

### OBJECTIVE OF THE COURSE

To teach the fundamental concepts of Chemistry and their applications, the syllabus pertaining to M.Sc. (2 Year Degree Course) in the subject of Chemistry has been prepared as per provision of the UGC module and demand of the academic environment. The syllabus contents are duly arranged unit wise and contents are included in such a manner that due importance is given to requisite intellectual and laboratory skills. This M.Sc course of chemistry consist of 2 year - course with semester system-in all 4 semesters (two semester in a year)

Total marks: 2000 (1000 per year and 500 per semester) of core and elective disciplines

#### MSc SEM I

S. No.	Paper	Paper Code	Max Marks (100)	
			Ext.	Int.
1	Inorganic Chemistry	CHC101	80	20
2	Organic Chemistry	CHC102	80	20
3	Physical Chemistry	CHC103	80	20
4	Group Theory and Instrumentation Techniques	CHC104	80	20
5	Lab Course (Inorganic Organic and physical))	CHC10P	80	20

#### MSc SEM II

S. No.	Paper	Paper Code	Max Marks (100)	
			Ext.	Int.
1	Inorganic Chemistry	CHC201	80	20
2	Organic Chemistry	CHC202	80	20
3	Physical Chemistry	CHC203	80	20
4	Spectroscopy and analytical methods	CHC204	80	20
5	Lab Course (Inorganic, Organic and Physical)	CHC20P	80	20

#### MSc SEM III [SPECIALIZATION IN INORGANIC CHEMISTRY]

S. No.	Paper	Paper Code	Max Marks	
			Ext.	Int.
1	Organometallic Chemistry	CHC301	80	20
2	Spectroscopy	CHC302	80	20
3	Analytical Chemistry	CHC303	80	20
4(i)	Chemistry of Biological System I (Bioinorganic)	CHC301	80	20
(ii)	Bioinorganic & Supramolecular Chemistry	CHC302	80	20
5	Lab Course (Inorganic)	ICHC30P	80	20

#### MSc SEM III [SPECIALIZATION IN ORGANIC CHEMISTRY]

S. No.	Paper	Paper Code	Max Marks	
			Ext.	Int.
1	Reagents in Organic Synthesis and Organometallics	CHC304	80	20

2	Spectroscopy	CHC302	80	20
3	Organic Photochemistry	CHC305	80	20
4(i)	Chemistry of Biological System I (Bioorganic)	CHE303	80	20
(ii)	Chemistry of Natural Products	CHE304	80	20
5	Lab Course (Organic)	(CHC30P	80	20

### MSc SEM III [SPECIALIZATION IN PHYSICAL CHEMISTRY]

S. No.	Paper	Paper Code	Max Marks	
			Ext.	Int.
1	Advanced Quantum Chemistry	CHC306	80	20
2	Spectroscopy	CHC302	80	20
3	Analytical Chemistry	CHC307	80	20
4(i)	Chemistry of Biological System I (Biophysical)	CHE305	80	20
(ii)	Nuclear Chemistry	CHE306	80	20
5	Lab Course (Physical)	PCHC30P	80	20

### MSc SEM IV [SPECIALIZATION IN INORGANIC CHEMISTRY]



S. No.	Paper	Paper Code	Max Marks	
			Ext.	Int.
1	Spectroscopy & Diffraction method	CHC401	80	20
2	Photo Inorganic Chemistry	CHC402	80	20
3	Inorganic Polymers	CHC403	80	20
4(i)	Nuclear Chemistry	CHE306	80	20
(ii)	Environmental Chemistry	CHE401	80	20
(iii)	Project work / Dissertation	CHE402	80	20
5	Lab Course (Inorganic)	ICHC40P	80	20

### MSc SEM IV [SPECIALIZATION IN ORGANIC CHEMISTRY]



S. No.	Paper	Paper Code	Max Marks	
			Ext.	Int.
1	Organic Synthesis	CHC404	80	20
2	Organic Spectroscopy	CHC405	80	20
3	Heterocyclic Compounds	CHC406	80	20
4(i)	Medicinal Chemistry	CHE403	80	20
(ii)	Environmental Chemistry	CHE401	80	20
(iii)	Project work / Dissertation	CHE404	80	20
5	Lab Course (Organic)	OCHC40P	80	20

### MSc SEM IV [SPECIALIZATION IN PHYSICAL CHEMISTRY]



S. No.	Paper	Paper Code	Max Marks	
			Ext.	Int.
1	Advanced Chemical Dynamics	CHC407	80	20
2	Advanced Spectroscopy	CHC408	80	20
3	Solid State Chemistry	CHC409	80	20
4(i)	Chemistry of Materials	CHE405	80	20

(ii)	Environmental Chemistry	CHE401	80	20
(iii)	Project work / Dissertation	CHE406	80	20
5	Lab Course (Physical)	PCIC40P	80	20

**Abbreviation:**

CHC = Chemistry Core course

CHE = Chemistry Elective Course

**Note:**

In III and IV semesters, the candidate shall have to opt for one elective papers of a particular specialization (Inorganic/Organic/Physical). The candidate shall not be allowed to opt elective papers from different specializations. Five lab experiments from the list of experiments given in the syllabus is the minimum requirement. He/ She can opt for Project/dissertation as an elective paper. The topic of the project will be decided by the Project Supervisor. Marks awarded for the project work shall be based on the novelty/quality of project work; it's presentation/viva-voice and social applicability. He/She will have to submit the project/dissertation not later than the date of his/her practical examination.




## SEM I

### (I) Inorganic Chemistry (CHC101)

#### 1. Stereochemistry and Bonding of

##### a) Main Group Compounds

Origin of VSEPR theory and its significance in main group structural chemistry, structure of  $SF_6$ ,  $TeF_6$ ,  $BrF_3$ ,  $ICl_3$ ,  $ICl_4^-$ ,  $OF_2$ ,  $OSF_4$ ,  $XeF_4$  and  $IF_7$ ,  $sp^3$  bonds, Bent rule and energetic of hybridization, some simple reactions of covalently bonded molecules.

##### b) Metal Borides, metal carbides and metal nitrides

Metal borides, carbides and nitrides: preparation, properties, structures and application.

#### 2. Metal-Ligand bonding in Coordination Chemistry

Crystal field theory, factors affecting the magnitude of  $\Delta_0$ , Consequences of crystal field splitting, Merits and limitations of CFT, Jahn-Teller distortion and its consequences on complex formation, Evidence of covalent character in Metal-Ligand bonding, Molecular orbital theory as applied to octahedral, tetrahedral and square planar complexes.

#### 3. Metal Ligand Equilibria in Solution

Concept of thermodynamic and kinetic stabilities of metal complexes, Stepwise and overall formation constants and their correlations, trends in stepwise constants, factors affecting the stability of metal complexes with reference to the nature of metal ion and ligand, chelate effect and its thermodynamic origin, determination of binary formation constants by pH-metry and spectrophotometry

#### 4. Reaction Mechanism of Transition metal Complexes

Energy profile of a reaction and reactivity of metal complexes, Inert and labile complexes, Ligand substitution reactions in octahedral complexes i.e.  $SN_1$ ,  $SN_2$  and  $SN_{ICB}$  mechanism, Anation reactions without metal ligand bond cleavage, Electron transfer reactions (Redox reactions), Outer and inner sphere mechanism (OSM and ISM), Reactions of coordinated ligands, Substitution reactions in square-planar complexes.

#### Books Recommended:

1. F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann, Advance Inorganic Chemistry, John Wiley & Sons, New York.
2. J. D. Lee, Concise Inorganic Chemistry, Oxford University Press.
3. Atkins, Overton, Rourke, Weller and Armstrong, Inorganic Chemistry, Oxford University Press.
4. J. E. Huheey, E. A. Keiter and R. L. Keiter, Inorganic Chemistry Principles of Structure and Reactivity, Pearson Education.
5. W. W. Porterfield, Inorganic Chemistry: A Unified Approach, Elsevier.
6. G. Wulfsberg, Inorganic Chemistry, Viva Books.
7. G. L. Miessler and D. A. Tarr, Inorganic Chemistry, Pearson Education.

### (II) Organic Chemistry (CHC102)

#### 1. Nature of Bonding in Organic Molecules

Delocalized chemical bonding conjugation, cross conjugation, resonance, hyperconjugation, bonding in fullerenes, tautomerism, Aromaticity in benzenoid and non-benzenoid compounds, alternant and nonalternant hydrocarbons, Hückel's rule, energy level of  $\pi$ -molecular orbitals.

annulenes, antiaromaticity,  $\psi$ -aromaticity, homo-aromaticity, PMO approach. Bond weaker than covalent bond, addition compounds, crown ether complexes and cryptands, inclusion compounds, cyclodextrins, catenanes and rotaxanes.

## 2. Stereochemistry of Organic compounds

Molecular symmetry and chirality: symmetry operations and symmetry elements, point group classification and symmetry number. Stereoisomerism: Classification, racemic modification, molecules with one, two or more chiral centres. Configuration, nomenclature, D, L, R, S and E, Z nomenclature. Axial and planar chirality and helicity (P & M); stereochemistry and configurations of allenes, spiranes, alkylidene, cycloalkanes, adamantanes, catenanes, biphenyls (atropisomerism), bridged biphenyls, ansa compounds and cyclophanes. Topicity and prostereoisomerism: Topicity of ligands and faces and their nomenclature, stereogenicity, cyclostereoisomerism: configurations, conformations and stability of cyclohexanes, (mono-, di- and tri-substituted), cyclohexenes, cyclohexanones, halocyclohexanones, decalines, decalols, decalones. Asymmetric induction; Cram's, Prelog's and Horeaus rules. Dynamic stereochemistry (cyclic and acyclic). Stereochemistry of compounds containing N, S and P, chirogenicity, pseudo asymmetry and stereogenic centre. Stereoselectivity, stereospecificity, regioselectivity and chemoselectivity. Enantiomeric and diastereomeric excess.

## 3. Reaction Mechanism: structure and reactivity

Types of mechanisms, types of reactions, thermodynamic and kinetic requirements, kinetic and thermodynamic control, Hammond's postulate, Curtin-Hammett principle. Potential energy diagrams, transition states and intermediates, methods of determining mechanisms, isotope effects. Effect of structure on reactivity - resonance and field effects, steric effect, quantitative treatments. Hammett equation and linear free energy relationship, substituent and reaction constants. Taft equation.

## 4. Aliphatic and Aromatic Nucleophilic Substitution and Mechanism of Carbocationic rearrangement reactions

The  $S_N^2$ ,  $S_N^1$ , mixed  $S_N^1$  and  $S_N^2$ ,  $S_N^1$  and SET mechanisms. Nucleophilic substitution at and allylic, aliphatic trigonal and a vinylic carbon. Reactivity effects of substrate structure, attacking nucleophile, leaving group and reaction medium, phase transfer catalysis and ultrasound, ambident nucleophile, regioselectivity. Neighbouring group mechanism, neighbouring group participation by  $\pi$  and  $\sigma$  bonds, anchimeric assistance. Classical and nonclassical carbocations, phenonium ions, norbornyl system.

Pinacol-Pinacolone rearrangement, Wagner-Meerwein rearrangement, Benzilic acid rearrangement, Allylic rearrangement, Hofman reaction, Schmidt reaction, Baeyer-Villiger oxidation, Cumene-Hydroperoxide rearrangement, Curtius rearrangements, Lossen rearrangement, Dakin reaction. Application of NMR Spectroscopy in detection of carbocations.

### BOOKS SUGGESTED:

1. Jerry March, Advanced Organic Chemistry Reactions, Mechanism and Structure, John Wiley.
2. R. T. Morrison and R. N. Boyd, Organic Chemistry, Prentice Hall.
3. C. K. Ingold, Structure and Mechanism in Organic Chemistry, Cornell University Press.
4. S. M. Mukherji and S. P. Singh, Reaction Mechanism in Organic Chemistry, Macmillan.
5. D. Nasipuri, Stereochemistry of Organic Compounds, New Age International
6. P. S. Kalsi, Stereochemistry of Organic Compounds, New Age International.
7. S. M. Mukherjee, Pericyclic Reactions, Macmillan, India.
8. F. A. Carey and R. J. Sundberg Advanced Organic Chemistry, Plenum.
9. Benjamin, Modern Organic Reactions, HO House.
10. Ernest L. Eliel and Samuel H. Wilen, Stereochemistry of Organic Compounds, Wiley



### (III) Physical Chemistry (CHC103)

#### 1. Quantum Chemistry

**Introduction:** De Broglie's equation and its physical significance. Time independent and dependent forms of Schrodinger equation. Operator and their algebra. Postulates of Quantum mechanics. Particle in one, two and three dimensional box. Harmonic oscillator. Rigid rotator. Hydrogen atom and shapes of orbitals.

**Approximate Methods:** Approximate methods of quantum mechanics: Variational method and Perturbation theory upto second order in energy and applications (Helium atom).

Angular Momentum and eigen function. Ladder operator. Addition of angular and spin momentum. Pauli exclusion principle. Fermions and bosons.

**Chemical Bonding:** Valence bond (VB) and molecular orbital (MO) approaches. VB treatment of Hydrogen molecule. Bonding and antibonding MO according to LCAO method. Huckel molecular orbital (HMO) theory and its application to ethene, butadiene etc.

#### 2. Chemical Thermodynamics

Basics of thermodynamics (laws of thermodynamics). Partial molar properties: Chemical potential and its determination and applications.

Concept of fugacity and its determination. Activity and activity coefficient. Debye-Huckel theory for activity coefficient of electrolytic solutions. Ionic strength.

#### 3. Chemical Dynamics

**Arrhenius equation, Kinetics of bimolecular reactions;** Collision theory of reaction rates. Activated complex theory. Kinetics of unimolecular reactions: Lindemann-Hinshelwood theory, RRKM treatment.

**Kinetics of Chain Reactions:** Hydrogen-bromine reaction, pyrolysis of acetaldehyde, decomposition of ethane.

**Kinetics of photochemical reactions:** Hydrogen-bromine and hydrogen-chlorine photochemical reactions.

**Oscillatory reactions:** Belousov-Zhabotinsky reaction

#### 4. Surface Chemistry and Micelles

**Adsorption:** Thermodynamics and kinetics of adsorption. BET method and its applications for estimation of surface area. Heterogeneous catalysis.

**Micelles:** Concept of Micellization. Critical micellar concentration (CMC). Factors affecting micelles formation. Thermodynamics of micellization. Solubilization. Reverse micelles.

#### BOOKS SUGGESTED:

1. Physical Chemistry, P.W. Atkins, ELBS.
2. Introduction to Quantum Chemistry, A.K. Chandra, Tata McGraw Hill.
3. Quantum Chemistry, Ira N. Levine, Prentice Hall. Coulson's Valence, R. McWeeny, ELBS.
4. B. R. Puri, L. R. Sharma and M. S. Pathania, Physical Chemistry, Milestone Publisher & Distributors, New Delhi.
5. K. L. Kapoor, Physical Chemistry: Macmillan Publishers India Limited.
6. K. J. Laidler, Kinetics, Pearson Education India.

### (IV) Group Theory and Analytical Techniques (CHC104)



## 1. Symmetry and Group Theory in chemistry

Symmetry elements and symmetry operation. Definition of group, subgroup. Point symmetry group. Matrix representation of groups ( $C_n$ ,  $C_{nv}$ ,  $C_{nh}$ ,  $D_n$  only). Character table. Character representation of (case of  $H_2O$  and  $NH_3$ ). Great orthogonality theorem (without derivation) and its applications. Applications of group theory in IR and Raman spectroscopy.

## 2. Chromatographic and Radio Analytical Methods

Basic principle and types of chromatography. Principle, instrumentation and applications of GC, LC, HPLC and Ion-exchange chromatography. Van-Deemter equation (without derivation).

Nuclear reactions and radiations. Measurement and detection of radiation. Principle of Isotopic dilution method and Neutron activation analysis (NAA).

## 3. Microwave, Infrared, Raman Spectroscopy

Classification of molecules. Principle of rotational spectroscopy. Energy, selection rule and spectroscopic frequency of rigid and non-rigid diatomic rotator. Population of states. Stark effect. Application of MW spectroscopy. Effect of isotopic substitution.

Principle of vibrational spectroscopy. Morse function and diagram. Vibrational energies, selection rules for diatomic harmonic and anharmonic oscillator. Overtones, hot bands, P-Q-R branch lines. Fundamental modes of vibrations, fundamental frequency and factors affecting it. Applications of IR, FTIR and its advantages.

Classical and Quantum theories of Raman effect. Pure rotational, vibrational and rotational-vibrational Raman spectroscopy. Stokes and anti-Stokes lines. Mutual exclusion principle. Applications.

## 4. Atomic and Molecular Spectroscopy

Energies of atomic orbitals. Spin and angular vector coupling for  $p^1$  and  $d^1$  system. Spectra of hydrogen atom and alkali metal atoms. Frank-Condon principle. Electronic spectrum of diatomic molecules. Vibrational (coarse) progressions and Rotational fine structures. Einstein's coefficients. Fluorescence, Phosphorescence and Stimulated emission.

### Books Suggested:

1. Modern Spectroscopy, J.M. Hollas, John Wiley.
2. Physical Methods for Chemistry, R.S. Drago, Saunders Company.
3. Chemical Applications of Group Theory, F.A. Cotton.
4. Introduction of Molecular Spectroscopy, G.M. Barrow, McGraw Hill.
5. Basic Principles of Spectroscopy, R. Chang, McGraw Hill.
6. Symmetry and Spectroscopy of Molecules, K. Veera Reddy, New Age International.

## (V) Lab Course (Inorganic, Organic and Physical) SEM I (CHC10P) (2×6 hours)

### I(a). Qualitative Analysis

Qualitative analysis of mixtures by semi-micro methods containing not more than six cations and anions including:

- (i). Rare-earth elements
- (ii). Anions, which have not been done in under graduate practicals.
- (iii). Insolubles

1×20 marks

**(b). Chromatography**

Separation of cations and anions by- Paper Chromatography, Thin Layer Chromatography  
Ion Exchange Chromatography

**2(a). Qualitative Analysis**

Separation, purification and identification of compounds of binary mixture (solid-solid or liquid and solid) using TLC and Paper Chromatography, Chemical tests and spectroscopic analysis.

**(b). Organic Synthesis**

1×20 marks

Acetylation: Acetylation

Oxidation: Adipic acid by chromic acid oxidation of cyclohexanol.

Grignard reaction: Synthesis of triphenylmethanol from benzoic acid.

Sandmeyer reaction: p-Chlorotoluene from p-toluene

**3(a). Chemical Kinetics**

- i. Determination of the effect of (a) Change of temperature (b) Change of concentration of reactants and catalyst and (c) ionic strength of the media on the velocity constant of Hydrolysis of an ester/ionic reactions.
- ii. Determination of the velocity constant of hydrolysis of an ester.
- iii. Determination of the rate constant for the oxidation of iodide ions by hydrogen peroxide studying the kinetics of the reaction.
- iv. Flowing clock reactions (Ref: Experiments in Physical Chemistry by Showmaker).
- v. Determination of the primary salt effect on the kinetics of ionic reactions and testing of the Bronsted relationship (iodide ion is oxidized by persulphate ion).

**(b). Electrochemistry**

1×15 marks

**Conductometry**

- i. Determination of the velocity constant, order of the reaction and energy of activation for saponification of ethyl acetate by sodium hydroxide conductometrically.
- ii. Determination of solubility and solubility product of sparingly soluble salts (e.g.,  $PbSO_4$ ,  $BaSO_4$ ) conductometrically.
- iii. Determination of the strength of strong and weak acids in a given mixture conductometrically.
- iv. To study the effect of solvent on the conductance of  $AgNO_3/CH_3COOH$  and to determine the degree of dissociation and equilibrium constant in different solvents and in their mixtures (DMSO, DMF, dioxane, acetone, water) and to test the validity of Debye-Huckel-Onsager theory.
- v. Determination of the activity coefficient of zinc ions in the solution of 0.002 M zinc sulphate using Debye Huckel's limiting law.
- vi.

4. Viva

10 marks

5. Record

15 marks

**SEM II**

**(I) Inorganic Chemistry (CHC201)**

**1. Electronic Spectra & Magnetic Properties of Transition Metal Complexes**

Spectroscopic ground states correlation, Orgel and Tanabe-Sugano diagrams for transition metal complexes ( $d^1-d^9$  states), calculations of  $Dq$ ,  $B$  and  $\beta$  parameters, charge transfer spectra, spectroscopic method of assignment of absolute configuration in optically active metal chelates and their stereochemical information, magnetic properties of complexes of various geometries based on CFT, spin free- spin paired equilibrium in octahedral stereochemistry, anomalous magnetic moments, magnetic exchange coupling and spin crossover.

**2. Metal- $\pi$  Acid Complexes and Organometallic compounds**



Metal carbonyl complexes. Preparation, properties and uses. Nature of bonding in metal carbonyls and carbon monoxide analogs i.e. nitrosyls and dinitrogen complexes. Evidence for back bonding in complexes. Nature of M-C bond. Synthesis, bonding and uses of organometallic compounds, two electron ligands (olefinic and acetylenic complexes), three electron ligands (allylic complexes), four electron ligand (butadiene and cyclobutadiene complexes), five electron ligand (ferrocene complexes).

### 3. Metal Clusters, Polynuclearmetalates and silicates

Higher boranes, carboranes, metalloboranes and metallocarboranes. Metal carbonyl and metalhalide clusters. Clusters with metal-metal multiple bonds. Isopoly and heteropoly acids and salts (or anions) with special reference to vanadium, molybdenum and tungsten. Nomenclature, classification, preparation and structural aspects of poly acids and polyanions.

### 4. Silicates

Principles of silicates. Structure and classification of silicates. Asbestos, Zeolites and Ultramarines as silicate materials. Silicates in technology.

### Books Recommended:

1. F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann, *Advance Inorganic Chemistry*, John Wiley & Sons, New York.
2. J. D. Lee, *Concise Inorganic Chemistry*, Oxford University Press.
3. Atkins, Overton, Rourke, Weller and Armstrong, *Inorganic Chemistry*, Oxford University Press.
4. J. E. Huheey, F. A. Keiter and R. L. Keiter, *Inorganic Chemistry Principles of Structure and Reactivity*, Pearson Education.
5. W. W. Porterfield, *Inorganic Chemistry: A Unified Approach*, Elsevier.
6. G. Wulfsberg, *Inorganic Chemistry*, Viva Books.
7. G. L. Miessler and D. A. Tarr, *Inorganic Chemistry*, Pearson Education.

## (II) Organic Chemistry (CHC202)

### 1. Free Radical Reactions

Types of free radical reactions, free radical substitution mechanism, mechanism of an aromatic substrate, neighboring group assistance. Reactivity for aliphatic and aromatic substrates at a bridgehead. Reactivity in the attacking radicals. The effect of solvents on reactivity. Allylic halogenation (NBS), oxidation of aldehydes to carboxylic acids, auto-oxidation, coupling of alkynes and arylation of aromatic compounds by diazonium salts. Sandmeyer reaction. Free radical rearrangement. Hunsdiecker reaction.

### 2. Electrophilic substitution reactions of

#### a) Aliphatic Organic Compounds

Bimolecular mechanisms-SE<sub>2</sub> and SE<sub>1</sub>. The SE<sub>1</sub> mechanism, electrophilic substitution accompanied by double bonds shifts. Effect of substrates, leaving group and the solvent polarity on the reactivity

#### b) Aromatic Organic Compounds

Orientation and reactivity, energy profile diagrams; The ortho/para ratio, ipso attack, orientation in other ring systems. Quantitative treatment of reactivity in substrate and electrophiles. Diazonium coupling, Vilsmeier Haack reaction, Gattermann-Koch reaction.

### 3. Addition Reactions and Elimination Reactions

#### (a) Addition reactions of carbon-carbon multiple bonds

Mechanism and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals, regio- and chemoselectivity, orientation and reactivity. Addition to cyclopropane ring. Hydrogenation of double and triple bonds, hydrogenation of aromatic rings. Hydroboration-Michael reaction. Sharpless asymmetric epoxidation.

#### (b) Addition reactions of $\pi$ -hetero multiple bonds

Mechanism of metal hydride reduction of saturated and unsaturated carbonyl compounds, acids, esters and nitriles; Wittig reaction. Mechanism of condensation reactions involving enolates-Knoevenagel, Claisen, Mannich Benzoin, Perkin and Stobbe reactions. Hydrolysis of esters and amides, ammonolysis of esters.

#### (c) Elimination Reactions

The E2, E1 and E1cB mechanisms and their spectrum. Orientation of the double bond. Reactivity-effects of substrate structures, attacking base, the leaving group and the medium. Mechanism and orientation in pyrolytic elimination.

#### 4. Pericyclic Reactions

Molecular orbital symmetry. Frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene and allyl system. Classification of pericyclic reactions, Woodward-Hoffmann. Correlation diagrams. FMO and PMO approach. Electrocyclic reactions-conrotatory and suprafacial additions,  $4n$ , and  $4n+2$  systems. Cycloadditions-antarafacial and suprafacial additions,  $4n$  and  $4n+2$  systems,  $2+2$  addition of ketenes, 1,3 dipolar cycloadditions and cheletropic reactions. Sigmatropic

rearrangements- suprafacial and antarafacial shifts of H, sigmatropic shifts involving carbon moieties, 3,3- and 5,5- sigmatropic rearrangements, Claisen, Cope and aza-Cope rearrangements. Fluxional tautomerism. Ene reaction.

#### BOOKS SUGGESTED:

1. Jerry March, Advanced Organic Chemistry-Reactions, Mechanism and Structure, John Wiley.
2. R. T. Morrison and R. N. Boyd, Organic Chemistry, Prentice Hall.
3. C. K. Ingold, Structure and Mechanism in Organic Chemistry, Cornell University Press.
4. S. M. Mukherji and S. P. Singh, Reaction Mechanism in Organic Chemistry, Macmillan.
5. D. Nasipuri, Stereochemistry of Organic Compounds, New Age International
6. P. S. Kalsi, Stereochemistry of Organic Compounds, New Age International.
7. S. M. Mukherjee, Pericyclic Reactions, Macmillan, India.
8. F. A. Carey and R. J. Sundberg, Advanced Organic Chemistry, Plenum.
9. Benjamin Modern Organic Reactions, HO House.
10. Ernest L. Eliel and Samuel H. Wilen, Stereochemistry of Organic Compounds, Wiley.
11. India
12. Ernest L. Eliel, Stereochemistry of Carbon Compounds, Tata McGraw Hill.

### (III) Physical Chemistry (CHC203)

#### 1. Statistical Thermodynamics

Most probable distribution. Ensemble averaging. Canonical, grand canonical and microcanonical ensembles. Partition functions. Translational, rotational and vibrational partition functions. Maxwell-Boltzmann, Bose-Einstein and Fermi-Dirac Statistics. Thermodynamic properties and partition functions. Applications of partition functions.

#### 2. Non-equilibrium Thermodynamics



Thermodynamical criteria for non-equilibrium states. Entropy production and entropy flow. Entropy balance equations for different irreversible processes (e.g. heat flow, chemical reaction etc.) transformations of the generalized fluxes and forces, non-equilibrium stationary states. Phenomenological equations, microscopic reversibility and Onsager's reciprocity relations. Electrokinetic phenomena, diffusion, electric conduction. Irreversible thermodynamics for biological systems, coupled reactions.

### 3. Electrochemistry

Basics of electrochemistry. Debye-Huckel-Onsager treatment for ion-solvent interactions. Structure of electrified interfaces: Gouy, Chapman and Stern. Over voltage and potential. Theories of over voltage. Exchange current density. Derivation of Butler-Volmer equation. Tafel plot. Polarography theoretical aspect. Ilkovic equation. Half potential and its significance. Applications. Corrosion. Theory of corrosion. Forms of corrosion. Monitoring and prevention of corrosion.

### 4. Macromolecules-Polymers

Classification. Kinetics of polymerisation. Number and mass average molecular mass. Molecular mass determination (osmometry, viscometry, diffusion and light scattering method). Chain configuration of macromolecules. Calculation of average dimensions of various chain structures.

#### BOOKS SUGGESTED:

1. Physical Chemistry, P.W. Atkins, ELBS.
2. B. R. Puri, L. R. Sharma and M. S. Pathania, Physical Chemistry, Milestone Publisher & Distributors, New Delhi.
3. K. L. Kapoor, Physical Chemistry, Macmillan Publishers India Limited.
4. K. J. Laidler, Kinetics, Pearson Education India

## (IV) Spectroscopy and Analytical Methods (CHE204)

### 1. Thermal Analytical methods and XRD

Methods of thermal analysis. Principle and instrumentation of TGA, DTA and DSC. Applications. X-ray diffraction and Bragg's equation. Principle of XRD and its application in crystal structure determinations. Principle of Auger emission spectroscopy (AES).

### 2. Electron Spin Resonance (ESR) and Nuclear Magnetic Resonance Spectroscopy (NMR)

Principle of ESR, Lande's g factor. Hyperfine splitting. Application to hydrogen atom, methyl free radical etc.

ENDOR and ELDOR. Applications. Principle of NMR. Nuclear spin, Population of states. Saturation, Chemical shift and its measurement. Factor affecting chemical shift, Spin-spin interaction, factors influencing coupling constant 'J'. Spin decoupling. NMR studies of nuclei other than proton- $^{13}\text{C}$ ,  $^{19}\text{F}$  and  $^{31}\text{P}$ . FT NMR, advantages of FT NMR. Instrumentation of NMR. Applications.

### 3. Mass Spectrometry

Principle of Mass spectrometry. Mass instrumentation. Ionisation methods: EI, CI, ESI & Desorption methods. Analyser: Magnetic sector, Quadrupole & Time-of Flight analyser.

### 4. Electroanalytical Methods

Principle of Potentiometry, Voltametry, Conductometry and pH-metry. Applications.

#### BOOKS SUGGESTED:

1. Pavia, Lampman, Kriz, Spectroscopy, Books/Cole: Vyvyan
2. PS Kalsi Spectroscopy of Organic Compounds, New Age International Publishers;
3. Silverstein, Robert M.; Webster, Francis X.; Kiemle, Spectrometric Identification of Organic Compounds, John Wiley;
4. ML Martin, JJDelpach and GJ Martin, Heyden, Practical NMR Spectroscopy.
5. Colin N. Banwell and Elaine M. Mc Cash, Fundamentals of Molecular Spectroscopy, Tata McGraw Hill.
6. RJ Abraham, J Fischer and P Loftus, Introduction to NMR Spectroscopy, Wiley.
7. DH Williams, I Fleming, Spectroscopic Method in Organic Chemistry: Tata MacGraw Hill.
8. Willard Merritt, Dean, Settle, Instrumental Method of Analysis: Seventh Edition, CBS, Publication.

**(V) Lab Course (Inorganic, Organic and Physical) SEM II (CHC20P)**  
**(2×6 hours)**

**1. Quantitative Analysis**

Quantitative Analysis of mixtures of two metal ions involving Volumetric (by complexometric titration using masking and demasking agents) and gravimetric analysis.

**2(a). Organic Synthesis**

**20 marks**

Acetoacetic ester Condensation: Synthesis of ethyl-n-butylacetoacetate by A.E.E. condensation. Cannizzaro reaction: 4-Chlorobenzaldehyde as substrate. Aromatic electrophilic Substitutions: Synthesis of p-nitroaniline and p-bromoaniline. The products may be characterized by Spectral Techniques where possible.

**(b). Quantitative Analysis**

**1×20 marks**

Determination of the percentage or number of hydroxyl groups in an organic compound by acetylation method. Estimation of amines/phenols using bromate bromide solution/or acetylation method. Determination of Iodine and Saponification values of an oil sample. Determination of DO, COD and BOD of water sample.

**3(a). Potentiometry/pH-metry**

- i. Determination of strengths of halides in a mixture potentiometrically.
- ii. Determination of the valency of mercurous ions potentiometrically.
- iii. Determination of the strength of strong and weak acids in a given mixture using a potentiometer/pH meter.
- iv. Determination of temperature dependence of EMF of a cell.
- v. Determination of the formation constant of silver-ammonia complex and stoichiometry of the complex potentiometrically.
- vi. Acid-base titration in a non-aqueous media using a pH meter.
- vii. Determination of activity and activity coefficient of electrolytes.
- viii. Determination of the dissociation constant of acetic acid in DMSO, DMF, acetone and dioxane by titrating it with KOH.
- ix. Determination of the dissociation constant of monobasic/dibasic by Albert-Serjeant method.

**1×15 marks**

**(b). Spectrophotometric (UV/VIS) Estimations**

(i) Amino acids

(ii) Ascorbic acid

(iii) Proteins

(iv) Aspirin

(v) Carbohydrates

(vi) Caffeine

(vii) Cholesterol

**4. Viva**

**10 marks**

**5. Record**

**15 marks**

**SEM III**  
**Specialization Inorganic Chemistry**



## (I) Organometallic Chemistry (CHC301)

- 1. Transition Metal  $\pi$ -Complexes and metal compounds with bonds to hydrogen**  
Transition Metal  $\pi$ -Complexes with unsaturated organic molecules. Alkenes, alkynes, allyl, diene, dienyl, arene and trienyl complexes; preparation, properties, nature of bonding and structural features. Important reactions relating to nucleophilic and electrophilic attack on ligands and to organic synthesis. Compounds of Metal Carbon Multiple Bonds and Metal Compounds with Bonds to Hydrogen
- 2. Organic Derivatives of Metals and Alkyls, Aryls and Acyls of Metals:**  
Metal beta-diketonates and thio-beta-diketonates; general chemistry, structural aspects and applications. Metal Alkoxides; general methods of preparation, reactivity, structure and applications. Alkyls, aryls and acyls of transition metals, nature of metal carbon bond, routes of synthesis, stability and decomposition pathways and structure, alkyls, aryls and acyls of s-block and p-block elements. Comparison of such transition and non-transition element derivatives. Organocopper in organic synthesis.
- 3. Homogeneous Catalysis and types of reactions:**  
Stoichiometric reactions for catalysis, homogeneous catalytic hydrogenation, Zeigler-Natta polymerization of olefins, catalytic reactions involving carbon monoxide such as hydrocarbonylation of olefins (oxo reaction), oxopalladation reactions. Activation of C-H bond. Oxidative-Addition and Migration (Insertion) Reactions, activation of small molecules by coordination
- 4. Fluxional Organometallic Compounds Fluxionality and dynamic equilibria in compounds such as  $\eta^3$ - allyl and dienyl complexes, their characterization.**

### Books Suggested:

1. Principle and Application of Organotransition Metal Chemistry, J.P. Collman, L.S. Heegsdus, J.P. Norton and R.G. Finke. University Science Books.
2. The Organometallic Chemistry of the Transition Metals, R.H. Crabtree, John Wiley.
3. Metallo-organic Chemistry, A.J. Pearson, Wiley.
4. Organometallic Chemistry, R.C. Mehrotra and A. Singh; New Age International.
5. Organometallic Compounds, N.H. Green, Chapman & Hall, U.K.
6. Principles of Organometallic Chemistry, G.E. Coates, M.H. Green, P. Powell, Chapman & Hall, U.K.

## (II) Spectroscopy (CHC302)

- 1. Photo-Electron Spectroscopy (PES) and Fluorometry and Phosphometry**  
Photoelectric effect. Principle of PES. Ionization process, Koopman's Theorem. Photoelectron spectra of simple molecules. ESCA. Chemical information from ESCA. Applications.  
Principles. Factors affecting fluorescence and phosphorescence. Total Luminescence spectroscopy. Applications
- 2. Nuclear Quadrupole Resonance (NQR)**  
Quadrupole nuclei, Quadrupole moment. Principle of NQR. Splitting of NQR spectra. Instrumentation.
- 3. Mossbauer Spectroscopy**

Principle of Mossbauer technique. Parameters in Mossbauer spectroscopy. Instrumentation. Applications.

#### 4. Optical Rotatory Dispersion (ORD) and Circular Dichroism (CD)

Principles of ORD and CD. Cotton effect. Octant rule for ketones. Applications

##### Books Suggested:

1. Physical Methods for Chemistry, R.S. Drago, Saunders Company.
2. Structural Methods in Inorganic Chemistry, E.A.V. Ehsworth, D.W.H. Rankin and S. Craddock, ELBS.
3. Craddock, ELBS.
4. Infrared and Raman Spectra: Inorganic and Coordination Compounds, K. Nakamoto, Wiley.
5. Inorganic Electronic Spectroscopy, A.P.B. Lever, Elsevier.
6. Symmetry and Spectroscopy, K. Veera Reddy, New Age International, 1998.
7. Instrumental Methods of Analysis, Willard et al., 7th Edn., CBS Publishers.

### (III) Analytical Chemistry(CHC303)

#### 1. Introduction

Role of analytical chemistry. Classification of analytical methods-classical and instrumental. Types of instrumental analysis. Selecting an analytical method. Neatness and cleanliness. Laboratory operations and practices. Analytical balance. Techniques of weighing, errors. Volumetric glassware-cleaning and calibration of glassware. Sample preparations-dissolution and decompositions. Gravimetric techniques. Selecting and handling of reagents. Laboratory notebooks. Safety in the analytical laboratory.

#### 2. Errors

Determinate and indeterminate errors. minimization of determinate errors, random distribution of indeterminate errors.

#### 3. Statistical data analysis

Accuracy and precision, significant figures and computations, mean and standard deviation, distribution of random errors, reliability of results, confidence interval, comparison of results, comparison of means of two samples, paired t-test, number of replicate determinations and its use, correlation and regression, linear regression, analysis of variance, rejection of data.

#### 4. Application of Analytical Chemistry

Application of analytical chemistry in the study of water and soil pollutions, analysis of fuel, body fluids and drugs

##### Books Suggested:

1. Analytical Chemistry, G.D. Christian, J. Wiley.
2. Fundamentals of Analytical Chemistry, D.A. Skoog, D.M. West and F.J. Holler, W.B. Saunders.
3. Analytical Chemistry-Principles, J.H. Kennedy, W.B. Saunders.
4. Analytical Chemistry-Principles and Techniques, L.G. Hargis, Prentice Hall.
5. Principles of Instrumental Analysis, D.A. Skoog and J.L. Lorry, W.B. Saunders.
6. Quantitative Analysis, R.A. Day, Jr. and A.L. Underwood, Prentice Hall.
7. Environmental Solution Analysis, S.M. Khopkar, Wiley Eastern.
8. Basic Concepts of Analytical Chemistry, S.M. Khopkar, Wiley Eastern.
9. Handbook of Instrumental Techniques for Analytical Chemistry, F. Settle, Prentice Hall.

### IV (i) Chemistry of Biological System I (Bioinorganic) (CHE301)

#### 1. Metal Ions in Biological Systems, Na<sup>+</sup>/K<sup>+</sup> Pump

- Essential and trace metals. Role of metal ions in biological processes.  $\text{Na}^+/\text{K}^+$  Pump.
- Bioenergetics and ATP Cycles**  
DNA polymerization, glucose storage, metal complexes in transmission of energy; chlorophylls, photo system I and photo system II in cleavage of water; Model systems.
  - Transport and Storage of Dioxygen**  
Heme proteins and oxygen uptake, structure and function of hemoglobin, myoglobin, hemocyanins and hemerythrin, model synthetic complexes of iron, cobalt and copper.
  - Electron Transfer in Biology and Nitrogenase**  
Structure and function of metalloproteins in electron transport processes-cytochromes and iron-sulphur proteins, synthetic models.  
Biological nitrogen fixation, molybdenum nitrogenase, spectroscopic and other evidence, other nitrogenases model systems.

#### BOOKS SUGGESTED

- P.S. Kalsi, Bioorganic, Bioinorganic and Supramolecular Chemistry, New Age International.
- I Bertoni, H.B. Gray, S.J. Lippard and J.S. Valentine, Bioinorganic Chemistry, University Science Books.
- Principles of Bioinorganic Chemistry, S.J. Lippard and J.M. Berg, University Science Books.
- Bioinorganic Chemistry: A Chemical Approach to Enzyme Action, Hermann Dugas and C. Penny, Springer-Verlag.

#### IV(ii) Bioinorganic & Supramolecular Chemistry (CHE302)

- Metal Storage Transport and Biomineralization**  
Ferritin, transferrin and siderophores.
- Calcium in Biology**  
Calcium in living cells, transport and regulation, molecular aspects of intramolecular processes, extracellular binding proteins.
- Metalloenzymes and Metal – Nucleic Acid Interactions**

Zinc enzymes— carboxypeptidase and carbonic anhydrase. Iron enzymes—catalase, peroxidase and cytochrome P-450. Copper enzymes— superoxide dismutase, Molybdenum oxotransferase enzymes— xanthine oxidase. Coenzyme vitamin B12.  
Metal ions and metal complex interactions, Metal complexes—nucleic acids

- Supramolecular Chemistry**  
Concepts and language. Molecular recognition: Molecular receptors for different types of molecules including arisonic substrates, design and synthesis of coreceptor molecules and multiple recognition. Supramolecular reactivity and catalysis. Transport processes and carrier design. Supramolecular devices. Supramolecular photochemistry. Supramolecular electronic, ionic and switching devices. Some example of self-assembly in supramolecular chemistry.

#### BOOKS SUGGESTED

- P.S. Kalsi, Bioorganic, Bioinorganic and Supramolecular Chemistry, New Age International.
- Understanding Enzymes, Trevor Palmer, Prentice Hall.
- Enzyme Chemistry: Impact and Applications, Ed. Collins J Sucking, Chapman and Hall.
- Enzymes Mechanism Ed, M.L. Page and A. Williams, Royal Society of Chemistry.
- Fundamentals of Enzymology, N.C. Price and L. Stevens, Oxford University Press.
- I Bertoni, H.B. Gray, S.J. Lippard and J.S. Valentine, Bioinorganic Chemistry, University Science Books.
- Principles of Bioinorganic Chemistry, S.J. Lippard and J.M. Berg, University Science Books.

8. Immobilized Enzymes: An Introduction and Applications in Biotechnology, Michael D. Trevan, John Wiley.
9. Enzymatic Reaction Mechanism, C. Walsh, W.H. Freeman.
10. Enzymatic Structure and Mechanism, W.H. Freeman.
11. Supramolecular Chemistry, J.M. Lehn, VCH.

### (V) Lab Course (Inorganic) SEM III (ICHC30P) (2×6 hours)

1. Analysis of the given sample (Ores): Both Qualitative and Quantitative Dolomite, Pyrolusite, Galena. 20 marks
2. Analysis of the given alloys: Coin, Gunmetal, Brads and Bronze. 20 marks

#### 3. Preparations

Preparation of selected inorganic compounds:

- (i) VO (aac)<sub>2</sub>
  - (ii) TiO (C<sub>6</sub>H<sub>5</sub>NO)<sub>2</sub> · 2H<sub>2</sub>O
  - (iii) cis-K[Cr(C<sub>2</sub>O<sub>4</sub>)<sub>2</sub> (H<sub>2</sub>O)<sub>2</sub>]
  - (iv) Na[Cr(NH<sub>3</sub>)<sub>3</sub>(SCN)<sub>3</sub>]
  - (v) Mn (aac)<sub>2</sub>
  - (vi) K<sub>3</sub>[Fe(C<sub>2</sub>O<sub>4</sub>)<sub>3</sub>] · 3H<sub>2</sub>O
  - (vii) Co [(NH<sub>3</sub>)<sub>6</sub>] Cl<sub>2</sub>
  - (viii) [Cu (en)<sub>2</sub> (H<sub>2</sub>O)<sub>2</sub>] I<sub>2</sub>
  - (ix) [Co (Py)<sub>2</sub>Cl<sub>2</sub>]
  - (x) Tris-(thiourea) copper (I) sulphate [Cu (tu)<sub>3</sub>] SO<sub>4</sub> · 2H<sub>2</sub>O
- And their characterization by following techniques:

1×20 marks

- i) Elemental analysis
- ii) Molar conductance values
- iii) I.R. Spectral interpretation
- iv) Thermal analysis
- v) UV-Visible Spectra

#### 4. Viva

10 marks

#### 5. Record

10 marks

## Specialization Organic Chemistry

### (I) Reagents in Organic Synthesis and Organometallics (CHC304)

#### 1. Determination of Reaction Mechanism

Classification, rate constants and life times of reactive energy states-determination of rate constants of reactions. Effect of light intensity on the rate of photochemical reactions. Types of photochemical reactions, photo-dissociation, gas-phase photolysis.

#### 2. Oxidation: Reduction and Reaction

Introduction. Different oxidative processes. Hydrocarbons-alkenes, aromatic rings, saturated C-H groups (activated & unactivated). Alcohols, diols, aldehydes, ketones, ketals and carboxylic acids, Amines, hydrazines and sulphides. Oxidation with ruthenium tetroxide, iodobenzene diacetate and thallium (III) nitrate.

Introduction. Different reductive processes.

Reduction of hydrocarbons- alkenes, alkynes and aromatic rings.

Reduction of carbonyl compounds (aldehydes, ketones, acids and their derivatives). Epoxides.

Reduction of nitro, nitroso, azo and oxime groups.



2. To make studies on gradient analysis.
3. To identify different forest types of the locale.
4. Calculate the Pateren week index of any natural forest stand.
3. Study ordination and continuum of different forest stands.
6. Study interspecific Association in forest stands using Plot less technique.
7. Calculate analytical and synthetic characters of different forest stands.
8. Prepare profile diagram of forest stands using Single Plot Method.

#### SUGGESTED READINGS:

1. Bir, S.S. and Chatha, G.S. 1988. Forest Vegetation Characteristics of Indian Hills. Today and Tomorrow's Printers & Publ., New Delhi.
2. Dwivedi, A.P. Forestry in India. Jugal Kishor and Company, Dehradun.
3. Misra, R. Ecology Work Book. Oxford & IBH Publishing Co. New Delhi.
4. Mishra, R. and Gopal, B. Recent Advances in Tropical Ecology: Part I & II. International Society for Tropical ecology, Varanasi.
5. Negi, S.S. 1983. Forest Ecology. Bishen Singh Mahendra Pal Singh, Dehradun.
6. Puri, G.S., Gupta, R.K., Meher-Homji, V.M. and Puri, S. 1989. Forest Ecology: Plant Form, Diversity, Communities and Succession. Oxford and IBH Publishing Co. Pvt. Ltd. New Delhi.
7. Puri, G.S., Meher-Homji, V.M., Gupta, R.K. and Puri, S. Forest Ecology: Vol I & II. Oxford and IBH Publishing Co. Pvt. Ltd. New Delhi.
8. Singh, G. 1987. Forest Ecology of India. Rawat Publications, Jaipur
9. Singh, J.S. and Singh, S.P. 1992. Forests of Himalaya. Consul Book Depot. Gyanodaya Prakashan, Nainital, India.
10. Singh, J.S. Singh, S.P. and Gupta, S.R. 2005. Ecology, Environment and Resource Conservation. Anamaya Publ., F-154/2 Ladosarai, New Delhi- 110 030
11. Singh, M.P. and Vishwakarma, V. 1997. Forest Environment and Biodiversity. Daya Publ. House, Delhi.
12. Wareing, R.H. and Schlesinger, W.H. 1985. Forest Ecosystems: Concepts and Management. Academic Press. New York.

#### Paper IV (b) (BOT404/E2): Industrial Microbiology

##### Unit 1

1. Introduction to industrial microbiology-Range of fermentation processes, microbial biomass, microbial enzymes, microbial metabolites and transformation processes.
2. Selection and strain improvement strategies - Isolation of industrially important microorganisms - primary and secondary screening. Detection and assay of fermentation products - physical-chemical, biological assays. Preservation of microbes - storage at reduced temperature, storage in dehydrated forms.

##### Unit 2

1. Types of fermentation - Solid state fermentation and submerged fermentation; batch, continuous and fed batch fermentation. Homo- and heterofermentation. Aerobic and anaerobic fermentation. Static and stirred fermentations. Media for microbial growth and fermentation - Typical media, media formulation; water, energy and carbon source, nitrogen sources, minerals and vitamins, buffers, precursors, metabolic regulators, oxygen requirement.
2. Bioreactors - Brief study on stirred tank fermenter, air-lift fermenter, packed tower fermenter, tray fermenter, rotary drum fermenter. Microbial fermentation- Sterilization -

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media, fermenter, air. Inoculum preparation, inoculation. Aeration, agitation, pH control, temperature control, antifoam agents. Process parameter optimization: One factor at a time and statistical optimizations (brief study only). Scale up of fermentation (lab scale, pilot plant, industrial scale).

#### Unit 3

1. Downstream processing. Separation of microbial cells – Filtration, precipitation, centrifugation.
2. Cell disruption – liquid shear, freezing-thawing, ultrasonication, osmotic shock, enzyme treatment. Concentrating and purifying the products - ultrafiltration, crystallization, solvent precipitation, reverse osmosis, chromatography. Production of industrially important products.

#### Unit 4

1. Antibiotics - Penicillin, Streptomycin. Amino acids - Lysine, Glutamic acid. Enzymes - Amylase, Cellulase, Pectinase, Organic acids - Lactic acid, Acetic acid, Gluconic acid. Biofuels – Bio-ethanol, Bio-butanol. Biopolymers - PHB, PLA. Alcoholic beverages - Wine, Beer. Microbial cells - SCP.
2. Baker's yeast. Immobilization of cells and enzymes- Methods of cell and enzyme immobilization. Applications of immobilized cells and enzymes.

#### Lab Course

1. Screening and isolation of microbes for production of organic acids and enzymes.
2. Preparation and maintenance of stock cultures (Bacteria and Fungi).
3. Preparation of bacterial inoculum by measuring OD and enumeration of bacterial cells by serial dilution and pour plate (or spread plate) method.
4. Solid state and Submerged fermentation for amylase (or any other enzyme) production and quantification of product by suitable assay methods.
5. Optimization of process parameters for enzyme production in submerged fermentation.
6. Partial purification of amylase (or any other enzyme) produced by microbial fermentation using acetone precipitation.
7. Immobilization of yeast cells and sugar fermentation using immobilized cells.

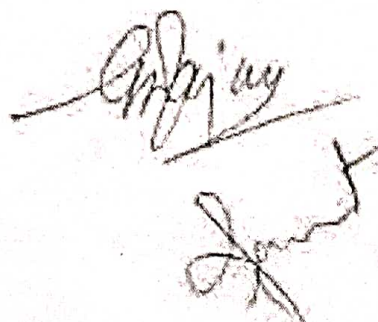
#### Suggested readings:

1. Madigan, M.T., J.M. Martink and J. Parker (1997). Brock Biology of Microorganism. Printice hall International, Inc., New, Jersey.
2. Prescott (2000). Microbiology.
3. Cruzer, W. and A. Cruzer (1990). A Textbook of Industrial Microbiology.
4. Alexander, M. (1977), Soil Microbiology. John Wiley and Sons, New York.
5. Dubey, R.C. and D.K. Maheshwari (2010). A Textbook of Microbiology. S. Chand and Co. Pvt. Ltd. New Delhi.

#### Paper IV (c) (BOT404/E3): Ethnobotany

##### Unit I

1. Introduction, concept, scope and objectives. Linkage of Ethnobotany with other sciences and disciplines in biology – food and nutrition, medicine, sociological and cultural practices, religions and social costumes and economic relations.
2. Ethnic groups and Ethnobotany: Major and minor ethnic groups of Uttarakhand and their life styles. Forest v/s Ethnic groups.



## Unit 2

1. Methodology of Ethnobotanical studies: Field work, Herbarium, Ancient Literature, Archaeological findings, Temples and sacred places, Protocols. Plants and Tribal medicine: Significance of *Circaea orchoides*, *Costus speciosus*, *Gloriosa superba*, *Butea monosperma*, *Wrightia tinctoria* and *Pongamia pinnata* in Ethno-medical practices along with a brief note on their habitat and morphology.
2. Medico-ethnobotanical research in Uttarakhand.

## Unit 3

1. Different systems of indigenous medicine (Traditional medicine, Ayurveda, Siddha, Unani), Homeopathy and Allopathy. Role of Phytomedicine in modern systems of medicine.
2. Classification of drugs; analytical methods – drug adulteration, drug evaluation, anatomical and phytochemical analysis of crude drugs; preliminary screening, fractionation and separation of different groups of biodynamic compounds and biological evaluation.

## Unit 4

1. Phytopharmaceuticals: Drugs of alkaloids, coumarins, volatile oils, tannins, resins and gums. Natural pesticides, antibiotics, allergens and poisonous plants. Economic potential of phytomedicine; potential drug yielding plants and their marketing avenues. IPR and patenting of active principles.
2. Ethnobotany and conservation of plants with special reference to Uttarakhand – mythology and conservation of ecosystems, conservation of selected plant species: sacred groves, forestry and unique ecosystems and their ethnobiological values, plants and animals in art, tradition and ethnography; methodologies in ethno-botanical research

## Lab Course:

1. Preparation of the herbarium specimen medicinally important plants.
2. Listing of plants used by villagers and on the basis of their local use to place them in the field of the study of ethnobotanical research.
3. Study of Economic potential of Phytomedicine and role of phytomedicine in modern system of medicine.

## Suggested Readings:

1. S.K. Jain, Manual of ethnobotany, scientific publishers, Jodhpur, 1995.
2. S.K. Jain (ed.) Glimpses of Indian Ethnobotany, Oxford and I B H, New Delhi, 1981.
3. S.K. Jain, (ed.) Methods and approaches in ethnobotany. Society of Ethnobotanists, Lucknow, India, 1989.
4. S.K. Jain, Contributions of Indian ethnobotany, Scientific Publishers, Jodhpur, 1990.
5. Colton C.M. Ethnobotany-Principles and applications. John Wiley and sons-Chichester, 1997.
6. Rama R. N. and A.N. Henry, The ethnobotany of Eastern Ghats in Andhra Pradesh, India. Botanical Survey of India, Howrah, 1996.
7. Rajiv K. Sinha, Ethnobotany-the renaissance of traditional Herbal Medicine-I N A- Shree publishers, Jaipur, 1996.

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## Paper IV (d) (BOT404/E4): PALYNOLOGY AND POLLINATION BIOLOGY

### Unit 1

1. General Introduction, trilete spores, microsporeogenesis, microspore tetrads and polarity of spores and pollen grains.
2. Pollen wall development and pollen chemistry. Chemical nature of sporopollenin, development of pollen wall, Utricle body, pollen wall proteins; origin and formation exineless pollen grains; pollen expressed and pollen specific genes.

### Unit 2

1. Spore-pollen morphology: Symmetry, shape, size, aperture patterns, NPC System for numerical expression of apertural details, exine stratification, surface structures and sculptures of sporoderm, LO-analysis and edge-analysis.
2. Palynotaxonomy: Systematic palynology, identification key and evolutionary trends among pollen grains based on palynotaxonomical works.
3. Aeropalynology with reference to allergy: Aeroallergens, introductory idea of Immune System with special reference to IgE. Study of airspores, identification of allergic taxa by *in vivo* and *in vitro* tests with spore-pollen extracts, chemical nature of exine-borne allergens, allergic taxa of North-West Himalaya.

### Unit 3

1. **Melissopalynology:** Indian species of honey bees, importance of pollen grains as constituent of bee-bread, pollen-collecting mechanism of honey bees, analysis of pollen load and honey sample in understanding bee forage, objectives of melissopalynological studies, important bee plants of North-West Himalaya.
2. **Palaeopalynology:** Introductory idea about palaeopalynological remains, significance of palaeopalynology.

### Unit 4

1. Forensic palynology: Definition and significance, a few well-known case studies.
2. Pollination Biology: Pollen dispersal units; pollination types, contrivances for cross- and self-pollination; pollen vectors, pollination modes and flora organization, Pollen viability and storage, evolutionary trends in pollination modes. Breeding systems, incompatibility and compatibility control with reference to pollen-pistil interactions and pollen biotechnology.

### Lab Course

1. Pollen morphological studies of some pteridophytes, gymnosperms, and angiosperms representing different morphological types using acetolysis / alkali maceration method.
2. Extraction of pollen grains from honey sample and study of the frequency of different morpho-types.
3. Study of *in vivo* and *in vitro* germination of pollen grains.
4. Morpho-anatomical study of stigma and style.
5. Study of the growth of pollen tube through stigma and style.
6. Study of allergy producing pollen morpho-types.

### SUGGESTED READINGS:

1. Crane, E.V., Walker, Penelope and Day Rosemary. 1984. Directory of Important World Honey Sources: International Bee Research Association, London.
2. Firdman, G. 1952. Pollen Morphology and Plant Taxonomy, Angiosperms; Almqvist and Wiksell, Stockholm.

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3. Knut Segril, Johnson Iverson. 1975. Text book of pollen analysis 3rd edition. Blackwell Publ.
4. Nair, P.K.K. 1966. Essentials of Palynology, Asia Publication House Lucknow.
5. Windhouse, R.P. 1935. Pollen Grains: Hafner Publication Co.

#### Paper IV (c) (BOT404/E5): Seed Pathology

##### Unit 1

1. Introduction, terminology and historical development, seed health and its importance.
2. Kinds of seed borne pathogens: fungi, bacteria, viruses, viroids and nematodes.
3. Types of damage caused by the seed borne fungi to seeds and crops.

##### Unit 2

1. Nature of seed infection. Systemic infection through flower, fruit and seed stock. Penetration through seed coat, natural openings and inflicted openings.
2. Longevity of seed borne pathogens. Factors influencing longevity.

##### Unit 3

1. Epiphytology of seed borne diseases, monocyclic and polycyclic diseases
2. Detection of seed borne pathogens, objectives of seed health testing. Testing methods for seed borne fungi, seed borne bacteria, seed borne viruses and seed borne nematodes.

##### Unit 4

1. Study of seed borne diseases of certain specific crops, cereals, millets, pulses, oil crops, fibre crops, and vegetable and timber crops
2. Control of seed borne pathogens: selection of seed production areas, crop management, seed treatment, certification, plant quarantine and disease resistance.

##### Lab Course

1. Isolation and inoculation of mycorrhiza.
2. Study of seed borne pathogen. Description of pathogen, symptoms and section cutting.
3. Isolation of some important pathogens.
4. Procedure of equipments uses.
5. To establish a plant disease clinic in the department for advise to local people.

##### SUGGESTED READINGS

1. Neegard P. 1977. Seed Pathology Vol I and II. MacMillan Press, London
2. Suryanarayan, D. 1978. Seed Pathology. Vikas Publ. House. Pvt. Ltd. New Delhi.
3. Jha, D.K. 1995. A Text Book of Seed Pathology. Vikas Publ. House. Pvt. Ltd. New Delhi.
4. Agarwal, V.K. 1978. Principles of Seed Pathology. In (ed.) James B.S. Sindsir, CRC Press, II Edition.
5. Desui, B.B. Seed Handbook. CRC Press.
6. Singh, Gurnam. Seed Pathology. Pointer Publisher, Jaipur.
7. Singh, T. Seed Technology and Seed Pathology. Pointer Publisher, Jaipur.
8. Nene, Y.L. and Agarwal, V.K. 1978. Some seed borne diseases and their control. ICAR, New Delhi

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**Lab Course : BOT40P\***

1. Emasculation, bagging and hand pollination techniques to study pollen germination.
- Application of common plant breeding techniques
2. Floral biology of local food, pulse, vegetable and horticultural crop
3. To test the goodness of fit and independent assortment using Chi-square method.
4. To study the pattern of regional biodiversity.
5. To study the Hot spots and key stone species.
6. Survey of biological resources.
7. Study of habitat loss with respect to plant species. To observe factors expediting habitat loss viz., floods, forest fires, landslides, natural and anthropological activities.
8. Visits to national parks, sanctuaries and biosphere reserves of Uttarakhand.
9. Visit to ecosystem restoration sites in mined areas in Uttarakhand Himalayas.
10. PTC – Laboratory organization, different sterilization/aseptic technique.
11. Preparation and sterilization of media
12. Callus culture (morphological and internal structure) and suspension cultures (growth curve)
13. Shoot tip, axillary bud, nodal explant culture.
14. Root tip and leaf culture.
15. Protoplast isolation and fusion
16. Somatic embryogenesis and production of artificial seeds.
17. Anther, pollen, ovule culture.

\*Additional lab course of selected elective paper.

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## Hydrogenolysis.

### 3. Organometallics in Synthesis:

Principle, preparations, properties and applications of the following in organic synthesis:  
Group I and II metal organic compounds Li, Mg, Hg and Zn compounds  
Transition metals: Pd, Ni, Fe, Ti, Cu, Rh and Cr compounds; Other elements: S, Si and B compounds

### 4. Metallocenes, Nonbenzenoid Aromatics and Polycyclic Aromatic Compounds:

General considerations, synthesis and reactions of some representative compounds.

#### Books suggested

1. Modern Synthetic Reactions, H.O. House, W.A. Benjamin.
2. Some Modern Methods of Organic Synthesis, W. Carruthers, Cambridge Univ. Press.
3. Advanced Organic Chemistry, Reactions Mechanisms and Structure, J. March, John Wiley.
4. Principles of Organic Synthesis, R.O.C. Norman and J.M. Coxon, Blackie Academic & Professional.
5. Advanced Organic Chemistry Part II, F.A. Carey and R.J. Sundberg, Plenum Press.
6. Rodd's Chemistry of Carbon Compounds, Ed. S. Coffey, Elsevier.
7. W. Carruthers, Some Modern Methods of Organic Synthesis, Cambridge Univ. Press.
8. J. Fuhrhop and G. Penzillin, Organic Synthesis- Concept, Methods and Starting Materials Verlag VCH.

## (II) Spectroscopy (CHC302)

### 1. Photo-Electron Spectroscopy (PES) and Fluorometry . Phosphometry

Photoelectric effect. Principle of PES. Ionization process. Koopman's Theorem. Photoelectron spectra of simple molecules. ESCA. Chemical information from ESCA. Applications.  
Principles. Factors affecting fluorescence and phosphorescence. Total Luminescence spectroscopy. Applications.

### 2. Nuclear Quadrupole Resonance (NQR)

Quadrupole nuclei. Quadrupole moment. Principle of NQR. Splitting of NQR spectra. Instrumentation.

### 3. Mossbauer Spectroscopy

Principle of Mossbauer technique. Parameters in Mossbauer spectroscopy. Instrumentation. Applications.

### 4. Optical Rotatory Dispersion (ORD) and Circular Dichroism (CD)

Principles of ORD and CD. Cotton effect. Octant rule for ketones. Applications.

#### Books Suggested:

1. Physical Methods for Chemistry, R.S. Drago, Saunders Company.
2. Structural Methods in Inorganic Chemistry, E.A.V. Ebsworth, D.W.H. Rankin and S. Craddock, ELBS.
3. Infrared and Raman Spectra: Inorganic and Coordination Compounds, K. Nakamoto, Wiley.
4. Inorganic Electronic Spectroscopy, A.P.B. Lever, Elsevier.
5. Symmetry and Spectroscopy, K. Veera Reddy, New Age International, 1998.
6. Instrumental Methods of Analysis, Willard et al., 7th Edn., CBS Publishers.

## (III) Organic Photochemistry(CHC305)

### 1. Basics of Photochemistry:

Absorption, excitation, photochemical laws, electronically excited states-life times, measurements of the times. Flash photolysis. Stopped flow techniques. Energy dissipation by radiative and non-radiative processes, absorption spectra, Franck-Condon principle, Photochemical stages- primary and secondary processes. Photo physical reactions, Jablonskii diagram, photosensitization, quantum yield and its determination, reactions of high and low quantum yields with suitable examples, fluorescence, phosphorescence and chemiluminescence with suitable examples

### 2. Photochemistry of Organic Compounds:

Photochemistry of alkenes; cis-trans isomerization, non-vertical energy transfer, photochemical additions; reactions of 1,3- and 1,4-dienes; dimerisation.

### 3. Photochemistry of Carbonyl Compounds:

Norrish type I & II reactions (cyclic and acyclic);  $\alpha,\beta$ -unsaturated ketones;  $\beta,\gamma$ -unsaturated ketones; cyclohexenones (conjugated); cyclohexadienones (cross-conjugated & conjugated); Paterno-Buchi reactions; photoreductions

### 4. Photochemistry of Aromatic Compounds:

Isomerisation, skeletal isomerisations, Dewar and prismanes in isomerisations. Singlet oxygen reactions; Photo Fries rearrangement of ethers and anilides; Barton reaction, Hoffmann-Löffler-Freytag reaction.

#### Books Suggested:

1. Fundamentals of Photochemistry, K.K. Rohtagi-Mukherji, New Age International
2. Essentials of Molecular Photochemistry, A. Gilbert and J. Baggott, Blackwell Scientific Publication
3. Molecular Photochemistry, N.J. Turro, W.A. Benjamin
4. Introductory Photochemistry, A. Cox and T. Camp, McGraw Hill
5. Photochemistry, R.P. Kundall and A. Gilbert, Thomson Nelson
6. Organic Photochemistry, J. Coxon and B. Hallon, Cambridge University Press.
7. W. M. Horspool, Aspects of Organic Photochemistry, Academic Press.

## IV (i) Chemistry of Biological System I (Bioorganic (CHE303))

### 1. Enzymes

Introduction and historical perspective, chemical and biological catalysis, remarkable properties of enzymes like catalytic power, specificity and regulation. Nomenclature and classification, extraction and purification. Fischer's lock and key and Koshland's induced fit hypothesis, concept and identification of active site by the use of inhibitors, affinity labeling and enzyme modification by site-directed mutagenesis. Enzyme kinetics, Michaelis - Menten and Lineweaver-Burk plots, reversible and irreversible inhibition.

### 2. Mechanism of Enzyme Action and Kinds of Reactions Catalysed by Enzymes

Transition-state theory, orientation and steric effect, acid-base catalysis, covalent catalysis, strain or distortion, Examples of some typical enzyme mechanisms for chymotrypsin, ribonuclease, lysozyme and carboxypeptidase A.

Nucleophilic displacement on a phosphorus atom, multiple displacement reactions and the coupling of ATP cleavage to endergonic processes. Transfer of sulphate, addition and elimination reactions, enolic intermediates in isomerization reactions,  $\alpha$ -cleavage and condensation, some isomerization and rearrangement reactions. Enzyme catalyzed carboxylation and decarboxylation.

### 3. Enzyme Models and Co-Enzyme Chemistry



Host-guest chemistry, chiral recognition and catalysis, molecular recognition, molecular asymmetry and prochirality. Biomimetic chemistry, crown ethers, cryptates. Cyclodextrins, cyclodextrin-based enzyme models, calixarenes, ionophores, micelles, synthetic enzymes or synzymes.

Cofactors as derived from vitamins, coenzymes, prosthetic groups, apoenzymes. Structure and biological functions of coenzyme A, thiamine pyrophosphate, pyridoxal phosphate, NAD<sup>+</sup>, NADP<sup>+</sup>, FMN, FAD, lipole acid, vitamin B12. Mechanisms of reactions catalyzed by the above cofactors.

#### 4. Applications of Enzymes

Large-scale production and purification of enzymes, techniques and methods of immobilization of enzymes, effect of immobilization on enzyme activity, application of immobilized enzymes, use of enzymes in food and drink industry-brewing and cheese-making, syrups from corn starch, enzymes as targets for drug design. Clinical uses of enzymes, enzyme therapy, enzymes and recombinant DNA technology.

#### BOOKS SUGGESTED

5. P.S. Kalsi, *Bioorganic, Bioinorganic and Supramolecular Chemistry*, New Age International.
6. *Understanding Enzymes*, Trevor Palmer, Prentice Hall.
7. *Enzyme Chemistry: Impact and Applications*, Ed. Collins J Suckling, Chapman and Hall.
8. *Enzymes Mechanism* Ed. M.I. Page and A. Williams, Royal Society of Chemistry.
12. *Fundamentals of Enzymology*, N.C. Price and L. Stevens, Oxford University Press.
13. I Bertoni, H.B. Gray, S.J. Lippard and J.S. Valentine, *Bioinorganic Chemistry*, University Science Books.
14. *Immobilized Enzymes: An Introduction and Applications in Biotechnology*, Michael D. Trevan, John Wiley.
15. *Enzymatic Reaction Mechanism*, C. Walsh, W.H. Freeman.
16. *Enzymatic Structure and Mechanism*, W.H. Freeman.
17. *Supramolecular Chemistry*, J.M. Lehn, VCH.

### IV(ii) Chemistry of Natural Products (CHE304)

#### 1. Terpenoids and Carotenoids

Classification, occurrence, isolation, general methods of structure determination, U.V., IR., NMR and Mass Spectra. Biosynthesis and synthesis of citral, geraniol,  $\alpha$ -terpineol, menthol, farnesol, zingiberene, santonine, longifolene, phytol, abietic acid,  $\beta$ -carotene and vitamin A.

##### Plant Pigments:

Occurrence, nomenclature, synthesis of Quercetin myricetin cyanidine hirsutidin Biosynthesis of plant pigments flavonoids, flavone, flavonol.

#### 2. Steroids

Occurrence, physiological action, basic skeleton, stereochemistry, structure determination of cholesterol by degradation experiments, synthesis and biosynthesis of cholesterol, bile acids, and rosterone, testosterone, estrone, progesterone, cortisone.

#### 3. Alkaloids

Occurrence, isolation, physiological action, general method structure elucidation, degradation, classification based on nitrogen heterocyclic ring structure, stereochemistry, synthesis and biosynthesis of ephedrine, coniine, Nicotine, atropine, quinine, morphine, chloroquin and prima quin, uses of strychnine brucin etc. in organic synthesis.

#### 4. Vitamins

Occurrence, deficiency, physiological effects and synthesis of B complex. E and K. Chemotherapy; Sulpha drugs, antibiotics Cell wall biosynthesis, inhibitors,  $\beta$ -lactam rings synthesis of penicillin G, V, ampicillin, amoxyceillin, chloramphenicol, cephalosporin, tetracyclin and streptomycin. Prostaglandins Biosynthesis, Synthesis of PGE2 and PGF22.

### Books Suggested

1. Natural Products: Chemistry and Biological Significance, J.Mann, R.S. Davidson, J.B. Hobbs, D.V. Banthorpe and J.B. Harborne, Longman, Essex.
2. Organic Chemistry, Vol 2, I.L. Finar, ELBS.
3. Stereoselective Synthesis: A Practical Approach, M. Nogradi, VCH.
4. Rodd's Chemistry of Carbon Compounds, Ed. S. Coffey, Elsevier.
5. Chemistry, Biological and Pharmacological Properties of Medicinal Plants from the Americas, Ed. Kurt. Hostettmann, M.P. Gupta and A. Marston, Harwood Academic Publishers.
6. Introduction to Flavonoids, B.A. Bohn, Harwood Academic Publishers.
7. New Trends in Natural product Chemistry, Atta-ur-Rahman and M.I. Chaudhary, Harwood Academic Publishers

### (V) Lab Course (Organic) SEM III (OCHC30P) (2x6 hours)

#### 1. Qualitative Analysis

Separation, purification and identification of the components of a mixture of three organic compounds (three solids or two liquids and one solid, two solids and one liquid), using TLC for checking the purity of the separated compounds. Preparation of derivatives and spectral analysis.

#### 2. Multi-step Synthesis of Organic Compounds

The exercise should illustrate the use of organic reagents and may involve purification of the products by chromatographic techniques. **2x30 marks**

#### 3. Photochemical conversions

- Benzophenone to Benzpinacol to Benzpinacolone
- Beckmann rearrangement: Benzanilide from benzene
- Benzene to Benzophenone to Benzophenone oxime to Benzanilide
- Benzilic acid rearrangement: Benzilic acid from benzoin
- Benzoin to Benzil to Benzilic acid

#### 4. Enzymatic Synthesis

Enzymatic reduction: Reduction of ethyl acetoacetate using Baker's yeast to yield enantiomeric excess of S (-) ethyl-3-hydroxybutanoate and determine its optical purity.  
Biosynthesis of ethanol from sucrose

#### 5. Viva

10 marks

#### 6. Record

10 marks

### Specialization Physical Chemistry

#### (I) Advanced Quantum Chemistry (CHC306)

#### 1. Theoretical and Computational (optional) Treatment of Atoms and Molecules, Hartree-Fock Theory

Review of the principles of quantum mechanics. Born-Oppenheimer approximation. Slater-Condon rules. Hartree-Fock equation. Koopmans and Brillouin theories. Roothan equation, Gaussian basis sets.

#### 2. Configuration Interaction and MC-SCF

Introduction to CI; full and truncated CI theories. Size consistency. Introductory treatment of coupled cluster and MC-SCF methods.

#### 3. Semi-Empirical Theories

A review of the Huckel, EHT and PPP treatments, ZIC approximation. Detailed treatment of CNDO and INDO theories. A discussion of electronic energies and properties.

#### 4. Density Functional Theory

Derivation of Hohenberg-Kohn theorem, Kohn-Sham formulation, N- and V- representabilities, review of the performance of the existing local (e.g. Slater X $\alpha$  and other methods) and non-local functionals, treatment of chemical concepts with the density functional theory.

### Books Suggested

1. Modern Quantum Chemistry, N.S. Ostlund and a. Szabo, McGraw Hill.
2. Methods of Molecular Quantum Mechanics, R. Mcweeny and B.T. Sutcliffe, Academic Press
3. Density Functional Theory of Atoms and Molecules, R.G. Parr and W. Yang, Oxford.
4. Exploring Chemistry with Electron Structure Methods, J.B. Foresman and e. Frish, Gaussian Inc.
5. Semi-empirical MO Theory, J. Pople and D.L. Beveridge.

## (II) Spectroscopy (CHC302)

### 1. Photo-Electron Spectroscopy (PES) and Fluorometry, Phosphometry

Photoelectric effect. Principle of PES. Ionization process. Koopman's Theorem. Photoelectron spectra of simple molecules. ESCA. Chemical information from ESCA. Applications.

Principles. Factors affecting fluorescence and phosphorescence. Total Luminescence spectroscopy. Applications.

### 2. Nuclear Quadrupole Resonance (NQR)

Quadrupole nuclei. Quadrupole moment. Principle of NQR. Splitting of NQR spectra. Instrumentation.

### 3. Mossbauer Spectroscopy

Principle of Mossbauer technique. Parameters in Mossbauer spectroscopy. Instrumentation. Applications.

### 4. Optical Rotatory Dispersion (ORD) and Circular Dichroism (CD)

Principles of ORD and CD. Cotton effect. Octant rule for ketones. Applications.

### Books Suggested:

1. Physical Methods for Chemistry, R.S. Drago, Saunders Company.
2. Structural Methods in Inorganic Chemistry, E.A.V. Ebsworth, D.W.H. Rankin and S.
3. Craddock, ELBS.
4. Infrared and Raman Spectra: Inorganic and Coordination Compounds, K. Nakamoto,
5. Wiley.
6. Inorganic Electronic Spectroscopy, A.P.B. Lever, Elsevier.
7. Symmetry and Spectroscopy, K. Veera Reddy, New Age International, 1998.
- Instrumental Methods of Analysis, Willard et al., 7<sup>th</sup> Edn., CBS Publishers.

## (III) Analytical Chemistry (CHC307)

### 1. Introduction

Role of analytical chemistry. Classification of analytical methods-classical and instrumental. Types of instrumental analysis. Selecting an analytical method. Neatness and cleanliness. Laboratory operations and practices. Analytical balance. Techniques of weighing, errors. Volumetric glassware-cleaning and calibration of glassware. Sample preparations-dissolution and decompositions. Gravimetric techniques. Selecting and handling of reagents. Laboratory notebooks. Safety in the analytical laboratory.

2. **Errors**  
Determinate and indeterminate errors, minimization of determinate errors, random distribution of indeterminate errors.
3. **Statistical data analysis**  
Accuracy and precision, significant figures and computations, mean and standard deviation, distribution of random errors, reliability of results, confidence interval, comparison of results, comparison of means of two samples, paired t-test, number of replicate determinations and its use, correlation and regression, linear regression, analysis of variance, rejection of data.
4. **Application of Analytical Chemistry**  
Application of analytical chemistry in the study of water and soil pollutions, analysis of fuel, body fluids and drugs.

**Books Suggested:**

1. Analytical Chemistry, G.D. Christian, J. Wiley.
2. Fundamentals of Analytical Chemistry, D.A. Skoog, D.M. West and F.J. Holler, W.B. Saunders.
3. Analytical Chemistry-Principles, J.H. Kennedy, W.B. Saunders.
4. Analytical Chemistry-Principles and Techniques, L.G. Hargis, Prentice Hall.
5. Principles of Instrumental Analysis, D.A. Skoog and J.L. Loary, W.B. Saunders.
6. Quantitative Analysis, R.A. Day, Jr. and A.L. Underwood, Prentice Hall.
7. Environmental Solution Analysis, S.M. Khopkar, Wiley Eastern.
8. Basic Concepts of Analytical Chemistry, S.M. Khopkar, Wiley Eastern.
9. Handbook of Instrumental Techniques for Analytical Chemistry, F. Settle, Prentice Hall.

**IV(i) Chemistry of Biological System I (Biophysical)(CHE305)**

1. **Biological Cell and its Constituents, Cell Membrane and Transport of Ions**  
Biological cell, structure and functions of proteins, Enzymes, DNA and RNA in living systems. Helix coil transition. Structure and functions of cell membrane, Ion transport through cell membrane.
2. **Bioenergetics and Statistical Mechanism in Biopolymers**  
Standard free energy change in biological reactions. Exergonic, endergonic. Hydrolysis of ATP. Synthesis of ATP from ADP.  
Chain configuration of macromolecules. Statistical distribution. End-to-end dimensions. Calculation of average dimensions for various chain structures. Polypeptide and protein structures. Introduction to protein folding problem.
3. **Biopolymer Interactions, Thermodynamics of Biopolymer Solutions**  
Forces involved in biopolymer interactions. Electrostatic charge and molecular expansion, hydrophobic forces, dispersion force interactions. Multiple equilibria and various types of binding processes in biological systems. Thermodynamics of biopolymer solutions, osmotic pressure, membrane equilibrium, muscular contraction and energy generation in mechanochemical system.
4. **Biopolymers and their Molecular Weights**  
Evaluation of size, shape, molecular weight and extent of hydration of biopolymers by various experimental techniques. Sedimentation equilibrium, hydrodynamic methods, diffusion, sedimentation velocity, viscosity, electrophoresis and rotational motions.

#### IV (ii) Nuclear Chemistry (CHE306)

- 1. Atomic Nucleus and Nuclear Models**  
Basics of atomic structure. Classification of nuclides. Nuclear stability. Mechanical effects due to orbiting and spinning nucleons. Magnetic quantum number. Total magnetic nuclear quantum number. NMR. Mossbauer effect. Parity. Quarks and Gluons.  
Shell model. Liquid drop model. Fermi gas model. Collective model. Optical model.
- 2. Radioactivity and Nuclear reactions**  
Radioactive decay. Kinetics. Alpha, beta decay. Nuclear deexcitation. Artificial radioactivity. Bethe's notation. Types. Reaction cross-section. Compound nucleus theory. Photoneuclear reactions. Thermonuclear reactions. Nuclear Fission, fission energy, cross-section and threshold. Neutron evaporation and spallation.
- 3. Detection and Measurement of Activity**  
Electrometer. Ionization chamber. Electron pulse counter. Scintillation detector. Semiconductors detectors. Thermoluminescence and neutron detector.
- 4. Radiation Chemistry**  
Interaction of radiation with matter. Interaction of neutrons and gamma radiations with matter. Units. Dosimetry. Radiolysis. Radiochemical and radiometric analysis in chemistry.  
**Book Suggested:**
  1. Essential of nuclear chemistry by H.J. Amikal (Wiley Publication)
  2. Modern nuclear chemistry by Walter Loveland and Water D. Loveland (Wiley Publication)
  3. Radio chemistry and nuclear chemistry by Gregory and Choppin (Wiley Publication)

#### (IV) Lab Course (Physical) SEM III((6×2 hours)

- 1. (a) Determination of transport number.**  
**(b) Determination of liquid junction potential.**  
**(c) Determination of the charge on colloidal particle.**  
**(d) Determination of partial molar volume of solute.**  
**(e) Determination of CMC of surfactants**  
**(f) Determination of solubility of sparingly soluble salts by the following methods:**  
Electrical Conductivity or E.M.F.  
**3×20 marks**
- 2. (a) Beer's law verification.**  
**(b) Decomposition of potential determination.**  
**(c) Validity of Freundlich's adsorption isotherm.**  
**(d) Dissociation constants of polybasic acids.**
- 3. Study of complex formation by the following methods and determination of stability constant wherever practicable:**  
**(a) Cryoscopic**  
**(b) Electrical Methods.**  
**(c) E.M.F.**
- 4. Polarography.** **10 marks**
- 5. Viva.** **10 marks**
- 6. Record**

#### MSc SEM IV

#### Specialization Inorganic Chemistry

#### (I) Spectroscopy & Diffraction method (CHC401)

#### 1. UV-Visible Spectroscopy

Electronic states in complexes. Selection rules. Orgel Diagram. Electronic spectrum of inorganic compounds.

2. **IR Spectroscopy**  
Vibrational frequencies of metal carbonyls, nitrosyls and phosphine derivatives. Effect of substitution and conjugation. IR spectrum of other inorganic compounds.
3. **Diffraction methods**
  - I. **X-Ray Diffraction**  
Miller indices, Laue method, Bragg method, Debye-Scherrer method of X-ray structural analysis of crystals, index reflections, identification of unit cells from systematic absences in diffraction pattern. Structure of simple lattices and X-ray intensities, structure factor and its relation to intensity and electron density, phase problem. Description of the procedure for an X-ray structure analysis, absolute configuration of molecules, Ramchandran diagram.
  - II. **Electron Diffraction**  
Scattering intensity vs. scattering angle, Wire equation, measurement technique, elucidation of structure of simple gas phase molecules. Low energy electron diffraction and structure of surfaces.
  - III. **Neutron Diffraction**  
Scattering of neutrons by solids and liquids, magnetic scattering, measuring techniques. Elucidation of structure of magnetically ordered unit cell.
4. **Atomic Absorption Spectroscopy (AAS) and Atomic Emission Spectroscopy (AES)**  
Principle of AAS. Interference. Applications. Principle of AES. ICP method of elemental analysis.

#### Books Suggested

1. Physical Method for Chemistry, R.S. Drago, Saunders Company.
2. Structural Method in Inorganic Chemistry, E.A.V. Ebsworth, D.W.H. Rankin and S. Craddock, ELBS
3. NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry, R.V. Parish, Ellis Horwood. Practical NMR Spectroscopy, M.L. Martin, J.J. Delpuech and G.J. Martin, Heyden.
4. Spectrometric Identification of Organic Compounds, R.M. Silverstein, G.C. Bassler and T.C. Morrill, John Wiley.
5. Introduction to NMR Spectroscopy, R.J. Abraham, J. Fisher and P. Lufius, Wiley.
6. Spectroscopic Methods in Organic Chemistry, D.H. Williams, I. Fleming, Tata McGraw-Hill. Introduction to Spectroscopy, D.L. Pavia, G.M. Lampman, G.S. Kriz, Thompson Asia Pvt. Ltd. Singapore.
7. Electronic spectroscopy, D.N. Sathyanarayan, Universities Press.
8. Interpretation of Mass Spectra, F.W. McLafferty, University Science Books, California.

### (II) Photo Inorganic Chemistry (CHC402)

1. **Basics of Photochemistry and Photochemical Reactions**  
Absorption, excitation, photochemical laws, electronically excited states-life times, measurements of the times. Flash photolysis, stopped flow techniques. Energy dissipation by radiative and non-radiative processes, absorption spectra, Franck-Condon principle, photochemical stages- primary and secondary processes.  
Interaction of electromagnetic radiation with matter, types of excitations, fate of excited molecule, quantum yield, transfer of excitation energy, actinometry. Singlet molecular oxygen reactions. Photochemical formation of smog. Photo-degradation of polymers. Photochemistry of vision.
2. **Excited States of Metal Complexes and Ligand Field Photochemistry:**  
Structure, dipole moment, acid-base strengths, reactivity. Photochemical kinetics-calculation of rates of radiative processes. Biomolecular deactivation-quenching. Excited states of metal complexes: comparison with organic compounds, electronically excited states of metal complexes. Charge-transfer spectra, charge transfer excitations, methods for obtaining charge-transfer spectra.

Photosubstitution, photooxidation and photoreduction, lability and selectivity, zero vibrational levels of ground state and excited state, energy content of excited state, zero-zero spectroscopic energy, development of the equations for redox potentials of the excited states.

### 3. Redox Reactions by Excited Metal Complexes:

Energy transfer under conditions of weak interaction and strong interaction; exciplex formation, conditions of the excited states to be useful as redox reactants, excited electron transfer, metal complexes as attractive candidates (2,2'-bipyridine and 1,10-phenanthroline complexes), illustration of reducing and oxidizing character of  $Ru^{2+}$ -bipyridal complex (comparison with  $[Fe(bipy)_3]^{3+}$ ); role of spin-orbit coupling-life time of these complexes. Application of redox processes of electronically excited states for catalytic purpose, transformation of low energy reactants into high energy products, chemical energy into light.

### 4. Metal Complex Sensitizers and Determination of Reaction Mechanism :

Metal complex sensitizer, electron relay, metal colloid system, semiconductor supported metal or oxide systems, water photolysis, nitrogen fixation and carbon dioxide reduction. Classification, rate constants and life times of reactive energy states-determination of rate constants of reactions. Effects of light intensity on the rate of photochemical reactions. Types of photochemical reactions; photo-dissociation, gas-phase photolysis

#### Books Suggested:

1. Concepts of Inorganic Photochemistry, A.W. Adamson and P.D. Fleischauer, Wiley, Inorganic Photochemistry, J. Chem. Educ., vol. 60, no. 10, 1983.
2. Progress in Inorganic Chemistry, vol. 30, ed. S.J. Lippard, Wiley.
3. Co-ordination Chem. Revs., 1975, 15, 321; 1981, vol. 39, 121, 131; 1990, 97, 313.
4. Photochemistry of Co-ordination Compounds, V. Balzani and V. Carassiti, Academic Press.
5. Elements of Inorganic Photochemistry, G.J. Ferraudi, Wiley.
6. Fundamentals of Photochemistry, K.K. Rohtagi-Mukherji, Wiley-Eastern.
7. Essentials of Molecular Photochemistry, A. Gilbert and J. Baggott, Blackwell Scientific Publication.
8. Molecular Photochemistry, N.J. Turro, W.A. Benjamin.
9. Introductory Photochemistry, A. Cox.

## (III) Inorganic Polymers (CHC403)

### 1. Introduction of Inorganic Polymers:

Importance of polymers, basic concepts, monomers, repeat units, degree of polymerization. Linear, branched and network polymers. Classification of polymers, polymerization: condensation, addition, radical chain-ionic and co-ordination and co-polymerization. Polymerization conditions and polymer reactions Kinetics of polymerization. Stereochemistry and mechanism of polymerization. Polymerization in homogeneous and heterogeneous systems. Comparison with organic polymers.

### 2. Polymer Characterization:

Polydispersion, average molecular weight concept: number average, weight average and viscosity average molecular weights. Polydispersity and molecular weight distribution. The practical significance of molecular weight. Measurement of molecular weight: end-group, viscosity, light scattering, osmotic and ultracentrifugation methods. Analysis and testing of polymers, chemical analysis of polymers, spectroscopic methods, X-ray diffraction study, Microscopy. Thermal analysis and physical testing- tensile strength Fatigue impact. Tear resistance. Hardness and abrasion resistance.

### 3. Structure, Properties and Polymer Processing

Morphology and order in crystalline polymers-configurations of polymer chains: Crystal structures of polymers. Morphology of crystalline polymers, strain-induced morphology, crystallization and melting. Polymer structure and physical properties-crystalline melting point(T<sub>M</sub>); melting points

of homogeneous series, effect of chain flexibility and other steric factors, entropy and heat of fusion. The glass transition temperature ( $T_g$ ) relationship between  $T_m$  and  $T_g$ , effects of molecular weight, diluents, chemical structure, chain topology, branching and cross linking. Property measurements and polymer utilization.

Plastics, elastomers and fibres. Compounding. Processing techniques: calendaring, die casting, rotational casting, film casting, injection moulding, extrusion moulding, thermoforming, foaming, reinforcing and fibre spinning.

#### 4. Boron Based Polymers, Silicon Based Polymers, Phosphorous Based Polymers and Coordination Polymers:

Borazine, substituted borazines, boron nitride. Boron-oxygen-silicon and boron-oxygen-phosphorus polymers. Polyhedrafluorane anions. Silica, feldspars and ultramarines, silicones, phosphorus polymers. Polyhedrafluorane anions. Silica, feldspars and ultramarines, silicones, silicone fluids, silicone rubbers, silicone greases, silicone resins and metallosiloxanes. Silicon-nitrogen polymers and silazenes. Metaphosphates, polyphosphates, cross-linked phosphates. Phosphonitrilic halides and related polymers. Phosphorous-sulphur polymers. Factors affecting formation of coordination polymers. Types of coordination polymers. Metal halides. Metal pseudohalides, metal alkoxides, metal carboxylates and metal chelates.

#### Books Suggested

1. Textbook of Polymer Science, F.W. Billmeyer Jr, Wiley.
2. Polymer Science, V.R. Gowarikar, N.V. Viswanathan and J. Sreedhar, Wiley-Eastern.
3. Functional Monomers and Polymers, K. Takemoto, Y. Inaki and R.M. Ottonbrine.
4. Contemporary Polymer Chemistry, H.R. Alcock and F.W. Lampe, Prentice Hall.
5. Physics and Chemistry of Polymers, J.M.G. Cowie, Blackie Academic and Professional.
6. F.W. Billmeyer Jr, Text Book of Polymer Science, Wiley.
7. N.H. Ray, Inorganic Polymers, Academic Press, N. York.
8. J.M. Lehn, Supramolecular Chemistry, VCH.

### IV (i) Nuclear Chemistry (CHE306)

#### 1. Atomic Nucleus and Nuclear Models

Basics of atomic structure. Classification of nuclides. Nuclear stability. Mechanical effects due to orbiting and spinning nucleons. Magnetic quantum number. Total magnetic nuclear quantum number. NMR. Mossbauer effect. Parity. Quarks and Gluons.

Shell model. Liquid drop model. Fermi gas model. Collective model. Optical model.

#### 2. Radioactivity and Nuclear reactions

Radioactive decay. Kinetics. Alpha, beta decay. Nuclear deexcitation. Artificial radioactivity.

Bethe's notation. Types. Reaction cross-section. Compound nucleus theory. Photoneuclear reactions. Thermonuclear reactions. Nuclear Fission, fission energy, cross-section and threshold. Neutron evaporation and spallation.

#### 3. Detection and Measurement of Activity

Electrometer. Ionization chamber. Electron pulse counter. Scintillation detector. Semiconductors detectors. Thermoluminescence and neutron detector.

#### 4. Radiation Chemistry

Interaction of radiation with matter. Interaction of neutrons and gamma radiations with matter. Units. Dosimetry. Radiolysis. Radiochemical and radiometric analysis in chemistry.

#### Book Suggested:

7. Essential of nuclear chemistry by H.J. Amikal (Wiley Publication)
8. Modern nuclear chemistry by Walter Loveland and Water D. Loveland (Wiley Publication)
9. Radio chemistry and nuclear chemistry by Gregory and Choppin (Wiley Publication)



## (IV) Environmental Chemistry(CHE401)

### 1. Introduction to Environmental Chemistry and Description of Atmosphere

Concept and scope of environmental chemistry. Environmental terminology and nomenclatures. Environmental segments. The natural cycles of environment (Hydrological, Oxygen, Nitrogen). Atmosphere, environmental segments, composition of the atmosphere, earth's radiation balance, particulates, ions and radicals and their formation, chemical and photochemical reactions in the atmosphere, air pollution, oxides of C,N,S and their effects, acid-rain, smog formation, Green house effects (global warming and ozone depletion), air pollution controls and introduction to analytical methods for monitoring air pollution.

### 2. Hydrosphere and Lithosphere:

Chemical composition of water bodies-lakes, streams, rivers, sea etc, hydrological cycle, complexation in natural and waste water and microbially mediated redox reactions. Water pollution-inorganic, organic, pesticides, industrial and radioactive materials, oil spills and oil pollutants, eutrophication, acid-mine drainage, waste water treatment, domestic waste water(aerobic and anaerobic treatment), and industrial waste water treatment.

Inorganic and organic components in soil, acid-base and ion-exchange reactions in soil, micro and macro nutrients, nitrogen pathways and NPK in soil.

### 3. Water quality parameters and standards:

Analytical methods for measuring DO, BOD, COD, fluoride, oils and grease and metals (As, Cd, Rg, Pb, Zn,Cu,Cr). Biochemical effects of As, Cd, Hg, Pb, Cr, CN and pesticides.

### 4. Air Pollution and Water Pollution:

Particulates, aerosols, SO<sub>x</sub>, NO<sub>x</sub>, CO<sub>x</sub> and hydrocarbon. Photochemical smog, air-quality standards.

#### Books suggested

1. Environmental Chemistry, S.E. Manahan, Lewis Publishers.
2. Environmental Chemistry, Sharma and Kaur, Krishna Publishers.
3. Environmental Chemistry, A.K. De, Wiley Eastern.
4. Environmental Pollution Analysis, S.M. Khopkar, Wiley Eastern.
5. Standard Method of Chemical Analysis, F.J. Welcher Vol. III, Van Nostrand Reinhold Co.
6. Environmental Toxicology, Ed. J. Rose, Gordon and Breach Science Publication.
7. Elemental Analysis of Airborne Particles, Ed. S. Landsberger and M. Creatchman, Gordon and Breach Science Publication.
8. Environmental Chemistry, C. Baird, W.H. Freeman.

### IV (iii) Project Work /Dissertation (CHE402)

### (V) Lab Course (Inorganic) SEM IV (ICH40P) (2×6 hours)

#### 1. Spectrophotometric Determinations

- (a) Manganese/chromium/vanadium in steel sample.
- (b) Nickel/molybdenum/tungsten/vanadium/uranium by extractive Spectrophotometric method.
- (c) Fluoride/nitrite-phosphate.
- (d) Iron-phenanthroline complex: Job's Method of continuous variation.
- (e) Zirconium-alizarin Red-S complex: Mole-ratio method.
- (f) Copper-ethylene diamine complex: Slope -ratio method.

#### 2. Flame Photometric Determinations

- (a) Sodium and Potassium when present together.
- (b) Lithium/Calcium/barium/strontium.
- (c) Cadmium and magnesium in tap water.

#### 3. Nephelometric Determinations

27 | P a g e

3×20marks

- (a). Sulphate
- (b). Phosphate
- (c). Silver

**4. Chromatographic separations: Paper or TLC and determination of Rf values:**

- (a). Cadmium and Zinc.
- (b). Silver, Lead and Mercury.
- (c). Nickel, Magnesium, Cobalt and Zinc.

- 5. Viva
- 6. Record

10 marks

10 marks

## Specialization Organic Chemistry Organic Synthesis (CHC404)

(I)

**1. Disconnection Approach**

An introduction to synthons and synthetic equivalents disconnection approach, functional group interconversions, the importance of order of events in organic synthesis, one group C-X and two group C-X disconnections, chemoselectivity, reversal of polarity, cyclisation reactions and amine synthesis.

**2. One Group and Two Group C-C Disconnections**

Alcohols and carbonyl compounds regioselectivity, Alkene synthesis, use of acetylenes and aliphatic nitro compounds in organic synthesis. Diels-Alder reaction, 1,3-difunctional compounds,  $\alpha,\beta$ -unsaturated carbonyl compounds, control in carbonyl condensations, Micheal addition and Robinson annelation.

**3. Ring Synthesis and Protecting Groups**

Saturated heterocycles, synthesis of 3-, 4-, 5- and 6-membered rings, aromatic heterocycles in organic synthesis.  
Principles of protection of alcohol, amine, carbonyl and carboxyl groups

**4. Synthesis of Some Complex molecules**

Application of the above in the synthesis of following compounds: Camphor, Longifoline, Cortisone, Reserpine, Vitamin D, Juvabione, Aphidicolin and Fredericamysin A.

**Books Suggested**

- 1. Modern Synthetic Reactions, H.O. House, W.A. Benjamin.
- 2. Some Modern Methods of Organic Synthesis, W. Carruthers, Cambridge Univ. Press.
- 3. Advanced Organic Chemistry, Reactions Mechanisms and Structure, J. March, John Wiley.
- 4. Principles of Organic Synthesis, R.O.C. Norman and J.M. Coxon, Blackie Academic & Professional.
- 5. Advanced Organic Chemistry Part B, F.A. Carey and R.J. Sundberg, Plenum Press.
- 6. Rodd's Chemistry of Carbon Compounds, Ed. S. Coffey, Elsevier.
- 7. Designing Organic Synthesis, S. Warren, Wiley.
- 8. Organic Synthesis-Concept, Methods and Starting Materials, J. Fuhrhop and G. Penzillin, Verlag VCH.

## (II) Organic Spectroscopy(CHC405)

**1. UV-Visible Spectroscopy**

Electronic transitions in organic compounds. Factors affecting absorption maximum and molar extinction coefficient. Solvent effects. Woodward Fieser rules for conjugated dienes and carbonyl

compounds. UV-Visible spectrum of alkenes, carbonyl compounds, alcohol/phenol, Aromatic compounds (characteristic features).

## 2. IR Spectroscopy

Effect of Hydrogen Bonding and solvent polarity of IR spectrum of organic compounds. Characteristic features of IR spectrum of aliphatic/aromatic hydrocarbons, alcohols/phenols, amines, carbonyl compounds, carboxylic acid and derivatives. Effect of conjugation on vibrational frequencies.

## 3. Nuclear magnetic resonance

### Proton-NMR Spectroscopy

Chemical shift values for protons bonded to carbon (aliphatic, olefinic, aldehydic and aromatic) and other nuclei (alcohols, phenols, carboxylic acids, amines, amides). Chemical exchange. Effects of deuteration. Karplus curve-variation of coupling constant with dihedral angle.

### Carbon-13 NMR Spectroscopy

Characteristics of CMR. Chemical shift (aliphatic, olefinic, alkyne, aromatic, heteroaromatic and carbonyl compound). Coupling constants. Advantages and disadvantages.

### Fluorine -19 NMR Spectroscopy

Characteristic features of F19-NMR. Chemical shifts and Coupling constants.

Introduction of DEPT, COSY and 2D NMR spectroscopy.

## 4. Mass Spectrometry

Fragmentation Pattern: Isotopic studies. Characteristics of Mass spectrum of aliphatic, olefinic, aromatic, carbonyl compounds, alcohols, phenols, carboxylic acids, amines and amides.

### Books Suggested

1. Pavia, Lampman, Kriz and Vyvyan Spectroscopy, Books/Cole
2. P. S. Kalsi, Spectroscopy of Organic Compounds, New Age International Publishers.
3. Robert M. Silverstein, Francis X. Webster, and D. J. Kiemle Spectrometric Identification
4. of Organic Compounds, John Wiley.
5. M. L. Martin, J. J. Delpuech G. J. Martin and Heyden, Practical NMR Spectroscopy.
6. Colin N. Banwell and Elaine M. McCash, Fundamentals of Molecular Spectroscopy, Tata McGraw Hill.
7. R. J. Abraham, J. Fischer and P. Loftus, Introduction to NMR Spectroscopy, Wiley.
8. D. H. Williams and I. Fleming, Spectroscopic Method in Organic Chemistry, Tata Mac Graw Hill.
9. H. H. Willard, Jr. L. L. Merritt, J. A. Dean and Jr F. A. Settle, CBS Publication, Instrumental Method of Analysis: Seventh Edition,

## (III) Heterocyclic Compounds (CHC406)

### 1. Aromatic and Non-aromatic Heterocycles

Replacement and Systematic nomenclature (Hantzsch-Widman system) for monocyclic, fused and bridged heterocycles

General chemical behaviour of aromatic heterocycles, classification (structural type), Heteroaromatic reactivity and tautomerism in aromatic heterocycles Strain -bond angle and torsional strains and their consequences in small ring heterocycles. Conformation of six-membered heterocycles with reference to molecular geometry, barrier to ring inversion, pyramidal inversion and 1,3-diaxial interactions. Stereo-electronic effects, aromatic and related effects. Attractive interactions - hydrogen bonding and intermolecular nucleophilic, electrophilic interactions.

### 2. Small Ring and Benzo-Fused Five-Membered Heterocycles

Three-membered and four-membered heterocycles-synthesis and reactions of aziridines, oxiranes, thiiranes, azetidines, oxetanes and thietanes

Synthesis and reactions including medicinal applications of benzopyrroles, benzofurans and benzothiophenes

### 3. Six-Membered Heterocycles with One, Two or More Heteroatoms

Synthesis and reactions of pyrylium salts and pyrones and their comparison with pyridinium & thiopyrylium salts and pyridines. Synthesis and reactions of quinolizinium and benzopyrylium salts, coumarins and chromones. Synthesis and reactions of diazines, triazines, tetrazines and thiazines

### 4. Seven- and Large-Membered Heterocycles

Synthesis and reactions of azepines, oxepines, thiepinines, diazepines, thiazepines, azocines, diazocines, dioxocines and dithiocines

#### Books Suggested:

1. Heterocyclic Chemistry Vol. 1 & 2, R.R. Gupta, M. Kumar and V. Gupta, Springer Verlag
2. The Chemistry of Heterocycles, T. Eicher und S. Hauptmann, Thieme.
3. Heterocyclic Chemistry, J.A. Joule, K. Mills and G.F. Smith, Chapman and Hall.
4. Heterocyclic Chemistry, T.L. Gilchrist, Longman Scientific Technical
5. Contemporary Heterocyclic Chemistry, G.R. Newkome and W.W. Paudler, Wiley-Inter Science.
6. An introduction to the Heterocyclic Compounds, R.M. Acheson, John Wiley
7. Comprehensive Heterocyclic Chemistry, A.R. Katritzky and C.W. Rees, eds. Pergamon
8. Natural Products: Chemistry and Biological Significance, J.Mann, R.S. Davidson, J.B. Hobbs, D.V. Banthrope and J.B. Harborne, Longman, Essex.
9. Organic Chemistry, Vol 2, I.L. Finar, ELBS.
10. Stereoselective Synthesis: A Practical Approach, M. Nogradi, VCH

## (IV) Medicinal Chemistry (CHE403)

### 1. Drug Design

Development of new drugs, procedures followed in drug design, concepts of lead compound and lead modification, concepts of prodrugs and soft drugs, structure-activity relationship (SAR) factors affecting bioactivity, resonance, inductive effect, isosterism, bio-isosterism, spatial considerations. Theories of drug activity: occupancy theory, rate theory, induced fit theory. Quantitative structure activity relationship. History and development of QSAR. Concepts of drug receptors. Elementary treatment of drug receptor interactions. Physico-chemical parameters: lipophilicity, partition coefficient, electronic ionization constant, steric, Shelton and surface activity parameters and redox potentials. Free Wilson analysis, Hansch analysis, relationships between Free-Wilson and Hansch analysis. LD-50, ED-50 (Mathematical derivations of equations excluded).

### 2. Pharmacokinetics

Introduction to drug absorption, disposition, elimination using pharmacokinetics, important pharmacokinetic parameters in defining drug disposition and in therapeutics. Mention of uses of pharmacokinetics in drug development process.

### 3. Pharmacodynamics

Introduction, elementary treatment of enzyme stimulation, enzyme inhibition, sulphonamides, membrane active drugs, drug metabolism, xenobiotic, biotransformation, significance of drug metabolism in medicinal chemistry.

### 4. Antineoplastic Agents and Antibiotics

Introduction, cancer chemotherapy, special problems, role of alkylating agents and antimetabolites in treatment of cancer. Mention of carcinolytic antibiotics and mitotic inhibitors. Synthesis of mechlotethamine, cyclophosphamide, melphalan, uracil, mustards, and 6-mercaptopurine. Recent development in cancer chemotherapy. Hormone and natural products.

Cell wall biosynthesis inhibitors,  $\beta$ -lactam rings, antibiotics inhibiting protein synthesis. Synthesis of penicillin G, penicillin V, ampicillin, amoxycillin, chloramphenicol, cephalosporin, tetracycline and streptomycin.

### Books suggested

1. Introduction to Medicinal Chemistry, A. Gringuage, Wiley-VCH.
2. Wilson and Gisvold's: Text Book of Organic Medicinal and Pharmaceutical Chemistry, Ed. Robert F. Dorge.
3. An Introduction to Drug Design, S.S. Pandeya and J.R. Dimmock, New Age International.
4. Burger's Medicinal Chemistry and Drug Discovery, Vol-I, Ed. M.E. Wolff, John Wiley.
5. Goodman and Gilman's Pharmacological Basis of Therapeutics, McGraw-Hill.
6. The Organic Chemistry of Drug Design and Drug Action, R.B. Silverman, Academic Press.
7. Strategies for Organic Drug Synthesis and Design, D. Lednicer, John Wiley.

## IV(ii) Environmental Chemistry (CHE401)

### 1- Introduction to Environmental Chemistry and Description of Atmosphere

Concept and scope of environmental chemistry. Environmental terminology and nomenclatures. Environmental segments. The natural cycles of environment (Hydrological, Oxygen, Nitrogen). Atmosphere, environmental segments, composition of the atmosphere, earth's radiation balance, particulates, ions and radicals and their formation, chemical and photochemical reactions in the atmosphere, air pollution, oxides of C, N, S and their effects, acid-rain, smog formation, Green house effects (global warming and ozone depletion, air pollution controls and introduction to analytical methods for monitoring air pollution.

### 2-Hydrosphere and Lithosphere:

Chemical composition of water bodies-lakes, streams, rivers, sea etc. hydrological cycle, complexation in natural and waste water and microbially mediated redox reactions. Water pollution-inorganic, organic, pesticides, industrial and radioactive materials, oil spills and oil pollutants, eutrophication, acid-mine drainage, waste water treatment, domestic waste water (aerobic and anaerobic treatment), and industrial waste water treatment. Inorganic and organic components in soil, acid-base and ion-exchange reactions in soil, micro and macro nutrients, nitrogen pathways and NPK in soil.

### 3-Water quality parameters and standards:

Analytical methods for measuring DO, BOD, COD, fluoride, oils and grease and metals (As, Cd, Hg, Pb, Zn, Cu, Cr), Biochemical effects of As, Cd, Hg, Pb, Cr, CN and pesticides.

### 4-Air Pollution and Water Pollution:

Particulates, aerosols, SO<sub>x</sub>, NO<sub>x</sub>, CO<sub>x</sub> and hydrocarbon. Photochemical smog, air-quality standards.

### Books suggested

1. Environmental Chemistry, S.E. Manahan, Lewis Publishers.
2. Environmental Chemistry, Sharma and Kaur, Krishna Publishers.
3. Environmental Chemistry, A.K. De, Wiley Eastern.
4. Environmental Pollution Analysis, S.M. Khopkar, Wiley Eastern.
5. Standard Method of Chemical Analysis, F.J. Welcher Vol. III, Van Nostrand Reinhold Co.
6. Environmental Toxicology, Ed. J. Rose, Gordon and Breach Science Publication.
7. Elemental Analysis of Airborne Particles, Ed. S. Landsberger and M. Creatchman, Gordon And Breach Science Publication.
8. Environmental Chemistry, C. Baird, W.H. Freeman.

## IV (iii) Project Work /Dissertation (CHE404)

## (V) Lab Course (Organic) SEM IV (OCHC40P) (2×6 hours)

### 1. Spectroscopy



2(a). Extraction of Organic Compounds from Natural Sources

20 marks

- i. Isolation of caffeine from tea leaves.
- ii. Isolation of casein from milk (the students are required to try some typical colour reactions of proteins).
- iii. Isolation of lactose from milk (purity of sugar should be checked by TLC and PC and Rf value reported).
- iv. Isolation of nicotine dipicrate from tobacco.
- v. Isolation of cinchonine from cinchona bark.
- vi. Isolation of piperine from black pepper.
- vii. Isolation of lycopene from tomatoes.
- viii. Isolation of  $\beta$ -carotene from carrots.
- ix. Isolation of oleic acid from olive oil (involving the preparation of complex with urea and separation of linoleic acid).
- x. Isolation of eugenol from cloves.
- xi. Isolation of limonene from citrus fruits.

2x20 marks

(b). Synthesis of heterocyclic compounds

Skraup synthesis: Preparation of quinoline from aniline. Fisher-Indole synthesis: Preparation of 2-phenyl indole from phenylhydrazine.

(c). Spectrophotometric (UV/VIS) Estimations

- i. Amino acids
- ii. Proteins
- iii. Carbohydrates
- iv. Cholesterol
- v. Ascorbic acid
- vi. Aspirin
- vii. Caffeine

3. Viva

10 marks

4. Record

10 marks

Specialization Physical Chemistry

(I) Advanced Chemical Dynamics (CHC407)

1. Thermodynamics

Thermodynamical properties of Solids: Crystal symmetry and Macroscopic properties. Microscopic theory of thermal properties. Contribution of Anharmonicity. Properties of Complex Solids and imperfect solids.

Phase rule: Phase diagram of  $\text{CO}_2$ ,  $\text{H}_2\text{O}$  and He. Thermodynamical aspects of phase transitions. Liquid-Solid phase diagrams, Eutectics, Incongruent melting Ternary systems, partially miscible liquids.

2. Kinetics

Interactions between reacting molecules (Quantum mechanical aspect). Methods of determinations of rate of fast reactions. Fluctuations in chemical kinetics. Symmetry rules.

Electron transfer in homogeneous systems. role of electron tunnelling, reorganization energy.

Kinetics of electrode reactions: Rates of adsorption and desorption.

3. Liquids

Thermodynamical properties of Liquids: Bulk properties. Relation between structure and thermodynamic properties of simple liquids. Molecular theory of monatomic liquids:

Molecular interactions in liquids, radial distribution, Liquid-surface interface, surface tension, curved surface and capillary action. Thermodynamics of surface layers. Condensation.

4. Non-equilibrium phenomena

Transport parameters in gases, diffusion coefficient, thermal conductivity, viscosity and effusion.

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Liquid viscosity, Mobility of ions, drift speed, mobility and conductivity, Einstein relations.

Thermodynamical and statistical view of diffusion.

#### Book Suggested

- i. Chemical Kinetics and Reaction Dynamics – Upadhyay, Santosh K. (Springer)
- ii. Chemical Kinetics and Dynamics – Jeffrey I. Steinfeld's Books
- iii. C.M Guldberg and P.Waage- Studies concerning affinity.
- iv. Atkins P. and de Paula J.-Physical Chemistry
- v. Steinfeld J.I., Francisco J.S. and Hase W.L.- Chemical Kinetics and Dynamics (Prentice-Hall)

### vi. Advanced Spectroscopy(CHC408)

#### 1. Molecular Spectroscopy

Anharmonicity, convergence of energy levels. Resonance Raman spectroscopy, Coherent anti-Stokes Raman spectroscopy.

LASER, Pulsed LASER, Time-resolved spectroscopy, Examples of LASER, Applications. Instrumentation of IR and UV-Visible spectrometers.

#### 2. Magnetic Resonance

Nuclear Overhauser effect. Pulse Sequence, Magnetization vectors, DEPT, Two-dimensional NMR. Solid state NMR.

#### 3. X-Ray Diffraction

Miller indices, Laue method, Bragg method, Debye-Scherrer method of X-ray structural analysis of crystals, index reflections, identification of unit cells from systematic absences in diffraction pattern. Structure of simple lattices and X-ray intensities, structure factor and its relation to intensity and electron density, phase problem, Description of the procedure for an X-ray structure analysis, absolute configuration of molecules, Ramchandran diagram.

#### 4. Electron Diffraction and Neutron Diffraction

Scattering intensity vs. scattering angle, Wire equation, measurement technique, elucidation of structure of simple gas phase molecules. Low energy electron diffraction and structure of surfaces. Scattering of neutrons by solids and liquids, magnetic scattering, measuring techniques. Elucidation of structure of magnetically ordered unit cell.

#### Books Suggested

1. Physical Method for Chemistry, R.S. Drago, Saunders Company.
2. Structural Method in Inorganic Chemistry, E.A.V. Ebsworth, D.W.H. Rankin and S. Cradock, ELBS
3. NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry, R.V. Parish, Ellis Horwood.
4. Practical NMR Spectroscopy, M.L. Martin, J.J. Delpuech and G.J. Martin, Heyden.
5. Spectrometric Identification of Organic Compounds, R.M. Silverstein, G.C. Bassler and T.C.
6. Morrill, John Wiley.
7. Introduction to NMR Spectroscopy, R.J. Abraham, J. Fisher and P. Loftus, Wiley.
8. Inorganic Electronic Spectroscopy, A.P.B. Lever, Elsevier.
9. Solid State Chemistry and its Applications, A.R. West, Plenum.
10. Solid State Chemistry, D.K. Chakrabarty, New Age International.
11. Symmetry and Spectroscopy, K. Veera Reddy, New Age International, 1998. Instrumental Methods of Analysis, Willard et al., 7th Edn., CBS Publishers.

### III Solid State Chemistry(CIIC409)

- 1. Crystalline solids and Solid preparations**  
Basics of solids, Crystalline solids, Crystal systems, Defects in solids, Methods of crystallization, Doping, Intercalation compounds, Deposition methods, Preparation of thin films and monolayers.
- 2. Advanced solid materials**  
Fullerenes, Nanomaterials-definition and classification, Carbon nanomaterials, Ceramics and their uses, Intercalation compounds of transition elements.
- 3. Solid State Reactions**  
General principles, experimental procedures, co-precipitation as a precursor to solid state reactions, kinetics of solid state reactions.
- 4. Electrical and magnetic properties of solids**  
Electrically conducting solids, Electrical properties of fullerenes and doped fullerenes carbon nanotubes, Magnetism in inorganic and organic materials, Superconductivity in inorganic and organic compounds, Solids used in rectifiers, transistors, switches and sensors.

#### Books Recommended

1. G.W. Castellan, Physical Chemistry, 4th Ed. Narosa.
2. R.G. Mortimer, Physical Chemistry, 3rd Ed. Elsevier, NOIDA, UP.
3. Solid State Chemistry and its Applications, A.R. West, Plenum.
4. Solid State Chemistry, D.K. Chakrabarty, New Age International.

### IV (i) Chemistry of Materials (CHE405)

- 1. Glasses, Ceramics, Composites and Nanomaterials**  
Glassy state, glass formers and glass modifiers, applications, Ceramic structures, mechanical properties, clay products, Refractories, characterizations, properties and applications.  
Microscopic composites; dispersion-strengthened and particle-reinforced, fibre-reinforced composites; macroscopic composites, Nanocrystalline phase, preparation procedures, special properties, applications.
- 2. Thin Films, Langmuir-Blodgett Films and Liquid Crystals**  
Preparation techniques; evaporation/sputtering, chemical processes, MOCVD, sol-gel etc.  
Langmuir-Blodgett (LB) film, growth techniques, photolithography, properties and applications of thin and LB films.  
Mesomorphic behavior, thermotropic liquid crystals, positional order, bond orientational order, nematic and smectic mesophases; smectic-nematic transition and clearing temperature-homeotropic, planar and schlieren textures, twisted nematics; chiral nematics, molecular arrangement in smectic C phases, optical properties of liquid crystals, Dielectric susceptibility and dielectric constants, Lyotropic phases and their description of ordering in liquid crystals.
- 3. Ionic Conductors**  
Types of ionic conductors, mechanism of ionic conductors, interstitial jumps (Frenkel); vacancy mechanism, diffusion superionic conductors; phase transitions and mechanism of conduction in superionic conductors, examples and applications of ionic conductors.



#### 4. High Tc Materials

Defect perovskites, high Tc superconductivity in cuprates, preparation and characterization of 1-2-3 and 2-1-4 materials, normal state properties; anisotropy; temperature dependence of electrical resistance; optical phonon modes, superconducting state; heat capacity; coherence length, elastic constants, position lifetimes, microwave absorption-pairing and multigap structure in high Tc materials, applications of high Tc materials.

##### Books Suggested

1. Solid State Physics, N.W. Ashcroft and N.D. Mermin, Saunders College.
2. Material Science and Engineering, An Introduction, W.D. Callister, Wiley.
3. Principles of the Solid State, H.V. Keer, Wiley Eastern.
4. Materials Science, J.C. Anderson, K.D. Leaver, J.M. Alexander and R.D. Rawlings, ELBS.
5. Thermotropic Liquid Crystals, Ed., G.W. Gray, John Wiley.
6. Handbook of Liquid Crystals, Kelker and Hutz, Chemie Verlag.
7. Inorganic Materials:Recent Advances,Editors D.Bahadur *et al.*, Narosa
8. Ion Conducting Materials: Theory and Applications, Editor A. R. Kulkarni, Narosa.

### IV(ii) Environmental Chemistry(401)

#### 1-Introduction to Environmental Chemistry and Description of Atmosphere

Concept and scope of environmental chemistry.Environmental terminology and nomenclatures. Environmental segments. The natural cycles of environment (Hydrological, Oxygen, Nitrogen). Atmosphere, environmental segments, composition of the atmosphere, earth's radiation balance, particulates, ions and radicals and their formation, chemical and photochemical reactions in the atmosphere, air pollution, oxides of C,N,S and their effects, acid-rain, smog formation, Green house effects (global warming and ozone depletion, air pollution controls and introduction to analytical methods for monitoring air pollution.

#### 2-Hydrosphere and Lithosphere:

Chemical composition of water bodies-lakes, streams, rivers, sea etc, hydrological cycle, complexation in natural and waste water and microbially mediated redox reactions. Water pollution-inorganic, organic, pesticides, industrial and radioactive materials, oil spills and oil pollutants, eutrophication, acid-mine drainage, waste water treatment, domestic waste water(aerobic and anaerobic treatment), and industrial waste water treatment. Inorganic and organic components in soil, acid-base and ion-exchange reactions in soil, micro and macro nutrients, nitrogen pathways and NPK in soil.

#### 3-Water quality parameters and standards:

Analytical methods for measuring DO, BOD, COD, fluoride, oils and grease and metals (As, Cd, Hg, Pb, Zn,Cu,Cr), Biochemical effects of As, Cd, Hg, Pb, Cr, CN and pesticides.

#### 4-Air Pollution and Water Pollution:

Particulates, aerosols, SO<sub>x</sub>, NO<sub>x</sub>, CO<sub>x</sub> and hydrocarbon. Photochemical smog, air-quality standards.

##### Books suggested

1. Environmental Chemistry, S.E. Manahan, Lewis Publishers.
2. Environmental Chemistry, Sharma and Kaur, Krishna Publishers.

3. Environmental Chemistry, A.K. De, Wiley Eastern.
4. Environmental Pollution Analysis, S.M. Khopkar, Wiley Eastern.
5. Standard Method of Chemical Analysis, F.J. Welcher Vol. III, Van Nostrand Reinhold Co.
6. Environmental Toxicology, Ed. J. Rose, Gordon and Breach Science Publication.
7. Elemental Analysis of Airborne Particles, Ed. S. Landsberger and M. Creatchman, Gordon and Breach Science Publication.
8. Environmental Chemistry, C. Baird, W.H. Freeman.

**IV (iii) Project Work / Dissertation (CHE406)**


**(V) Lab Course (Physical) SEM IV (PCHC40P) (2×6 hours)**

1. Verification of the law of photochemical equivalence.
2. Order of reaction by:
  - (a). Isolation Method.
  - (b). Half life period method
  - (c). Integration method
  - (d) Temperature coefficient of a reaction.
  - (e) Energy of activation of a reaction.
  - (f) Entropy of a reaction.
3. Determination of pH by following methods:
  - (a). Electrical Conductivity.
  - (b). E.M.F.
  - (c). Polarography
4. Hydrolysis of the salts by following methods:
  - (a). Cryoscopic
  - (b). Electrical Conductivity.
  - (c). E.M.F.
5. Viva
6. Record

3×20 marks

10 marks  
10 marks



  
Prof. S. S. Janghwan