero atoms

CPI - 52: Larger ring and other heterocycles

#### **CPI - 49: Non aromatic heterocyclics & Aromaticity**

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

**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.

#### **CPI - 50: Five and six membered heterocyclics with two hetero atoms**

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.

#### **CPI - 51: Heterocyclics with more than two hetero atoms**

Synthesis, reactivity, aromatic character and importance of the following Heterocycles: 1,2,3-triazoles, 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. Synthesis of Caffeine, theobromine and theophylline.

#### **CPI - 52: Larger ring and other heterocycles**

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

#### **Recommended Books:**

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

## PAPER- IV : CH(CPD)404 T

### ELECTIVE 4B

#### **Green chemistry and Organic materials**

CPI - 53: Principles of Green chemistry

CPI - 54: Green Synthesis

CPI - 55: Organic nanomaterials

CPI - 56: Supramolecular chemistry

#### **CPI - 53: Principles of Green chemistry**

**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.

#### **CPI - 54: Green Synthesis**

**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 dihydroxylation reactions.

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

**iv) Green Catalysts in organic synthesis:** introduction

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

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

#### **CPI - 55: Organic nanomaterials**

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

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

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

Structures of aromatics belts, nano car and molecular machines.

**Optoelectronic molecules:** OLEDs, Organic Solar Cells (Basic OLED mechanism and structures) - Natural Benz heterazoles and their synthetic modifications as optoelectronic molecules.



## **CPI - 56: Supramolecular chemistry**

**Introduction:** Supramolecular interactions (ion-ion, ion-dipole, H-bonding, cation- $\pi$ , anion- $\pi$ ,  $\pi$ - $\pi$  and Van der Waals interactions), Ionophore and molecular receptors.

**Host-Guest Chemistry:** Lock and key analogy, Structures and applications of Cryptands, Spherands, Calixerenes, Cyclodextrins, Cyclophanes, Carcerands and hemicarcerands.

**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 framework, Chiral receptor from Kemp's triacid. Chiral receptors for tartaric acid.

### **Recommended books:**

1. P.T. Anastas & J.K. Warner: Oxford Green Chemistry- Theory and Practical, University Press (1998).
2. A.S. Matlack: Introduction to Green Chemistry, Marcel Dekker, (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 Dalco, 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.

**SEMESTER -IV**  
**PRACTICALS**

**Paper-V: CPI – 451P: Quantitative Analysis of Pharmaceuticals**

**Assay of pharmaceuticals - Redox titrations**

Assay of analgin in tablets by iodometry

Assay of ascorbic acid in raw material by iodometry

Assay of ascorbic acid in tablets by cerimetry

Determination of hydrogen peroxide in medicament by Permanganometry

**Assay of pharmaceuticals - Complexometric titrations**

Assay of Calcium in Calcium gluconate

Assay Zinc in Bacitracin zinc

**Assay of pharmaceuticals - Non-aqueous titrations:**

Assay of diphenylhydramine hydrochloride in tablets

Assay of ephedrine hydrochloride in capsules

Assay of Ibuprofen in tablets

**Assay of pharmaceuticals – Potentiometry/Conductometric**

Potentiometric estimation of Sulphanilamide

Potentiometric estimation of Atropine

Conductometric estimation of analysis Amidazophen (aminophenazone)

Conductometric estimation of analysis Aspirin

**Assay of pharmaceuticals - UV-Visible Spectrophotometry**

Assay of Riboflavin in tablets

Assay of Diazepam in tablets

Assay of Nimuselide in nimuselide tablets

**Assay of pharmaceuticals – by other methods**

Dissolution profile of paracetamol & ampicillin

Determination of Sodium and potassium ions in pharmaceuticals by flamephotometry

Determination of Quinine sulphate & Riboflavin by florimetry.

**Identification of unknown pharmaceuticals and intermediates by interpretation of IR, UV, <sup>1</sup>H and <sup>13</sup>C NMR and Mass spectra**

**Chromatography:**

1. Identification of unknown organic compounds by interpretation of IR, UV, <sup>1</sup>H -NMR, <sup>13</sup>C-NMR and mass spectral data. A minimum of 08 simple organic molecules should be studied initially as examples along with the spectral elucidation of the drugs as mentioned below to be studied.

(Asprin, p-Chloroacetophenone, clofibrate, Ibuprofen, Phenylacetic acid, p-MethylBenzoylchloride, L-Dopa, Benzocaine)

2. Thin layer chromatography: Determination of purity of a given sample, monitoring the progress of chemical reactions, identification of unknown organic compounds by comparing the R<sub>f</sub> values of known standards.

3. Separation by column chromatography: Separation of a mixture of *ortho* and *para* nitroanilines using silicagel as adsorbant and chloroform as the eluent. The column chromatography should be monitored by TLC.

**Paper-VI: CPI - 452P: PROJECTWORK**