

Course Code	Course Title	T/P	Credits	Evaluation (MM=100)			
				Internal		External	
				CIE	Practical	ETE	
<b>Semester-I</b>							
CHE-501	Core	INORGANIC CHEMISTRY	T	5	25	-	75
CHE-502	Core	ORGANIC CHEMISTRY	T	5	25	-	75
CHE-503	Core	PHYSICAL CHEMISTRY	T	5	25	-	75
CHE-504	Core	TECHNIQUES OF CHEMISTRY-I	T	5	25	-	75
CHE-531	Core	FIELD WORK/MINOR PROJECT/PRACTICAL	P	4	-	100	-
<b>Semester-II</b>							
CHE-505	Core	INORGANIC CHEMISTRY	T	5	25	-	75
CHE-506	Core	ORGANIC CHEMISTRY	T	5	25	-	75
CHE-507	Core	PHYSICAL CHEMISTRY	T	5	25	-	75
CHE-508	Core	TECHNIQUES OF CHEMISTRY-II	T	5	25	-	75
CHE-532	Core	FIELD WORK/MINOR PROJECT/PRACTICAL	P	4	-	100	-
<b>Semester-III</b>							
CHE-601	Core	SPECTROSCOPY	T	5	25	-	75
CHE-602	Core	MOLECULAR REARRANGEMENTS & PHOTOCHEMISTRY	T	5	25	-	75
CHE-651	Electives (Select any two)	POLYMER CHEMISTRY	T	5	25	-	75
CHE-652		ELECTROCHEMISTRY	T	5	25	-	75
CHE-653		HETEROCYCLIC CHEMISTRY	T	5	25	-	75
CHE-654		QUANTUM CHEMISTRY	T	5	25	-	75
CHE-655		ANALYTICAL CHEMISTRY	T	5	25	-	75
CHE-631	Core	FIELD WORK/MINOR PROJECT/PRACTICAL	P	4	-	100	-
<b>Semester-IV</b>							
CHE-603	Core	ORGANOMETALLIC CHEMISTRY	T	5	25	-	75
CHE-604	Core	SOME SPECIFIC REACTIONS AND REAGENTS IN CHEMISTRY	T	5	25	-	75
CHE-656	Electives (Select any two)	INORGANIC SPECTROSCOPY	T	5	25	-	75
CHE-657		CHEMISTRY OF NATURAL PRODUCTS	T	5	25	-	75
CHE-658		SUPRA-MOLECULAR CHEMISTRY AND STRATEGIES IN CHEMICAL SYNTHESIS	T	5	25	-	75
CHE-659		MEDICINAL CHEMISTRY	T	5	25	-	75
CHE-660		NANO MATERIALS & SOLID STATE CHEMISTRY	T	5	25	-	75
CHE-632	Core	FIELD WORK/MINOR PROJECT/PRACTICAL	P	4	-	100	-

There is:

CIE: Continuous Internal Evaluation.

Practical: 100% Internal

ETE: End Term Examination (University Examination).

**SEMESTER -I**  
**Paper First -CHE – 101**

**INORGANIC CHEMISTRY**

**I. Stereochemistry and Bonding in main group compounds:**

VSEPR, Walsh diagrams (tri-and penta-atomic molecules),  $d\pi$ - $p\pi$  bonds, Bent rule and energetics of hybridization, some simple reactions of covalently bonded molecules.

**II. Metal-Ligand Bonding in Transition Metal Complexes**

Limitation of crystal field theory, molecular orbital theory, octahedral, tetrahedral and square planar complexes,  $\pi$ -bonding and molecular orbital theory and Jahn-Teller distortion.

**III. Molecular symmetry and character tables**

Symmetry elements and symmetry operations, symmetry groups, defining properties of a group, character tables and its applications.

Symmetry considerations in simple inorganic and coordination compounds.

**IV. Chemistry of f-Block Elements**

Comparative study of lanthanides and actinides. Electronic configuration, Oxidation state, Ionic radii (lanthanide contraction), complex formation, Structure of complexes, spectral properties and magnetic properties. General chemistry of actinides including E.M.F. diagrams, Extraction and metallurgy of thorium and uranium. Separation of transamericium elements.

**V. Metal ligand equilibria in solution:**

Stepwise and overall formation constant, trends in stepwise constant, factors affecting the stability of metal complex with reference to the nature of metal ion and ligand, chelate effect and its thermodynamic origin.



**SEMESTER- I**  
**Paper-Second -CHE-102**

**ORGANIC CHEMISTRY**

**I- Nature of bonding in organic molecules:**

Delocalised chemical bonding-conjugation, crossconjugation, resonance, hyperconjugation, Aromaticity in benzenoid and non-benzenoid compounds, alternant and non-alternant hydrocarbons, Huckel's rule, energy of pi-molecular orbitals, annulenes, anti-aromaticity, homo-aromaticity. Bonding in fullerenes.

**II - Reaction Mechanism: Structure and Reactivity:**

Generation, structure stability and fate of reaction intermediates: carbocation(including nonclassical carbocation, phenonium ion, and norbornyl system), carbanion (including enolate ions), carbene, nitrenes, free radicals(allylic halogenation) and arynes. Hammond's postulate, Curtin-Hammett principle. Potential energy diagrams, transition states and intermediates. Methods of determining mechanism-isotope effects, product analysis. Kinetic and stereochemical studies.

**III. Stereochemistry**

Conformational analysis of cycloalkanes-disubstitutedcyclohexanes, decalins, effect of conformation on reactivity.

Elements of symmetry, chirality, molecules with more than one chiral centre, threo and erythro isomers, optical purity, enantiotopic and diastereotopic atoms, group and faces, regiospecific, stereospecific and stereoselective synthesis, Asymmetric synthesis. Optical activity in the absence of chiral carbon (biphenyls, allenes and spiranes), chirality due to helical shape. R/S nomenclature, chiral centres and chiral molecules.

**IV Aliphatic Nucleophilic Substitution**

The  $S_N^1$ ,  $S_N^2$ , mixed  $S_N1'$ ,  $S_N2'$ ,  $S_N'$  and SET mechanisms.

neighbouring group participation by pi and sigma bonds, anchimeric assistance. Nucleophilic substitution at allylic, aliphatic trigonal and vinylic carbon. Effects of substrate structure, attacking nucleophile, leaving group and reaction medium on reactivity. Phase transfer catalysis, ambident nucleophile and regioselectivity. Stereochemistry of  $S_N^1$  and  $S_N^2$  reactions.

**V. Aromatic Electrophilic Substitution**

The arenium ion mechanism, orientation and reactivity, energy-profile diagrams. The ortho/para ratio, ipso attack. Diazonium coupling, Vilsmeier reaction, Gatterman-Koch reaction..

**VI. Aromatic Nucleophile Substitution**

The  $ArSN^1$ ,  $ArSN^2$  &  $ArSN^1$  via benzyne mechanisms. Effect of substrate structure, leaving group and attacking nucleophile on reactivity. The Von Richter, Sommelet-Hauser and Smiles rearrangements.

**SEMESTER- I**  
**Paper-Third -CHE-103**

**PHYSICAL CHEMISTRY**

**I. Partial Molar Properties, Nernst Heat Theorem (NHT) and Third Law of Thermodynamics:**

Partial molar properties, Chemical potential and other thermodynamic functions, Fugacity of real gases, Nernst Heat Theorem and its application to non-condensed systems. Statement of the third law of thermodynamics. Derivation of unattainability of absolute zero. The relationship between entropy constant and Nernst chemical constant. Determination of entropy from the Third Law using the correction due to gas imperfections.

**II. Statistical Thermodynamics:**

Quantum states and complexions. The combinatory rule, system with definite total energy. Degeneracy of energy levels, probability and most probable distribution, in distinguishability, Maxwell-Boltzmann statistics, partition function, translational, rotational, vibrational, nuclear and electronic partition functions. Internal energy and heat capacity in terms of partition function.

**III. Spectroscopy:**

**Molecular Spectra**-Basic concepts of molecular spectroscopy. Classification of spectra, characterization of electromagnetic radiations. Regions of the spectrum.

**Rotation Spectra**-Rigid and non-rigid rotation spectra, selection rule, centrifugal distortion, isotopic shift. Spectra of polyatomic molecules, rotational constant. Experimental techniques.

**Vibration rotation spectra** -Simple harmonic oscillator, vibrational energy, anharmonicity, principle of vibration-rotation spectra, selection rule, PQR branches. Vibration in polyatomic molecules, effect of nuclear spin, isotopic shift, group frequency. Experimental techniques.

**IV Chemistry of Macromolecules:**

Introduction, type of polymers. Step polymerization, kinetics of step polymerization. Statistical approach to Gelation, Molecular weight distribution in linear poly condensation (Derivation of size distribution), Molecular weight averages. Methods of determining molecular weight by osmotic pressure, light scattering, sedimentation and viscosity methods.

**SEMESTER-I**  
**Paper-Fourth -CHE-104**  
**Techniques of Chemistry-I**

**1. Data handling in Analysis:**

Accuracy and precision. Errors, determinate and indeterminate errors, significant figures. Rounding off figures, standard deviation, regression analysis.

**2. Separation Techniques:**

Principles and applications of solvent extraction. Quantitative treatments of extraction equilibria. Solvent extraction of metals. Solid phase extraction.

**3. Chromatography:**

Introduction, principle, and experimental setup of chromatography. Partition and Adsorption chromatography: Principle of partition and adsorption chromatography. Mobile and stationary phases. liquid-liquid, gas-liquid, gas-solid and liquid-solid chromatography. Reversed phase partition chromatography, paper and thin layer chromatography Applications of partition and adsorption chromatography., HPLC.

**4. Ion Exchange resins:**


Mechanism of ion exchange. Factors affecting the selection of ion exchange resins. Techniques in ion exchange methods and analytical applications.

**5. Spot tests:**

Spot tests for metal ions, spot tests for identification of functional groups-hydroxyl, carboxylic, nitro, nitroso, azo and amino.

**6. Thermal Methods of Analysis:**

Principle, methodology and applications: Thermogravimetric and differential thermal Analysis, thermometric titrations. Thermal stability of polymers. Decomposition Pattern and decomposition reactions- examples.



**SEMESTER II**  
**PAPER First -CHE-201**  
**INORGANIC CHEMISTRY**

**I. Term Symbols and Basic Principles of Electronic Spectroscopy:**

Frank - Condon principle, spin and Laporte selection rules, band intensities, band-width. Number of microstates and term symbols for gaseous atoms/ions. Spin-orbit coupling in spectroscopic ground state of  $p^2$  and  $d^2$  configurations and energies of J levels.

**II. Electronic Spectra of Transition Metal Complexes:**

Interpretation of electronic spectra using Orgel and Tanabe - Sugano diagram for 3d transition metal complexes. Calculations of crystal field and ligand field parameters ( $Dq$ ,  $B$  and  $\beta$  parameters), nephelauxetic series and charge transfer spectra.

**III. Reaction mechanism of transition metal complexes(octahedral)**

Energy profile of reaction, reactivity of metal complexes, inert and labile complexes. Mechanism and kinetics of substitution reaction. Acid hydrolysis, factors affecting acid hydrolysis, base hydrolysis, conjugate base mechanism, direct indirect evidence in favour of conjugate mechanism.

**IV. Reaction mechanism of transition metal complexes(square planer)**

Mechanism and kinetics of substitution reaction. The trans effect, redox reactions, electron transfer reactions, mechanism of one electron transfer reactions, outer-sphere type reactions, cross reactions and Marcus-Hush theory, inner-sphere type reactions.

**V. Metal Clusters:**

Higher boranes, carboranes, metalloboranes and metallocarboranes.

Metal carbonyls and halide clusters.

Compounds with metal-metal multiple bonds

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**SEMESTER II**  
**Paper –Second -CHE-202**

**ORGANIC CHEMISTRY**

**I. Addition to Carbon-Carbon Multiple Bonds**

Mechanistic and stereochemical aspect of addition reaction involving electrophiles, nucleophiles and free radicals, regio and chemoselectivity, orientation and reactivity. Addition to cyclopropane ring. Hydroboration, Michael reaction, Sharpless asymmetric epoxidation, stereochemistry of epoxidation and halolactonisation.

**II. Addition to Carbon-Hetero atom Multiple Bonds**

Generation of enolate ions and their Synthetic applications. Stereochemistry of Wittig reaction and Aldol condensation. Stobbe condensation reactions. Hydrolysis of esters.

**III. Elimination Reactions**

The E1, E2 and E1cB mechanisms, their stereochemistry and orientation. Effects of substrates, attacking base, the leaving group and the medium on reactivity. Mechanism and orientation in pyrolytic elimination. Peterson elimination, Stereochemistry of E2 reactions and pyrolytic eliminations.

**IV. 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 disrotatory motions.  $4n$ ,  $4n+2$  and allyl systems. Cycloadditions - antarafacial and suprafacial additions,  $4n$ ,  $4n+2$  system,  $2+2$  addition of ketenes.  $1-3$  dipolar addition and chelotropic reactions.

**V. Sigmatropic rearrangement**

Suprafacial and antarafacial shift of H, sigmatropic shifts involving carbon moieties, retention and inversion of configuration.  $[3,3]$  and  $[5,5]$  sigmatropic rearrangements. Detailed treatment of Claisen and Cope-rearrangements. Fluxional tautomerism, Aza-Cope rearrangements. Introduction to Ene reaction. Simple problems on pericyclic reactions.

**SEMESTER II**  
**Paper –Third -CHE-203**

**PHYSICAL CHEMISTRY**

- I. Quantum Chemistry:** Origin of quantum theory. Black body radiation. Wien and Rayleigh-Jeans laws, Planck's law and energy of harmonic oscillator. Postulates of quantum mechanics. Three dimensional time independent Schrodinger wave equation, Eigen functions and Eigen values. Normalization and Orthogonally conditions. One dimensional harmonic oscillator. Tunnel effect. Eigen function and Eigen value of H-atom (Solutions not required), shapes of s, p, d and f- orbitals  
**Approximate Methods-**Vibrational principle and its application to ground state H-atom. Radial and Angular distribution curves for H-atom
- II. Chemical Kinetics:** Thermodynamic formulation of rate constant. Comparison of collision and absolute reaction rate theories. Calculation of transmission coefficient. Transition State theory in solution. Primary and secondary salt effects in the light of mechanistic tests. The theory of Absolute reaction rates - for reactions between atoms and reactions between molecules in terms of partition function. Influence of ionic strength and dielectric constant. Explosive reactions.
- III. Electrolytes:** Limitation of Arrhenius theory of electrolytic dissociation. Role of solvent and inter-ionic forces. Activity and activity coefficients, determination of activity coefficients, Debye- Huckel Theory of the structure of dilute ionic solution, charge density and electrical potential. Properties of ionic cloud, activity coefficients from Debye-Huckel theory. Limiting law and its verification. Debye-Huckel theory to more concentrated solutions. Partial molar quantities of electrolytic solutions, determination of partial molar volume.
- IV. Solid State:** Crystal structures, Bragg's law and applications. Band structure of solid.





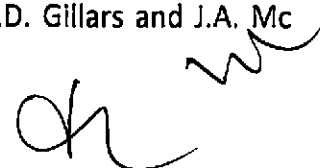
**SEMESTER-II**  
**Paper-fourth (CHE-204)**

**Techniques of Chemistry-II**

1. **Interaction of electromagnetic radiation with matter:** Electromagnetic spectrum, mode of absorption of radiation by matter. Electronic, vibrational & rotational transitions.
2. **Absorption Laws:** Grothus-Draperis Law, Einstein's Law of photochemical equivalence, Quantum efficiency, Reasons for low & high quantum yields, photoelectric cell & photosensitization Lambert-Beer's Law.
3. **Spectrophotometric instrumentation:** Monochromators, sample cell, detectors types of instruments-single beam and double beam spectrophotometers. Applications of spectrophotometric methods in analysis.
4. **Conductometric methods:** Principle of analysis, measurement of conductance, analytical applications of conductometry, conductometric titrations.
5. **Sensors:** Chemical sensors: classification. sensitivity and limit of detection. Potentiometric sensors, gas sensors, Volta metric sensors.  
**Biosensors:** The enzyme electrode, biosensor based on ion-selective electrodes. Applications of enzyme electrodes. Biosensors based on plant and animal tissues. Applications of chemical and biosensors in agriculture, medicine and biochemical analyses.

**BOOKS SUGGESTED – (CHE-101, CHE-201)**

1. Advanced Inorganic Chemistry, F.A. Cotton and Wilkinson, John Wiley.
2. Inorganic Chemistry, J.E. Huhey. Harpes & Row.
3. Chemistry of the Elements, N.N. Greenwood and A. Earnshaw, Pergamon.
4. Inorganic Electronic Spectroscopy, A.B.P. Lever, Elsevier.
5. Magnetochemistry, R.L. Carlin, Springer Verlag.
6. Comprehensive Coordination Chemistry ed., G. Wilkinson, R.D. Gillars and J.A. McCleverty. Pergamon.



### BOOKS SUGGESTED – (CHE-102, CHE-202)

1. Advanced Organic Chemistry-Reactions, Mechanism and Structure, Jerry March, John Wiley.
2. Advanced Organic Chemistry, F.A. Carey and R.J. Sundberg. Plenum.
3. A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, Longman.
4. Structure and Mechanism in Organic Chemistry, C.K. Ingold, Cornell University press.
5. Organic Chemistry, R.T. Morrison and R.N. Boyd. Prentice Hall.
6. Modern Organic Reaction H.O. House, Benjamin
7. Principles of Organic Synthesis, R.O.C. Normon and J.M. Coxon, Blackie Academic and professionla.
8. Perricyclic Reactions. S.M. Mukherji, Macmillan India.
9. Reaction Mecnanism in Organic Chemistry S.M. Mukherji and S.P. Singh, Macmillan.
10. Stereochemistry of Organic Compounds D. Nasipuri, New Age International.
11. Stereochemistry of Organic Compounds, P.S Kalsi, New Age International.
12. Advanced Organic Chemistry, J.Singh and L.D.S Yadav, Pragati Prakashan, India.

### BOOKS SUGGESTED – (CHE-103, CHE-203)

1. Physical Chemistry P.W. Atkins, ELBS.
2. Introduction to Quantum Chemistry, A.K. Chandra, Tata Mc Graw Hill.
3. Quantum Chemistry, Ira N. Levine. Prentice Hall.
4. Coulson's Valence, R.Mc Weeny, ELBS.
5. Chemical Kinetics, K.J. Laidler, Megraw-Hill.
6. Kinetics and Mechanism of Chemical Transformations J. Rajaraman and J.Kuriacose Mc Millan.
7. Micelles, Theoretical and Applied Aspects, V. Moroi, Plenum.
8. Modern Electrochemistry Vol. I and Vol. II J.O.M. Bockris and A.K.N. Reddy, Plenum.
9. Introduction to Polymer Science V.R. Gowarikar, N.V. Vishwanathan and J.Sridhar, Wiley Eastern.
10. Elements of Physical Chemistry, S. Glasstone and D.Lewis., McMillan, London.



#### BOOKS SUGGESTED – (CHE-104)

1. Chromatographic Methods, A. Baithwaite and F.J.Smith., Chapman Hall, London.
2. Chromatography, E. Heftmann., Reinhold, Newyork.
3. Chromatographic Adsorption Analysis, H.H. Strain., Interscience, Newyork.
4. Modern Practice of Gas Chromatography, R.L.Grob., Wiley- Interscience, Newyork.
5. Techniques of Liquid Chromatography, C.F.Simpson., Wiley.
6. Practice of High Performance Liquid Chromatography, H.Engelhardt., Springer-Verlog, Berlin.
7. Practice of Thin Layer Chromatography, J.C. Touchstone and M.F. Dobbins., Wiley, Newyork.
8. Techniques of Chemistry, Ed.A. Weissberger., Interscience, London.
9. Ion Exchange: Theory and Practice, Friedrich helfferich., Dover Publications, New-york.
10. Ion Exchange in Analytical Chemistry, William Rieman and Herold F.Walton., Pergemon Press.
11. Encyclopedia of Analytical Chemistry, vol.1-15, R.A. Meyers., John Wiley.
12. Instrumental Methods of Chemical Analysis, G.W. Ewing, McGraw Hill.

#### BOOKS SUGGESTED – (CHE-204)

1. Visible And Ultraviolet Spectroscopy, R.C.Denney and R. Sinclair., Wiley, Chichester.
2. Elementary Organic Spectroscopy: Principles & Chemical Application, Y.R. Sharma., S. Chand, Ram Nagar, New Delhi.
3. Theory and Applications of Ultraviolet Spectroscopy, H.H. Jaffe and M. Archin., Wiley, Newyork,
4. Vogel's Textbook of Quantitative Inorganic Analysis, Eds J. Basset, R.C. Denney, G.H. Jeffrey and J. Mendhem., Longman, London.
5. Chemical Sensors and Biosensors, Rene Lalauze., Wiley.
6. Chemical Sensors and Biosensors, Brian R. Eggins., Wiley.
7. Biosensors, Rajmohan Joshi., Rediff books.

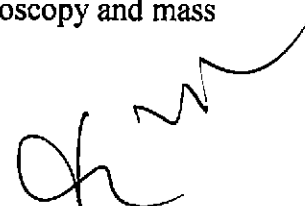


## SEMESTER III

### Paper-First (Compulsory)- CHE-301

#### SPECTROSCOPY

- I. Ultraviolet and Visible Spectroscopy:**  
Various electronic transitions (185-800 nm). Beer-Lambert Law, effect of solvent on electronic transitions, ultraviolet bands for carbonyl compounds, unsaturated carbonyl compounds, dienes, conjugated polyenes. Fisher-Woodward rules for conjugated dienes and carbonyl compounds. Ultraviolet spectra of aromatic and heterocyclic compounds. Steric effect in biphenyls.
- II. Infrared Spectroscopy:**  
Vibrational transitions, modes of vibrations, selection rules. Characteristic vibrational frequencies of alkanes, alkenes, alkynes, aromatic compounds, alcohols, ethers, phenols and amines. Detailed study of vibrational frequencies of carbonyl compounds (ketones, aldehydes, esters, amides, acids, anhydrides, lactones, lactams and conjugated carbonyl compounds). Effect of hydrogen bonding and solvent effect on vibrational frequencies. Overtones, combination bands and Fermi resonance. FTIR.
- III. Proton Magnetic Resonance Spectroscopy ( $^1\text{H}$  NMR) :**  
General introduction and definition, chemical shift, spin-spin interaction, shielding mechanism, measurement of chemical shift values and correlation for protons bonded to carbon (aliphatic, olefinic, aldehydic and aromatic) and other nuclei (alcohols, phenols, enols, carboxylic acids, amines, amides & mercapto), chemical exchange, spin-spin interaction and *j-j* coupling, dihedral angle. nuclear magnetic double resonance, solvent effects. Fourier transform technique, nuclear Overhauser effect (NOE).  
Use of NMR in medical diagnostics.
- IV. Carbon-13 NMR Spectroscopy:**  
General considerations, chemical shift (aliphatic, olefinic, alkyne, aromatic, hetero aromatic and carbonyl carbon), coupling constants.  
An Introduction to Two dimensional NMR spectroscopy - COSY, NOESY and INADEQUATE techniques.
- V. Mass Spectrometry:**  
Introduction, ion production . Factors affecting fragmentation, ion analysis, ion abundance. Mass spectral fragmentation of organic compounds. Common functional groups, molecular ion peak, metastable peak, McLafferty rearrangement. Nitrogen rule. High resolution mass spectrometry. Examples of mass spectral fragmentation of organic compounds with respect to their structure determination.
- VI. Structural problems based on UV, IR,  $^1\text{H}$ NMR,  $^{13}\text{C}$ NMR spectroscopy and mass spectrometry.**



### BOOKS SUGGESTED – (CHE-301)

1. Physical Methods for Chemistry. R.S. Drago, Saunders Company.
2. An Introduction to Practical Infrsred Spectroscopy, A.D.Cross and R.A. Jones., Butterworths, London.
3. Infrsred Spectroscopy, W.O.George and P.S.McIntyre., Wiley, Chichester.
4. NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry, R.V. Parish, Ellis Horwood.
5. Practical NMR Spectroscopy. M.L. Martin, J.J. Delpeuch and G.J. Martin, Heyden.
6. Spectrometric Identification of Organic Compounds. RM. Silverstein. G.C. Bassler and T.C. Morill. John Wiley.
7. Introduction to NMR Spectroscopy. R.J. Abraham. J. Fisher and P.Loftus. Wiley.
8. Application of Spectroscopy of Organic Compounds. J.R. Dyer Prentice Hall.
9. Spectoscopic Methods in Organic Chemistry. D.H. Williams. Fleming. Tata Mc Graw-Hill.
10. Introduction to Mass Spectrometry, H.C. Hill.,Heyden, London.
11. Mass Spectrometry, R.Davis and M. Frearson., Wiley,, Chichester.
12. Interpretation of Mass Spectra, F.W.McLafferty., Benjamin.
13. Mass Spectrometry: Techniques and Applications, G.W.A.Milne., Wiley-Interscience, Newyork.

## SEMESTER-III

### Paper Second (Compulsory)-CHE-302

#### MOLECULAR REARRANGEMENTS AND PHOTOCHEMISTRY

##### Molecular Rearrangements:

General mechanistic considerations-nature of migration, migratory aptitude, memory effects.

##### I. Migration to electron deficient carbon atom:

Pinacol-Pinacolone rearrangement, Wagner-Meerwein rearrangement, Tiffenev-Demjanov ring expansion, Dienone-Phenol rearrangement, Benzil Benzilic acid rearrangement, Arndt-Eistert synthesis, Favorski rearrangement.

##### II. Migration to electron deficient nitrogen atom:

Wolf, Hofmann, Curtius, Losen, Schmidt and Beckmann rearrangements.

##### III. Migration to electron deficient oxygen atom:

Baeyer-Villiger rearrangement.

##### I. Photochemical Reactions:

Interaction of electromagnetic radiation with matter, types of excitations, fate of excited molecule, quantum yield, transfer of excitation energy, actinometry.

##### II. Photochemistry of Alkene:

Intermolecular reactions of the olefinic bond, geometrical isomerism, cyclisation reactions, rearrangement of 1,4- and 1,5-dienes.

##### III. Photochemistry of Aromatic Compounds:

Isomerisations, additions and substitutions.

##### IV. Photochemistry of Carbonyl Compounds: -

Cleavage, - cleavages and inter and intra molecular hydrogen abstractions of carbonyl. Intermolecular reactions of carbonyl compounds-saturated, cyclic and acyclic, unsaturated compounds, rearrangements of cyclohexanone and rearrangement of unsaturated ketones, cyclohexadienones, intermolecular cycloaddition reactions-dimerisations and oxetane formation. Norrish type-I and type-II reactions.

##### V. Miscellaneous Photochemical Reactions:

Photo-Fries reactions of annelids, Photo-Fries rearrangement, Barton reaction, Singlet molecular oxygen and its reactions, photochemical formation of smog, photo-degradation of polymers. Chemistry of vision.

### BOOKS SUGGESTED – (CHE-302)

1. Fundamentals of Photochemistry. K.K. Rohtagi Mukherji, Wiley Eastern.
2. Essentials of Molecular Photochemistry A.Gilbert, Baggot Blackwell Scientific Publication.
3. Introductory Photochemistry. A. Cox and T. Camp. McGraw Hill.
4. Photochemistry. R.P. Kundall and A.Gilbert. Thomson Nelson.
5. Organic Photochemistry. J. Coxon and B.Halton. Cambridge University Press.
6. Frontier Orbitals and Organic Chemical Reactions, I. Fleming.,Wiley, London.
7. Guide book to Mechanism in Organic Chemistry, P.Sykes., Longman, harlow.
8. Molecular Rearrangements in Organic synthesis by Christian M.Rojas, Wiley-VCH
9. Molecular Rearrangements by A.C. Knipe and J.M.Coxon, Wiley-VCH.

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**SEMESTER – III**  
**Paper-Third (Elective) –CHE-EL--303**  
**POLYMER CHEMISTRY**

**I. Basics**

Importance of polymers, basic concepts :monomers, degree of polymerization. Linear branched and network polymers. Classification of polymers. Polymerization: condensation, addition/radical chain-ionic and co-ordination and copolymerization. Polymerization conditions and polymer reactions.Polymerization in homogeneous and heterogeneous systems.

**II. Polymer Characterization**

Polydispersion-average molecular weight concept. Number, weight and viscosity average molecular weights. Polydispersity and molecular weight distribution. The practical significance of molecular weight. Measurement of molecular-weights. Endgroup, viscosity, light scattering, osmotic and ultracentrifugation methods.

**III. Analysis and testing of polymers**

Chemical analysis of polymers, spectroscopic methods, X-ray diffraction study. Thermal analysis and physical testing-tensile strength. Fatigue, impact tear resistance, hardness and abrasion resistance.

**IV. Inorganic Polymers**

A general survey and scope of inorganic polymers special characteristics, classification, homo and hetero atomic polymers. Structure, properties and applications of (1) Polymers based on boron-borazines, boranes and carboranes. (2) Polymers based on silicon, silicones, polymetalloxanes and polymetallosiloxanes, silazanes.

**V. Structure, Properties and Application of**

- a. Polymers based on Phosphorous-Phosphazenes, Polyphosphates.
- b. Polymers based on Sulphur-tetrasulphurtetranitride and related compounds.
- c. Co-ordination and metal chelate polymers.





**BOOKS SUGGESTED – (CHE-303)**

1. Textbook of Polymer Science, F.W. Billmeyer Jr. Wiley.
2. Polymer Science, V.R. Gowarker, N.V. Viswanathan and J Sreedhar, Wiley-Eastern.
3. Functional Monomers and Polymers. K. Takemoto, Y. Inaki and RM. Rttanbrite.
4. Contemporary Polymer Chamistry, H.R. Alcock and F.W. Lambe, Prentice Hall.
5. Physics and Chemistry of Polymer, J.M.G. Cowie, Blackie Academic and Professional.

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**SEMESTER-III**  
**Paper fourth (Elective)-CHE-EL-304**

**ELECTROCHEMISTRY**

- I. Conversion and Storage of Electrochemical Energy :** Present status of energy consumption: History of fuel cells, direct energy conversion by electrochemical means. Maximum intrinsic efficiency of an electrochemical converter. Physical interpretation of the Carnot efficiency factor in electrochemical energy converters. Power outputs. Electrochemical generators (Fuel Cells): Hydrogen oxygen cells, Hydrogen Air cell. Hydrocarbon air cell, Alkane fuel cell, Phosphoric fuel cell, direct NaOH fuel cells, applications of fuel cells.

**Electrochemical Energy Storage:**

Properties of Electrochemical energy storage : Measure of battery performance, Charging and discharging of a battery, Storage Density, Energy Density. Classical Batteries: (i) Lead Acid (ii) Nickel-Cadmium, (iii) Zinc manganese dioxide. Modern Batteries: (i) Zinc-Air (ii) Nickel-Metal Hydride. (iii) Lithium Battery. Future electricity storers: Storage in (i) Hydrogen, (ii) Alkali Metals, (iii) Non aqueous solutions.

- II. Corrosion and Stability of Metals:**

Surface mechanism of the corrosion of the metals; Thermodynamics of the stability of metals. Potential -pH (or Pourbaix) Corrosion current and corrosion potential - Evans diagrams. Measurement of corrosion rate: (i) weight loss method, (ii) electrochemical method.

**Inhibiting Corrosion :**

Cathodic and anodic protection, (i) Inhibition by addition of substrates to the electrolyte environment, (ii) by changing the corroding method from external source, anodic protection, organic inhibitors, the fuller Story Green inhibitors.

**Passivation :** Structure of Passivation films. Mechanism of passivation, Spontaneous Passivation. Nature's method for stabilizing surfaces.

- III. Bio-electrochemistry:**

Bio-electrodes, Membrane Potentials. Simplistic theory, Modern theory, Electrical conductance in biological organism: Electronic, Protonic electrochemical mechanism of nervous systems, enzymes as electrodes.

**Kinetic of Electrode Process :**

Essentials of electrode reaction, current density, overpotential, Tafel Equation, Butler Volmer equation. Standard rate constant (K) and transfer coefficient (a), exchange current.

**Irreversible Electrode processes:** Criteria of irreversibility, information from irreversible wave.

- IV. Methods of determining kinetic parameters for quasi-reversible and irreversible Electro catalysis:**

Chemical catalysts and Electrochemical catalysts with special reference to prostates, porphyrin oxides of rare earths. Electro catalysis in simple redox reactions, in reactions involving adsorbed species. Influence of various parameters.



### BOOKS SUGGESTED – (CHE-304)

1. An Introduction to Electrochemistry, Samuel Glasstone., East West Press.
2. Modern Electrochemistry, John O.M. Bockris., Springer.
3. Electrochemistry and Corrosion Science, Nestor Perez., Springer.
4. Electrochemistry: Principles , Methods and Applications, Christopher M.A. Brett and Ana Maria O. Brett., Oxford Science Publications.
5. Electrochemical Science and Technology: Fundamentals and Applications, Keith B. Oldham Jan C Myland alan M. Bond., wiley.
6. Fundamentals of Electrochemical Corroison ,E.E. Stansbury.R.A. Buchanan., ASM International.

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**SEMESTER-III**  
**Paper Fifth (Elective)-CHE-EL-305**

**HETEROCYCLIC CHEMISTRY**

**I. Nomenclature of Heterocyclic Compounds**

Replacement and systematic nomenclature (Hantzsch MCH-Widman system) for monocyclic, fused and bridged heterocyclic compounds.

**Aromatic Heterocycles**

General chemical behaviour of aromatic heterocycles, classification (structural type), criteria of aromaticity (bond lengths, ring current and chemical shifts in  $^1\text{H}$ NMR spectra, empirical resonance energy, delocalization energy and Dewar resonance energy, diamagnetic susceptibility exaltations). Reactivity and tautomerism in aromatic heterocycles.

**II. Small Ring Heterocycles**

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

**Benzo-Fused Five-Membered Heterocycles**

Synthesis and reactions including medicinal applications of benzopyrroles, bezofurans and benzothiophenes.

**III. Meso-Ionic Heterocycles**

General classification, chemistry of some important meso-ionic heterocycles of type-A and B and their applications.

**IV. Six-Membered Heterocycles with one Heteroatom**

Synthesis and reactions of pyrilium salts and pyrones and their comparison with pyridinium & thiopyrylium salts and pheridones. Synthesis and reactions of quinolinium and benzopyrylium salts, coumarins and chromones. Six Membered Heterocycles with two or more Heteroatoms: Synthesis and reactions of diazines, triazines, tetrazines and thiazines.

**V. Seven-and large-membered heterocycles:**

Synthesis and reactions of azepines, oxepines, thiapines, diazepinesthiazepines, azocines, diazocines, dioxocines and dithiocines.



**BOOKS SUGGESTED – (CHE-305)**

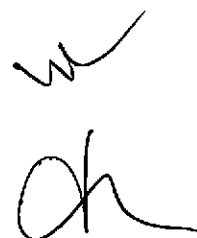
1. "Heterocyclic Chemistry" Vol, 1-3 R.R. Gupta, M. Kumar and V.Gupta, Springer, Verlag.
2. The Chemistry of Heterocyclic, T.Eicher and S. Hauptmann, Thieme.
3. Heterocyclic Chemistry, J.A. Joule, K. Mills and G.F. Smith, Chapman and Hall.
4. Heterocyclic Chemistry, T.L. Gilchrist, Longman Scientific 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 Press.



**SEMESTER III**  
**Paper Sixth (Elective)-CHE-EL-306**

**QUANTUM CHEMISTRY**

- I. Time - independent perturbation theory for non - degenerate states (first order correction to energy and wave function), and its application to particle in a one - dimensional box, ground state helium atom (without spin consideration) and perturbed harmonic – oscillator. Vibrational method: theory and application to ground state hydrogen and helium atoms and one - dimensional oscillator.
- II. **Theory of time - dependent quantum approximation technique.** Fermi Golden Rule. Radiation - Matter interaction (induced emission and absorption of radiation). Einstein's transition probabilities. Determination of selection rules in respect of rigid rotation and harmonic - oscillator approximation.
- III. **Quantum - mechanics of multielectron atoms:** Hartree self - Consistent method. Hartree - Fock self - Consistent (HFSCF) method. Rootham's method. Correlation energy (CE) and configuration interaction (CI), Koopmann's theorem. Basic idea of Density Functional Theory (DFT): Kohn - Sham equation.
- II. **Quantum - mechanical treatment of diatomic molecules:** The Born Oppenheimer approximation and its formulation. The valence - bond treatment of hydrogen molecule. Heitler - London treatment and ionic contribution. Molecular Orbital Theory (MOT) of  $H_2^+$ . MOT with configuration interaction (CI). Hybridization ( $sp$ ,  $sp^2$  &  $sp^3$ ) from a quantum - mechanical view - point.
- V. **Quantum - mechanical treatment of  $\pi$  - electron systems.** The  $\pi$ - electron approximation . Free electron molecular orbital (FEMO) method and its application to polyenes. The Huckel - Molecular Orbital Theory (HMOT) for conjugated hydrocarbons and cyclic conjugated systems. Huckel calculations for ethylene, allyl systems, cyclobutadiene and benzene. Calculation of electron density, charge distribution and bond orders.



### BOOKS SUGGESTED – (CHE-306)

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. JB. Foresman and E.Frish.  
Goussian Inc.
5. Semi-empirical MO theory. J. Pople and D.D. Beveridge.
6. Introduction to Quantum Chemistry, A.K. Chandra., Tata Mc Graw Hill.
7. Introduction to Quantum Chemistry, R.K. Prasad., New Age International.
8. Coulson 's Valence, R.C. Weeny., ELBS.

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**SEMESTER III**  
**Paper Seventh (Elective)-CHE-EL-307**

**ANALYTICAL CHEMISTRY**

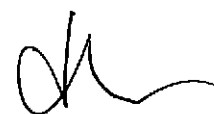
- I. **Introduction:** Role of analytical chemistry. Classification of analytical methods-classical and instrumental.Types of instrumental analysis.Neatness and cleanliness. Laboratory operations and practices, analytical balance. Gravimetric techniques.Selecting and handling of reagents.Laboratory notebooks.Safety in the analytical laboratory.
- II. **Food Analysis:** Analysis of moisture, ash, crude protein, fat, crude fibre. carbohydrates. calcium, potassium, sodium and phosphate in food products. Food adulteration-common adulterants in food, contamination of food stuffs. Microscopic examination of foods for adulterants. Pesticide analysis in food products. Extraction and purification of sample. HPLC, Gas chromatography for organophosphates. Thin-layer chromatography for identification of chlorinated pesticides in food products.
- III. **Analysis of Water Pollution:** Origin of waste water, types water pollutants and effects. Sources of water pollution –domestic, industrial and agricultural . Soil and radioactive wastes as sources of pollution. Parameters for analysis -colour, turbidity total solids conductivity, hardness, chloride, sulphate. Metal/heavy metal pollution due to cadmium, chromium, copper, lead, zinc, manganese, mercury and arsenic. Measurements of DO, BOD and COD. Pesticides as water pollutants and analysis Water pollution laws and standards.
- IV. **Analysis of Soil:** Moisture, pH, total nitrogen, phosphorus, silican, lime, magnesia, manganese, sulphur and alkali salts.
- IV. **Analysis of Drug:** Narcotics and dangerous drugs. Classification of drugs. Screening by gas and thin-layer chromatography and (spectrophotometric) measurements.





### BOOKS SUGGESTED – (CHE-307)

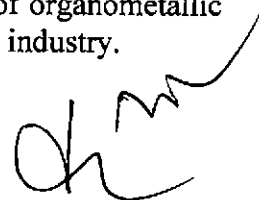
1. Analytical Chemistry, G.D. Christian, J.Wiley.
2. Fundamentals of Analytical Chemistry D.A. Skoog D.M. West and F.J. Holler W.B. Saunders.
3. Analytical Chemistry-Principles J.S. Kennedy, W.B. Saunders.
4. Analytical Chemistry-Principles and Techniques. L.G. Hargis Prentice Hall.
5. Principles of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



**SEMESTER IV**  
**Paper First (compulsory)-401**

**ORGANOMETALLIC CHEMISTRY**

- I. Organometallic Compounds of transition elements:**  
General introduction of ligands, classification and nomenclature. 2-6 electron donor ligands with special reference to  $\pi$ -allyl, cyclopentadienyl and arenes.
- II. Synthesis, structure and bonding aspects of organometallic compounds with:**
- (a)  $\sigma$ -bonded alkyl groups as ligands. ( $\beta$ -Hydride elimination,  $\sigma$ -bonded  $\eta^1$ -aryl ligands)
  - (b) Olefinic and acetylic groups as ligands.
  - (c) Cyclic and acyclic polyenyl  $\pi$ -bonded ligands: ( $\pi$ -allyl, butadiene cyclobutadiene, cyclopentadienyl and arenes as ligands)
- III. Reactions in Organometallic Chemistry:**  
Oxidative addition, Oxidative coupling, Reductive elimination, Migratory insertion reactions, Coupling reactions (Palladium catalysed C-C and C-N couplings, Stille coupling, Heck coupling, Suzuki-Miyaura coupling, Sonogashira coupling, Negishi coupling, Hiyama coupling)
- IV. Homogeneous and heterogeneous transition metal catalysis:**  
General considerations, Reason for selecting transition metals in catalysis (bonding ability, ligand effects, variability of oxidation state and coordination number), Homogeneous hydrogenation of unsaturated compounds (alkenes, alkynes, aldehydes and ketones). Asymmetric hydrogenation. Phase transfer catalysis.
- V. Some important homogeneous and heterogeneous catalytic reactions:**  
Ziegler Natta polymerization of ethylene and propylene, oligomerisation of alkenes by aluminium alkyl, Wacker acetaldehyde synthesis, hydroformylation of unsaturated compounds using cobalt and rhodium complexes, Monsanto acetic acid synthesis, carboxylation reactions of alkenes and alkynes using nickel carbonyl and palladium complexes. Carbonylation of alkynes (acetylene) using nickel carbonyls or Palladium complexes.
- VI. Metal-metal bonding in carbonyl and halide clusters:**  
Polyhedral model of metal clusters, effect of electronic configuration and coordination number. Structures of metal carbonyl clusters of three atoms  $M_3(CO)_6$  ( $M = Fe, Ru \& Os$ ), Four metal atoms (tetrahedra)  $[M_4(CO)_6]$  ( $M = Co, Rh \& Ir$ ) and octahedron of type  $M_6(CO)_6$  [ $M = Co \& Rh$ ], and halide derivatives of Rhenium (III) triangles, metal carbonyls involving bridged-terminal exchange and scrambling of CO group.  
**Metal Carbonyls and Nitrosyl:** Classification, bonding, factors affecting the magnitude of stretching frequency, Synthesis of metal carbonyls, Fluxionality, properties and reactions.  
**Fluxional Organometallic Compounds:** Fluxionality and dynamic equilibrium in compounds such as  $\eta^2$  olefine,  $\eta^3$ -allyl and dienyl complexes.
- V. Transition Metal-Carbon multiple bonded compounds:**  
Metal carbenes and carbynes (preparation, reactions, structure and bonding considerations). Biological applications and environmental aspects of organometallic compounds, Organometallic compounds in medicine, agriculture and industry.



**BOOKS SUGGESTED – (CHE-401)**

1. Principles and application of Organotransition Metal Chemistry J.P. Collman. L.S. Hegsdus. J.R. 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. Organotransition Metal Chemistry, S.G. Davies., Pergamon Press Oxford.
6. Organometallics in Organic Synthesis, E.I. Negishi.,Wiley, NewYork.

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**SEMESTER -IV**  
**Paper Second (Compulsory)-CHE-402**

**SOME SPECIFIC REACTIONS AND REAGENTS IN CHEMISTRY**

**I. Some Name Reactions:**

Bamford-Stevens reaction, Chichibabin reaction, Cope elimination reaction, Dakin oxidation, Mannich reaction, Meerwein-Ponndorf-Verley reduction, Mitsunobu reaction, Nef reaction, Oppenauer oxidation, Perkin reaction, Peterson olefination, Reformatsky reaction, Robinson annulations, Favorskii reaction, Birch reduction, Knoevenagel condensation, Stork- enamine reaction, Stetter reaction, Baylis-Hillman reaction and Wittig reaction.

**II. Reagents in Organic Synthesis:**

Use of following reagents in organic synthesis and functional group transformation.

- A.** Organometallic reagents – Organolithium reagents, Organomagnesium reagents, Organotitanium reagents, Organozinc reagents, Organoboron reagents, Organosilicon reagents, Palladium-catalyzed Coupling Reactions.
- B.** DEAD, Tebbe's reagent, Hydrazine and phenylhydrazine, DCC, DDQ, Nucleophilic heterocyclic carbenes, 1, 3- Dithiane (Umpolung reactivity), Lithium diisopropyl amide (LDA), Selenium dioxide
- C.** Complex metal hydrides-  $\text{NaBH}_4$ ,  $\text{LiAlH}_4$ , DIBAL, diborane, disoamylborane, tetrylborane, 9-BBN, and isopinocampheylborane.

**III. Organic Reagents in Inorganic Chemistry:**

Chelation, factors determining the stability of chelates (effect of ring size, oxidation state of the metal, coordination number of the metal); Use of the following reagents in analysis:

- (a) Dimethylglyoxime (in analytical chemistry)
- (b) EDTA (in analytical chemistry and chemotherapy)
- (c) 8-Hydroxyquinoline (in analytical chemistry and chemotherapy)
- (d) 1,10-Phenanthroline (in analytical chemistry and chemotherapy)

*W*  
*dh*

### BOOKS SUGGESTED (CHE-402)

1. Reagents for Organic Chemistry, L.F. Fieser and M. Fieser., Wiley, New York.
2. Organometallic Chemistry, R.C. Mehrotra and A. Singh., Wiley, Eastern.
3. Organotransition Metal Chemistry, S.G. Davies, Pergamon Press, Oxford.
4. Modern Synthetic Reactions, H.O. House, W.A. Benjamin, California.
5. Organic Chemistry, vol. I and II, I.L. Finar, Longman.
6. Comprehensive Organic Chemistry, D. Barton and W D Wallis., Pergamon Press, Oxford.
7. Advanced Organic Chemistry-Reaction Mechanism & Structure. Jerry March., John Wiley.
8. Advanced Organic Chemistry, F.A. Carey and R.J. Sundberg., Plenum.
9. A Guide book to Mechanism in Organic Chemistry, Peter Sykes., Longman.
10. Structure and Mechanism of Organic Chemistry, C.K. Ingold., Cornell University Press.

**SEMESTER -IV**  
**Paper Third (Elective)-CHE-EL-403**

**INORGANIC SPECTROSCOPY**

**I. Electronic Spectroscopy:**

Electronic spectral studies for  $d^1$ -  $d^9$  systems in octahedral, tetrahedral and square planer complexes,

**II. Vibrational Spectroscopy**

Symmetry and shapes of  $AB_2$ ,  $AB_3$ ,  $AB_4$ ,  $AB_5$  and  $AB_6$ . Mode of bonding of ambidentate ligands, nitrosyl, ethylenediamine and diketonato complexes. Application of resonance. Raman spectroscopy and its applications.

**III. Electron Spin Resonance Spectroscopy:**

Hyperfine coupling, spin polarization for atoms and transition metal ions, spin-orbit coupling and significance of g-tensors. Application to transition metal complexes (having one unpaired electron) including biological systems and to inorganic free radicals such as  $PH_4$ ,  $F_2$  and  $[BH_3]$ .

**IV. Nuclear Magnetic Resonance Spectroscopy-I (Paramagnetic Substances in Solution):**

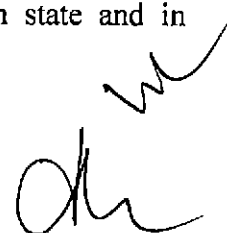
The contact and pseudo contact shift, factors affecting nuclear relaxation, some applications including biochemical systems, an overview of NMR of metal nucleides with emphasis on  $^{195}Pt$  and  $^{119}Sn$  NMR.

**V. Nuclear Magnetic Resonance Spectroscopy - II**

Chemical exchange, effect of deuteration, complex spin - spin interaction between two, three, four and five nuclei ( $I^{\text{st}}$  order spectra), stereochemistry, hindered rotation, Karplus curve-variation of coupling constant with disordered angle, NMR shift reagents, solvent effects, Nuclear Overhauser effect (NOE).

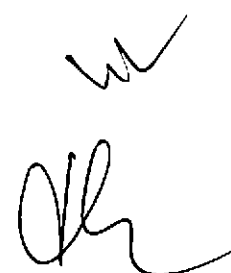
**VI. Mossbauer Spectroscopy**

Basic principles, spectral parameters and spectrum display. Application of the technique to the studies of (1) bonding and structures of  $Fe^{+2}$  and  $Fe^{+3}$  compounds including those of intermediate spin, (2)  $Sn^{+2}$  and  $Sn^{+4}$  compounds: nature of M-L bond, coordination number, structure and (3) detection of oxidation state and in equivalent MB atoms.



### BOOKS SUGGESTED (CHE-403)

1. Structural Methods in Inorganic Chemistry, E.A.V. Ebsworth, Rankin and Cradock-ELBS.
2. Infrared and Raman Spectra Inorganic and Coordination compounds. K. Nakamoto. Willey.
3. Progress in Inorganic Chemistry vol. 8cd. F.A. Cotton. vol. 15 ed S.J. Lippard. Wiley.
4. Transition Metal Chemistry ed R.L. Carlin vol. 3 Dekker.
5. Inorganic Electronic Spectroscopy,. A.P.B. Lever. Elsevier.

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**SEMESTER- IV**  
**Paper fourth (Elective)- CHE-EL-404**

**CHEMISTRY OF NATURAL PRODUCTS**

**I. Terpenoids and Carotenoids:**

Classification, nomenclature, occurrence, isolation, general methods of structure determination, isoprene rule. Stereochemistry and synthesis of the following representative molecules:  $\alpha$ -Terpineol, camphor and Farnesol . Biogenesis of Terpenoids & alkaloids.

**II. Alkaloids**

Definition, nomenclature and physiological action, occurrence, isolation, general methods of structure elucidation, degradation. Classification based on nitrogen heterocyclic ring, role of alkaloids in plants. Structure, stereochemistry & synthesis of the following: Ephedrine, Nicotine and Morphine.

**III. Steroids**

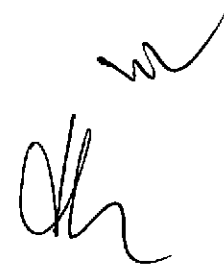
Occurrence, isolation and nomenclature. Diel's hydrocarbon. Basic skeleton and biological significance of sterols, bile acids, estrone, progesterone, aldosterone and testosterone. Photoproducts of ergosterol-vitamin D. Structure determination of cholesterol.

**IV. Prostaglandins**

Occurrence, nomenclature, classification, and physiological effects. Syntheses of PGE<sub>2</sub> and PGF<sub>2a</sub>.

**V. Anthocyanins:**

Methods of isolation, basic structural features of coumarins, flavones, chromones and isoflavones. Structural elucidation of quercetin .





### BOOKS SUGGESTED – (CHE-404)

1. Natural Products: Chemistry and Biological Significance, J.Mannm R.S. Davidson, J.B. Hobbs, D.V. Banthrope 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 of Flavonoids, B.A. Bohm, Harwood Academic Publishers.
7. New Trends in Natural Product Chemistry, Atta-ur-Rahaman and M.I. Choudhary, Harwood Academic Publishers.
8. Insecticides of Natural Origin, Sukh Dev, Harwood Academic Publishers.
9. Organic Chemistry, Vol.II, I.L. Finar, Longman.



## SEMESTER-IV

### Paper Fifth (Elective)EL--405

#### Supramolecular Chemistry and Strategies in Chemical Syntheses

##### A. Supra molecular Chemistry:

- i Molecular Recognition: Molecular receptors for different types of molecules including arisonic substrates, design and synthesis of co receptor molecules and multiple recognition.
- ii. Supramolecular reactivity and catalysis.
- iii. Transport processes and carrier design.
- iv Supramolecular devices: Supramolecular photochemistry, supramolecular electronic, ionic, and switching devices. Some examples of self-assembly in Supramolecular chemistry.

##### B. Strategies in Syntheses:

###### I. Disconnection Approach:

An introduction to synthons and synthetic equivalents. functional group inter conversions, the importance of the order of events in organic synthesis, chemo selectivity, reversal of polarity (Umpolung reactivity).

###### II. One Group C-C Disconnections:

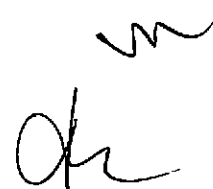
Alcohols and carbonyl compounds, regioselectivity. alkene synthesis. use of acetylenes and aliphatic nitro compounds in organic synthesis.

###### III. Three group C-C disconnections:

Diels-Alder reaction, 1-3 difunctionalised compounds,  $\alpha$ - $\beta$ -unsaturated carbonyl compounds. control in carbonyl condensations, 1-5- difunctionalised compounds.

##### C. Protecting Groups:

Principle of protection of alcohols and diols as acetals, amine, carbonyl, double bond, triple bond and carboxyl group.



### BOOKS SUGGESTED – (CHE-405)

1. Designing organic Synthesis, S. Warren. Wiley.
2. Organic Synthesis-Concept, methods and Starting Materials, J.Fuhrhop and G. Penicillin. Verlage VCH.
3. Some modern methods of organic Synthesis. W. Carruthers Cambridge Univ. Press.
4. Modern Synthetic Reaction, H.O. House W.A. Benjamin.
5. Advanced Organic Chemistry: Reactions, Mechanisms and Structure, J. March. Wiley.
6. Advanced Organic Chemistry Part B. F. A. Carey and R.J. Sundberg. Plenum Press.
7. Physical Organic Chemistry, N.S. Isaacs, ELBS. Longman.
8. Super molecular Chemistry: Concept and perspectives, J.M. Lehn, VCH
9. Bioinorganic, Bioorganic and Supramolecular Chemistry, P.S.Kalsi and J.P. Kalsi., New Age International.



## SEMESTER IV

### Paper Sixth (Elective)-CHE-EL-406

#### NANO MATERIALS AND SOLID STATE CHEMISTRY

1. **Nano-materials:** Introduction and classification, Preparation and characterization of different types of nano structures-nanoparticles, nano clustures, nanowires, nanorods, nanofilms, nanotubes.
2. **Nano-catalysts:** Mode of action of catalysts, classification and comparison of nano-catalysis with homogeneous and heterogeneous catalysts. Specificity, shapes, surface area of nano-catalysts. Role of size, shape and surface area of nanoparticles in catalysts. Langmuir Hinshelwood mechanism on nano-catalysts.
3. **Liquid crystals:** Types of liquid crystals, Nematic, Smectic, ferroelectric and antiferro electric liquid crystals. Theories of LCs, liquid crystal display. New materials as liquid crystals.
4. **Solid State Reactions:** General principle, experimental procedure. Co-precipitation as a precursor to solid state reactions. Kinetics of solid state reactions.
5. **Organic Solids:** Electrically conducting solids, organic charge transfer complexes, organic metals, new superconductors.
6. **Crystal Defects and Non-Stoichiometry :** Perfect and imperfect crystals, intrinsic & extrinsic defects - point defects, line and plane defects, vacancies - Schottky defects & Frenkel defects.

#### BOOKS SUGGESTED –CHE-406

1. Solid State Chemistry and its Applications A.R. West, Plenum.
2. Principles of the Solid State H.V. Keer Wiley Eastern.
3. Solid State Chemistry, N.B. Hannay.
4. Solid State Chemistry D.K. Chakrabarty, New Age International.
5. Principles of the Solid State, H.V. Keer. Wiley Eastern.
6. Thermotropic Liquid Crystalism Ed. G.W. Gray. John Wiley.
7. Handbook of Liquid Crystals. Kelker and Hafz. Chemie Verlag.
8. Nanomaterials, Dieter Vollath, 2<sup>nd</sup> Edition, Wiley, VCH.
9. Nanomaterials: Science and Applications, Deborah Kane, Adam Micolich and Peter, Roger., CRC Press Books.

**SEMESTER –IV**  
**Paper Seventh (Elective) CHE-EL-407**

**MEDICINAL CHEMISTRY**

**I. Drug Design**

Development of new drugs, procedures followed in drug design, concept of lead compound and end modification, concepts of prodrugs and soft drugs, structure-activity relationship (SAR). Factors affecting bioactivity: Theories of drugs activity- occupancy theory, rate theory, induced fit theory. Quantitative structure activity relationship. History and development of QSAR. Concepts of drugs receptors and drug receptors. Elementary treatment of drug interactions. Physico-chemical parameters: lipophilicity, partition coefficient, electronic ionization constants, steric, Shelton surface activity parameter and redox potentials. LD-50, ED-50 (Mathematical derivations of equations excluded). Basic ideas about Pharmacokinetics and Pharmacodynamics.

**II. Antineoplastic Agents**

Introduction, cancer chemotherapy. Role of alkylating agents and antimetabolites in treatment of cancer. Mention of carcinolytic antibiotics and mitotic inhibitors. Synthesis of mechlorethamine, mustards and 6- mercaptopurine. Recent developments in cancer chemotherapy.

**III. Cardiovascular Drugs**

Introduction, cardiovascular diseases, drug inhibitors of peripheral sympathetic function. Central intervention of cardiovascular output. Direct acting arteriolar dilators. Synthesis of amyl nitrate, hydrolaxine methyldopa and diazoxide propanol.

**IV. Local Anti-infective Drugs**

Anti-tubercular drugs and Anti-malarial drugs: Introduction and general mode of action. Synthesis of sulphonamides, norfloxacin, dapson, chloroquin and primaquin.

**V. Psychoactive Drugs-The Chemotherapy of mind**

CNS depressants, general anesthetics, mode of action, hypnotics, sedatives, anti-anxiety drugs, benzodiazepines, antipsychotic drugs. Synthesis of diazepam, alprazolam and barbiturates.

**VI. Antibiotics**

General introduction, structure and synthesis of penicillin G & chloramphenicol.

**VI. Metals in Medicines**

Metal deficiency and diseases, toxic effects of metals, metals for diagnosis and chemotherapy.

**BOOKS SUGGESTED – (CHE-407)**

1. Introduction to Medicinal Chemistry: How Drugs Act and Why?, A. Gringuaz., John Wiley and Sons.
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. Pandey and J.R. Dimmock, New Age International.
4. Burger's Medicinal Chemistry and Drug Discovery, Vol-1 (Chapter-9 and Ch-14) 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.
8. Organic Chemistry Vol.II, I.L. Finar., Longman.
9. Inorganic Biochemistry vol.I and II, G.L. Eichborn., Elsevier.



## M.Sc. CHEMISTRY PRACTICALS:

There will be one practical examination in each of the semesters I, II & III of 100 marks. The students will have to complete 4 exercises in examination selecting at least one experiment from each section/specialized branch. Duration of examination will be of 12 hours spread over two days. The practical examination in semester IV will be of 75 marks & its duration will be of 7 hours. In each practical exam the board of examiners will comprise of one external examiner and one internal examiner.

Distribution of Marks:

### For Semesters I, II and III

Each experiment of 20 marks (Four Experiments)	total =	<b>80 marks</b>
Viva-Voce		<b>15 marks</b>
Record		<b>05 marks</b>
	<b>Total=</b>	<b>100 marks</b>

### For Semester IV

Each experiment 20 marks (Three Experiments)	total =	<b>60 marks</b>
Viva-Voce		<b>10 marks</b>
Record		<b>05 marks</b>
	<b>Total =</b>	<b>75 marks</b>

**Internal assessment** **25 marks**



**SEMESTER - I**  
**CHEMISTRY PRACTICAL**  
**CHE - PR - I**  
**Inorganic :**

**a) Qualitative Analysis :**

- Qualitative mixture analysis for seven radicals including two rare elements (Mo, W, Ti, Zr, Th, Ce, V) in cationic and anionic forms.
- b) Quantitative separation and determination of the following pairs of metal ions using gravimetric & volumetric methods.
- (i)  $\text{Ni}^{++}$  and  $\text{Cu}^{++}$
  - (ii)  $\text{Cu}^{++}$  and  $\text{Zn}^{++}$
  - (iii)  $\text{Ag}^+$  and  $\text{Cu}^{++}$
  - (iv)  $\text{Ag}^+$  and  $\text{Ca}^{++}$

**Organic**

- a) Separation and identification of organic compounds using chemical methods from binary mixture.
- b) Isolation of
- (i) Caffeine from tea leaves
  - (ii) Eugenol from cloves
  - (iii) Casein from milk
  - (iv) Lycopene from Tomatoes

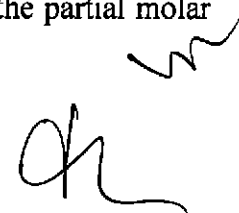
**Physical**

**Chemical Kinetics :**

1. Kinetic studies of a reaction between acetone and iodine catalyzed by  $\text{H}^+$  ions.
2. Kinetics of oxidation of reducing sugars by potassium ferricyanide in presence of ammonium hydroxide or sodium hydroxide.
3. Determination of rate constant and order of reaction between  $\text{H}_2\text{O}_2$  and HI
4. Determination of velocity constant of hydrolysis of an ester/ionic reaction in micellar media.
5. Determination of the effect of a) change of temperature, b) ionic strength of media, c) change of concentration of reactants and catalysts on the velocity constant of hydrolysis of an ester/ionic reaction.

**Thermodynamics**

1. Determination of partial molar volume of solute (e.g. KCl) and solvent in a binary mixture.
2. Determination of the temperature dependence of the solubility of a compound in two solvents having similar inter molecular interactions and to calculate the partial molar heat of solution.





**SEMESTER - II**  
**CHEMISTRY PRACTICAL**  
**CHE - PR - II**  
**Inorganic :**

- A. Preparation of coordination complexes and their characterization by recorded UV, visible, IR spectra, molar conductivity measurement values etc.
- (a) VO (acac)<sub>2</sub>
  - (b) K<sub>3</sub> [Cr(C<sub>2</sub>O<sub>4</sub>)<sub>3</sub>]. 3H<sub>2</sub>O
  - (c) K<sub>3</sub> [Fe(C<sub>2</sub>O<sub>4</sub>)<sub>3</sub>]
  - (d) [Ni (NH<sub>3</sub>)<sub>6</sub>]Cl<sub>2</sub>
  - (e) [Cu(NH<sub>3</sub>)<sub>4</sub>]. SO<sub>4</sub>.6.H<sub>2</sub>O
  - (f) Cis and trans copper glycolates.
- B. Paper chromatography separation of a mixture of the following and measurement of R<sub>f</sub> values.
- (a) Pb<sup>++</sup>, Ag<sup>+</sup>, Hg<sup>++</sup>
  - (b) Co<sup>++</sup>, Ni<sup>++</sup>, Cu<sup>++</sup>
  - (c) Ba<sup>++</sup>, Ca<sup>++</sup>, Sr<sup>++</sup>

**Organic**

- A. Preparation of various organic compounds involving two or three steps :
- (a) Dibenzal acetone from benzaldehyde
  - (b) Adipic acid by chromic acid oxidation of cyclohexanol.
  - (c) p-chlorotoluene from p-toluidine
  - (d) Benzilic acid from benzoin
  - (e) m-nitro aniline from acetanilide
  - (f) Anthranilic acid from phthalic anhydride
- B. Quantitative estimation:
- (i) Determination of the percentage or number of hydroxyl groups in an organic compound by acetylation method.
  - (ii) Determination of iodine number & saponification values of an oil sample.
  - (iii) Estimation of amine/phenols using bromate bromide solutions or acetylation method.
  - (v) Estimation of carbonyl groups
  - (vi) Estimation of glycine (Sorensen's method)

**Physical**

**Electrochemistry conductometry :**

- (a) Determination of the velocity constant, order of reaction and energy of activation for



saponification of ethyl acetate by sodium hydroxide conductometrically.

- (b) Determination of strength of strong and weak acids in a given mixture conductometrically.
- (c) Determination of solubility and solubility product of sparingly soluble salts (eg  $\text{PbSO}_4$ ,  $\text{BaSO}_4$ ) conductometrically.
- (d) Estimation of glucose by conductometric method

**Potentiometry/ PH metry**

- (a) Determination of strength of halides in a mixture potentiometrically.
- (b) Determination of strength of strong and weak acids in a given mixture using potentiometer/pH meter.
- (c) Acid-Base titration in non-aqueous media using pH meter.
- (d) Determination of temperature dependence of EMF of a cell.



**SEMESTER - III**  
**CHEMISTRY PRACTICAL**  
**CHE - PR - III**

**Any four experiments selecting at least one from each section**

**Section - I**

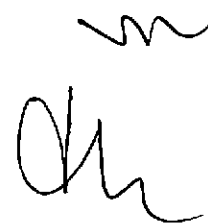
- (i) Ion exchange method of separation :  
Separation of  $Zn^{++}$  and  $Mg^{++}$  on an ion exchanger.  
Separation of  $Co^{++}$  &  $Ni^{++}$  on an ion exchanger.
- (ii) Spectrophotometric determinations:  
Iron-phenanthroline complex : Job's Method  
Manganese / chromium / vanadium in steel / water sample.
- (iii) Thin layer chromatographic separation of cations like  $Ni^{++}$ ,  $Mn^{++}$ ,  $Co^{++}$  &  $Zn^{++}$  etc. and determination of their  $R_f$  values.

**Section - II**

- (i) Separation & identification of organic compounds using chemical methods from organic mixtures containing upto three components.
- (ii) Paper chromatography : Separation and identification of the sugars present in the given mixture of glucose, fructose and sucrose by paper chromatography & determination of  $R_f$  values.

**Section - III**

- (i) Verification of Lambert-Beer's law and to determine concentration of unknown sample.
- (ii) Flame emission photometric determination of ions e.g. sodium potassium etc.
- (iii) Polari metric determination of rate constant for hydrolysis/inversion of sugar.
- (iv) Polarimetric study of Enzyme kinetics-inversion of sucrose.



**SEMESTER - IV**  
**CHEMISTRY PRACTICAL**  
**CHE - PR - IV**

**Any three experiments from the following.**

1. Identification of organic compounds/biologically important compounds from the recorded data of NMR, UV & IR spectroscopy and mass spectrometry.
2. Polarography :  
Estimation of  $Pb^{++}$  &  $Cd^{++}$ ,  $Zn^{++}$  &  $Ni^{++}$  ions in a mixture of  $Pb^{++}$  and  $Cd^{++}$ ,  $Zn^{++}$  &  $Ni^{++}$  by polarography.
3. Determination of stoichiometry and stability constant of inorganic (e.g. ferric - salicylic acid) and organic (e.g. amine iodine) complexes by colorimeter.
4. Electrophoresis experiments.
5. Water analysis : determination of pH, DO, COD & BOD of water sample.
6. Determination of molecular weight of non volatile and nonelectrolyte/electrolyte by cryoscopy method.
7. To construct the phase diagram for three component system (e.g. chloroform- acetic acid -water).
8. To synthesise ethanol from sucrose enzymatically i.e. biosynthesis of ethanol from sucrose.
9. Nephelometric determination of sulphate, phosphate, silver ions etc.
10. Synthesis of heterocyclic compounds -
  - Skroup synthesis: preparation of quinoline from aniline
  - Fischer indole synthesis - preparation of 2-phenyl indole from phenyl hydrazine.

**BOOKS SUGGESTED – (CHE-PR)**

1. Inorganic Experiments. J. Derek Wooline VCH
2. Microscale Inorganic Chemistry, Z Szafarsn R.M. Pike, M.M. Singh. Wiley.
3. Practical Inorganic Chemistry, G. Mar and B.W. Bookett. Van Nostrand.
4. The Systematic Identification of Organic Compounds R.L. Shnier and D.Y. Curtin.
5. Semimicro Qualitative Organic Analysis, N.D. Cheronis, J.B. Entnkin and E.M. Hodentt.
6. Experimental Organic Chemistry, M.P. Doyte and W.S. Mungall.

