# MANGALORE UNIVERSITY

## M. Sc. Degree Programme in Applied Chemistry:

### CHOICE BASED CREDIT SYSTEM (CBCS) SEMESTER SCHEME

### C O U R S E  P A T T E R N  AND  S C H E M E  OF  E X A M I N A T I O N

(Year 2014-15 onwards)

| Semester | Paper | Instruction hrs/week | Duration of Exam(hrs) | Marks | | | Credits |
|---|---|---|---|---|---|---|---|
| | | | | IA | Exam | Total | |
| I/II | 4Theory Papers | 4x4 | 4x3 | 4x30 | 4x70 | 4x100 | 4x4 |
| | 3 Practicals and 1 theory paper of 2 hours duration/ week | 3x4<br>1x2 | 3x4<br>1x2 | 3x15<br>1x15 | 3x35<br>1x35 | 3x50<br>1x50 | 3x2<br>1x2 |
| | Semester Total 18T+12P | | | 180 | 420 | 600 | 24 |
| | | | | | | | |
| III/IV | 4Theory Papers | 4x4 | 4x3 | 4x30 | 4x70 | 4x100 | 4x4 |
| | 3 Practicals | 3x6 | 3x5 | 3x25 | 3x50 | 3x75 | 3x3 |
| | Seminar | 1 | - | 25 | - | 25 | 1 |
| Semester Total 16T+18P | | | | 220 | 430 | 650 | 26 |
| Grand Total | | | | | | | 100 |
| In the III Semester, there will be a choice based course in lieu of one of the theory papers and in the IV Semester, there may be a project work/dissertation in lieu of 1 or 2 Practicals. | | | | | | | |

## M. Sc. DEGREE PROGRAMMES IN APPLIED CHEMISTRY,

The First, Second and Third Semesters of the course involve theory and practicals, while the IV Semester involves theory, practicals and project work. The project work shall be carried out for 6 to 8 weeks (at least 30 hrs per week), after the Second Semester of the course, either in the concerned Department or in an Approved Industry or in both, under the supervision of a teacher and submit a project report. Experts from the industries may also be involved in the project work as co-guides and in the evaluation of project reports.

**BASIS FOR INTERNAL ASSESSMENT:**

Internal assessment marks in theory papers shall be based on tests. The tests may be conducted 8 and 12 weeks after the start of a semester. Practical internal assessment marks shall be based on test and records. The practicals test may be conducted 10 weeks after the

start of a semester. The Seminar shall be of at least 45 minutes duration. The project report shall be evaluated for 75 marks. The Seminar in IVSemester shall be related to the project.

**THEORY QUESTION PAPERS PATTERN**

The Syllabus of each paper shall be grouped into units of 14 teaching hours. All the papers, except, Environmental Chemistry (1st semester) and Diffraction & Electroanalytical Techniques (2nd Semester) shall contain four such units each. Question Papers in all the four semesters shall consist of Parts A and B. Part A shall contain twelve (12) very short answer objective type questions carrying 2 marks each drawn from all the four units of the syllabus (3 questions per unit). Ten (10) questions out of Tweleve (12) are to be answered. Part B shall contain eight (8) brief and/or long answer questions carrying 10 marks each drawn from all the four units of the syllabus (2 questions per unit). There may be a maximum of three sub-divisions per question, carrying 3 or more marks per sub-division. Five (5) out of eight (8) questions are to be answered.

The Syllabi of the papers, in AC 405/OC 405/CA 405 - Environmental Chemistry (1st semester) and in in AC 455/OC 455/CA 455 - Diffraction & Electroanalytical Techniques (2nd Semester) shall also be grouped into units of 14 teaching hours. They shall contain two such units each. Question Papers in AC 405/OC 405/CA 405 and AC 455/OC 455/CA 455 shall also consist of Parts A and B. Part A shall contain six (6) very short answer objective type questions carrying 2 marks each drawn from both the units of the syllabus (3 questions per unit). Four (4) questions are to be answered. Part B shall contain five (5) brief and/or long answer questions carrying 9 marks each drawn from both the units of the syllabus (2 questions per unit and a combined question from both the units). There may be a maximum of three sub-divisions per question, carrying 3 or more marks per sub-division. Three (3) out of five (5) questions are to be answered.

**PRACTICALS EXAMINATION PATTERN**

In the I& II semesters, the 35 marks shall be awarded based on the experiment. But in the III & IV semesters, out of 50 marks, 10 marks are for the viva to be conducted during the practical examinations and 40 marks for the experiment.

## Applied Chemistry Course

| Description of Papers | Teaching Hrs/week | Hrs.of Exam | Max Marks: Exam+IA | Credits for the Course |
|---|---|---|---|---|
| **I Semester: i)Theory** | | | | |
| AC 401 : Inorganic Chemistry | 4 | 3 | 70+30 | 4 |
| AC 402 : Organic Chemistry | 4 | 3 | 70+30 | 4 |
| AC 403 : Physical Chemistry | 4 | 3 | 70+30 | 4 |
| AC 404 : Molecular Spectroscopy | 4 | 3 | 70+30 | 4 |
| AC 405**:** Environmental Chemistry | 2 | 2 | 35+15 | 2 |
| **ii) Practicals** | | | | |
| AC 406 : Inorganic Chemistry Practicals-I | 4 | 4 | 35+15 | 2 |
| AC 407 : Organic Chemistry Practicals-I | 4 | 4 | 35+15 | 2 |
| AC 408 : Physical Chemistry Practicals-I | 4 | 4 | 35+15 | 2 |
| **II Semester: i) Theory** | | | | |
| AC 451 : Advanced Inorganic Chemistry | | | | |
| AC 452 : Advanced Organic Chemistry | 4 | 3 | 70+30 | 4 |
| AC 453 : Advanced Physical Chemistry | 4 | 3 | 70+30 | 4 |
| AC 454 : Molecular Symmetry & Spectroscopy | 4 | 3 | 70+30 | 4 |
| AC 455: CH 455: Diffraction and Electroanalytical Techniques | 4 | 3 | 70+30 | 4 |
| **ii) Practicals** | 2 | 2 | 35+15 | 2 |
| AC 456 : Inorganic Chemistry Practicals-II | | | | |
| AC 457 : Organic Chemistry Practicals-II | 4 | 4 | 35+15 | 2 |
| AC 458 : Physical Chemistry Practicals-II | 4 | 4 | 35+15 | 2 |
| **III Semester, i) Theory** | 4 | 4 | 35+15 | 2 |
| AC 501 : Choice Based Paper | | | | |
| AC 502 : Organometallic Chemistry | 4 | 3 | 70+30 | 4 |
| AC 503 : Dyes, Drugs and Heterocyclic Chemistry | 4 | 3 | 70+30 | 4 |
| AC 504 : Industrial Catalysis and Soft Materials | 4 | 3 | 70+30 | 4 |
| . Chemistry | 4 | 3 | 70+30 | 4 |
| **ii) Practicals** | | | | |
| AC 505: Analytical Chemistry Practicals | | | | |
| AC 506: Multistep Organic Synthesis | | | | |
| AC 507: Kinetic Methods & Allied Practicals | 6 | 5 | 50+25 | 3 |
| AC 508 : Seminars | 6 | 5 | 50+25 | 3 |
| **IV Semester, i)Theory** | 6 | 5 | 50+25 | 3 |
| AC 551 : Analytical Chemistry | 2 | | 25 | 1 |
| AC 552 : Synthetic and Natural Products Chemistry | | | | |
| AC 553 : Applied Electrochemistry and Reaction Kinetics | | 3 | 70+30 | |
| AC 554 : Polymer Chemistry | 4 | 3 | 70+30 | 4 |
| **ii) Practicals** | 4 | 3 | 70+30 | 4 |
| AC 555 : Environmental Chemistry Practicals | 4 | 3 | 70+30 | 4 |
| AC556: Electrochmistry, Polymers and Computer related Practicals | 4 | 5 | 50+25 | 4<br>3 |
| **iii) Project Work (6 to 8 weeks )** | 6 | 5 | 50+25 | 3 |
| AC 557 : Project Report | 6 | | | |
| AC 558 : Seminars | | | 75 | 3 |
| | 30 | | 25 | 1 |
| | 2 | | | |

# FIRST SEMESTER M. Sc. Course in Applied Chemistry

## AC 401: INORGANIC CHEMISTRY

**UNIT- I:** **[14 Hours]**

Ionic bond: Properties of ionic substances, coordination number of an ion, structures of crystal lattices- NaCl, CsCl, ZnS and rutile. Lattice energy- Born Lande equation, Born-Haber cycle, Uses of Born-Haber type of calculations. Ionic radii, methods of determining ionic radii, factors affecting ionic radii, radius ratio rule, covalent character in ionic bonds, hydration energy and solubility of ionic solids.

Covalent bond: valence bond theory, resonance, hybridisation, Bent's rules and enregetics of hybridization, Deduction of molecular shapes – VSEPR theory.

M.O.theory, application to homo- and hetero-diatomic and -triatomic molecules.

**UNIT -II:** **[14 Hours]**

Alkali and alkaline earth metal complexes of crown ethers, cryptands and calixarenes and their biological significance.

Halogens and Noble gas chemistry –interhalogens, psuedohalogens, polyhalide ions, oxyhalogen species, xenon oxides and fluorides. Oxy- and peroxy acids of N, P and S.

Graphitic compounds, carbides, pure silicon, silica and silicates, zeolites.

**UNIT- III:** **[14 Hours]**

Theories of acids and bases – Lux-Flood theory, Bronsted and Lewis acids and bases, gas phase vs. solution acidity, solvent leveling effects, hardness and softness, HSAB concept. super acids. Reactions in non-aqueous media: Liquid ammonia, anhydrous sulphuric acid, glacial acetic acid, anhydrous HF, bromine trifluoride, liquid sulphur dioxide and dinitrogen tetroxide. Reactions in molten salts.

**UNIT- IV:** **[14 Hours]**

Sampling techniques, preparation of samples for analysis. Nature of errors, statistical treatment of errors, the t- and F-tests, significant figures, rejection of data.

Precipitation phenomena: precipitation from homogeneous solutions, organic precipitants in inorganic analysis. Solvent extraction of metal ions, nature of extractant, distribution law, partition coefficients, types of extractions and applications.

Theories of redox indicators, titration curves, feasibility of redox titrations.

Chelometric titrations- titration curves with EDTA, feasibility of EDTA titrations, indicators for chelometric titrations, selective masking and demasking techniques, industrial applications of masking.

**References:**


1. J.E Huheey, Keiter, Keiter and Medhi: Inorganic Chemistry ( 4th ed.), Pearson Education, 2006.
2.Shriver, Atkins and Langford : Inorganic Chemistry ( 3rd edn.) OUP, 1999.
3.J.D.Lee: Concise Inorganic Chemistry, ( 5th edn.) Blackwell Science, 2000.
4.B.E.Douglas, D.McDaniel & A Alexander: Concepts & Models of Inorganic Chemistry, Wiley 2001
5.W.W.Porterfield: Inorganic chemistry – A Unified Approach, Elsevier, 2005.


## AC 402: ORGANIC CHEMISTRY

**UNIT –I: [14 Hours]**

**Nature of Bonding in Organic Molecules:** Hybridization and Index of Hybridization, Localized and delocalized bonding: Conjugation crossconjugation, resonance, hyper-conjugation and tautomerism. Huckel rule, Homo-aromatic, non-aromatic and anti-aromatic systems. Aromaticity in benzenoid and non-benzenoid molecules. Annulenes and hetero-annulenes. Physical methods to study aromaticity-UV, IR & $^{1}$H NMR. 7 hrs

**Bonds weaker than covalent:** Addition compounds, crown ether complexes, cryptands, inclusion compounds, catenanes, fluxional molecules. 2 hrs

**Acids and Bases:** Introduction to acids and bases, Bronsted-Lowry and Lewis acid- bases concept, organic acids and bases, pKa and pH, effect of solvent on acid and base strength, effect of structure of organic compound on acid & base strength. Running scale of acidity, General & specific acid-base catalysis. 5 hrs

**UNIT-II: [14 Hours]**

**Methods of Determining Reaction Mechanism:** Kinetic and non-kinetic methods, Identification of products, detection of intermediates, isotopic labeling, stereochemical evidences, cross-over experiments, Limitation of reactions, kinetic evidences and kinetic isotopic effects. 4 hrs

**Reaction Intermediates:** Generation, structure, stability, reactivity and detection of classical and non-classical carbocations, carbanions, free radicals, carbenes, nitrenes and arynes. Singlet oxygen-generation and reactions with organic molecules. 4 hrs

**Aliphatic Nucleophilic Substitution Reactions:** Mechanism and scope of aliphatic nucleophilic substitution reactions-$S_N1$, $S_N2$ and $S_Ni$. Stereochemistry of nucleophilic substitution reactions, allylic nucleophilic substitution reactions, Walden inversion, neighbouring group participation and anchimeric assistance. Factors influencing the rates of nucleophilic substitution reactions. 6 hrs

**UNIT-III: Stereochemistry [14 Hours]**

**Optical Isomerism:** Conformation and configuration of molecules, projection formulae, Fischer, Saw-horse, Newman and Flying wedge representations.Interconversion of these formulae. Absolute configuration (D,L) and (R,S) systems. Elements of symmetry,Psedoassymmetric centres, chirality, molecules with more than one chiral centre, threo and erythro isomers, methods of resolution, stereospecific and stereoselective synthesis, asymmetric synthesis, Cram's and Prelog's rules. Optical activity in the absence of chiral carbon-biphenyls, allenes and spiranes. Conformational analysis of cycloalkanes and decalins. Effect of conformation on reactivity. Acyclic & cyclic systems-Substituted cyclohexanes, cyclohexanones, cyclohexanols, Curtain-Hammet Principle. Stereochemistry of compounds containing nitrogen, sulphur and phosphorus.
11 hrs

**Geometrical Isomerism:** Cis-trans isomerism resulting from double bonds, monocyclic compounds & fused ring systems. E,Z-notations, determination of configuration of geometrical isomers, syn & anti isomers. 3 hrs

**UNIT-IV: Carbohydrates & Heterocycles [14 Hours]**

**Carbohydrates:** Introduction, Configuration and conformation of monosaccharides, Chemistry of important derivatives of monosaccharides-ethers, esters, acetals, ketals, deoxysugars, aminosugars, Structure of disaccharides-maltose, cellobiose and sucrose. General methods of structural degradation of polysaccharides-methylation, partial hydrolysis, periodate oxidation, Smith degradation and alkaline degradation techniques. Structures of cellulose, chitin, starch and glycogen.
8 hrs

**Heterocycles:** Introduction, Biologically important heterocycles, Synthesis and reactions of five membered simple and fused heterocycles-furan, pyrrole, thiophene, pyridine, benzofuran, benzothiophene & indole.
6 hrs

**References:**


1.Organic Chemistry-P.Y.Bruice (Pearson Education Pvt. Ltd.,New Delhi),2002.
2.Stereochemistry,Conformation and Mechanism-P.S.Kalsi (Wiley Eastern,New Delhi)1993.
3.Stereochemistry of Carbon Compounds-E.L.Eliel (Tata McGraw Hill, New. Delhi) 1994.
4.Advanced Organic Chemistry-Reactions, mechanisms & structure-J.March(Wiley, NY)2000.
5.Organic Chemistry-Vol. -1,2 &3-Mukherji, Singh and Kapoor. (Wiley Eastern,) 1994.
6.A guide book of mechanisms in Organic Chemistry-P.Sykes (Orient- Longman) 1985.
7.Organic Chemistry-R.T. Morrison and R.N. Boyd (Prentice Hall, New Delhi) 1994.
8.Organic Chemistry 4th Edn.–S.H. Pine et al (McGraw-Hill, London) 1987.
9.Advanced Organic Chemistry- R.A. Carey and R.J. Sundberg (Plenum, New York)1990.
10.Modern Concepts of Advanced Organic Chemistry-R.P. Narein (Vikas, Delhi) 1997.
11.A Text book of Organic Chemistry-Tewari, Vishnoi and Mehrotra (Vikas, New Delhi)1998.
12.A Text book of Organic Chemistry-3rd Edn.-R.K. Bansal, (New Age, New Delhi) 1997.
13.Organic Chemistry-3rd Edn- F.A. Carey (Tata McGraw Hill, New Delhi) 1996.
14.Stereochemistry by K.Mislow.

## AC 403: PHYSICAL CHEMISTRY

**UNIT – I : [14 hours]**

**Catalysis:** Homogeneous catalysis-equilibrium and steady state treatments, activation energies of catalysed reactions. Acid-base catalysis (general and specific), protolytic and prototropic mechanisms, catalytic activity and acid strength measurements. Kinetics of enzyme catalysed reactions-Michaelis-Menten equation. Effect of pH, temperature & inhibitors 7 hrs.

**Surface reaction kinetics:** A review of adsorption isotherms, uni- and bi-molecular reactions. multilayer adsorption-BET equation- application in surface area determination. Harkin–Jura equation-application. Desorption & heterogeneous catalysis–catalytic activity at surfaces, semiconductor catalysis, n-&p-type. Mechanism of surface reactions. . 7 hrs.

**UNIT - II: [14hours]**

**Chemical Kinetics:** Complex reactions- parallel, consecutive and reversible reactions. Chain reactions ($H_2$-halogen reactions). Branched chain reactions- general rate expression, explosion limits and Oscillatory reactions. 4 hrs.

**Reactions in solution**: Ionic reactions - salt and solvent effects. Substituent effects on the rates of reactions - Hammett and Taft equations, linear free energy relationships. 4 hrs.

**Fast reactions**-Introduction, Study of fast reactions by-flow, relaxation, molecular beam and photolysis and line broadening methods. 4 hrs

**Theories of Reaction Rates**: Collision theory of reaction rates, limitations and an introduction to transition state theory. 2hrs

**UNIT-III : [ 14hours]**

**Electrochemistry of solutions:** Ionic atmosphere-introduction, derivation and its effect on the theory of conductivity. Walden`s rule. Debye-Huckel limiting law (DHL)- Concept of Ionic strength and activity coefficient, derivation of DHL equation, modifications to DHL equation- qualitative tests and verification of DHL equation. Bjerrum theory of ion association, triple ion formation and significance, abnormal conductance 5hrs.

**Corrosion**: Introduction, principles, loss due to corrosion, Forms of corrosion (Galvanic, Atmospheric, stress, microbial, and soil). Corrosion rate measurement, EMF series &Galvanic series and their limitations. Thermodynamics (Pourbaix diagram) and Kinetics (mixed potential theory) of corrosion. Kinetics of passivity. Protection against corrosion (Design improvement, Anodic and cathodic protection, inhibitors, coating).Corrosion failure and its treatment. 9hrs.

**UNIT-IV** : **[ 14 hours]**

**Photochemistry**: Introduction to photochemistry. Actinometry. Frank-Condon principle. Absorption and emission spectra- effect of solute solvent interactions on electronic spectra-spectral shifts. Physicochemical properties of electronically excited molecules-excited state dipole moments, acidity constants. Flash photolysis technique.

Photophysical pathways- Jablonski diagram, Radiationless transitions and selection rules. Photochemical kinetics of unimolecular and bimolecular processes. Quenching-collisions in

the gas phase, solution (Stern-Volmer equation). Photoisomerization, photo Fries rearrangement and Norrish type cleavage reactions with specific examples.

**REFERENCES :**


1. Physical Chemistry, 5th Ed., - Atkins (ELBS) 1995.
2. Physical chemistry – G. M. Barrow (McGraw Hill, Int. St. Ed) 1988.
3.Fundamentals of Physical Chemistry – Maron and Lando (Collier, Macmillan) 1974.
4. Chemical Kinetics - K. J. Laidler (Harper and Row) 1987.
5. Kinetics of Chemical Reactions, S K Jain (Vishal Publications, Delhi) 1982.
7. Principles and Applications of Electrochemistry–Crow (Chapman hall, New York) 2014.
8. Electrochemistry and Corrosion Science-Nebtor Ferez (Springer Pvt.Ltd.), Delhi, 2010.
9. Fundamentals of Photochemistry – Rohatgi and Mukherje (New Age Bangalore), 2000.

# AC 404: MOLECULAR SPECTROSCOPY

**UNIT–I:** **[14 hours]**

**Unifying Principles** -Electromagnetic radiation, dual nature, regions of the spectrum, interaction of electromagnetic radiation with matter - absorption, emission, transmission, reflection, refraction, dispersion, polarization and scattering. Natural line width and broadening, intensity of spectral lines. Rotational, vibrational and electronic energy levels, selection rules.

**Microwave Spectroscopy**- The rotation and classification of molecules, rotation spectra of diatomic and polyatomic molecules. Rigid and non-rigid rotator models. Determination of bond lengths, isotope effect on rotation spectra. Stark effect, nuclear and electron spin interaction. Microwave Spectrometer.

**Vibrational Spectroscopy:** Vibration spectra of diatomic molecules - linear harmonic oscillator, vibrational energies, zero point energy, force constants & bond strengths; anharmonicity of molecular vibrations- Morse PE diagram, selection rules, fundamental, overtones and hot bands. Vibrations of polyatomic molecules- normal modes of vibrations & nature of molecular vibrations (Ex-$CO_2$& $H_2O$).

**UNIT–II :[14 hours]**

**Vibration-rotation spectra** of diatomic and polyatomic molecules, selection rules, PQR branches. IR Spectrophotometer-Instrumentation, sample handling techniques, FTIR Spectroscopy. Far IR region.

**Raman Spectroscopy**: Classical and quantum theories of Raman effect, concept of polarizability and polarizability ellipsoid. Rotational and vibrational Raman spectra, selection rules, Raman activity of vibrations, vibrational - rotational Raman spectra, selection rules, mutual exclusion principle, polarization of Raman lines. An introduction to Laser Raman Spectroscopy. Raman Spectrometer – instrumentation. Applications of IR and Raman spectroscopy in elucidation of molecular structure (Ex - $H_2O$, $N_2O$ & $CO_2$ molecules).

**UNIT–III: [14 hours]**

**Application of infrared spectroscopy** in the structural study-identity by finger printing and identification of functional groups. Characteristic vibrational frequencies of common functional groups (alkanes, alkenes, alkynes, aromatic compounds, alcohols, ethers, phenols and amines). Study of vibrational frequencies of carbonyl compounds (ketones, aldehydes, esters, amides and acids). Factors affecting band positions and intensities such as effect of hydrogen bonding, phase and solvent on vibrational frequencies, overtones, combination bands and Fermi resonance.

**Polarimetry:**Plane polarized light, instrumentation, acid-catalyzed muta rotation of glucose, inversing of cane sugar-relative strengths of acids. Optical rotatory dispersion &circular dichroism–introduction, selection rules, deduction of absolute configuration, octant rule for ketones and cotton effect.

**UNIT-IV: Nuclear Magnetic Resonance Spectroscopy** **[14 hours]**

Magnetic properties of nuclei, theory and measurement techniques, NMR spectrometer, FT NMR and its advantages. Solvents used, chemical shift and its measurements, factors affecting chemical shift. Integration of NMR signals, spin-spin coupling, coupling constant. Shielding and deshielding. Chemical shift assignment of major functional groups, Classification (ABX, AMX, ABC, $A_2B_2$), spin decoupling; effects of chemical exchange, fluxional molecules, Hindered rotation through NMR spectrum, Karplus relationships (Karplus curve–variation of coupling constant with dihedral angle), double resonance

techniques, NMR shift reagents, solvent effects and Nulear Overhauser Effect. High resolution $^{1}H$ NMR. Applications of NMR spectroscopy in structure elucidation of simple organic and inorganic molecules. $^{1}H$ NMR in the structural study of complex organic compounds. Pulse techniques in NMR, two dimensional and solid state NMR.Use of NMR in Medical diagnostics.

**REFERENCES:**

1.Fundamentals of Molecular Spectroscopy, Banwell & McCash (Tata McGraw Hill, New Delhi) 2007.
2. Spectroscopy, H. Kaur (Pragathi Prakashana,Meerut), 2012.
3.Spectroscopy, Donald L.Pavia (Cengage learning India Pvt.Ltd., Delhi), 2007.
4.Spectroscopy, B.K.Sharma (Goel prakashan, Meerut), 2013.
5. Organic Spectroscopy-3rd ed.-W.Kemp (Pagrave Publishers, New York), 1991.
6.Spectrometric Identification of Organic Compounds-Silverstein,Bassler&Monnill(Wiley)1981.

## AC 405: ENVIRONMENTAL CHEMISTRY

**UNIT-I:** **[14 hours]**

Environmental segments, evolution of earth's atmosphere. Air pollution : Air pollutants, prevention and control, Green house gases and acid rain. Carbon monoxide, industrial sources and tranportation sources. $SO_x$- sources, ambient concentration, test methods, control techniques - scrubbing, , limestone injection process. Ozone hole and CFC's. Photochemical smog and PAN. $NO_x$ - Sources, ambient concentration, test methods, $NO_x$, control techniques. Particulates : Size distribution, , particulate collection - settling chambers, centrifugal separators, wet scrubbers, electrostatic precipitators & fabric filters. Catalytic converters for mobile sources. Bhopal gas tragedy.

**UNIT-II:** **[14 hours]**

Hydrologic cycle, sources, chemistry of sea water, criteria and standards of water quality-safe drinking water, maximum contamination levels of inorganic and organic chemicals, radiological contaminants, turbidity, microbial contaminants. Public health significance and measurement of colour, turbidity, total solids, acidity, alkalinity, hardness, chloride, residual chlorine, sulphate, fluoride, phosphate and different forms of nitrogen in natural and polluted water. Chemical sources of taste and odour, treatment for their removal, sampling and monitoring techniques. Determination and significance of DO, BOD ,COD and TOC. Water purification for drinking and industrial purposes, disinfection techniques, demineralization, desalination processes and reverse osmosis.

**REFERENCES :**


1. A.K. De : Environmental Chemistry, (Wiley Eastern).
2. S.K.Banerji : Environmental Chemistry, ( Prentice Hall India), 1993.
3 S.D. Faust and O.M. Aly : Chemistry of Water Treatment, (Butterworths),1983.
4. G.D. Christian : Analytical Chemistry, (4th Ed.), (John Wiley)
5. Sawyer and McCarty, Chemistry for Environmental Engineering(McGraw Hill) 1978
6. I.Williams, Environmental Chemistry, John Wiley, 2001

## AC 406: INORGANIC CHEMISTRY PRACTICALS - I

1. Analysis of Hematite-insoluble residue by gravimetry and Iron by volumetry using $Ce^{4+.}$
2. Analysis of Dolomite - insoluble residue be gravimetry and Ca, Mg by complexometry.
3. Pyrolusite - Insoluble residue by gravimetry and Manganese content by oxalate method.
4. Analysis of solder - Pb and Sn by EDTA method.
5. Complexometric determination of Mn, Cu, Ni and Fe-Cr mixture
6. Hardness of water
7. Analysis of Halide Mixture - Iodide by $KIO_3$ and total halide by gravimetrically.
8. Colorimetric Determination of Iron by thiocyanate and Cu by aqueous ammonia.
9. Gravimetric Determinations of Mn, Ni, Mo, Pb/Cr, sulphide, thiocyanate.
10. Statistical Analysis of Data.

**Reference :**

1. Vogel's Text Book of Quantitative Chemical Analysis($5^{th}$ Ed), G.H.Jeffrey, J.Bassette, J.Mendham and R.C.Denny, Longman, 1999.

## *CH 407/AC 407/OC 407/CA 407 : ORGANIC CHEMISTRY PRACTICALS - I*

**Single and two stage organic preparations**

1. Electrophilic substitution reactions–Preparations of p-bromoaniline, p-nitroaniline, and picric acid
2. Alkylations–Preparations of nerolin and N-methyl anthranilic acid.
3. Acetylations–Preparations of β-D-glucose penta-acetate and 2-naphthyl acetate.
4. Reactions with ring formation–Preparations of 1,2,3,4–tetrahydrocarbazole and 7–hydroxy-4-methyl-coumarin.
5. Diazotisation reactions–Preparations of iodo, chloro and azo compounds.
6. Dehydration reactions–Preparations of cyclohexene and succinic anhydride
7. Condensation reactions–Condensations involving diethylmalonate and ethyl acetoacetate. Aldol condensation and Perkin reactions.
8. Halogenation reactions-Preparation of n-butylbromide &α,β-dibromocinnamic acid.
9. Reduction reactions–Reductions of nitro compounds and carbonyl compounds.
10. Oxidation reactions-Preparation of p-nitrobenzoic acid, p-benzoquinone and adipic acid.

**References :**

1. Laboratory Manual in Organic Chemistry–R. K. Bansal (New Age, New Delhi)1990.
2. Experimental Organic Chemistry–Vol. I & II–P. R. Singh et al (TMH New Delhi)1981
3. Laboratory Manual in Organic Chemistry–Dey &Sitaraman(Allied , New Delhi)1992.
4. Vogel's Text Book of Practical Organic Chemistry including Qualitative Organic Analysis-B. S. Furniss et al., (Longman - ELBS, London), 1989.

**AC 408 : PHYSICAL CHEMISTRY PRACTICALS** - I

Any 12 experiments are to be carried out

1. Potentiometric titration of halides in mixtures ( $Cl^-$, $Br^-$ and $I^-$) with silver nitrate
2. Potentiometric determination of redox potentials ($Fe^+$ Vs. $I^-$ $Mn^{+7}$, $Ce^{+4}$).
3. Potentiometric and conductometric acid –base titrations in partial, aqueous & non-aqueous media.
4. Conductometric titrations of displacement and precipitation reactions.
5. Determination of equivalent conductances and dissociation constants of weak acids.
6. Determination of solubility of lead iodide at different T & hence molar heat of solution
7. Determination of pH of buffer solutions with a pH meter & evaluation of $pK_a$ of acids
8. Verification of Walden`s rule (relation between viscosity of a solution and the electrical conductivity.
9. Study of variation of viscosity of a liquid with temperature
10. a)Determination of parachor value for $CH_2$ group by S.T method,
    b) Determination of the composition of a solution by S.T measurement and
    c) Determination of CMC of a soap solution by S.T measurement
11. Potentiometric determination of solubility of insoluble silver halide and the standard electrode potential using quinhydrone electrode
12. Determination of degree of hydrolysis of $CH_3COONa$ and $NH_4Cl$.
13. Determination of hydrolysis constant of aniline hydrochloride.
14. Verification of Nernst equation for $Ag^+$, $Cu^{2+}$and $Zn^{2+}$ species.

**References:**


1. Findlay's Practical Physical Chemistry- B. P. Levitt ( Longman, London).
2. Experiments in Physical Chemistry– James and Prichard.
3. Experimental Physical Chemistry - Daniels et al.
4. Experimental Physical Chemistry-Das & Behera (Tata McGraw Hill, New Delhi)1983.
5. Advanced Practical Physical Chemistry–Yadav (1989).
6. Experiments in Physical Chemistry–J. C. Ghosh ( Bharathi Bhavan)1974.

# SECOND SEMESTER M. Sc. Course in Applied Chemistry

## AC 451: ADVANCED INORGANIC CHEMISTRY

**Unit -I: [14 Hours]**

Chemistry of higher boranes, classification, structures and M.O. description of bonding, framework electron counting, Wade's rules, chemistry of $B_5H_9$, $B_{10}H_{14}$ and $B_nH_n^{2-}$. Carboranes and metallocarboranes. Cyclophosphazenes, phosphazene polymers, P-O and P-S cage compounds. S-N compunds : binary sulphur nitrides- $S_4N_4$, $S_2N_2$ and $(SN)_x$. Borazines and boron nitride, Isopoly and heteropoly acids of transition metals.

**Unit -II: [14 Hours]**

Coordination numbers 2-10 and their geometry, crystal field theory of coordination compounds, d-orbital splittings in octahedral, square planar and tetrahedral fields, spectrochemical series, and Jahn-Teller effect.

Structural evidences for ligand field splittings – hydration, ligation and lattice energies, site preference energies. MO theory of coordination compounds- MO energy level diagrams for octahedral and tetrahedral complexes.

Stepwise and overall formation constants, factors affecting stability of metal complexes, determination of binary formation constants by pH-metry and spectrophotometry.

**Unit-III: [14 Hours]**

Metal Pi-acceptor complexes: metal carbonyls – preparative methods, structure and bonding, vibrational spectra of metal carbonyls for bonding and structural elucidation, magnetic and X-ray evidences of structures, M.O.representation of bi- and tri-nuclear carbonyls,. Reactions of metal carbonyls. Metal carbonylates and carbonyl halides – preparation and important reactions. Chemistry of metal nitrosyls – preparation, structure and bonding; dinitrogen and dioxygen complexes. Metal-metal bonding in carbonyls and halides evidences for M-M bonding, factors favouring M-M bond formation. Metal clusters- bi-, tri-, tetra-, penta- and hexanuclear metal clusters, bonding in metal clusters. Zintl ions and Chevrel phases.

**Unit -IV: [14 Hours]**

Methods of reduction of oxide ores, Ellingham diagram, chemical and electrolytic reductions, reduction potentials, Latimer and Frost diagrams, effect of complexation on potential.

Trends in oxidations states, stereochemistry and ionic sizes of metals, comparison of 3d, 4d and 5d series by taking Ti subgroup as example. Lanthanides and actinides: electronic structure, oxidation states, extraction and separation of lanthanides, stereochemistry, spectral and magnetic properties of lanthanide and actinide complexes, lanthanide complexes as NMR shift reagents. Comparison with d-block ions.

**References:**


1. J.E Huheey, E.A..Keiter, R.L.Keiter& O K Medhi: Inorganic Chemistry ( 4th edn.), Pearson, 2006.
2. Shriver, Atkins and Langford : Inorganic Chemistry ( 3rd edn.) OUP, 1999.
3. J.D.Lee: Concise Inorganic Chemistry, ( 5th edn.) Blackwell Science, 2000.
4. B.E.Douglas, D.McDaniel &A Alexander: Concepts & Models of Inorganic Chemistry, Wiley 2001
5. W.W.Porterfield: Inorganic chemistry – A Unified Approach, Elsevier, 2005.


## AC 452: ADVANCED ORGANIC CHEMISTRY

**UNIT - I:** **[14 Hours]**

**Aliphatic Electrophilic Substitution Reactions:** Bimolecular mechanisms-$S_E1$, $S_E2$ and $S_Ei$ mechanism. Electrophilic substitution reactions accompanied by double bond shifts. 3 hrs

**Aromatic Electrophilic and Nucleophilic Substitution Reactions:** Mechanism of aromatic electrophilic substitution reactions, Arenium ion mechanism, orientation and reactivity, energy profile diagram. The ortho/para ratio, ipso attack, orientation in other ring systems. Mechanism of Vilsmeir-Haack reaction, Pechmann reaction and Fries rearrangement. Mechanisms of aromatic nucleophilic substitution reactions- $S_NAr$, $S_N1$ & aryne mechanism. Von-Richter rearrangement, Sommelet-Houser rearrangement, Smiles rearrangement.

11 hrs

**UNIT- II:** **[14 Hours]**

**Free Radical Reactions:** Types, mechanisms of free radical substitution reactions & neighbouring group assistance. Reactivity for the aliphatic and aromatic substances at a bridgehead. Reactivity of attacking radical. Effect of solvent on reactivity. Auto-oxidation, coupling of alkynes. Arylation of aromatic compounds by diazonium salts. Sandmeyer, Ullmann & Hunsidiecker reactions.

5 hrs

**Elimination Reactions:** Discussions of E1, E2 and E1cB mechanisms. Orientation during elimination reactions. Saytzeff and Hofmann rules. Reactivity-effects of substrate structures, attacking base, leaving group and solvent medium. 5 hrs

**Pyrolytic Eliminations:** Mechanisms of pyrolysis of esters of carboxylic acids. Chugaev reactions, Hofmann degradation, Cope elimination and xanthate pyrolysis. 4 hrs

**UNIT- III:** **[14 Hours]**

**Formation and Hydrolysis of Esters:** Plurality of mechanism. Mechanism of esterification reactions. Ester hydrolysis-$A_{AC}2$, $B_{AC}2$, $A_{AC}1$ & $A_{AL}1$ mechanism. Transesterification.4 hrs

**Addition to Carbon-Carbon Multiple Bonds:** Addition reactions involving electrophiles, nucleophiles and free radicals. Cyclicmechanisms. Orientation and stereochemistry. Addition of halogens, hydrogen halides, carboxylic acids and amines. Addition to cyclopropanes, hydroboration, Michael addition. Addition of oxygen across double bonds. 6 hrs

**Addition to Carbon-Hetero Multiple Bonds:** Electrophilic, nucleophilic and free radical additions to C=O and C=N systems. Addition of Grignard reagents. Reformasky reaction, aldol condensation, Knoevenagel condensation, Perkin reaction and Wittig reactions. 4 hrs

**UNIT- IV: Chemistry of Heterocyclic Compounds** **[14 Hours]**

Synthesis and reactions of three membered heterocycles-aziridines, oxiranes, episulfides, diaziridines, oxazirines and diazirines. Synthesis and reactions of four membered heterocycles-oxetanes, azetidines and thietanes. Synthesis & reactions of selenophenes, tellurophenes, oxazoles, imidazoles, thiazoles and oxazines..

**References:**

1.Organic Reactions and Their Mechanisms- P.S. Kalsi (New Age, New Delhi),1996.
2.Advanced Organic Chemistry 4th Edn- J. March (Wiley, NY) 2000.
3.Organic Reaction Mechanisms- Bansal (Tata McGraw Hill, New Delhi) 1978.
4.Organic Chemistry-Vol.–I & II-Mukherji, Singh and Kapoor(Wiley Eastern, New Delhi) 1985.

5.Mechanism and Theory in Organic Chemoistry-Lowry and Richardson Harper and Row, 1987.
6.An Introduction to the Chemistry of Heterocyclic Compounds-Acheson (Wiley–Eastern) 1987.
7. Heterocyclic Chemistry-J. Joule & G. Smith, (Van-Nostrand, ELBS), 1978.
8. Reaction Mechanisms in Organic Chemistry-Mukherji, Singh and Kapoor (McMillan) 1978.
9. Organic Chemistry-P.Y. Bruice (Pearson Education, New Delhi) 2002.

# AC 453: Advanced Physical Chemistry

**UNIT - I:** **[14 hours]**

**Chemical Thermodynamics** : Entropy, dependence of entropy on variables of a system (S,T & V; S,T and P). Thermodynamic equations of state. Irreversible processes-Clausius inequality.

Free energy, Maxwell relations and significance, temperature dependence of free energy-Gibbs Helmholtz equation, applications of Gibbs Helmholtz equation.

Partial molar quantities, chemical potential and Gibbs-Duhem equations, determination of partial molar volume and enthalpy.

Fugacity, relation between fugacity and pressure, determination of fugacity of a real gas.

Activity. variation of fugacity and activity with temperature and pressure.

Thermodynamics of mixing, Gibbs-Duhem-Margules equation, Henry's law.

Excess thermodynamic functions-free energy, enthalpy, entropy and volume, Determination of excess enthalpy and volume.

Chemical affinity and thermodynamic functions, effect of temperature and pressure on chemical equilibrium-vant Hoff reaction isochore and isotherm.

Third law of thermodynamics, Nernst heat theorem, determination of absolute entropies using third law, entropy changes in chemical reactions.

**UNIT - II: Statistical and Irreversible thermodynamics [ 14 hours]**

**Statistical Thermodynamics :** Basic terms: Probability, cell, phase space, micro and macro states, thermodynamic probability, statistical weight factor, statistical equilibrium, assembly, ensemble and its classification, Derivation of Boltzmann-Maxwell, Bose-Einstein and Fermi-Dirac statistics, partition function and derivations of translational, rotational, vibrational and electronic partition functions, thermodynamic functions such as internal energy, heat capacity,

entropy, work function, pressure, heat content, etc. Partition function and third law of thermodynamics, applications of partition function to mono atomic gases, diatomic molecules, equilibrium constant.Heat capacity of solids -the vibrational properties of solids, Einsteins theory and its limitations, Debye theory and its limitations. 9hrs.

**Irreversible Thermodynamics**-Thermodynamics of irreversible processes with simple examples. Uncompensated heat and its physical significance. Entropy production-rate of entropy production, entropy production in chemical reactions, the phenomenological relations. The principle of microscopic reversibility, Onsager reciprocal relations – validity (linear and non-linear rections) and application (Electrokinetic, Thermoelectric phenomena).

**UNIT-III: Quantum Chemistry-1** **[14 hours]**

Particle waves and Schrödinger wave equation, wave functions, properties of wave functions, Normalization and orthogonality of wave functions. Operators and their algebra, linear and hermitian operators, operators for the dynamic variables of a system such as, position, linear momentum, angular momentum, total energy, eigen functions, eigen values and eigen value equation. Quantum numbers and their characteristics.

Shrodinger wave equation- significance and derivation. Eigen values and eigen functions. Statistical interpretation of $\psi$. Solution of SWE for simple systems-particle in a box(1D & 3D), particle in a ring, harmonic oscillator, rigid rotor, the H atom (solution of $r,\theta,\Phi$ equations), tunneling the harmonic oscillator, the rigid rotator, and the hydrogen atom. Quantum numbers and their characteristics.

**UNIT-IV: Quantum Chemistry-II [14 hours]**

Approximates methods of solving SWE- Principle of Variation and Perturbation methods. Application of variation method to H and He atoms. Secular equations and determinants.

Chemical Bonding: Covalent bond-Valence bond and molecular orbital approaches with comparison. Application of VBT to $H_2$.

MO theory applied to homonuclear and heteronuclear diatomic molecules –calculation of BO.

Hybridisation-construction of wave function of hybrid orbitals (sp, $sp^2$ and $sp^3$). Calculation of bond angle between hybrid orbitals.

Huckel molecular orbital theory of conjugated systems - secular equations and determinants. Applications to linear (ethane, allyl, 1-3 butadiene) and cyclic (benzene ) systems.

Calculation of charge density, bond order, free valence and delocalisation energy.

**References:**


1. Physical Chemistry, 5th Ed., - Atkins, (ELBS) 1995
2. Physical Chemistry, 4th ed.,Ignacia Tinowa Jr, Kenneth Sauer etal., (Pearson), 2011.
3. Chemical Themodynamics, Rajaram and Kuriokose (East-West)Pearson, Chennai, 2013.
4. Thermodynamics, 3rd Ed., R.C. srivastava and Subit K Saha (Prentice-Hall of India, Delhi), 2007.
5. Statistical Thermodynamics, M. C. Gupta (Wiley eastern Ltd.) 1993.
6. Advanced Physical Chemistry- Gurdeep R Chatwal (Goel Publishes, Meerut), 1992.
7. Introductory Quantum Chemistry – A.K.Chandra (Tata McGraw Hill) 1994.
8.Quantum Chemistry, A.B.Sannigrahi (Book and Allied Pvt.Ltd., Kolkatt), 2013.
9. Quantum Chemistry, Donald A.P (Viva Books, Delhi), 2013.
10. Physical Chemistry, 4th Edn., K.J. Laidler, J.H. Meiser, B.C.Sanctuary(Houghton Mifflin), 2003

## AC 454: MOLECULAR SYMMETRY AND SPECTROSCOPY

**UNIT- I: Symmetry and Group Theory [14 Hours]**

Definitions of group, subgroup, relation between orders of a finite group and its subgroup. Conjugacy relation and classes, symmetry elements and symmetry operations, Schonflies symbols, Matrix representations of symmetry operations, products of symmetry operations, some properties of matrices and vectors, classification of molecules into point groups. Reducible and irreducible representations. The Great Orthogonality theorem (without proof), character tables. The direct product. Applications of group theory - Molecular vibrations, group theoretical selection rules for electronic transitions, for infra red and Raman spectra. Hybrid orbitals and Molecular orbitals, transformation properties of atomic orbitals.

**UNIT- II: [14 Hours]**

**Electron Spin Resonance Spectroscopy:** Basic principles, hyperfine couplings, the 'g' values, factors affecting 'g' values, isotropic and anisotropic hyperfine coupling constants, Zero Field splitting and Kramer's degeneracy. Measurement techniques and Applications to simple inorganic and organic free radicals and to inorganic complexes. 4 hrs

**NQR Spectroscopy:** Quadrupolar nuclei, electric field gradient, nuclear quadrupole coupling constants, energies of quadrupolar transitions, effect of magnetic field. Applications.3 hrs

**Mössbauer Spectroscopy:** The Mössbauer effect, chemical isomer shifts, quadrupole interactions, measurement techniques and spectrum display, application to the study of $Fe^{2+}$ and $Fe^{3+}$ compounds, $Sn^{2+}$ and $Sn^{4+}$ compounds( nature of M-L bond, coordination number and structure), detection of oxidation states and inequivalent Mössbauer atoms. 4 hrs

**Photoelectron spectroscopy**: Basic principles, valence &core binding energies, shifts in energies due to chemical forces, Photoelectron spectra of simple molecules, Auger transitions, measurement techniques. Applications. 3 hrs

**UNIT- III: [14 Hours]**

**UV/Electronic Spectroscopy**: Basic principles, Beer-Lambert law, molar absorptivity, energy levels, types of electronic transitions. Franck - Condon principles, ground and excited electronic states of diatomic molecules. Chromophores, auxochromes, electronic spectra of polyatomic molecules. Emission spectra, spectra of transition metal complexes, charge transfer spectra. Instrumentation and application. Factors affecting the positions of UV bands. Electronic transitions and empirical correlations of predicting $\lambda_{max}$ of organic compounds. Woodward–Fieser rules. UV absorption of aromatic compounds - effect of substituents and solvent effects. Emperical rules to calculate $\lambda_{max.}$ Application of UV spectroscopy in the structural study of organic molecules.

7 hrs

**NMR of nuclei other than proton:** $^{13}C$ chemical shift & factors affecting it Coupling constants. Decoupling-Noise decoupling & broad band decoupling. Off-resonanceproton decoupling-some representative examples. $^{19}F$ &$^{31}P$ NMR- Predicting the spectra of simple inorganic compounds, NMR of paramagnetic complexes. 7 hrs

**UNIT- IV:** **[14 Hours]**

**Mass Spectrometry**: Basic principles, Instrumentation -Mass spectrometer, interpretation of mass spectra, resolution, exact masses of nucleides, molecular ions, meta-stable ions and isotope ions. Fragmentation processes-representation of fragmentation, basic fragmentation types and rules. Factors influencing fragmentations and reaction pathways. McLafferty rearrangement. Fragmentations (fragmentation of organic compounds with respect to their structure determination) associated with functional groups- alkanes, alkenes, cycloalkanes, aromatic hydrocarbons, halides, alcohols, phenols, ethers, acetals, ketals, aldehydes, ketones, quinines, carboxylic acids, esters, amides, acid chlorides, nitrocompounds, amines & nitrogen heterocycles. Fragmentation patterns of carbohydrates, terpenoids, alkaloids, steroids, peptides & proteins-some representative examples, ion analysis, ion abundance, retro Diels-Alder fragmentation. Application in structure elucidiation and evaluation of heats of sublimation & ionization potential. Nitrogen rule. High resolution mass spectroscopy. 9 hrs

Composite problems involving the applications of UV, IR, $^{1}H$ and $^{13}C$ NMR and mass spectroscopic techniques. Structural elucidation of organic molecules. 5 hrs

**REFERENCES:**


1. Fundamentals of Molecular Spectroscopy, Banwell & McCash (Tata McGraw Hill)2001.
2. Organic Spectroscopy-3rd Ed.-W.Kemp(Pagrave Publishers, New York), 1991.
3. Spectrometric Identification of Organic Compounds - Silverstein, Bassler & Monnill (Wiley)1981.
4. Applications of Absorption Spectroscopy of Organic Compounds-Dyer(Prentice Hall,NY) 1965.
5. Spectroscopy of Organic Compounds-3rd Ed.-P.S.Kalsi (New Age, New Delhi) 2000.
6. E.A.V.Ebsworth, D.W.H.Ranklin and S.Cradock: Structural Methods in Inorganic Chemistry, Blackwell Scientific, 1991.
7. R.S.Drago: Physical Methods for Chemists, Saunders College Publishing, 1992.
8. D.N.Satyanarayana: ElectronicAbsorption Spectroscopy and Related Techniques,
9. G.Aruldhas, Molecular Structure and Spectroscopy, Prentice Hall, 2001
10. J. A. Iggo: NMR Spectroscopy in Inorganic Chemistry, Oxford University Press, 1999.
11. C.N.R.Rao and J.R. Ferraro: Spectroscopy in Inorganic Chemistry, Vol I&II(Academic)1970
12. Analytical Chemistry-Open Learning : Mass spectrometry.
13. Spectroscopic Methods in Organic Chemistry - Williams and Fleming, TMH.

## AC455: Diffraction and Electroanalytical Techniques

**UNIT-I: [14 hours]**

**Diffraction Techniques:** Introduction, production of X-ray, X-ray diffraction-Bragg`s law, Laue equations, Ewald`s diagram, X-Ray diffraction experiments-Powder method (Debye-Scherrer and photographic methods), Interpretation of power patterns. Single crystal technique- :Laue and Rotation photographic methods). Moving Film method (Weissenberg method). X-ray diffractometers. Systematic absences. Intensities of diffracted X-rays and structural analysis, X-ray scattering by atoms and molecules, Factors affecting X-ray intensities, Crystal structure analysis. 10 hrs

Electron Diffraction: Scattering intensity vs. scattering angle, qualitative aspects of Wierl equation, measurement technique, Elucidation of structure of simple gas molecules, Low Energy Electron Diffraction and structure of surfaces.

Basic theory and applications of Neutron diffraction. 4 hrs

**UNIT- II: [14 hours]**

**Electroanalytical Techniques:** Theory of classical polarography, polarograhic measurements, polarograms, polarographic currents. Factors influencing diffusion currents, advantages and limitations of using dropping mercury electrode. half wave potential, oxygen interference, Applications of polarographic measurements. Modern Polarography : Necessity and development of new voltammetric techniques and their comparison with classical polarography. Fundamentals of DC polarography (Tast), oscilliography, differential and derivative voltammetry, cyclic, pulse, alternating current and square wave polarography.

Cyclic Voltammetry: Principle, Instrumentation, current-potential relation applicable for Linear Sweep Voltammetry (LSV) and Cyclic Voltammetry (CV), interpretation of cyclic voltammograms and parameters obtainable from voltammograms.

Principle, measurement technique and the applications of Coulometry, Amperometry and Electrogravimetry.

Chrono Methods: Basic concepts and applications of chronopotentiometry, chronoampermetry.

**References:**


1. A Basic Course in Crystallography, JAK Tareen and TRN Kutty, University Press, Hyderabad (2001).
2. Essentials of Crystallography, M.A. Waheb, Narosa Publishing House, New Delhi (2009),
3. Polarography and Allied Techniques, V. Suryanarayana Rao (University Press, Hyderabad), (2002).
5. Principles of Instrumental Analysis, D.A. Skoog, F.J. Holler and T.A. Nieman, 5th Ed. , (Saunders College Publishing, Harcourt Brace & Company, U.S.A.) 1998.
6. Electrochemical Methods: Fundamentals and Applications, A.J. Bard and L.R. Faulkner, 2nd Ed. ( Wiley, New York), 2000.


## *AC 456 : INORGANIC CHEMISTRY PRACTICALS-II*

Qualitative Analysis of mixtures of Inorganic Salts containing 4 metal ions and 2 anions (2 less common metal ions like Tl, W, Mo, V, Zr, Th, U, Ce, Ti and Li to be

included among anions organic acid radicals, phosphate, borate and fluoride separation included).

**References:**

1. Vogel's Text Book of Quantitative Chemical Analysis (5th Ed), G. H. Jeffrey, J. Bassette, J.Mendham and R. C. Denny, Longman, 1999
2. Vogel's Qualitative Inorganic Analysis (7th Ed), G. Svehla, Longman (2001).

## AC 457: ORGANIC CHEMISTRY PRACTICALS-II

SEPARATION AND SYSTEMATIC QUALITATIVE ANALYSIS OF BINARY MIXTURES OF ORGANIC COMPOUNDS CONTAINING BOTH MONO AND BIFUNCTIONAL GROUPS AND PREPARATION OF SUITABLE DERIVATIVES.

**References:**

1.Practical Organic Chemistry-F .G. Mann and B. C. Saunders (ELBS, England), 2001.
2. Practical Organic Chemistry - A. I. Vogel (Longman-ELBS, England), 1971.
3. Experimental Organic Chemistry–Vol.I&II Singh et al(TMH, New Delhi)1981.
4. Semimicro Qualitative Organic Analysis–Cheronis etal Wiley-Eastern, New Delhi) 1964.
5. Vogel's Text Book of Practical Organic Chemistry Including Qualitative Organic Analysis- B. S. Furniss et al (Longman-ELBS, England), 1978.

## *AC 458 : PHYSICAL CHEMISTRY PRACTICALS - II*

**At least 12 experiments are to be carried out**

1. Determination of cryoscopic constants of solvents and molecular weight of non volatile substances by thermal method.
2. Determination of degree of dissociation & Vant Hoff factor of an electrolyte by cryoscopic method.
3. Heat of solution of substances by solubility method.
4. Phase diagram of two component systems by thermal analysis.
5. Kinetics of acid catalysed hydrolysis of methyl acetate and determination of (a) order and rate constant, (b) Relative strength of two acids and (c) Energy of activation.
6. First and second order kinetics of reaction between potassium persulphate and KI.
7. Kinetics of (a) inversion of cane sugar, (b) sodium formate–iodine reaction.
8. Determination of heat of neutralisation, integral and differential heat of solution calorimetrically.
9. Thermometric titration of an acid with a base.
10. Direct determination of the latent heat of evaporation of carbon tetrachloride.
11. Measurement of the vapour pressure and latent heat of vapouration of Benzene using tensemeter.
12. Detn.of association constants carboxylic acids in organic solvents by distribution method.
13. Preparation of colloidal solutions.
14. Verification of F & L adsorption isotherms for acetic acid on activated charcoal.
15. To study the adsorption of iodine on charcoal from alcoholic solution.
16. To study the effects of gelatin solution on the precipitation values.
17. To determine the surface and interfacial tension and the effect of detergents.
18. Thermodynamic prediction and measurement of the solubility of naphthalene in benzene.
19. Study of association of benzoic acid in benzene/toluene.

Any other relevant experiments of interest.

**References:**

1. Findlay's Practical Physical Chemistry- B. P. Levitt ( Longman, London).
2. Experiments in Physical Chemistry–James and Prichard.
3. Experimental Physical Chemistry - Daniels et al.
4. Experimental Physical Chemistry-Das & Behera (Tata McGraw Hill, New Delhi) 1983.
5. Advanced Practical Physical Chemistry–Yadav (1989).
6. Experiments in Physical Chemistry–J. C. Ghosh (Bharathi Bhavan) 1974.

# THIRD SEMESTER M.Sc. Course in APPLIED CHEMISTRY

## AC 501: CHOICE BASED COURSE

## AC 502: ORGANOMETALLIC CHEMISTRY

**UNIT- I:** **[14 Hours]**

Historical development- classification and nomenclature, bond energies and stability.

Transition metal alkyls and aryls- types, routes of synthesis, stability and decomposition pathways,. Nucleophilic and electrophilic cleavage of metal-carbon sigma bonded compounds. Alkane activation.

Transition metal to carbon multiple-bonded compounds- carbenes, carbynes, synthesis, nature of bond, agostic interactions, structural characteristics and reactivity. Transition metal hydrides – synthetic routes, structure and reactivity, synthetic applications.

**UNIT-II:** **[14 Hours]**

Transition metal-carbon pi complexes: Preparative methods, nature of bonding, structural features of olefinic, acetylenic, allylic, butadiene, cyclobutadiene, $\eta^5$- cyclopentadienyl, $\eta^6$-benzene and other arenes, cycloheptatriene and cyclooctatetraene complexes.

Important reactions relating to nucleophilic and electrophilic attack on ligands.

Fluxional isomerism in olefin, allyl, dienyl and cyclopentadienyl complexes.

Isolobal concept.

**UNIT- III:** **[14 Hours]**

Catalysis by organometallic compounds:16- and 18-electron rules, oxidative addition, insertion, deinsertion and reductive elimination reactions.

Homogeneous catalysis by organometallics- hydrogenation, hydrosilation, hydrocyanation and isomerization of olefins, immobilisation of homogeneous hydrogenation catalysts,

Hydrocarbonylation of olefins (oxo reaction–cobalt and rhodium oxo catalysts), carbonylation of alcohols- Monsanto acetic acid process. Polymerization of olefins and acetylenes: Ziegler-Natta catalyst systems. Fischer – Tropsch reaction , Water Gas Shift reactions.

**UNIT- IV:** **[14 Hours]**

Organometallics in Organic Synthesis: Main group organometallics- preparation, properties and applications of organometallic compounds of Li, Mg, Hg, Zn, Cd and Sn. Synthetic applications of organo-transition metal compounds: organocuprates. Hydrozirconation, transmetallation reactions by organopalladiums and organonickels, carbonylation by metal carbonylates, decarbonylation, carbene complexes and metallacycles, arene complexes.

**References:**


1.J.P.Collman, L.S.hegedus, J.R.Norton and R.G.Finke: Principles and Applications of
2.Organotransition Metal Chemistry, University Science Books, 1987.
3.R.C.Mehrotra and A.Singh: Organometallic Chemistry, New Age International, 1999.
4.R.H.Crabtree:Organometallic Chemistry of Transition Metals, Wiley , 1999.
5.F.A.Cotton and G.Wilkinson : Advanced Inorganic Chemistry, Wiley, 1991.

## AC 503: DYES, DRUGS AND HETEROCYCLIC CHEMISTRY

**UNIT- I: [14 Hours]**

**Drugs:** Introduction, Classification and nomenclature of drugs. Theories of drug action such as Occupancy theory, Rate theory, Induced fit theory and Perturbation theory. Analogues and Prodrugs, Factors governing drug design. Rational approach to drug design, Variation method of drug designing, tailoring of drugs, Physico-Chemical factors and biological activities. Factors governing the ability of drugs, Isosterism and Bio-isosterism.

**Antipyretic Analgesics:** Classification, synthesis of Phenacetin, Aspirin, Cinchophen, Phenazone and Mefenamic acid, mode of action. **General Anesthetics:** Introduction and classification, synthesis of anesthetic ether, Thiopental sodium and Fentanyl citrate, Mode of action.

**Local anesthetics:** Introduction and classification, synthesis of benzocaine, α-Eucaine, Lignocaine hydrochloride and Dibucaine hydrochloride, Mode of action

**UNIT- II: [14 Hours]**

**Dyes:** Colour and constitution (electronic concept). Classification of dyes, methods of applying dyes to the fabrics. A general study of Azo dyes, Orange –II, Mordant brown, Congo red and methyl orange; Triphenylmethane dyes-Malachite green, Rosaniline, Crystal violet and Phenolphthalein; Cyanin dyes-Ethyl Red, Cyanin blue and Quinaldine; Reactive dyes and Optical brighteners-Tinapal and Blankophor. **Pigments:** Fast violet, Lake red and Orange R.

**Pesticides and Insecticides:** Introduction and classification. Natural insecticides-Nicotine, Pyrethrins, Rotenone and Allethrin. Organic insecticides-DDT, Methoxychlor, BHC, Aldrin, Malathion and Parathion. Fumigants and repellants.

**UNIT- III: Heterocyclic Chemistry-I [14 Hours]**

Nomenclature of Heterocycles, Replacement and systematic nomenclature, Hantzsch-Widman system for monocyclic, fused and bridged heterocycles. Structure, synthesis and reactions of six membered heterocycles- α- and γ-Pyrones, Pyrazines, Pyridazines, Pyrimidines. Synthesis and reactions of seven membered heterocycles-Azepines, Oxepines and Thiepines. Synthesis and reactions of fused heterocycles-Quinolines, Isoquinolines, Coumarins, Naphthyridines and Purines.

**UNIT-IV: Heterocyclic Chemistry-II [14 Hours]**

**Mesoionic compounds**: Introduction, Synthesis and reactions of sydnones.

**Anthocyanins and Anthocyanidins**: Introduction and general methods of synthesis.

**Flavones, Flavonols and Isoflavones**: Introduction and synthesis of flavone, flavonal and quercetin. Structural elucidation and synthesis of Uric acid, Caffeine.

**Heterocycles in functional group and ring transformations:** Alkanes from thiophenes, dienes from pyrroles, alcohols from isooxazolines, conversion of coumarin to benzofuran, sydnone to pyrazole, chromones to pyrazoles, furans to pyridines, pyrrole to pyridines, pyrimidine to pyrazole, isatins to quinolines, indoles to quinoline. Dimroth and related rearrangements.

**References:**


1 An Introduction To the Chemistry of Heterocyclic Compounds- Acheson (Wiley Eastern), 1997.
2. Heterocyclic Chemistry- J.Joule & G.Smith (Van Nostrand ELBS), 1978.
3. Comprehensive Heterocyclic Chemistry Vol-I-VI Ed. Katritzky & Rees (Pergamon), 1984.
5. Synthetic Dyes – Vol-I- Venkataraman, 1999.

6. Medicinal Chemistry- Ashutoshkar (New Age.), 2005, 2. Medicinal Chemistry- G. R.Chatwal (Himalaya) 2002.
7. Natural Products Chemistry, Vol-I-II- G.R.Chatwal (Himalaya), 1990.
8. Principles of Drug Action- II Ed. A.Goldstein Lewis Arnold & Suner M. Kalman (Wiley Int.Ed.)

## AC 504:INDUSTRIAL CATALYSIS and SOFT MATERIALS CHEMISTRY

**Unit 1:** **[14 Hours]** Preparation of catalyst and their behavior: Introduction, role of supports-preparation and structure of supports, silica, alumina, silica-alumina, zeolites, carbon, Catalyst manufacture, catalyst size and shape, pre-treatments, deactivation process, sintering, poisoining and catalyst fouling. 6 hrs. **Techniques in Catalysis-Surface Investigations**: Electron diffraction, scanning tunnelling microscopy (STM), X-ray and UV photoelectron spectroscopy (XPS & UPS), Auger electron spectroscopy (AES)-basic principles &applications.

3hrs**Applications in Fertiliser and Petrochemical Industry:** Catalytic reforming and refining, catalytic cracking, hydro-treatment, steam reforming, hydrocarbon from synthesis gas, Fischer-Tropsch process. Mobil process for conversion of methanol to gasoline. 5hrs

**UNIT-II:** **[14 Hours]** Nano Materials :Introduction, Definition and terminology, consequences of the nanoscale (Nanoparticle, Morphology, Geometric structure, Electronic structure, Optical properties), Nanolayers, Carbon nanotubes, Nanowires, Quantum dots.Nanotechnology and its business applications, Introduction to nanoscale, Potential applications of nanomaterials, Challenges and opportunities scope of nanotechnology, Commercialization scope Nanotechnology research in 21st century, Basic nanotechnology science and chemistry concepts, basic nanostructures , nanocomposites, Thin films, nanofoam, nanoclusters, smart nanostructures, manufacturing techniques of nanomaterials. 10hrsSupra Molecular ChemistryIntroduction, Cryptands, Cyclophanes, Crown ether, Calixerenes, Cyclodextrines, Molecular self assembly: Catenens and Rotaxenes, Supramolecular reactivity and catalysis, Supramolecular devices. 4hrs

**UNIT-III:** **[14 Hours] Crystal Defects and Non-Stoichiometry:** Perfect and imperfect crystals, intrinsic and extrinsic defects- point, line and plane defects.Vacancy, Schottky and Frenkel defects. Thermodynamics of Schottky and Frenkel defect formation, colour centres, non-stoichiometry and defects – Structures of $UO_2$, FeO and TiO. 5 hrs**Solid State Reactions**: General Principles, Wagner's theory. Order - disorder transitions in solids- Bragg- William's theory Mechanism of diffusion , Kirkendall effect. 4 hrs **Preparative Methods:** Ceramic, sol-gel, precursor and chemical vapour deposition (CVD) methods. Nucleation & crystal growth techniques-pulling, zoning, flame fusion & skull melting. Basic methods of preparation of thin films . 5 hrs

**UNIT – IV :** **[14 Hours]Ionic Conductors:** Types of ionic conductors, mechanism of ionic conduction, diffusion superionic conductors; phase transitions and mechanism of conduction in superionic conductors, examples- β-alumina, AgI, halide and oxide ion conductors. 4 hrs**Superconductivity:**Meisner effects; Types I and II superconductors, Features of superconductor, isotope effect, high $T_c$ materials. Principle of low temperature superconductivity. 4 hrs **New Materials:** An introduction toZeolites and Organic conducting materials-polyacetylenes, polyparaphenylenes and polyanilines. 2 hrs **Liquid Crystals:** Mesomorphic behaviour, 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 arrangements in smectic A and smectic C phases. Optical properties of liquid crystals. 4 hrs

**References:**1. Solid state Chemistry, D. K. Chakrabarty (New Age) 1996.
2. Principles of the solid state, H.V.Keer ( Wiley Eastern ) 1993.
3. Solid state chemistry and its applications, A.R.West (Wiley) 1984.
4. L.Smart and E. Moore, Solid State Chemistry –An Introduction (Chapman &Hall)1992.
5 V. Raghavan, Material science and Engineering (3rd Ed), (Prentice Hall India)1993.
6. Thermotropic Liquid Crystals, Ed. G.W. Gray, Wiley.
7. S.Chandrasekhar, Liquid Crystals, Cambridge University Press (2nded), 1994.
8. Basics of Nano Chemistry, Mamta V Sachdeva, Anmol Publishers, New Dlhi. 2011.
9. Modern heterogeneous Oxidation Catalysis, Wd.Noritaka Miguno, Wiley, Weinheim, 2009.
10.Nanoscale materials, Ed-L.M.Liz-Marzan and P.V.Kamath (Kulwer), 2003.
11. Introduction to Nanotechnology, C P Poole and F J Owens (Wiley Intersci), 2006.
12. Introduction to Petrochemicals, Sukumar Maiti (Oxford & IBH, Delhi), 1992.

## AC 505: ANALYTICAL CHEMISTRY PRACTICALS

1. Analysis of brass–Cu gravimetrically using ∝-Benzoinoxime & Zn complexometrically.
2. Analysis Cu-Ni alloy .
3. Analysis of Stainless Steel – Insoluble residue by gravimetry, Ni gravimetrically using DMG, Fe volumetrically using Ce(IV) & Cr volumetrically by persulphate oxidation.
4. Analysis of Type metal –Sn gravimetrically, Pb electrogravimetrically and Sb titrimetrically using $KBrO_3$
5. Quantitative analysis of the constituents & mixtures containing the following radicals
   (i) Cu(II) + Fe(II) - Cu gravimetrically as CuSCN and Fe using Ce(IV).
   (ii) Fe(II) + Ni(II) – Fe gravimetrically as $Fe_2O_3$ and Ni using EDTA.
   (iii) Fe(III) + Ca(II) - Fe gravimetrically as $Fe_2O_3$ and Ca using EDTA.
   (iv) Cr(III) + Fe(III) – Using EDTA by Kinetic masking method.
6. Analysis of chalcopyrites, magnetite and ilmenite.
7. Ion-exchange chromatography: Separation and determination of $Mg^{2+}$ / $Zn^{2+}$, $Zn^{2+}$ /$Cd^{2+}$; $Cl^-$ / $Br^-$
8. Separation of cations using column and paper chromatography
9. Determination of the ion exchange capacity of a resin

**REFERENCES:**


1. A.I. Vogel : A Text book of Quantitative Inorganic Analysis, (ELBS), 1978.
2. I. M. Kolthof and E.P. Sandell: Quantitative Chemical Analysis.McMillan,1980
3. Lobinski and Marczenko, Comprehensive Analytical Chemistry, Vol.30, Elsevier,1996.

## AC 506: MULTISTEP ORGANIC SYNTHESIS

Preparation of Ethyl resorcinol from Resorcinol, 3-Bromo-4-methyl benzaldehyde from p-Toluedine, ε-Caprolactam from cyclohexanone, p-Aminobenzoic acid from p-Nitrotoluene, s-Tribromobenzene from aniline, o-hydroxyacetophenone from phenol, Benzanilide from Benzophenone, Benzylic acid from Benzoin, Benzopinacolone from Benzophenone, p-Chlorotoluene from p-Toludine, 2,5-Dihydroxyacetophenone from Hydroquinone, 2,4-Dinitrophenylhydrazine from Chlorobenzene, m-Nitrobenzoic acid from Benzoic acid, 2,4-Dinitrophenol from Chlorobenzene, o-Aminobenzoic acid from Phthalic acid, 2-Carbethoxycyclopentanone from Adipic acid, α-Acetylaminocinnamic acid from Glycine, p-Aminoazobenzene from Aniline.

Separation of components from mixture of organic compounds by fractional crystallization, fractional distillation, adsorption, Paper, TLC and column chromatography. The purification and characterizationof organic compounds.

Applications of computers in the study of conformation and geometry of some simple organic molecules.

**References:**


1. Elementary Practical Organic Chemistry-Vol. III quantitative Organic Analysis- A.I Vogel
2. Experimetal Organic Chemistry- Vol. I &II- P.R.Singh, Tata McGraw-Hill , 1981.
3. Practical Organic Chemistry- IV Ed- Dey &.Sitaraman (Allied)
4. Laboratory Experiments in Organic Chemistry-Adam, Johnson &Wicon(McMillan, London), 1979.
5. Experimental Organic Chemistry- H.D.Durst &G.E.Goke(McGraw-Hill)1980.

## AC 507: KINETICS METHODS AND ALLIED PRACTICALS

**A. Kinetics and Catalysis (Any FOUR of the following reaction systems to be studied)**
(Determination of reaction order and activation parameters, study of salt/solvent/catalytic effects and formulation of reaction scheme and deduction of rate laws ).

1. Kinetics of acid-base catalysed reactions. Acid catalysed hydrolysis of methyl acetate.
2. Saponification of ethyl acetate by conductivity method.
3. Reaction betweem potassium persulphate and potassium iodide (including the study of salt effect, dielectric constant effect and catalysis by $Ag^{+}$/ $Fe^{2+}$ / $Cu^{2+}$ ions).
4. Decomposition of diacetone alcohol by NaOH.
1. Kinetics of (i) Reaction between iodine and acetone and (ii) iodination of aniline.
2. Decomposition of $H_2O_2$ (including the study of catalytic effect).
3. Reaction between Chromic acid and oxalic acid
4. Iodine clock reactions.
9 Heterogeneous decomposition of ammonia.
10. Surface tension-concentration correlation for solutions (Gibbs equation).
11. Determination of activity of surfaces , free volumeof catalysts and surface area of catalysts.

**B. Thermodynamics Experiments** (**AnyFour**experiments to be carried out)

1. Determination of activities of an electrolyte and non – electrolyte by cryoscopy.
2. Determination of partial molar volumes of (a) Salts – water and (b) alcohol – water (methanol & ethanol) systems by density method.
3. Determination of specific heat of liquids and solutions by calorimetry.
4. Determination of stepwise neutralisation of acids.
5. Study of phase diagram of a ternary aqueous system of potassium chloride and water.
6. Determination of heat of solution of $KNO_3$ in water, integral heat of dilution of $H_2SO_4$ and heat of ionization of acetic acid and ammonium hydroxide calorimetrically.
7. Cryoscopic and ebullioscopic analysis of the given mixture of urea and glucose.
8. Determination of heat of neutralisation of two acids and hence their relative strength.
9. Study of adsorption of picric acid on charcoal using a calorimeter,

**C. Spectrophotometry (Any Two experiments are to be carried out)**

1. Determination of pKa values of indicators.
2. Determination of Hammett's acidity function.
3. Spectroscopic investigation of partition coefficient of iodine between $H_2O$ and $CHCl_3$.
4. Study of the effect of ionic strength on the pH of the given acid with the help of indicators using buffer solution by colorimetric method.
5. Determinationmof composition and stability consatant of metal complexes by ($Fe^{3+}$ ans salislic acid, Ni (II) and 1,10 phenanthroline).

**References:-**


1.Willard, Merrit, Dean & Settle:Instrumental Methods of analysis(Van Nostrand.NY)1981.
2. Sawyer and Roberts : Experimental Electrochemistry for Chemists (Wiley , N.Y)1974.
3. B.P.Levitt : Findlay's Practical Physical Chemistry, (Longman, London), 1973.
4. J. B. Yadav : Advanced Physical Chemistry Experiments ( Goel Publishing House), 1988.
5. F. J. Welcher(Ed): Standard methods of Chemical Analysis (Kriegen, N.Y)1975

# FOURTH SEMESTER M.Sc. course in APPLIED CHEMISTRY

## AC 551 : ANALYTICAL CHEMISTRY

**UNIT - I : [14 Hours]**

**Ion exchange chromatography** : Structures of resins, selectivity, capacity of resins, ion exchange equilibria, applications - removal of interfering ions, concentration and recovery of traces, anion and cation separations and application for the separation of lanthanides and actinides. Techniques of column chromatography, size exclusion chromatography.

**Gas Chromatography** : Principles, columns, detectors - TCD, FID, ECD, GC-MS column efficiency, capacity factors, resolution. Practical aspects of GC.

**HPLC** : Principles, equipment, columns, detectors, choice of column, materials.

**Paper chromatography**: Theory and principle. Techniques; one, two- dimensional and circular paper chromatography. Mechanism of separation, structure of cellulose and types of paper. Methodology- Factors affecting RF values. Advantages and applications. Thin layer chromatography, efficiency of TL plates, selection of stationary and mobile phases. Qualitative and quantitative analysis.

**UNIT – II : [14 Hours]**

**Atomic Absorption Spectrometry**: Theory, working of AAS instruments, analytical applications, interferences.

**Emission Spectroscopy**: Flame Emission Spectroscopy, plasma emission spectrometry, basic principles of flame photometry, evaluation methods in flame photometry, interferences.

**Molecular Luminescence Spectroscopy**: Theory of fluorescence and phosphorescence, fluorimetry in quantitative analysis, instruments, flourescence and structure, fluorescence quenching, phosphorescence method, applications in quantitative analysis.

**Light-Scattering methods** : Nephelometry and turbidimetry- theory, effects of concentration, particle size and wavelength on scattering, instrumentation and application. Activation analysis.

**UNIT - III**: [**14 Hours]**

**Thermal methods:** Thermogravimetric analysis, Instumentation, factors affecting the results and applications.Differential thermal analysis, simultaneous DTA-TGA curves. Differential scanning calorimetry, applications.

**Electrophoresis**: Theory and classification. Factors influencing mobility, macromolecular size and charge, interaction with supporting electrolyte, pH and concentration discontinuities. Factors affecting electrophoretic phenomena, electrolysis, electroosmosis, temperature and supporting media. Instrumentation, methodology, preparation of gels, staining and destaining. Applications.

**UNIT – IV: [14 Hours]Radiochemical Methods of Analysis**

Introduction, the nature of radioactivity, radiometric units, detection and measurements of radioactivity. Disintegration theory, rate of disintegration, radioactive tracers, tracer techniques. Application in analytical chemistry, isotopic dilution analysis, activation analysis and prompt gamma neutron activation analysis (PGNAA). Radiometric analysis, radiometric titrations and applications.

**REFERENCES:**

1. G.D. Christian : Analytical Chemistry, (4th Ed.), (John Wiley ),1986.
2. R.A.Day and A.L. Underwood : Quantitative Analysis, 5th Ed. (Prentice Hall, India), 1998.
3. H.H.Wlliard, L.L.Merrit and J.J.Dean, Instrumental methods of analysis,(7th Ed.) 1988
4. B.K.SHARMA, Instrumental Methods of Chemical Analysis (Goelpublishing), 2000.
5. Skoog, Holler and Nieman: Principles of Instrumental Analysis, (Harcourt Afca), 2001
6. Friedlander, Kennedy and Miller: Nuclear and Radiochemistry.
7.Arnikar :Nuclear and Radiochemistry, 8..Sood, Ramamoorthy &.Reddy :Principles of Radiochemistry.

## AC 552: SYNTHETIC & NATURAL PRODUCTS CHEMISTRY

**UNIT-I:** [**14Hours**]**Reduction**

**Reactions:** Catalytic hydrogenation: Introduction, catalysts and solvents employed reduction of functional groups, mechanisms and stereochemistry of catalytic hydrogenations, Hydrogenolysis and homogeneous catalytic hydrogenation.

**Metal hydride reduction:** Reduction with $LiAlH_4$ and $NaBH_4$, Stereo chemistry of reduction, Functional group transformation during reduction, Reduction with diborane and related reactions.Reduction in Biological systems-NADH,FAD.

**Dissolving Metal Reductions:** Mechanisms of reduction of conjugated system and carbonyl compounds, Bimolecular reductions of esters, Birch reduction, Wolf-Kishner reduction and related reactions, Reaction with diimide and related compounds.

**UNIT- II:** **[14 Hours]**

**Oxidation reactions:** Introduction and different oxidative processes, Mechanism of oxidation reactions with chromium and manganese salts, peracids and peresters, periodic acid, Lead tetra acetate, Ozone, Osmium tetroxide and their synthetic importance in functional group transformation.

**Halogenation:** Halogenation of olefins, carbonyl compounds, Benzyllic and Allylic halogenation, Dehalogenation reactions. Dehydrogenation with S, Se, Pt, Pd, Ni.

**UNIT –III:** **[14 Hours]**

**Alkaloids**: Introduction of isolation, classification, general methods of structure illucidation. Structure and synthesis of the following alkaloids: Papaverine, Adrenaline, Ephedrin, Morphine,Yohimbine,Reserpine.

**Terpenoids**: Introduction, classification, isoprene rule, methods of structure determination. Structure and synthesis of Geraniol, Menthol, α -Pinene, Camphor, Zingiberene and α-Santonin.

**UNIT- IV:** **[14 Hours]**

**Steroids:** Introduction and Nomenclature of steroids, Blanc's rule, Barbier-Wieland degradation, Oppenauer oxidation, Diel's hydrocarbon, Chemistry of Cholestrol, Ergosterol, Vitamin-D &bile acids.

**Steroidal Hormones:** Chemistry of Oestrone, Oestradiol, Oestriol and their chemical relationship. Chemistry of Progesterone, Androsterone and Testosterone. Structure and Synthesis of Cortisone, Cortisol and Aldosterone. Transformations in steroids and hormones.

**References :**


1. Modern Organic Reactions- H.O.House.
2. Advanced Organic Chemistry-IV-Ed. Part A &B-F.J.Carrey &R.J.Sundberg(Kluwer) 2001.
3. Modern Methods of Organic Synthesis-N.Carruthers (Cambridge University), 1996.
4. Natural Products Chemistry Vol-I & II. G. R. Chatwal (Himalaya Bombay) 1990.
5. Chemistry of Natural Products – Vol-I & II – O. P. Agarwal(Goel Gorakhpur), 1985.
6. Organic Chemistry-Vol-I-II- I. L. Finar (Longmann ELBS London), 2000.

## AC 553: APPLIED ELECTROCHEMISTRY & REACTION KINETICS

**UNIT-I : [14 Hours]**

**Electrochemical Energy System :**Limitations of chemical energy sources. Electricity storage-Importance, storage density, battery characteristics, Primary battery (Laclanche-dry cell and Alkaline cell). Secondary battery (acid and alkaline). Reseve batteries. Lithium batteries-(primary and secondary and lithium based conducting polymer battery). Fuel cells – introduction, classification, $H_2$-$O_2$ , methanol, solid polymer electrolyte fuel cell and bio-cells. Solar energy conversion.

**Bio-electrochemistry**- Introduction, Membrane potential-theoretical and modern approach. Electrical conduction in biological organism,Electrochemical communication in biological organisms.

**Sensors:Biosensors:** Introduction electrochemical bio-sensors- characteristics, use as a transducer, types (glucose, urea and alcohol sensors). **Ion-Sensors**: Io-n:selective electrode: Introduction, Types - Glass membrane electrodes, solid state ion exchange electrodes, solid state crystal electrodes, liquid membrane electrodes, and gas sensing electrodes. Analytical and biological applications of sensors.

**UNIT-II :[14 Hours]**

**Metallurgical Processing**: Electroplating-fundamentals, mechanism of electrodeposition of metals, role of anode and plating bath, anode efficiency-throwing power, effielectroplating practice, fault analysis in electroplating, electroplating process control, application of electroplating.Brief account of Electroless plating, Conversion coatings, Electrophoretic painting.

**Metals and materials processing**-theory and applications of Electroforming and Electrochemical etching. Production of metals by electrowinning and electrorefining.

**Electrochemistry of Environment**: Introduction, Global warming. Electrochemistry in - transport system, fixing of $CO_2$, sewage disposal, treatment of waste, Metal ion removal and metal recovery. Treatment of liquors containing dissolved chromium. Electrolytic methods of phase separation-electroflotation and electrophoretic separation

**UNIT-III: [14 Hours]**

**Electrochemical Engineering**: General considerations, costing and technology of electrolytic process, electrolysis parameters, principles of cell design, laboratory data and scale-up, performance and figures of merit. 5hrs

**Industrial Electrochemistry:** Fundamentals, electro- organic synthesis (Kolbes synthesis, oxidation and reduction of hydrocarbons, reduction of nitro-compounds); Indirect eletrosynthesis. Electro inorganic synthesis of fluorine, chlorates and ozone. Synthesis of metal salts via anodic dissolution. 5hrs

**Industrial applicfation**-A Case study:- The chlor-alkaly industry: Introduction, Generaal concepts of brine elecrolysis, modern technological developments (electrode materials, membrane), chlorine cell technologies (diaphragm ceslls, membrane cell). 4hr

**UNIT -IV: Reaction Kinetics [14 Hours] Theories of Reaction Rates**- Introduction, activation and thermodynamic parameters. conventional transition state theory (CTST) - statistical mechanisms and chemical equilibrium, derivation of rate equation. Some applications of conventional transition state theory (reaction between atoms and reaction

between molecules). Termodynamic formulation of conventional transition state theory. 6hrs

**Potential energy surfaces** and construction of them. Theoretical calculation of energy of activation.**Theory of Unimolecular Reactions**-Lindemann & Hinshelwood`s theory and their limitations. 5hr

**Kinetics of Composite Reactions**: Gold-Finger –Letort –Niclause rules, Inorganic reaction mechanism- (decomposition of $N_2O_5$ and phosgene). Organic reaction reaction mechanism - (decomposition of acetaldehyde ad combustion of hydrocarbon). 3hrs

**References:**


1. Modern Electrochemistry, 2nd Ed. Vol.1,2A&2B, Bockris & Reddy (Plenum, NY) 1998
2. Chemical &Electrochemical Energy Systems, R. Narayan &B. Viswanathan (University Press), 1998.
3. Industrial Electrochemistry, D. Peltcher & F. C. Walsh (Chapman & Hall)1990.
4. Biosensors-theory and Applications, Donald G. Burek, (Technomic), 1993.
5. Principles and Applications of Electrochemistry–Crow (Chapman hall, New York) 2014
6.Fundamentals of Electrochemistry, Fulkner and A. J.Bard, Wiley India, 2006.
7. Chemical Kinetics, K. J. Laidler, Pearson Education, Anand Sons(India) 3rd ed., 2008.
8. Fundamentals of Chemical Kinetics, M.R.wright, Harwood Publishing, Chichesrer, 1999.
9. Kinetics & Mechanisms of Chemical Transformations, J Rajaram & J C Kuriacose, Macmillan, Delhi, 2007.

# AC 554:POLYMER CHEMISTRY

**UNIT- I:[14 Hours]**

**Terminology and basic concepts**: Monomers, Functionality, repeat units, degree of polymerization.General structure and naming of polymers. Average molecular weight and average chain dimension concept.

**Classification** based on various considerations-source, preparation methods, thermal behavior, chain structure etc**.**

**Types** –Homopolymers and copolymers; linear, branched and network polymers.

**Techniques of polymerization**: Techniques of preparation of addition and condensation polymers.

**Kinetics of polymerization:**Kinetics of additionand condensationpolymerization. Kinetics of copolymerization.

**UNIT- II: [14 Hours]**

**Stereochemistry of polymers**: Geometric and optical isomerism in polymers. Structure, properties and preparation of stereoregular polymers.

**Expressions for average molecular weighs. Molecular weight distribution and Polydispersity.**

**Fractionation of polymers-** Different methods

**Determination of molecular weight:** Osmometry, viscometry, ultracentrifugation and GPC methods

**Thermal Characterization**: Glass Transition and melting-correlation with structure- Factors affecting Tg and Tm. Techniques of thermal characterization: DSC, DTA , DTG and TGA techniques.

**Unit- III**: **[14hours]**

**Analysis of Polymers-**Chemical analysis-spectroscopic methods. X-ray diffraction study. Microscopic analysis.

**Solution Properties of polymers**-Dissolution of polymers. Criteria of polymer dissolution, thermodynamics of dissolution, Flory Huggin's Theory . Size and shape of polymer molecules in solution, theta conditions. Solution viscosity.

**Polymer degradation and stability**-Thermal, oxidative, photo, chemical and radiation affected degradation. Plastic waste management-Incineration, recycling and biodegradation.

**UNIT-IV**: **[14hours]**

**Structural features, properties and uses of commercial polymers:** polyethylene, polystyrene, PVC, polyesters, polyamides, polyurethanes and polycarbonates.Cellulose polymers. Polymer fibers-natural ands synthetic fibers.

**Properties and uses of Specialty polymers**-Liquid crystalline polymers, , conducting polymers and biomedical polymers.

**Polymer processing Techniques**-Compounding- role of additives. Casting, calendaring, moulding , foaming, reinforcing and spinning techniques.

**Polymeric Reagents**: Important polymeric reagents used for oxidation and reduction.

Polymers as supports in solid phase peptide, protein and nucleotide synthesis. Polymeric supports, their merits and limitations in the solid phase strategy of organic synthesis

**REFERENCES:**

1. Text book of Polymers- F.W.Billmeyer (Wiley)
2. Contemporary Polymer Chemistry-H.R. Allcock and F.W. Lampe (Prentice Hall).
3. Polymer Science and Technology-J.R. Frird (Prentice Hall).
4. Polymer Science: V.R. Gowariker, N.V.Viswanathan & T.Sreedhar
5. Principles of Polymer Science- P.Bahadur and N.V.Sastry(Narosa Publishers)

## AC 555: ENVIRONMENTAL CHEMISTRY PRACTICALS

1. Determination of COD of a water sample,
2. Determination of dissolved oxygen (DO) by Winkler's method
3. Determination of nitrate & nitrite in water samples and sea water.
4. Analysis of heavy metals in waste water, sea water (Pb, Hg etc. By spectrophotometry)
5. Determination of available K in soil, 6. Determination of organic carbon in soil samples
7. Nephelometric determination of sulphate / phosphate.
8. Determination of alkalinity of water samples
9. Determination of fluoride in drinking water by spectrophotometry & ion selective electrode
10. DETERMINATION OF PHOSPHORIC ACID CONTENT IN SOFT DRINKS
11 Spectrophotometric determination of sulphur and phosphorus present in soil.
12. Determination of phosphates in detergents
13. Any other experiment of interest.

## AC 556: ELECTROCHEMISTRY, POLYMER& COMPUTER related PRACTICALS

**A. Electrochemistry :** (**Any EIGHT experiments are to be carried out**).

1. (a) Determination of transport number of $Cd^{2+}$ and $SO_4^{2-}$ ions by EMF method.
   (b) Determination of thermodynamic parameters of a cell reaction by EMF method.
2. Electroplating of (i)Nickel, (ii)Chromium,(iii) Aluminum and iv)copper on a copper plate.
3. (a) Verification of Tafel equation of hydrogen evolution reaction.
   (b) Determination of rate of corrosion by weight loss method.
4. (a) Identification of deposites by chemical spot tests.
   (b) Determination of electrochemical equivalent of copper.
5. (a) Identification of metal ions in a mixture polarographically.
   (b) Qualitative determination of electroreducible substances of (i)lead ion with dichromate & (ii)ferric ion with titanous ion and (c) Verification of Ilkovic equation.
6. Determination of (i) stability constant of a metal complex (lead oxalate or copper glycinate) and (ii) concentration of metal ions polarographically.
7. Kinetics of corrosion of mild steel and accelerated corrosion resistance tests.
8. Electrolytic preparation- peroxydisulphate, chlorate and perchlorate, calcium gluconate & tetrachloroquinine.
9. Determination of pK values of maleic acid/malonic and phosphoric acid bypotentiometric titration with sodium hydroxide using glass electrode.
10. Potentiometric titration of (a) Non aqueous sytem and (b) mixture of strong (HCl) and weak (HAC) acid with NaOH / NH4OH and find the strength of the acids in mixture.
11. Determination of decomposition potential of an aqueous electrolytic solution.
12. Determination of the potential of an electrochemical cell and mean ionic activity coefficient.
13. Determination of pKa values of di and tri-acid base potentiometrically and pH metrically.
14. Determination of acidic and basic dissociation constants and isoelectric point an amino acid pH metrically..
15. pH titration of (a) HCl versus NaOH, (b) $CuSO_4$ versus NaOH and (c) HOAC versus NaOH and (d) lead nitrate versus potassium chromate, Titration of mixture of bases ($Na_2CO_3$& $NaHCO_3$) with standard HCl and find the concentration of bases.
16. Determination of activity coefficient of an electrolyte at different molalities.

**B. Polymers : (Any FOUR experiments to be carried out).**

1. Preparation of polymers by condensation and free radical methods.

2. Study of kinetics of polymerization, 3. Thermal analysis of polymers.
4. Analysis of phenol-formaldehyde reaction products by TLC
5. Measurement of stress relaxation, creep & recovery of typical elastomers& plastics
6. Determination of molecular weight and size parameters of polymers by viscometryand turbidimetry.
7.Determination of sequences in polyvinylalcohol by viscometry.
8.Determination of molecular weight of a polymer by turbidimetry.
9. Preparation of Polymethylmethacrylate by suspension polymerization / polystyrene by free radical polymerization / Nylon by interfacial polymerization / Polyacrylamide by solution polymerisation method / polyvinylalcohol from polyvinylacetate / Phenol formaldehyde/ urea formaldehyde resins.

**C. Computer related experiments**

The following exercise may be given to illustrate the use of Softwares such as Excel and Origin in calculation and plotting curves using the data generated in regular lab experiments.

1. Use of mathematical functions to calculate parameters such as ionic strength, rate constants, dissociation constants, energy of activation, standard deviation, average molecular weights of polymer samples or any other similar calculation.
2. Use of software to make linear plots and calculate constants from slopes and intercepts- data from experiments such as verification of beer's law, determination of pKa of weak acids from pH data, determination of energy of activation , viscosity with concentration for determination of unknown concentration/ average molecular weight of polymers or any other similar data sets.
3. Use of software to fit multiple set of data obtained in different series of experiments on the same chart- pka of differen weak acids, kinetic data with different ionic strength conditions etc-or any other series of data may be given.
4. Use of software to fit non-linear curves with data from experiments such as absorbance vs. wavelength, first derivative curves of potentiometric and pH titrations, radioactive decay or any other similar experiments.
5. Programme writing and numerical analysis.
   Use of commercial software packages such as Mathcad, Matlab, Aspan Plus, Design II, Use of Chem draw and Chem sketch for construction of molecules. Use of Window excel for drawing graphs estimation of slope intercept.

**REFERENCES:-**

1.Willard, Merrit,Dean& Settle:Instrumental Methods of analysis(Van Nostrand.NY)1981.
2. Sawyer and Roberts : Experimental Electrochemistry for Chemists (Wiley , N.Y)1974.
3. B.P.Levitt : Findlay's Practical Physical Chemistry, (Longman, London), 1973.
4. J.B. Yadav :Advanced Physical Chemistry Experiments ( Goel Publishing House), 1988.
5. F. J. Welcher(Ed): Standard methods of Chemical Analysis (Kriegen, N.Y)1975.
6. Computers and their applications to Chemistry, Ramesh Kumari, Narosa
7. Theory and Problems of Programming with Basic, Mc graw Hill, NY,1987.
8. Computer programming in Fortran IV,V , Rajaraman, Prentice Hall of India, 1987.
9.Computers in Chemistry & Instrumentation,Vol.1-5 Mattson, Marcel Dekker, NY,1974