DR. BABASAHEB AMBEDKAR MARATHWADA UNIVERSITY, AURANGABAD

DEPARTMENT OF CHEMISTRY

Credit based syllabus

M.Sc. Chemistry I & II Semester

Effective from June 2011

DR. BABASAHEB AMBEDKAR MARATHWADA UNIVERSITY, AURANGABAD

DEPARTMENT OF CHEMISTRY

Syllabus Based upon Credit System

The department of Chemistry conducts four specializations namely Analytical, Inorganic, Organic and Physical Chemistry.

The M. Sc. Chemistry program is divided into Four Semesters with minimum 108 credits, comprising of 18 theory courses and 12 laboratory courses including projects, seminars and tutorials.

The 18 theory courses of each specialization include:

Core Courses: 09

Specialized Courses: 06

Elective Courses: 02

Service Courses: 01

The 12 laboratory course includes:

Core Courses: 06

Specialized Courses: 06

Credit System and Cafeteria approach

- The credit system with cafeteria approach has been adopted by the department.
- Students will have to learn at least 108 credits for the award of M. Sc. Degree.
- Out of 108 credits students will have to learn at least 36 credits of core courses, 24 credits of specialized courses and 12 credits of elective/service courses.
- Along with these credits of theory courses students are required to earn at least 36 credits of laboratory courses.

-

The following will be the structure for revised syllabus for M. Sc. Chemistry I & II semester effective from June 2011

Semester	Paper No.	Title	Total number of teaching hours	Credits
Semester- I	CHE-101	Analytical chemistry	60 hrs	4
	CHE-102	Inorganic Chemistry	60 hrs	4
	CHE-103	Organic Chemistry	60 hrs	4
	CHE-104	Physical Chemistry	60 hrs	4
	CHE(a)210	Laboratory course (Inorganic)	90 hrs.	3
	CHE(a)211	Laboratory course (Organic)	90 hrs.	3
	CHE(a)212	Laboratory course (Physical)	90 hrs.	3
Semester -II	CHE-205	Spectroscopic methods of analysis	60 hrs	4
	CHE-206	Inorganic Chemistry	60 hrs	4
	CHE-207	Organic Chemistry	60 hrs	4
	CHE-208	Physical Chemistry	60 hrs	4
	CHE (a)-209	Laboratory course (General)	90 hrs	3
	CHE(b)210	Laboratory course (Inorganic)	90 hrs.	3
	CHE(b)211	Laboratory course (Organic)	90 hrs.	3
	CHE(b)212	Laboratory course (Physical)	90 hrs.	3

CHE-101 ANALYTICAL CHEMISTRY

Teaching hours : 60 Clock Hrs **Credits: 04**

Unit- I. Basic concepts of Analytical Chemistry: **12 hrs**

The nature of analytical chemistry, the role of analytical chemistry, qualitative and quantitative analytical methods, a typical quantitative analysis - sampling and treatment of samples, validation of a method.

Statistical Treatment of analytical data:

Introduction, types of errors, significant figures, precision and accuracy, methods of expressing accuracy, methods of expressing precision, the confidence limit, tests of significance- the F test, the student T test, rejection of results - the Q test.Statistics for small data sets, linear least squares, correlation coefficient, using spreadsheets for plotting calibration curves, slope, intercept and coefficient of determination, numericals.

Unit - II. Basic Separation techniques: Distillation and Solvent and Solid Phase extraction: **12hrs**

Distillation: Fractional distillation, distillation under vacuum, theory of operation of distillation methods, some practical considerations.

Solvent and Solid Phase extraction: Phase equilibrium, the partition coefficient the distribution ratio, theory of phase contact methods, single equilibrations, repeated equilibrations, counter current distribution, practical aspects and applications - extraction of metals, extraction of molecular species, Ion pair extractions, Accelerated and microwave assisted extraction, solid phase extraction, Numericals.

Unit - III. Chromatography **12 hrs**

Introduction, basic principles and theory of chromatographic techniques, plate theory of chromatography, rate theory of chromatography, other factors in zone broadening, Development of the chromatogram - Frontal analysis, elution analysis displacement analysis, selection of chromatograph system, qualitative and quantitative analysis by chromatography.

Unit - IV. Chromatographic Systems **12 hrs**

(a) Thin layer Chromatography:

Basic principles, experimental techniques, solvent systems, plate development, detection of components, evaluation of chromatogram by different methods, applications of TLC.

(b) Liquid-Liquid partition chromatography:

Introduction, theory, solid supports, selection of stationary and mobile phases, reverse phase chromatography, choice of adsorption or partition, applications of partition chromatography.

(c) Column Chromatography:

Principle, experimental details, theory of development, column efficiency, factors affecting column efficiency, and applications.

(d) Gel permeation Chromatography:

Principle materials, gel preparation, column packing, detectors and applications.

(e) Ion Exchange Chromatography:

Ion Exchange resins, ion exchange equilibria, ion exchange capacity of resins and its determination, applications of ion exchange resins to chromatography, ion chromatography based on suppressors

Unit- V.

(a) Gas Chromatography: **12 hrs**

Introduction, principles of gas-liquid chromatography, instrumentation - Carrier gas, sample introduction system, columns, detectors, substrates, temperature control, evaluation

Retention volume, resolution, branches of gas chromatography, applications, numericals.

(b) High Performance Liquid Chromatography:

Principle, instrumentation - column, column packing, mobile phone, pumping system, detector system, practical procedure, applications, HPLC adsorption and partition chromatography.

Reference Books:

1. Fundamental of Analytical Chemistry 8th Edn. Skoog, West Hollar, Couch.
2. Analytical Chemistry 6th Edn., G.D. Christian
3. Chemical Separations and Measurements, D.G. Peters, J.M. Hayes and G.M. Hieftie
4. Instrumental Method of Chemical Analysis, G.R. Chatwal & S.K.Anand.

-

CHE-102 INORGANIC CHEMISTRY

Teaching hours: 60 **Credit : 04**

Unit -I & II: Group theory and symmetry concepts **24 hrs.**

Introduction to symmetry operations, symmetry elements, point group, classifications of point groups, point group of H_2O, NH_3, CO_2, BF_3, C_2H_4, PCl_3, PCl_5, C_6H_6, $[PtCl_4]^{--}$,$[PtCl_2(NH_3)]$, $[CoCl_2(NH_3)_4]$ HCl, BeF_2, CO, $[FeF_6]$, $C_2H_2Cl_2$, o, m, & p substituted benzene molecule.(AB_2, AB_3, AB_4,AB_5 and AB_6 type molecules) Application of point group, definition of group, properties of group ,

Group multiplication table, matrix representation of symmetry elements. Reducible and irreducible representation, character of representation, character of matrix, Conjugate matrix, Properties of irreducible representations, Great orthogonality theorem (without proof) and it's importance, construction of character table of C_{2v} & C_{3v} point group. Mulliken symbolism rules for irreducible representations & it's applications with examples. Standard reduction formula direct product and uses.

Unit III : Reaction mechanism of transition metal complexes. **12 hr**

Classification of inorganic reactions, ligand substitution reaction and their mechanisms of octahedral complexes, acid hydrolysis, factors affecting the acid hydrolysis base hydrolysis, conjugate base mechanism, Electron transfer teaction: mechanism of inner and outer sphere electron transfer reactions in octahedral complexes.

Unit IV : Metal ligand equilibria in solution: **12 hrs**

Definition of stability constant, step wise and overall formation constant, factors affecting the stability of metal complexes with reference to the nature of metal ion and ligand. Determination of formation constant for binary complexes using pH-metric technique.

Unit V : Inorganic chemistry in biological systems **12 hr**

Essential and trace elements in biological systems and their functions , structure and function of metalloenzymes, metallodrugs and metalloporphyrins , Role of Rhodium, Gold, Copper and cobalt complexes as anticancer agents, Electron transfer, Respiration and photosynthesis reaction, Metal deficient diseases of Fe, Zn, Cu and Mn and their theraphy.

Reference books:

1. Symmetry and Spectroscopy of Molecules, K.Veera Reddy.
2. Group Theory and symmetry in Chemistry, Gurdeep Raj.Ajay Bhagi and Vinod Jain.
3. Inorganic Chemistry, J.E.Huhey and Keiter R. L
4. Mechanism of Inorganic Reaction. II Edn. Fred Basolo and R.G.Pearsons.
5. Selected Topic in Inorganic Chemistry, Wahid U. Malik, G.D.Tuli and R.D.Madan.
6. Advanced Inorganic Chemistry, F.A.Cotton and Wilkinson.
7. Advanced Inorganic Chemistry, Satyaprakash, G.D.Tuli, S.K.Basu and R.D.Madan.
8. Advanced Inorganic Chemistry, Volume I and II Gurdeep Raj.
9. Concise Inorganic Chemistry, J.D.Lee.
10. A Textbook of bioinorganic chemistry, A. K. Das

-

CHE-103 ORGANIC CHEMISTRY

Total teaching hrs: 60 **Credits: 04**

Unit-I: Nature of Bonding in Organic Molecules: [12 hrs]

Delocalized chemical bonding, conjugation, cross conjugation, resonance, hyperconfugation, bonding in fullerenes, tautomerism.

Aromaticity in benzenoid and non-benzenoid compounds, alternant and non-alternant compounds, Huckel rule, energy level of π-molecular orbitals, annulenes, aromaticity, homo-aromaticity, ψ-aromaticity, PMO approach; Bonds weaker than covalent - addition compounds, crown ether complexes and cryptands, inclusion compounds, cyclodextrius, catenanes and rotaxanes.

Unit-II: Reaction Mechanism : Structure and Reactivity [12 hrs]

Types of Mechanisms, Types of reactions, Thermodynamic and Kinetic requirements, Kinetic and Thermodynamic control, Hammond's postulate, Curtin-Hammett Principle, Potential energy diagrams, transition states and intermediates, methods of determining mechanisms, isotope effects, hard and soft acids and bases, Generation, structure, stability and reactivity of carbocations, Carbanions, free redicals, carbenes and Nitrenes. Effect of structure on reactivity, resonance and field effect, steric effect quantitative treatment, The Hammett equation, Linear free energy relationship, substituent and reaction constants, Taft equation.

Unit-III & IV: Stereo-chemistry: [24 hrs]

Elements of symmetry, chirality, Enantiomeric and diastereomeric relationships, R and S, E and Z nomenclature. Molecules with more than one chiral center, Threo and Erytano isomers, Prochiral relationships, groups and faces, stereospecific and stereoselective reactions. Optical activity in the absence of Chiral Carbon (Biphenyls, allenes and Spiranes), Chirality due to helical shape. Methods of resolution, optical purity, stereochemistry of the compounds containing Nitrogen, Sulphur and phosphorous. Conformational analysis of cycloalkanes, Mono and disubstituted cyclohexanes, decalins, effect of conformation on reactivity.

Unit-V: Aliphatic Nucleophilic and Electrophilic Substitutions: [12 hrs]

Nucleophilic: The SN^2, SN^1 mixed SN^1 and SN^2 and SET mechanisms. The neighbouring group mechamism, Neighbouring group participation by π and 6-bonds, anchimeric assistance. The SN^i mechanism. Nucleophilic Substitution at an allylic aliphatic trigonal and a vinylic carbon.

Reacivity : Effect of substrate structure, attacking nucleophile, leaving group and reaction medium. Phase transfer catalysis, Ambident nucleophiles, regioselectivity.

Electrophilic: Bimolecular mechanisms-SE^2 and SE^i. The SE^1 mechanisms. Electrophilic substitution accompanied by double bond shifts.

Reference Books:

1. Advanced Organic Chemistry, IV Edition: J. March
2. Stereochemistry of Carbon Compounds: E. L. Eliel
3. Advanced organic Chemistry, Part-A and Part-B: F. A. Carey, & R. J. Sundburg.
4. A Guide Book to Mechanisum in Organic Chemistry: Peter Sykes.
5. Synthetic Organic Chemistry: H. O. House
6. Principles of Organic Synthesis: R. O. C. Norman
7. Stereochemistry of Organic Compounds: D. Nashipuri
8. Organic Chemistry: Clayden and Greeves
9. Mechanism and Structure in Organic Chemistry: E. S. Gould

CHE-104 PHYSICAL CHEMISTRY

Total Teaching Hours : 60 **Credits: 04**

Unit I: Ionic Equilibria and Biological Reactions **12 hrs.**

Exact treatment of the dissociation of week acids and bases, Dissociation constant of polyprotic acids, Statistical effects in polyprotic acids, Dissociation constant of complex ions, Logarithmic expression for pH and pOH, Calculations involving buffer solution, buffer capacity and buffer index, Salt effect and solubility product and its applications.

Thermodynamics of biochemical reactions, Binding of oxygen by myoglobin and hemoglobin, Reaction between microscopic and macroscopic dissociation constant.

Unit II: Chemical Dynamics **12 hrs.**

Collision theory, modified collision theory, weakness of the collision theory, Theory of absolute reaction rates, equilibrium hypothesis, Derivation of the rate equation, statistical mechanical derivation and thermodynamic formulation. Isotope effect on reaction rate. Primary salt effect, secondary salt effect.

Dynamics of uni-molecular reactions, Lindmann and Hinshelwood theory

Kinetics of fast reactions, study of fast reactions by flow method, relaxation method, flash photolysis and NMR method.

Reactions in solution: Reaction between ions, influence of solvent-double sphere model, single sphere model, influence of ionic strength, numericals.

Unit III: Classical Thermodynamics **12 hrs.**

Nernst heat theorem, the third law of thermodynamics, determination of absolute entropies of solids, liquids and gases. Partial molar properties : Partial molar free energy, chemical potential, partial molar volume and partial molar heat content and their significance, determination of these quantities, concept of fugacity and determination of fugacity.

Thermodynamic probability of a system of a distinguishable and indistinguishable particles, Sterling approximation, Boltzmann distribution law, Bose Einstein distribution law and Fermi – Dirac distribution law, partition function, energy in terms of partition function, entropy in terms of partition function, translational partition function, entropy for monoatomic gases, Sakur-Tetrode equation, rotational partition function, vibrational partition function, numerical.

Unit IV: Surface Chemistry: **12 hrs.**

Surface tension, capillary action, pressure difference across curved surface (Laplace equation) vapour pressure of droplets (Kelvin equation) Gibbs adsorption isotherm, estimation of surface area (BET equation), surface films on liquids (Electro kinetic phenomenon), catalytic activity at surfaces, numericals.

Colloidal electrolytes, Types of micelles in colloidal electrolytes, Micellization, Thermodynamics of micellization, Mechanism of Micellization, critical micellar concentration, Determinations of critical micellar concentration, Surface active agents, Classifications of surface active agents, Reverse micelles, Solubilization

Unit V: Electro-Chemistry **12 hrs.**

Debye-Huckel theory of strong electrolytes, Debye-Huckel-Onsager equation Testing of the equation, Debye-Falkenhagen effect, Wein effect, activity coefficient, mean ionic activity coefficient; Debye-Huckel limiting law ionic strength. Electrocapillary phenomena, and its measurements. Effect of anions, cations and molecules on electrocapillary curves. Electrocapillary properties of mercury-solution interface.

Polarography: the Ilkovic equation and its derivation, concentration polarization, instrumentation, advantages of DME, half wave potential. Applications of polarography, numerical.

-

References books:

1. Chemical Kinetics - Laidler (McGraw-Hill)
2. Kinetic and Mechanism of Chemical Transformations - J. Rajaram and J.C. CURIACOSE (Macmillan India Ltd.)
3. Physical Chemistry - Alkins (Oxford)
4. Thermodynamics for Chemists - S. Glasstone (EWP, New Delhi)
5. Physical Chemistry - G. M. Barrow
6. Advanced Physical Chemistry - Gurdeep-Raj (Pelenum)
7. Micelles : Theoretical and Applied Aspects - V. Moroi (Plenum)
8. Text Book of Physical Chemistry - S.Glasstone (McMillan)
9. An Introduction to Electrochemistry - S. Glasstone (EWP, New Delhi)
10. Physical chemistry – Robert A .Alberty ., Robert J .Silbey
11. Statistical Thermodynamic – M. C. Gupta

-

CHE-205 SPECTROSCOPIC METHODS OF ANALYSIS

Teaching hours : 60 hrs **Credits : 04**

Unit -I : General introduction of spectral methods of analysis. **12 hrs**

Characterization of electromagnetic radiations, Regions of the spectrum, Interaction of radiations with matter - absorption, emission, transmission, reflection, dispersion, polarization and representation of spectra. resolving power, signal to noise ratio. line width, and intensity of spectral lines. Energy levels. Components of spectrometer and their functions.

Microwave spectroscopy: Rotation of molecules, rotational spectra, diatomic molecules - rigid diatomic molecules, effect of isotopic substitution, non-rigid rotator, the spectrum of non-rigid rotator, instrumentation and applications, numerical problems.

Unit – II : Vibrational and Raman spectroscopy **12 hrs**

Review of linear harmonic oscillator, the vibrating diatomic molecule, the simple harmonic oscillator, the anharmonic oscillator, the diatomic vibrating rotator, the vibration-rotation spectrum of carbon monoxide, breakdown of the Born-Oppenhemier approximation, the vibration of polyatomic molecules, overtones and combination frequencies, the influence of rotation on the spectra of polyatomic molecules, the influence of nuclear spin, symmetric top molecules, analysis by Infra-red technique - Group frequencies, outline of technique and instrumentation. **Raman spectroscopy: T**heories of Raman effect, pure rotational, Vibrational and Vibrational-rotational. Raman spectra, rule of mutual exclusion, overtone and combination vibrations, Rotational fine structure, Instrumentation and applications.

Unit –III : **12 hrs**

Photoelectron spectroscopy : Basic principles, ESCA- Introduction - ESCA - ESCA satellite peaks spectral splitting ESCA chemical shifts, instrumentation, applications, Auger electron spectroscopy (brief review)

Thermal methods of analysis :

Thermogravimetry, principles, factors affecting thermal curve and application. Differential thermal analysis - principles, factors affecting DTA curve, applications. Differential scanning colorimetry - principles, instrumentation and applications. thermometric titrations, numerical.

Unit -IV. **12 hrs**

Ultraviolet- Visible Spectroscopy :

Various Electronic transitions, chromophores, Auxochromers, Bathochromic and Hypsochromic Shifts, Effect of solvent on electronic transitions, Woodward-Fieser rules for dienes, enones and aromatic compounds, Applications of U.V.

Infrared Spectroscopy

Characteristic vibrational frequencies of alkenes, alkynes, aromatic compounds, Carbonyl compounds, hydroxy compounds, amines and metal-ligand complexes. Factors affecting IR group frequencies, overtones, combination bands and Fermi resonance. Applications of IR.

Unit- V.

Nuclear Magnetic Resonance Spectroscopy **12 hrs**

Elementary Ideas, Chemical Shifts, Factors affecting chemical shifts, Spin-Spin couplings and coupling constants (J), Integration. Problems based on combined applications of UV, IR and NMR.

References Books :

1. The Determination of Molecular Structure : P. J. Wheatley
2. Physical Chemistry : G. M. Barrow
3. Instrumental Methods of Chem. Analy. Chatwal and Anand.
4. A Text book of Phy. Chem. : A.S. Negi & S. C. Anand
5. Instrumental Methods of Chemical Analysis - Willard, Merritt, Dean & Seatle
6. Instrumental Methods of Chemical Analysis - Chatwal, Anand
7. Instrumental Methods of Chemical Analysis - B.K. Sharma
8. Instrumental Methods of Chemical Analysis -R.D. Braun
9. Analytical Chemistry : Skoog and West
10. Principles of Instrumental Analysis : Skoog and West.
11. Fundamentals of Molecular Spectroscopy : Banwell.
12. Atomic and Molecular Structure : Manas Chanda
13. Molecular Spectroscopy : B.D. Acharya
14. Molecular Spectroscopy : Dyer.
15. Organic Spectroscopy : P.S. Kalsi (6th Edition).
16. Spectroscopic Methods in Organic Chemistry : D.H. Williams and I.Fleming.
17. Spectrometric Identification of Organic Compounds : R.M. Silverstein, Morril and G.C. Bassler
18. Introduction to Spectroscopy : Pavia, Lampman and Ktiz (3rd Edition)
19. Organic Spectroscopy : William Kemp (3rd Edition).
20. Quantum Chemistry- B. K. Sen
21. Inorganic Chemistry - Atkin and Shriver.

-

CHE-206 INORGANIC CHEMISTRY

Teaching hours: 60 **Credit : 04**

Unit -I : Spectroscopic term symbols: 12 hrs.

Terms, Inter-electronics repulsion, spin orbit coupling, ground terms, determination of terms symbol for d^1 to d^5 Configuration / complexes, Hunds rule, microstates. Racah Parameter. Weak and stronger field approach, correlation diagram of d^1, d^2, d^8 and d^9 configuration in octahedral and tetrahedral environments, Non-crossing rule, Orgel diagram of d^1 to d^9 configuration in an octahedral and tetrahedral environments, Tanabe Sugano diagram of d^2 and d^3 configuration of an octahedral environments.

Unit II : Electronic Spectra and magnetic properties of metal complex : **12 hrs.**

Types of experimental recording of the spectra, interpretation of electronic spectrum of transition metal complex with suitable examples, Band intensities, intensity of d-d bands, intensity of change transfer bands. Calculation of D_q, B and β parameters. Classification of charge transfer transitions and their mechanisms with suitable examples. Magnetic moment, electronic spectrum and structure of cobalt and Nickel complexes. ferromagnetic and anti-ferromagnetic behavior of compounds. Magnetic exchange coupling,

Unit III : Chemistry of Metal Carbonyls 12 hrs.

Classification; Chemistry of carbonyl group Preparation, properties, structures and bonding in - iron carbonyls, $Ni(CO)_4$, $Co_2(CO)_8$, $Mn_2(CO)_{10}$, $Cr(CO)_6$, $Mo(CO)_6$ and $W(CO)_6$, $Co_4(CO)_{12}$ and $V(CO)_6$. EAN rule applied to these carbonyls structures of mixed carbonyls of transition metals and EAN rule applied to these carbonyls. Preparations carbonyl halides

Unit IV: Metal nitrosyl compounds 12hrs.

Preparations and properties of Nitrosyl halides (NOX), Metal nitrosyl halides, compounds containing NO- group, Compounds containing NO+ groups, Preparation, structure and application of sodium Nitropruside. EAN and Eighteen electron rules applied to: Nitrosyl compounds of Cobalt, iron and Manganese. Significance of NO for the life of living animals

Unit-V : Dioxygen and Dinitrogen Complexes: 12 hrs.

Preparation of Cobalt containing dioxygen complexes, structural and functional analogy of cobalt dioxygen complexes with naturally occurring dioxygen complexes.

Preparation, properties and structures of dinitrogen complexes of Molybdenum, Structural and functional similarities with naturally occurring hemoglobin and nitrogenase protein and enzymes. Preparation, structure and bonding in Non-carbonyl metal clusters viz. Binuclear $(Re_2Cl_8)^{2-}$, Trinuclear $('ReCl_3)_3$, Tetranuclear $(W_4(OR)_6)$ and Hexanuclear $(Mo_6Cl_6)^{4+}$ ions. Preparation , properties and structures of Zintl anions & cation of the metal Ge, Sn, Pb, Sb, Bi

References Books:

1.Advanced Inorganic Chemistry Vol. I & Vol. II - By - Gurdeep and Raj.
2. Inorganic Chemistry (Principles, Structures and Reactivity) (Fourth Edition) By - J.E. Hubeey, E.A. Keitler, R.L. Keitler.
3. Inorganic Chemistry (IIIrd Edition) - By G.Y. Miessler and D.A. Tarr.
4. Advanced Inorganic Chemistry - Vol. I - By Satyaprakash, Tuli, Basu and Madan.
5. Selected Topics in Inorganic Chemistry - By W.U. Malik, G.D. Tuli & R.D. Madan.
6. Chemistry of the Elements - By N. N. Greenwood and A. Earnshaw.
7. Inorganic electronic spectroscopy, - A.B.P. Lever.
8. Symmetry and Spectroscopy of Molecules - K. Veera Reddy.
9. Physical Chemistry through problem - Dogra and Dogra.
10.Inorganic Chemistry - Attkin and Shriver.
11.Concise Inorganic Chemistry - By J.D. Lee.
12.Element of Magnetochemistry - By A.Samal & R. L. Datta.
13.Some aspect of Crystal Field theory- T. M. Dunn, D.S.Mcclure & R. G. Person
14.Introduction to Magnotochemistry- Alan Earnshaw
15.Introduction to Ligand Field - B. N. Figgis.-

CHE-207 ORGANIC CHEMISTRY

Teaching hrs: 60 **Credits: 04**

Unit-I: Aromatic Electrophilic and Nucleophilic Substitutions: [18 hrs]

Electrophilic Substitutions: The arenium ion mechanisum, orientation and reactivity, energy profile diagram. The ortho/para ratio, IPSO substitution, orientation in other ring system, Recapitulation of halogenation, nitration, sulphonation and Fridel Craft's reaction, diazonium coupling. **Nucleophilic Substitution:** The SN^{Ar}, SN^{1}, benzyne mechanisum, Effect of substrate structure, leaving group and attacking nucleophile on reactivity.

Unit-II: Addition to Carbon –Carbon multiple bond: [12 hrs]

Mechanisum and stereochemical aspect of addition reaction involving electrophile, nucleophile and frr radicals. Regioselectivity and chemoselectivity, orientation and reactivity, Michael addition, Sharpless asymmetric epoxidation.

Unit-III: Addition to Carbon–Hetero Multiple bond: [12 hrs]

Mechanisum of metal hydride reduction of saturated and unsaturated carbonyl compounds, acid, ester and nitriles. Addition of Grignard reagent, Organo zinc and organo lithium reagent to carbonyl and unsaturated carbonyl compounds. Wittig reaction. Mechanisum of condensation reaction involving enolates – Aldol, Knovenagel, Claisen , Mannich, Benzoin, Perkin, Stobbe reaction. Hydrolysis of esters and amides.

Unit-IV: Elimination Reactions: [12 hrs]

The E_1, E_2, and E_{1CB} mechanisum, orientation of double bond. Reactivity: effect of substrate structure, attacking base, the leaving group and the medium, pyrolytic elimination.

Unit-V: Rearrangements: **[06 hrs]**

General mechanistic consideration, nature of migration, migratory aptitude, memory effect, pinacole.pinacolone, Benzil–Bezilic acid, Beckmann, Hoffman and Fries rearrangements.

Reference Books:

1. Advanced Organic Chemistry, IV Edition: J. March
2. Advanced organic Chemistry, Part-A and Part-B: F. A. Carey, & R. J. Sundburg.
3. A Guide Book to Mechanisum in Organic Chemistry: Peter Sykes.
4. Synthetic Organic Chemistry: H. O. House
5. Principles of Organic Synthesis: R. O. C. Norman
6. Organic Chemistry: Clayden and Greeves
7. Mechanism and Structure in Organic Chemistry: E. S. Gould

CHE-208 PHYSICAL CHEMISTRY

Teaching Hours : 60 **Credits: 04**

Unit - I: Quantum Chemistry: I **12 hrs.**

The Schrodinger equation, particle in a one dimensional box, Eigen values and Eigen functions, operators, properties of quantum mechanical operators, Hermitian, Linear, Ladder, Hamiltonian and angular momentum operators.

Particle in three dimensional box, harmonic oscillator, rigid rotator and numericals.

Unit - II: Quantum Chemistry: II **12 hrs.**

Term symbols and selection rules, spin-orbital coupling, the variation theorem, non-degenerate perturbation theory and applications. Huckel molecular orbital theory of conjugated systems, application to ethylene, butadiene, cyclopropenyl radical , cyclobutadiene and benzene, numericals.

Unit –III : Phase Rule: **12 hrs.**

Recapitulation of phase rule and terms involved in it, one component system, two component systems (solid-solid, solid-liquid and liquid-liquid), reduced phase rule, three component systems, partially miscible three liquid systems : one partially miscible pair, two partially miscible pairs, three partially miscible pairs, systems composed of two solids and a liquid : crystallization of pure components only, formation of binary compounds, formation of ternary compounds, formation of solid solutions, partial miscibility of solid phases, numericals.

Unit –IV : Crystallography **12 hrs**

Classification of solids on the basis of shapes, and bonding, crystal lattice and unit cell, laws of crystallography crystal symmetry, symmetry elements, lattice planes and their designations, liquid crystals.

Principle of crystal structure. close packing of atoms, packing of equal sized spheres in HCP, CCP, BCC structures. packing in ionic solids, ionic radius, radius ratio rule, (3, 4, 6, 8 coordinate structures). octahedral and tetrahedral voids, isomorphism and polymorphism, numericals.

Unit –V : Photochemistry **12 hrs.**

Absorption of light and nature of absorption spectra, electronic transitions. photo-dissociation and pre-dissociation. photo-oxidation, photo-reduction and photo-dimerization. photo-physical phenomenon. Jablonski diagram. photo-physical pathways of molecular de-excitation, difference between delayed fluorescence and phosphorescence, Stern-Volmer equation, deviations from Stern-Volmer equation, concentration dependence of quenching and eximer formation, quenching of fluorescence formation of excimer and exciples.

References Books:

1.Quantum Chemistry : Ira N. Levine
2.Quantum Chemistry : R.K. Prasad
3.Quantum Chemistry : B.K. Sen
4.Principles of Physical Chemistry : Puri, Sharma, Pathania
5.Advanced Physical Chemistry : Gurdeep - Raj, Plenum.
6.Physical Chemistry : Maron and Prutton
7.Introduction to Molecular Photo-chemistry : C.H.J. Wells
8.Fundamentals of Photo-chemistry : Rohatgi-Mukherjee.
9.Photo-chemistry : J.G. Calvert & J.N. Pitts.
10.Ptoho-luminiscence of solutions : C.A. Parker.
11.Photo-chemistry : A. Singh and R. Singh
12Atkin's Physical Chemistry : Peter Atkins

13.Solid State Chemistry : D.K. Chakraborti
14.Solid State Chemistry and its applications : A.R. West.
15.The Determination of Molecular Structure : P.J. Wheatley.
16.Solid State Chemistry : N.B. Hannary.
17.Principles of Solid State : H.V. Keer.
18.Physical Chemistry : G.K. Vemulapalli.

-

CHE -210 (A & B) LABORATORY COURSE (INORGANIC)

Laboratory work hours: 180 hrs. **Credit : 06**

List of experiments

I) Semi micro Qualitative Inorganic analysis. **08 mixtures**

Identification of basic radicals including one rare earth and three common metal ion and one interfering acidic radical using semi micro qualitative analysis method

Note : Each mixture should contain different rare earth elements

II) A. Separation and estimation of metal ions from the following binary mixture solutions : **Any[04]**

1. Copper- Nickel 2. Copper- Iron 3. Nickel- Zinc
4. Iron- Magnesium 5. Copper- Barium 6. Iron –Aluminium

III).Synthesize, characterization and estimation of metal ion from the metal complexes. **Any [07]**

1. $Ti(C_9H_8NO)_2.2H_2O$ 2.$VO(acac)_2$ 3.Cis-$K[Cr(C_2O_4)_2(H_2O)_2]$
4. $[Mn(acac)_3]$ 5.$K_3[Fe(C_2O_4)_3]$ 6.$[Co(II)(Py)_2Cl_2]$
7. $[Co(III)(NH_3)_6]Cl_3$ 8.$[Co(III)(NO_2)(NH_3)_5]Cl_2$ 9.$[Ni(NH_3)_6]Cl_2$

Note : i).Synthesis should be carried out using (0.02 to 0.06 mole) of the starting materials.
ii). Practical Yield, % yield, theoretical yield and percentage of metal ion content should be recorded

IV) Paper Chromatography : **Any [02]**

1.Determine the R_f Values of Silver lead and Mercury by paper Chromatographic method.
2.Determine the R_f Values of Copper, Cadmium and Mercury by paper Chromatographic method
3.Determine the R_f Values of Nickel, Manganese and Zinc by paper Chromatographic method
4.Determine the R_f Values of Barium, Calcium and Strontium by paper Chromatographic method
Note : Submit the Paper chromatograph for verification with R_f values.
Note : Student will not be allowed for practical examination if his/her record book is not completed and certified.

Reference Book:

1. A Text book of Micro and Semi micro Qualitative Inorganic Analysis ; IV edn, A. I. Vogel
2. A Text book of Quantitative Inorganic Analysis; A. I. Vogel
3. Practical Inorganic Chemistry; Pass Geoffrey and Haydn Sutcliffe.
4. Advanced Practical Inorganic Chemistry; Gurudeep Raj;.
5. Vogel's Qualitative Inorganic Analysis, D. Svehla, VII Edn.Orient Longman Ltd.

Scheme of Marking:

I Semi micro Inorganic analysis: 25 Marks

i). Preliminary Test : [max. marks:02]
ii). Group identification: [max. marks:06]
iii). Step wise analysis of groups : [max. marks:05]
iv).C.T of Acidic/Basic radicals : [max. marks:06]
v). Spot test : [max. marks:06]
Note : At least one spot test for each radical should be performed and be reported

II) Separation and Estimations: 20 Marks

i). Flow chart of separation : [max. marks;02]
ii). Estimation of first component by gravimetric / volumetric method , observation table, : [max. marks:08]
iii). Estimation of second component by gravimetric / volumetric method, observation table : [max. marks:08]
iv). Correct calculation & reporting results : [max. marks:07]

III) Synthesis & estimation of Metal Complexes 20 Marks

i). Spectral Analysis (UV/IR) : [max. marks :04]
ii). Yield of complexes : [max. marks: 04]
iii). Estimation of metal percentage by gravimetric / volumetric method, observation table, : [max. marks: 08]
iv). Correct calculation & reporting of results : [max. marks: 04]

IV) Paper Chromatography : **10 Marks**

i) Submission of paper chromatograph: [max.marks:05]
ii). Correct calculation & reporting of results : [max. marks:04]
V) Record Book & Viva : [max .marks 05]

CHE -211 (A & B) LABORATORY COURSE (ORGANIC)

Laboratory work hours: 180 hrs. **Credit : 06**

List of experiments:

1) Qualitative Organic Analysis: **[30 Marks]**

Separation, purification and identification of binary mixtures.
The separation should be carried out using ether/ dichloromethane.
The two components may be solid-solid, solid-liquid or liquid-liquid (non-volatile).
The water soluble solid/liquid should also be given.
Student should submit the purified samples of the separated compounds and prepare a suitable derivative of the two compounds separated out.

Note : Analysis of at least ten mixtures should be carried out.

1) **Single Stage Preparations**: [**15 Marks]**

i) Benzaldehyde to cinnamic acid (Perkin Reaction).
ii) o-Iodo or o-chlorobenzoic acid from Anthranilic Acid.
iii) β-benzoyl propionic acid from succinic anhydride and benzene (Friedel-Craft reaction)
iv) p-nitro acetanilide from acetanilide.
v) p-nitrobromobenzene from bromobenzene.
vi) Dibenzal acetone from Benzaldehyde
vii) Salicylaldehyde from phenol (Reimer-Tiemann Reaction**).**

Note:

i) The preparations should be carried out using (0.02 to 0.05 mole) of the starting material.
ii) The yield, melting point and TLC of the recrystalised product should be recorded.
iii) The sample of the purified product and TLC plate should be submitted for inspection.

Note : Student will not be allowed for practical examination if his/her record book is not completed and certified.

Scheme of Marking:

1. Qualitative Organic Analysis

	Marks
Type of the mixture	06
i). Analysis of the individual components:	
ii). Detection of Elements	03
iii). Detection of functional groups	02
iv). Determination of MP/BP	03
v). Preparation of the derivative	02
vi). Identification (Spotting)	02
2. Preparation	
i). Yield of the recrystallized product	05
ii). MP of the recrystallized product	05
iii). TLC of the recrystallized product	05
3) Record Book + Viva voce	05

CHE -212 (A & B) LABORATORY COURSE (PHYSICAL)

Laboratory work hours: 180 hrs. **Credit : 06**

List of experiments

A. Instrumentation.

1.Determination of strengths of halides in a mixture potentiometrically.
2.Determination of dissociation constants of phosphoric acid potentiometrically.
3.Determination of dissociation constants of weak acid potentiometrically.
4.Determination of acidic and basic dissociation constants of an amino acid and its isoelectric point.
5.Determination of the strength of strong and weak acid in a given mixture conductometrically.
6.Determination of solubility and solubility product of sparingly soluble salt $BaSO_4$.
7.Study of kinetics of inversion of cane sugar.
8.Determination of equilibrium quotient for the formation of monothiocynato iron (III) complex.
9.Determine the indicator constant of given indicator by colorimetric measurements.
10.Determine the pK_1 and pK_2 value of phosphoric acid by pH metry.
11.To study the kinetics of mutarotation of glucose/fructose potentiometrically.

B. Non-Instrumentation.

1. Determine the molecular refraction of methyl acetate, ethyl acetate, n-hexane and carbon tetrachloride and calculate the refraction of CH_2, C, H and O atoms.
2. To study the effect of surfactants (sodium chloride) on surface tension of given liquid.
3. To determine the radius of molecule by viscosity measurements.
4. To study the adsorption of acetic acid from aqueous solution by activated charcoal and examine the validity of Freundlich and langmuir's isotherm.
5. To construct the phase diagram for three component system (chloroform-acetic acid-water).
6. Determine the solubility of benzoic acid in water at different temperature and hence its heat of solution.
7. Determine the velocity constant of hydrolysis of ester.
8. To study auto catalysis reaction between potassium permanganate and oxalic acid.
9. Determine the rate constant of the reaction between potassium persulphate and potassium iodide having equal/unequal concentration of the reacting species.
10. Determine the formula of the complex formed between Cu(II) and ammonia by distribution method.
11. To study the variation of viscosity with the composition of mixtures (ethanol-water-HNO_3-chloroform) and to determine the formation of complex between two liquids.

-

Note : Student will not be allowed for practical examination if his/her record book is not completed and certified.

Scheme of marking :

1) Experiment I (Instrumentation)	Max .Marks	Experiment -II (Non-instrumentation) Max. Marks
i) Observation :	10	0 8
ii) Calculation :	05	04
iii) Graph :	05	04
Accuracy& Results :	05	04
Record book & Viva :	05	05

DR. BABASAHEB AMBEDKAR MARATHWADA UNIVERSITY, AURANGABAD

Department of chemistry

Revised Syllabus

M.Sc. III & IV Semester Inorganic Chemistry

Effective from June 2012

Effective from June 2012

The following will be the structure for revised syllabus for M. Sc. Inorganic Chemistry III & IV semester effective from June 2012

Semester	Paper Nos.	Title of Paper	Durations (Hr)	Max. Marks	Credits
III- Semester	CHE-313		60	50	4
	CHEI- 314	Bioinorganic and supramolecular Chemistry	60	50	4
	CHEI-315	Applied Inorganic Chemistry	60	50	4
	CHEI-316	Chemistry of materials	60	50	4
	CHEI-317	Theoretical and structural Inorganic Chemistry	60	50	4
IV semester	CHEI: 418	Nuclear Chemistry	60	50	4
	CHEI: 419	Photo-inorganic Chemistry	60	50	4
	CHEI: 420	Therapeutic Bioinorganic and Chemistry of Forensic materials	60	50	4
	CHEI: 421	Organo-transitionmetal chemistry	60	50	4
	CHEI (PR) (a&b)- 422	Inorganic Chemistry Practical	180	50	6
	CHEI (PR) (a&b)- 423	Inorganic Chemistry Practical	180	50	6
	CHEI (PR) (a&b)- 424	Inorganic Chemistry Practical	180	50	6

CHEI- 314 Bioinorganic and Supramolecular Chemistry

Duration : 60 hrs **Marks : 50 Credit : 04**

.

Unit- I . Metalloenzymes: [12 hrs]

Structural and functional relationships and mechanisms of enzymatic reaction in the following metalloenzymes. **Zinc Enzymes:** carbonic anhydrase and carboxypeptidases, **Copper Enzymes**: super oxide dismutases **Iron Enzymes:** catalase and peroxidases, **Molybdenum Enzymes:** nitrogenase and xanthanine oxidase,**Coenzyme Vitamin:** B-12

Unit-II. Metal Nucleic Acid Interactions: [12 hrs.]

Introduction, nucleic acid structures, structures and binding sites in nitrogen bases, phosphates and sugar base. Coordination complexes of nucleic acids and their bases with metal ions. Hydrogen bonding, redox reaction and hydrolytic reaction of nucleic acids mechanisms of these reactions, natures role, pharmaceutical role, catalytic role

Unit-III . Molecular Recognition: [12 hrs]

Basic concepts and principles of supramolecular chemistry, Host-Guest interactions, spherical recognition, anionic receptors, porphyrin-sapphyrin systems, organometallic receptors, tetrahedral multiple and neutral molecular cleft recognition, enzyme models, molecular receptors, design and synthesis.

Unit - IV. Supramolecular reactions and catalysis [12hrs]

a. Catalysis by anion, cation and metal receptor molecules and co catalysis.

b. Molecular and supramolecular devices : likes Photonic, Electronic and ionic devices..

Unit-V: Techniques in Bioinorganic chemistry: **[12hrs]**

Principles and applications of electronic spectroscopy, IR spectroscopy, NMR spectroscopy, Raman spectroscopy

Reference Books:

1. Bioinorganic chemistry By:-Bertini Ivano, Gray H. B., Lippard S. J. & Valentine J. S.
2. Principles of Bioinorganic chemistry By:- S. J Lippard & M. J. Berg
3. Inorganic Biochemistry, (Vol.I & II) By:- G. L. Eicchorn.
4. Bioinorganic chemistry :- A. K. Das.
5. Bioinorganic chemistry - R. W. Hay.
6. Bioinorganic chemistry - Chatwal G. R. & A. K. Bhagi.
7. Supramolecular chemistry -Lehn J. M.
8. Bioinorganic & Supramolecular chemistry - Chatwal G. R. & A. K. Bhagi.
9. Bioinorganic, Bioorganic & Supramolecular chemistry By:-Kalasi P. S.
10. Supramolecular organometallic chemistry By:- j. L. Atwood and Jonathava W. steed, Macel Jekkar Publisher
11. Supramolecular Organometallic chemistry -Jean Marie-Lehn.

.

-

CHEI-315 Applied Inorganic chemistry

Duration : 60 hrs **Marks : 50 Credit : 04**

Unit -I. Basic concept of zeolites: [12 hrs]

Introduction, definition, classifications on the basis of morphological appearance, SBU, substitution of other iso-electronic metal ions, types of pore size. Lowenstein's rule. pore and channels, channel dimensions, shape of the pore opening, nomenclature of zeolites, structural aspect of zeolites, acidity of zeolite, identification of acidic sites, nature of active sites, synergetic effects, shape selectivity.

Unit-II Synthesis of zeolites [12 hrs]

General methods for synthesis of zeolite, hydrothermal treatment, mechanism of aluminosilicate formation during Sol-Gel, co-precipitation process, factors affecting the zeolite formation, Needs of modification of zeolites, general procedure for modification of zeolites, Oswald's rules of successive transformation, crystallization and its identification, factors affecting crystallization, template theory, organic additives, crystallizing zeolites, ZSM-5 from an organic free solvent system, synthesis in nonaqueous solvents.

Unit -III Characterization and applications of zeolite [12 hrs]

General characterization techniques used for analysis of zeolites, Details on FTIR, Pyridine adsorbed- IR analysis, XRD analysis, ^{27}Al MAS NMR and ^{29} Si MAS NMR analysis , Temperature programmed desorption (TPD), probe molecules for TPD analysis , measurement and analysis with suitable examples. Application of zeolites: softening of water, Agriculture, catalyst in organic transformations at least ten examples.

Unite -IV. Basic Chemical Calculations: [12 hrs.]

Moles**,** mole percent composition, mole fraction, weight & volume percent analysis of solid in composition, **Material balance involving chemical reaction:** Introduction, material balances, definition of terms, Concept of Selectivity, Conversion, Principle of green chemistry, Atom economy, numericals.

Unit-V. A). Manufacturing process : [12 hrs.]

Hydrochloric acid, Sulphuric acid, Nitric acid, Calcium carbonate, Alum

B). Explosive and propellant: General characteristics, Classification, Manufacturing process in outline.

C). Pigment and Paints: Introductions, white pigments, Manufacturing process and properties of blue pigment, red pigment, green pigment, yellow pigment. Paints: Constituent of Paint, manufacture of paints, requirement of good paints, paints failure, different type of paints.

Reference Books:

1.Molecular sieves: Principles of synthesis and Identifications R-Szostak.

2. Atlas of zeolite framework type; Ch. Barlocher, W M. Meier , D. H. Olson; 5th rev. Ed. Elsevier Amsterdam 2001

3.Stoichometry (SI Units): B.I. Bhatt & S.M. Vora.

4. Molecular Sieves Science and technology ; H. G. Karge, J Weitkamp Vol I to V , Springer

4.Industrial chemistry: B.K. Sharma, Goel publishing house, Meerut,

-

CHEI-316 : Advances in material chemistry

Duration : 60 hrs **Marks : 50 Credit : 04**

Unit- I : General introduction & synthesis of nanomaterials by physical methods: [12 hrs]

Objective of study, synthesis of nanoparticles by physical method, mechanical methods- high energy ball milling, melt mixing, method based on evaporation, physical vapour deposition with consolidation. Ionized cluster beam deposition. Laser vaporization, Laser pyrolysis, sputter diposition, electric arc deposition, Chemical Vapour Deposition (CVD).

Unit- II : Synthesis of Nanomaterials by Chemical Methods : [12hrs]

Introduction, colloids and colloids in solution, interaction of colloids and medium, colloids in vacuum, colloids in medium, effect of charge on colloids, stearic repulsion, synthesis of colloids, growth of nanoparticles, synthesis of metal and semiconductor nanoparticles by colloidal route, Langmuir-Blodgett (L-B) method, sol gel method, electrochemical method.

Unit-III : Analysis Technique : [12hrs]

Introduction, microscopes, electron microscopes,SEM, TEM, Scanning probe microscope (SPM), Scanning Tunnelling microscope, Atomic force microscope, X-ray diffraction, UV-visible and IR spectroscopy.

Unit-IV : Properties, types and application of Nanomaterials: [12hrs]

i).Properties of nanomaterials – Mechanical, electrical, optical, magnetic, semiconductor.

ii).Some special nanomaterials – Carbon nanotubes, porous silicon, Arogels, Zeolites.

iii).Application – Electronic, energy automobiles, sport and toys, textile, cosmetics, domestic appliances, biotechnology, medical, space, defence & environment.

Unit-V : Imperfections in solids: [12hrs]

Perfect and inperfect crystal, point defects, stichometric defects, Schootky & Frankle defects, thermodynamics of their formation, colour centres, Non-stichometric defects, metal excess and metal deficiency defects, line inperfections, Edge dislocation, Screw dislocation, Burgers circuits, Surface inperfections, grain bounderies & stacking falts.

Theories of solid states – free electron theory, band theory, refinement to simple band theory.

Reference Books:

1) Solid State Chemistry and applications- A.R. West (John Wiley and Sons)
2) Principles of the Solid State- H.V. Keer (Wiley Eastern Limited)
3) Nanotechnology: Principles and practices- Sulabha K. Kulkarni (capital Pub. Co.)
4) NANO- The next revolution –Mohan Surendra Rajan(Natioinal book Trust, India)
5) The British Glass Website- Types of Glass://www.britiglass.org.uk.
6) Fundamental of Nanotechnology – Gabor L. Hornyak, John J. Moore, Harry F. Tibbals, Joydeep Dutta.
7) Recent advances in the liquid phase synthesis of Inorganic Nanoparticles- B. L. Cushing , 8) V. L. Kolesmichenko & C.J.O".Connor Chemical Review 104, 3893-3946.(2004)

--

CHEI-317 Theoretical and structural inorganic chemistry

Duration : 60 hrs **Marks : 50 Credit : 04**

Unit- I Applications of theoretical models to chemical compounds. [12 hrs.]

Valence bond model: theoretical concept of hybridization, construction of wave functions for sp, sp^2, sp^3, dsp^2 and d^2sp^3 hybridizations. Identification of nature of bonds, Application of VSEPER theory to covalent bonded anionic compounds.

Unit- II Crystal field theory : [12 hrs.]

Important feature of CFT, crystal field splitting d orbital in octahedral , tetrahedral, square planer and tetragonal complexes, factors affecting 10Dq, application of CFT , CFSE and their uses, limitation of CFT

Unit III. Molecular orbital Theory : **[12 hrs.]**

Basic principles of MOT, linear combination of atomic orbitals, construction molecular orbital wave function of H_2, H_2^+, H_2^- HCl. Molecular orbital energy level diagram of poly atomic molecules (NH_3, BF_3, BeH_2, CO_2, H_2O, NO_2^-, CO_3^{--}, octahedral , tetrahedral , square planer complexes).

Donor acceptor chemistry of NH_3: BF_3, BF_3 : $O(C_2H_5)_2$, Br_2 : CH_3OH adducts. π- Molecular orbitals of planer C_nH_n molecules, HOMO -LUMO energy, correlation of HOMO- LUMO energies with ionization energy, electron affinity, hardness and reactivity of molecules. Overviews on computational approaches for calculation of molecular properties. Molecular term symbols with suitable examples.

Unit IV –Chemical forces and its importance: **[12 hrs.]**

Types of chemical forces, covalent bonding, ionic bonding, dipole-dipole interaction, induced dipole interactions, dipole-induced dipole interactions, with suitable examples, interpretation of hydrogen bonding interactions in common organic compounds , solubility of ionic substances, ion solvent interactions with examples, Polarity of solvent, factors affecting the polarity of solvents, importance of polar and non polar solvent in chemical reactions.

Unit -V Chemistry of main group elements [12 hrs]

Synthesis, structure and properties of Borazines, phosphazenes and their polymers, Hetrocyclic inorganic systems, Sulfur- nitrogen chain and ring compounds, Xenon compounds, interhalogens compounds, Structural aspect of oxy acid of phosphorous, sulfur, nitrogen and halogens

References books:

1. Inorganic Chemistry - J E Huheey
2. Concept and models of Inorganic chemistry – Bodil E Douglas and Darl H McDaniel , Oxford & IBH Pub. Co.
3. Inorganic chemistry- Gary L Miessler, Donald A Tarr 3rd Edn
4. Inorganic chemistry – Puri and Shrma
5. Inorganic chemistry – J D Lee
6. Inorganic chemistry- Attken
7. Quantum chemistry and spectroscopy- Engel
8. Physical chemistry - A molecular approach – Donald A McQuarrie , John D Simon

--

CHEI: 418 Nuclear Chemistry

Period : 60 hrs. **50 Marks** **Credit : 04**

Unit- I Nuclear particles and its properties **[12 hrs]**

The fundamental particles, roll call of elementary particles, composition of the nucleus, theories of nuclear composition, nuclear properties, mass defect and binding energy, nuclear stability explained by different factors.

Nuclear size and density, mechanical effects due to orbiting and spinning of nucleons, orbital angular momentum of the nucleons, Total angular momentum of the nucleons, magnetic quantum numbers, principal and radial quantum numbers, total angular momentum of nucleus, total magnetic nuclear angular momentum quantum number, magnetic properties of the nucleous, the neutron magnetic moment, the structure of nucleon the net magnetic moments, The spin of odd Z odd N nuclei, The Nordhein rule.

Unit- II Nuclear models : **[12 hrs.]**

The shell model and its salient features, periodicity in nuclear properties- magic numbers, forces of nuclear potential, energy level in nuclear potential well, the sequence of filling the orbital including models, nuclear configuration. The liquid drop model, and its details and The Fermi gas model.

Unit III Radioactivity: **[12 hrs.]**

Historical, background, natural radioactive elements, general characteristics of α, β, γ rays, detection and measurement of radioactivity, the theory of radioactive disintegration, decay kinetics, units of radioactivity, parent daughter growth relationship- secular and transient equilibrium, theory of α decay, β decay – energetics of β decay problems of β decay, fermis theory of β decay, nuclear de-excitation – emission, numerical

Unit-IV Nuclear Reactions. **[12 hrs.]**

Definition and Bethes notation, nuclear reaction energetic, nuclear reaction and threshold energy, characteristics of nuclear reactions, types of nuclear reactions, conservation in nuclear reactions, nuclear reactions cross section, cross section and reaction rate, the compound nucleus theory, general properties of compound nucleus, optical model, direct interaction model, specific nuclear reactions- photonuclear reactions, stripping and pickup reactions evaporation, spallation, fragmentation, direct nuclear reactions, thermonuclear reactions.

Unit - V Radiation chemistry and its applications **[12hrs]**

A. Introduction of radiation with matter, primary effects due to charged particle/radiation, Linear energy transfer(LET), Bethes equation for LET, Bremsstrahulung, the cerenkov radians, interactions of electron with matter, interaction of neutrons with matter, interaction of heavy charged particles with matter, interaction of rays with matter, units for measuring radiation absorption, absorption in water **B.** Typical reactions involved in the preparations of isotopes: the scillard-chalmers reactions, radiochemical principles in the use of tracers, typical application of radioisotopes as tracers- chemical investigation, physio-chemical research, analytical applications, agricultural applications, industrial applications, use of nuclear radiations, radioisotope as a source of electricity

Reference Books.

1. Source of Atomic energy by s. Glasstance, D. Van Nostrand co. INC
2. Essentials of nuclear chemistry by H.J. Arnikar 4th Edn, New Age International(p) Ltd.
3. Introduction to Nuclear By chemistry B. G. Harvey,
4. Nuclear chemistry by M. G. Arora & M. Singh Anmol publication, New Delhi
5. Elements of nuclear chemistry by A. K. Srivastav, P. C. Jain, S. Chand & Co.
6. A text book of Nuclear chemistry by C.V. Shekar Deminant publication & distribution, New Delhi.
7. Radiochemistry & nuclear chemistry, 3rd edn G. chappin, Butterwerth-Heinemann.

CHEI :419 Photoinorganic Chemistry

Duration : 60 hrs **Marks : 50 Credit : 04**

Unit –I Basic concept of Photo Chemistry: [12hrs]

Introduction to photochemistry, laws of photochemistry, Quantum yield, deviation in quantum yield, Experimental determination of quantum yield, Quantum yield and reactivity, life time of electronically excited state, kinetic aspects of photochemical reactions, temperature dependence of photochemical reaction, Methods used to study the kinetics of photochemical reaction: Flow methods, flash photolysis methods, numerical on quantum yield calculations.

Unit- II Physical properties of electronically excited molecules : [12 hrs]

Nature of changes on electronic excitation, potential energy diagram, shapes of absorption bands and franck condon principal, emission spectra, environmental effect on absorption and emission spectra. **Photo physical process in electronically excited molecule:**Types of physical pathways, Jablonski diagram, theory of radiationless transition, theory of radiative process, bimolecular quenching, experimental results.

Unit III. Excited States of Metal Complexes: [12 hrs.]

Ground and Excites states of d1 to d10 configurations, Ligand field excited states of Co(II), Cr(III), Ru(II), Ru(III), Fe(II) and Rh(III) in an octahedral omplexes, Excited states of organic ligand with examples, selection rules for electronic transitions. **Charge transfer photochemistry** : Introduction, charge transfer absorption spectra, types of charge transfer excitations and their energy level scheme for charge transfer excitations, Types of reactions observed by CTTM, Models of photoredox system.

Unit-IV. Ligand field photo chemistry of transition metal complexes : [12hrs]

Photochemistry Cr(III) of complexes : Photo-substitutions, properties of ligand field excited states ,Photo aquation reactions, photolysis rule , photoisomerization , photo recimization, photoanation reactions, sensitizer, energy transfer process, Mechanism of photo sensitization, photo reactive excited state, The Doublet hypothesis, Role of quartet excited states, Photochemistry of Co(III) complexes : Introduction, energy level diagram, Photoaquations in Co(III) amine, Co(III) cynide complexes, Fe(II) low spin complexes., Ru(II) ammine derivative complexes, Photo redox properties of (Ru(III) complexes, Ce(III) and Ce(IV) complexes, photochemistry of Cu(II) (1,3 diketone) complexes,

Unit-V. Photochemical reactions on solid surface: [12hrs]

Introduction, photo electron transfer mechanism, energy level diagram of solid acceptor and donor levels, Examples of photo catalytic metal/mixed metal oxides and their applications, semiconductor supported metal oxides for Photolysis of water, Decomposition of organic pollutants, experimental setup, and end product of organic moieties. OLED, Solar energy conversion and its storage.

Reference Books :

1. Concepts of Inorganic Photo chemistry, W. Adamson ,
2. Inorganic spectroscopy , A. B. P. Lever
3. Symmetry and spectroscopy of Molecule, K. Veera Reddy,
4. Inorganic Chemistry, J. E. Huhey
5. Fundamental of Photochemistry, Rohatgi Mukherjee
6. Inorganic chemistry , Attkin and shriver
7. Advanced Inorganic Chemistry, Gurdeep Raj.
8. A. W. Maverick and Harry B. Gray , Pure and applied chemistry, 52, 2339- 2348
9. Peter C Ford, The Photosubstitution Reactions of Rhodium (III) Ammine complexes, Journal of Chemical Education, 60, 10, 831, (1983).
10.Richard J Watts, Ruthenium Polypyridyls, Journal of Chemical Education, 60, 10, 835, (1983).
11.J. N. Demas, Photophysical Pathways in metal complexes, Journal of Chemical Education, 60, 10, 803, **(1983)**
12.L. D. Kirk, , Chromium Ammines and Acidoammines, Journal of Chemical Education, 60, 10, 843, **(1983)**
13. D. Chatterjee , Visible light induced photo degradation of organic pollutants on dye Adsorbed TiO_2 surface : Bull. Cat. Soc. of. India 2,,56-58, **2004**

M. Sc. Inorganic chemistry Semester -IV

CHEI- 420 Therapeutic Bioinorganic and chemistry of forensic materials

Duration : 60 hrs **Marks : 50 Credit : 04**

Unit- I: Metal ions in carcinogenesis: [12 hrs.]

General and biochemical aspects of cancer, carcinogens and anticancer agents. Carcinogenesis and its mechanism. Role of metal complexes and Pt(II) and (IV) as anticancer agents, anticancer activity of rhodium, gold, copper, and cobalt complexes. Selenium and its biochemical role and its mechanism of cacinostatic actions. Some representative metallodrugs containing arsenic, antimony, gold, mercury and tin metal. Antibacterial, antifungal and antiviral activity of metal; complexes.

Unit- II: Chemistry of Forensic Materials [12 hrs]

Forensic toxicology, legal definition of poison and toxinology, human and cattlepoison, and its antidotes. Principle underlying removal of poison from the body and use of antidotes, corrosivepoison and its classification. Common household poisons. Characteristic sign, symptoms, treatment and medicolegal aspects of common household poisons, classifications of poisons according to their mode of action.

Unit- III: Concepts on metal ion toxicity [12 hrs]

Metal ion toxicity in man and animals. Introduction, general aspects of Pb(II), Cd(II), and Hg(II), biochemical and physiological effects caused due to Pb(II), Cd(II), and Hg(II) ion toxicity. Detoxifications of this metals using chelating agents.

Unit- IV: Interactions of metal ions and metal complexes [12 hrs]

Structure and functions of amino acids, proteins, peptides, enzymes nucleoside, nucleotide and comparative study of structures and functions of these biomolecules. Metal ion binding sites present in amino acids, peptides, proteins,enzymes, nucleoside and nucleotide. Interactions of metal ion and metal complexes with these biomolecules.

Unit – V Physical methods in Bioinorganic chemistry : [12 hrs]

A). Electrophoresis method : Types of electrophoresis , principles and applications of capillary electrophoresis , analysis of bands using different methods **B). Centrifugation methods** : Basic principles of sedimentation, types of centrifuges and rotors, types of centrifugations and applications.C). Spectrophotometerics method : UV- visible spectroscopic techniques and their applications.

Books Suggested

1. Inorganic biochemistry – by Guther L. Eicchornvol 1 and 2 volume (Elsevier Scientific Publishing Company Amsterdam 1973, London New York.
2. Pharmacological basis of therapeutic, 5th and 6th edition by –Louis S. Goodman, (Macmillan Publishing company…INC, New York, Toronto and London)
3. Metal ions in biological system by- Helmut Sigel. Vol. l9 21, 22 - (Marcel Dekker INC, New York and Basel)
4. Metal ions in biological system (Concepts on metal ion toxicity) by Helmut Sigel. Vol.7- (Marcel Dekker INC, New York and Basel)
5. Modi's Medical Jurisprudence and Toxicology 22nd Edition.
6. Parikh's Textbook of Medical Jurisprudence, Forensic Medicine and Toxicology (Six Edi8tion) By C. K. Prikh. (CBS Publishers & distributors 4596/1A 11, Daryagaing New Delhi- 11002
7). Bioinstrumentations – L Veerakumari , MJP publisher Chennai
8). Principles of bioinorganic chemistry – S. J Lippard & J M Berg , Mill Valley californua
9) Elements of BVioinorganic - G N Mukherjii, and Arbinda Das U N Dhur and Sons Pvt. Ltd Kolkatta

CHEI: 421 Organotransition Metal Chemistry

Period : 60 hrs. **50 Marks**

Unit- I .A). General Properties of Organotransition Metal Compounds [12 hrs]
Definition, Classification based on the number of coordinated carbon (Hapticity), number of electrons donated by ligands, and type of bonding. Nomenclature, 16, 17, 18 Electron complexes and ligand substitutions, electron counting for common ligands and geometry of organo tranisition metal compounds.

B)

Unit – II .A) Alkyl ,aryl Carbene and carbine transition metal compounds. [12 hrs]
General method of synthesis of alkyl and aryl transition metal compounds, (i.e Ti, V, W, Mn, Ir, Co, Fe), Chemical properties, stability and decomposition pathways.

Carbene transition compounds: Types of carbine compounds, properties of carbene ligands, Synthesis of Fischer type carbine compounds, Chemical reaction on coordinated carbine compounds **.Carbyne transition metal compounds :** Synthesis and chemical properties

Unit- III.Transition metal compounds with Unsaturated organic molecules: [12 hrs.]
η^1 alkene transition metal compounds : General methods of the synthesis, Chemical properties: Reaction with nucleophiles and Electrophiles, Structure and bonding (DCD model) **η^2 alkyne transition metal compounds:** Introductions, preparation, chemical properties, Structure and bonding. **η^3 allyl transition metal compounds:** Introduction, Structural verities in allyl transition metal compounds, General methods of preparation, chemical properties, structure and bonding.**η^4 butadiene transition metal compounds:** Introduction, General methods of preparation, reaction on coordinated ligand, structure and bonding. **η^4 Cyclobutadiene transition metal compounds:** Preparation and chemical properties of $(C_4H_4)Fe(CO)_3$, structure and bonding.**η^5Cyclopentadienyl transition metal compounds:** Introduction, classification of η^5- Cyclopentadienyl derivatives, Preparation and chemical properties of $(\eta^5\text{-}C_5H_5)_2Mn$, $(\eta^5\text{-}C_5H_5)Mn(CO)_3$, structure and bonding in Ferrocene.

Unit- IV Synthetic and catalytic aspects of organotransition metal compounds [12hrs]
Introduction, catalyst, catalysis, homogeneous and heterogeneous catalyst, stoichiometric reagent, role and limitations of stoichiometric reagents, applications of organoboron, organocopper, organoaluminium in organic synthesis.

Unit- V) Organotransition metal compound as catalysts and synthetic reagents [12 hrs]
Activation process: consequent changes in the coordinated ligand reactivity, template effect. **Protection:** Sterric control, facilitation of nucleophilic addition reactions. **Product isolation:** Reductive elimination, β-eliminations, radical formation, alkene or arene displacement by competing ligand, electron transfer from metal atom to an oxidant, release of carbenoid ligands. **Catalytic processes involving organotransition metal compound:** Hydrogenation of alkene using wilkinson's catalysts, hydrosilation reaction, hydroformulation of alkene (oxo process) Ziegler Natta polymerizations. Fischer Tropsch process, water gas shift reaction. Monsanto process for acetic acid synthesis., Wacker process of oxidation of alkene.

Reference Books:

1. Organo metallic Chemistry, R. C. Mehrotra, & A. Singh
2. Principal and applications of organotransition metal Chemistry, J. P. Collman, L. S. Hegedus, J. R. Norton
3. Inorganic Chemistry , Attkin and Shriver
4. Advanced Inorganic Chemistry, Gurdeep Raj.
5. Inorganic Chemistry, J. E. Huhey

Inorganic Chemistry Practical CHI (PR) - 422

6 hrs/week **Max Marks : 50**

I. List of metal complexes to be prepared (any 06)

1.Tris (thiourea) Copper(II) Sulphate
2. Bis (thiourea) Zinc (II) sulphate
3. $NH_4[(Cr(III)(C_2O_4)_3]$
4. [Ni(II) (Salicyldoxime)$_2$]
5. [Copper (II) (Acetyl acetone)$_2$]
6. Manganese (II) Phthalocyanine
7. Mercury(II) Dithizonate
8. Preparation of Schiff base ligands and their complexes of using first transition metal ions.
9. Designing and synthesis of macro-cyclic ligands using Schiff base and their any two transition metal complexes

II Inorganic composite materials.

1. Preparation and magnetic properties of Zinc ferrite, Cobalt ferrite and Nickel ferrite
2. Preparation and catalytic applications of alumino-silicates compound
3. Preparation and photo degradation studies of modified TiO_2
4. Preparation and catalytic applications of sulphated zirconia .
5. Preparation and characterization of Al_2O_3 , CdS ZnO , Fe_2O_3,
6. Preparation of Nickel , silver and copper nano particles.
6. Preparation of Phosponitryl chloride $(PNCl_2)_3$ and its derivatives.
7. Preparation and properties of ferrocene

III. Preparation of copper carbonate from copper sulphate and Quantitative determination of reacted and un -reacted materials after completion of chemical reactions.

Scheme of marking

* UV-Vis and IR analysis of all the prepared compounds are compulsory (05 Marks)
* Record book and viva- voce examination – 05 marks
* Preparation , characterization and estimation of % of metal ions in Complex – 20 marks
* Inorganic composite materials – 20 marks

Reference Books:

1. Nano technology: Principles and Practices-Sulbha K. Kulkarni
2. A Text book of Quantitative Inorganic Analysis; A. I. Vogel
3. Practical inorganic chemistry; Pass Geoffrey and haydn Sutcliffe.
4. Advanced Practical inorganic chemistry; Gurudeep Raj.
5. Vogel's Qualitative Inorganic Analysis, D. Svehla, VII Edn. Orient Longman Ltd.

Scheme of marking

1. Preparation, characterizations and estimation % of metal ion in the complexes. (25 marks)
2. preparation ans application of inorganic materials (20 marks)
3. Record book and viva voce [05 marks]

Inorganic Chemistry Practical CHI (PR) – 423

06 hr per week **50 marks**

I Spectrophotometer:

1. Estimate the amount of copper and bismuth ions using EDTA, photometric titration method
2. Determine the stability constant, empirical formula, λ max. by job's method, mole ratio and slope ratio method.
3. Determine the $_pKa$ of Methyl red indicator
4. Simultaneous determination of MnO^-_4 and $Cr_2O_7^-$
5. Determination of Fe(II) by using O-phenanthroline reagent.

II. P^H metrically

1. Determine the Pk value of benzoic acid by using irrivaing Rossotgi method. By P^H metric method and metal ligand stability constant of its complex.
2. Determine the Pk value of Phthallic acid by using irrivaing Rossotgi methodby P^H metric method and metal ligand stability constant of its complex.
3. Determine the Pk value of Glycine by using irrivaing Rossotgi method. by P^H metric
4. Determine the metal ligand stability constant of copper benzoate complex by pH metric method.
5. Determine the metal ligand stability constant of copper phthalate complex pH metric method.
6. Determine the metal ligand stability constant of copper glycinato complex by pH metric method.

III. Conductometry

1. Analyze the acid mixture hydrochloric acid and acetic acid by conductometric method.
2. Analyze the mixture of copper sulphate, hydrochloric acid and acetic acid by conductometric method.
3. Determine the stability constant and composition/formula of lead oxalate by conductometric method.
4. Determine the solubility and solubility product of sparingly soluble salt by conductometric method.

IV. Potentionmetry

1. Determine the redox potential of Fe(II)/Fe(III) system and hence determine the number of electron involved in the system using $K_2Cr_2O_7$ by potentiometric method.
1. Determine the amount of chloride, bromide and iodide in the given sample by potentiometric method.
2. To determine the stability constant of $[Ag(NH_3)_2]^+$ complex by potentiometric method.
3. To determine the stability constant of silver thiosulphate complex by Potentiometric method.

V. Turbidometry

1. Determine the sulphate content of the given sample using turbidometric titration.

VI. Flame photometry:

1. Estimate the amount of sodium/potassium from the given sample

VII. Application of Computer in Chemistry: at least 05 expt

A. Application of Microsoft EXCEL in Chemistry (Attach the printed sheet in your record book)

1. Calculate the excess molar volume of given data 02
2. Calculate the excess viscosity of given data 02
3. Calculate the excess free energy of given data 02
4. Plot graph between x= sinθ Vs Y = Cosθ, θ= 0 - 360^0
5. Plot the Neat labeled graph from given data 06
6. Arrange the data increasing order of trend. 02

Reference Books/ Journals:

7. Systematic experimental physical chemistry – T. K. Chondhekar & S.W. Rajbhoj
8. Experiments in chemistry – D.V. Jahagirdar
9. Textbook of quantitative Inorganic Analysis – IV Edn. J. Bassett, R. C. Denny, G.H.Gefery and J. Mendham
10. Journal of Chemical Engineering Data, India. Journal of Chemistry, Journal of Indian Chemical Society, (Note: Data collection for computer practical)

Scheme of marking

1. Experiment on Spectrophotometer/ PH meter/ Conductometry / Potentiometer / Turbidometry / Flame photometry [30 marks]
2. Experiment on applications of Excel [15 marks]
3. Record book and Viva Voce [05 marks]

=

Inorganic Chemistry Practical CHI (PR) – 424

06 hr per week **50 marks**

1. Magneto chemistry : at least 10 sample

1. Determine the number of unpaired electron in the given sample by Gouy's balance method

Select the sample : Copper sulphate, sodium sulphate, calcium carbonate, potassium ferrocynide, potassium ferricynide, coordination complexes

2. To verify the Weidemann's law using nickel chloride solution and determine number of unpaired electron in it.

2. Alloy analysis : any 02

i. Solder alloy analysis
ii. Stainless steel alloy analysis
iii. Brass and bronze alloy analysis.
iv. Copper nickel alloy
v. Qualitative analysis of soil

3 Ore analysis : 02

i. Analysis of dolomite ore
ii. Analysis of calcite ore
iii. Analysis of Haematite ore
iv. Analysis of bauxite ore.

4. Analysis of metals in drug sample

i. Analysis of calcium from given drug sample
ii. Analysis of Iron from given drug sample
iii. Analysis of water soluble vitamin forms the given sample.
iv. Determination of number of water molecules present in given samples

5. Analysis of forensic toxic metal ion
6. Analysis of soil

7.. Project works presentation: **select any 01**

1. Water analysis **2**.soil analysis **3**. Designing of the experimental setup for preparation of thin film of semiconductor materials. **4**. UV absorption spectral studies of metal complexes. **5**. Synthesis and characterization of metal complexes. **6.** Synthesis and application of metal oxide/ zeolites. **7.** Synthesis, characterization and applications of nano composite materials. **8**. water analysis 9. Soil analysis of different places.

Scheme of marking

1. Analysis of given sample (25 marks)
2. Project work presentation (20 marks)
3. Record book and viva voce [05 marks]

DR. BABASAHEB AMBEDKAR MARATHWADA UNIVERSITY, AURANGABAD

Department of chemistry

Revised Syllabus

M.Sc. III & IV Semester Organic Chemistry

Effective from June 2012

Effective from June 2012

The following will be the structure for revised syllabus for M. Sc. Organic Chemistry III & IV semester effective from June 2012

Semester	**Paper Nos.**	**Title of Paper**	**Durations (Hr)**	**Max. Marks**	**Credits**
III- Semester	CHE-313	Structural Elucidation by Spectral Methods	60	50	4
	CHEO-314	Organic Synthesis - I	60	50	4
	CHEO-315	Organic Synthesis - II	60	50	4
	CHEO-316	Bioorganic and Green Chemistry	60	50	4
	CHEO-317	Photochemistry, Free radicals and Pericyclic Reactions	60	50	4
IV semester	CHEO- 418	Organic Synthesis: Retrosynthetic Approach	60	50	4
	CHEO-419	Heterocyclic and Polymer Chemistry	60	50	4
	CHEO-420	Chemistry of Natural Products	60	50	4
	CHEO-421	Medicinal Chemistry	60	50	4
	CHEO(a&b)-422	Organic Chemistry Laboratory Course- I	180	50	6
	CHEO(a&b)-423	Organic Chemistry Laboratory Course- II	180	50	6
	CHEO(a&b)-424	Organic Chemistry Laboratory Course- III	180	50	6

Third Semester **CHE-313** **Credits: 04**

STRUCTURAL ELUCIDATION BY SPECTRAL METHODS

UNIT-I ***Nuclear Magnetic Resonance Spectroscopy (^{1}H NMR)***

Elementary ideas (Recapitulation); Spin-spin couplings, Different types of couplings, factors affecting on coupling constants, Karplus equation, Spin systems (AB, AX, ABX, AMX), Rate processes, spin decoupling, shift reagents, Nuclear Overhauser effect (NOE), INEPT and INADEQUATE.

UNIT-II ***^{13}C Nuclear Magnetic Resonance Spectroscopy***

Elementary ideas, instrumental problems, chemical shifts (aliphatic, olefinic, alkyne, aromatic, heteroaromatic and carbonyl carbons); Effect of substituents on chemical shifts.

UNIT-III ***Mass Spectroscopy***

Introduction, ion production (EI, CI, FD and FAB), ion analysis, ion abundance, factors affecting on fragmentation, fragmentation of different functional groups, molecular ion peak, isotopic peaks, metastable peak, Nitrogen rule, McLafferty rearrangement, Retro-Diels-Alder reaction.

UNIT-IV

Problems based on joint applications of UV, IR, ^{1}H NMR, ^{13}C NMR and Mass spectroscopy.

UNIT-V

(A) Mossbauer Spectroscopy: Principle, factors affecting the line position and shape, isomer shift and Quadrupole splitting for iron salt like compounds, complexes, carbonyl compounds, temperature dependence of isomer shift and Quadrupole splitting in simple compounds and coordination, polynuclear complexes, numericals.

(B) Electron Spin Resonance Spectroscopy: Introduction, principle of ESR spectroscopy, presentation of spectrum, hyperfine splitting in various structures, hyperfine splitting digram of representative examples, factors affecting the magnitude

of ‘g’ values, Zero field splitting, Kramer’s degeneracy, Anisotropy in the hyperfine coupling constant, electron delocalization, instrumentation and applications.

Reference Books:

1. Introduction to Spectroscopy: D. L. Pavia, G. M. Lampman, G. S. Kriz
2. Spectrometric Identification of Organic Compounds: R. M. Silverstein & F. X. Webster
3. ^{13}C NMR Spectroscopy: G. C. Levy, R. L. Lichter, G. L. Nelson
4. Spectroscopic Methods in Organic Chemistry: D. H. Williams & I. Flemming
5. Absorption Spectroscopy of Organic Compounds: V. M. Parikh
6. Mass Spectrometry: K. G. Das & James
7. Coordination Chemistry by Experimental Methods: K. Berger
8. Coordination Chemistry vol. I: E. Martell
9. Physical Methods for Chemistry: R. S. Drago
10. Structural Methods in Inorganic Chemistry: E. A. V. Ebsworth & D. W. H. Rankin
11. Organic Structure Analysis: Philips Crews

Third Semester **CHEO-314** **Credits: 04**

ORGANIC SYNTHESIS-I

UNIT-I *Oxidation*

(a) Oxidation of alcohol to aldehyde, ketone or acid: Jones reagent, Swern oxidation, Collins reagent, Fetizones reagent, PCC, PDC, PFC, IBX, Activated MnO_2, Chromyl chloride (Etard reaction), TEMPO, CAN, NMO.

(b) Oxidative cleavage of Carbon-Carbon double bonds: $KMnO_4$, Ozonolysis.

(c) Allylic Oxidation: SeO_2, PhSeBr.

(d) Selective cleavages at functional groups: Cleavage of glycols, IO^-_4, $Pb(OAc)_4$.

UNIT-II *Reductions*

(a) Catalytic Hydrogenation; (b) Reduction of nitriles, oximes and nitro compounds; (c) Reduction of acids and Esters; (d) Reduction with metal hydride- Sodium cyanoborohydride, Diborane, L- & K-Selectrides, $LiBH_4$, DIBAL-H; (e) Reduction by dissolving metals- Sodium-alcohol, Sodium-Liq. Ammonia, Mg, Zinc-HCl or Acetic acid, Sn/Fe-HCl; (f) Reduction of aldehyde and ketones- Platinum, Raney nickel, $NaBH_4$, $LiBH_4$; (g) Birch reduction and related reactions, Luche reagent, Wolf-Kishner reduction, Clemmenson reduction, Wilkinson catalyst, TBTH.

UNIT-III *Organic Reagents*

Gilbert, DCC, EDC, DDQ, 1,3 Dithiane, LDA, DMDO, OsO_4, RuO_4, SmI_2, Dess-Martin Periodinane, Borane Complexes, Diazomethane, Lawesson's reagent, Bobbitt's reagent, Moffatt oxidation, Mosher's reagent, Baker's yeast, Merrifield resin.

UNIT-IV *Rearrangements*

Pummerer, Payne, Eschenmoser fragmentation, Brook, Anchimeric assistance (Neighbouring group participation) related rearrangement, Wagner-Meerwein, Wolf, Semipinacol, Epoxide rearrangement with lewis acid, Dienone-Phenol rearrangement, Tiffeneau-Demjanov, Favorskii,

von Richter, Wittig, Neber, Smiles, Fries, Curtius, Lossen, Schmidt, Steven, Hofmann, Iodolactonisation.

UNIT-V ***Name Reactions***

Arndt-Eistert, Hunds-Diecker reaction, Baeyer-Villiager, Dakin, Gabriel synthesis, Michael, Darzen, Prins, Henry, Reimer-Tiemann, Hoffmann–Loffler–Freytag, Dieckmann cyclization, Chichibabin, Vilsmeier, Ene, Ullmann reaction

Reference Books:

1. Organic Chemistry: Clayden, Greeves, Warren and Wothers
2. Stereochemistry of Organic Compounds (Principle and application): D. Nasipuri
3. Stereochemistry of Organic compounds: Ernest L. Eliel / Samuel H. Wilen
4. Organic Synthesis: W. Carruthers
5. Organic Reagents: Fieser & Fieser
6. Organic Synthesis: M. B. Smith
7. Advanced Organic Chemistry; Part A and B: F. A. Carey & R. J. Sundberg
8. Modern Organic Synthesis: An Introduction: G. S. Zweifel & M. H. Nantz
9. A Guidebook To Mechanism In Organic Chemistry: Peter Sykes
10. Organic Synthesis Concepts, Methods, Starting Materials: J. Fuhrhop, G. Penzlin
11. Name Reactions and Reagents in Organic Synthesis: B. P. Mundy, M. G. Ellerd, F. G. Favaloro
12. Organic Chemistry: An Intermediate Text: Robert V. Hoffmann
13. Multicomponent Reactions: J. Zhu, H. Bienayme (Wiley-VCH)
14. Advanced Organic Chemistry: Jerry March
15. Organic Synthesis: R. O. C. Norman and Coxan
16. Name Reactions: Jie Jack Li

Third Semester **CHEO-315** **Credits: 04**

ORGANIC SYNTHESIS-II

UNIT-I *Advanced Name Reactions*

Bamford-Steven, Baylis-Hillmann, Horner-Wadsworth-Emmons, Corey-Fuchs Reaction, Julia Olefination, Mukaiyama aldol, Mitsunobu, Peterson olefination, Corey-Winter olefination, Woodward and Prevost dihydroxylation, Shapiro, Ritter, Pauson-Khand, Stille, Heck, Sonogashira, Suzuki, Wacker, Duff, Chugaev, Petasis, McMurry reaction and Coupling.

UNIT-II *Reaction Intermediates*

(a) Ylides: Preparation and their synthetic applications along with their stereochemical aspects of Phosphorous, Sulphur and Nitrogen ylides.

(b) Enamines: Generation & application in organic synthesis with mechanistic pathways, stork enamine reaction.

(c) Enolates: Generation & reaction of enolates with aldehydes and ketones, Robinson annulations, Reformatsky reaction.

UNIT-III *Formation of Carbon-Carbon bonds via organometallic reagents*

Synthesis and applications of organo Lithium, Magnesium, Titanium, Cerium, Copper, Chromium, Zinc, Boron, Silicon, Cadmium, Rhodium.

UNIT-IV *Advanced Organic Chemistry*

(a) Ring closing metathesis (Grubb's metathesis)

(b) Tandem/Domino reaction: Aldol-Tishchenko reaction (Evans-Tishchenko reaction).

(c) Multicomponent reactions: Ugi, Passerini, Biginelli, Mannich, Hantzsch, Strecker amino acid synthesis.

UNIT-V *Asymmetric Synthesis*

Chiral pool, Chiral auxiliary, Enantio- & Diastereoselective synthesis, Chiral reagent and chiral catalyst including CBS reagent, NADH, Asymmetric hydrogenation including BINAP, Hydroboration- Ipc_2BH, $IpcBH_2$, Asymmetric epoxidation- (+) DET & (-) DET, Sharpless, Jacobson, Asymmetric dihydroxylation- $(DHQD)_2PHAL$ & $(DHQ)_2PHAL$, Felkin-Anh model, Zimmermann-Traxler transition state model, Proline catalyzed asymmetric reactions.

Reference Books:

1. Organic Chemistry: Clayden, Greeves, Warren and Wothers
2. Stereochemistry of Organic Compounds (Principle and application): D. Nasipuri
3. Stereochemistry of Organic compounds: Ernest L. Eliel / Samuel H. Wilen
4. Organic Synthesis: W. Carruthers
5. Organic Reagents: Fieser & Fieser
6. Organic Synthesis: M. B. Smith
7. Advanced Organic Chemistry; Part A and B: F. A. Carey & R. J. Sundberg
8. Modern Organic Synthesis: An Introduction: G. S. Zweifel & M. H. Nantz
9. A Guidebook To Mechanism In Organic Chemistry: Peter Sykes
10. Organic Synthesis Concepts, Methods, Starting Materials: J. Fuhrhop, G. Penzlin
11. Name Reactions and Reagents in Organic Synthesis: B. P. Mundy, M. G. Ellerd, F. G. Favaloro
12. Organic Chemistry: An Intermediate Text: Robert V. Hoffmann
13. Multicomponent Reactions: J. Zhu, H. Bienayme (Wiley-VCH)
14. Advanced Organic Chemistry: Jerry March
15. Organic Synthesis: R. O. C. Norman and Coxan
16. Name Reactions: Jie Jack Li

Third Semester **CHEO-316** **Credits: 04**

BIO-ORGANIC AND GREEN CHEMISTRY

UNIT-I *Introduction to Bioorganic chemistry*

Basic concepts, Proximity effects in organic chemistry, Molecular adaptation, Molecular recognition.

UNIT-II *Enzyme Chemistry*

Nomenclature, Classification and Extraction of enzymes, Structural outlines of enzymes (proteins); Introduction to catalysis and enzymes; Multifunctional catalysis, Intramolecular Catalysis, Molecular asymmetry and prochirality, Mechanism of enzyme action, Factors responsible for enzyme specificity, Enzyme activity and kinetics (Michaelis Menten and Lineweaver–Burk plots), Enzyme Inhibitions (Reversible and irreversible), Structure, Mechanism of action and applications of α-Chymotrypsin, Ribonuclease, lysozyme and Carbopeptidase-A. Enzymes in synthetic organic chemistry. [Additions, eliminations, substitutions, condensations, cyclocondensations, oxidations, reductions and rearrangement reactions are to be covered]

UNIT-III *Co-Enzyme Chemistry*

Introduction to co-enzymes, Cofactors, prosthetic groups and apoenzymes, Chemical structures of co-enzymes and cofactors, Oxidoreduction (NAD^+, $NADP^+$), Pyridoxal phosphate (PLP), Thiamine pyrophosphate (TPP), Biotin (CO_2 carrier), Haemoglobin (O_2-carrier), Flavin (FMN, FAD, $FADH_2$), Oxene Reactions, Lipoic acid, Mechanisms of reactions catalyzed by co-factors.

UNIT-IV Supramolecular Chemistry and Biomimetic Chemistry (Enzyme Models)

Host-Guest approach, Chiral recognition, Designing Enzyme Models, Ionophores, Crown ethers, cryptands, Micelles, Cyclodextrins, calixarenes, polymers.

UNIT-V Green Chemistry

Introduction, Need of green chemistry, Principles of green chemistry, Atom Economy,

Green concerns of water, Benefits and applications of Green chemistry.

Green Protocols: (a) Solvent free reactions (b) Reactions in aqueous media (Green solvent) (c) Ionic liquids (d) PEG and Water

Newer Techniques in organic synthesis: (i) Microwave irradiation (MWI) (ii) Ultrasonication (iii) Grinding (iv) Heterogeneous Catalysis / Immobile Catalysis

Reference Books:

1. Bioorganic chemistry (A chemical approach to enzyme action): Hermann Dugas.
2. Biotransformation in Organic chemistry: K. Faber.
3. Enzyme structure and Mechanism: Alan Fersht.
4. Enzyme catalysis in organic synthesis vol.1: Karlheinz Drauz and Herbert Waldmann.
5. Bioorganic, Bioinorganic and supramolecular chemistry: P. S. Kalsi and J. P. Kalsi.
6. Organic chemistry IVth Edn.: G. Marc Loudon.
7. Microwave synthesis: Brittany L. Hayes.
8. Green Chemistry (Theory and Practice): Paul T. Anastas and John C.Warner.
9. Green Chemistry: Rashmi Sanghi and M. M. Srivastava.
10. Handbook of Green chemistry and Technology: James Clark and Duncan Macquarrie.

Third Semester **CHEO-317** **Credits: 04**

PHOTOCHEMISTRY, FREE RADICALS AND PERICYCLIC REACTIONS

UNIT-I *Pericyclic Reactions-I*

Features and classification of pericyclic reactions, Phases, nodes and symmetry properties Of molecular orbital in ethylene, 1,3-butadiene, 1,3,5-hexatriene. Allyl cation, allyl radical, pentadienyl cation and pentadienyl radical. Thermal and photochemical reactions.

Electrocyclic reactions: Con-rotation and dis-rotation, electrocyclic closure and opening in 4n and 4n+2 systems, Woodward-Hoffmann selection rules for electrocyclic reactions. Explanation for the mechanism of electrocyclic reactions by: (i) Symmetry properties of HOMO of open chain partner; (ii) Conservation of orbital symmetry and orbital symmetry correlation diagram and (iii) Huckel-Mobius aromatic and antiaromatic transition state method.

UNIT-II *Pericyclic Reactions-II*

Cycloaddition reactions: Suprafacial and antarafacial interactions. (π) and (π cycloadditions. Cycloreversions. Stereochemical aspects in supra–supra, antara-supra and antara-antara (π and (π4cycloadditions. Diels-Alder reaction. Woodward-Hoffmann selection rules for cycloaddition reactions. Explanation for the mechanism of cycloaddition reactions by 1) Conservation of orbital symmetry and orbital symmetry correlation diagrams 2) Fukui Frontier Molecular Orbital (FMO) theory and (3) Huckel-Mobius aromatic and antiaromatic transition state method. Endo-exo selectivity in Diels-Alder reaction and it's explanation by FMO theory. Examples of cycloaddition reactions.

Sigmatropic reactions: [1,j] and [i,j] shifts. Suprafacial and antarafacial shifts. Selection rules for [i,j] shifts. Cope, degenerate Cope and Claisen rearrangements. Explanation for the mechanism of sigmatropic reactions by 1) symmetry properties of HOMO 2) Huckel-Mobius aromatic and antiaromatic transition state method. Introduction to chelotropic reactions and the explanation of mechanism by FMO theory.

UNIT-III *Photochemistry-I*

Photochemistry of (π, π^*) transitions: Excited state of alkenes, cis-trans isomerisation, photochemistry state, electrocyclisation and Sigmatropic rearrangements, di π-methane rearrangement.

Intermolecular reactions: photocycloadditions, photodimerasation of sample and conjugated olefins, addition of olefins to α, β unsaturated carbonyl compounds, excimers and exiplexes. Photoaddition reactions. Excited states of aromatic compounds, photodimerisation of benzene, photosubstitution reactions of aromatic compounds and Photo-Fries rearrangement.

UNIT-IV *Photochemistry-II*

Photochemistry of (n, π^*) transitions: Excited state of carbonyl compounds, hemolytic cleavage of α-bond-Norrish type I reaction in acyclic, cyclic ketones and strained cycloalkanediones.

Intermolecular abstraction of hydrogen: Photo reduction and photo oxidation-influence of temperature, solvent, nature of hydrogen donors and structure of the substrate.

Intramolecular abstraction of hydrogen: Norrish type II reaction in ketones, esters and 1, 2-diketones.

Addition to C-C multiple bonds: Paterno-Buchi reaction, photodecarboxylation, photochemistry of alkyl peroxides, hypohalites and nitriles. Barton reaction. Photochemistry of azo compounds, diazo compounds, azides and diazonium salts. Singlet oxygen-photo oxygenation reactions. Ene reaction, formation of dioxetanes and endoperoxides. Chemiluminescent reactions. Oxidative coupling.

UNIT-V *Free radical reactions*:

Introduction, generation, stability, reactivity, characteristics, structural and stereo chemical properties of free radicals. Persistent free radicals.

Reaction of free radicals: Addition, substitutions, fragmentations (Norrish-I, II, Mclafferty rearrangement), Oxidations and reductions, Neighbouring group assistance. Detection of free radicals, Homolysis and free radical displacement. Radical chain reactions, Addition and rearrangements, radical cyclization, reactivity of aliphatic and aromatic substrates at bridgehead, Coupling of alkynes and arylation of aromatic compound by diazonium salt, Sandmeyer reaction,

Hunsdieker reaction, Allylic halogenations, McMurry reaction, Acyloin condensation, Birch reduction, Bouveault-Blank reduction.

Reference Books:

1. Advanced Organic Chemistry Part A & Part B: F. A. Carey & R. J. Sundberg
2. Advanced Organic Chemistry: Jerry March
3. Organic Chemistry: Clayden, Greeves, Warren & wother.
4. Organic Chemistry: Stanley H. Pine
5. Organic Synthesis: W. Carruthers
6. Organic Synthesis: Norman and Coxon

Fourth Semester **CHEO-418** **Credits: 04**

ORGANIC SYNTHESIS: RETROSYNTHETIC APPROACH

UNIT-I *Disconnection Approach*

Introduction to:

(i) Grounding of organic chemistry for understanding retrosynthesis;

(ii) Retrosynthetic analysis and designing of the synthesis;

(iii) Disconnection approach: An introduction to synthons, synthetic equivalents, disconnection approach, functional group interconversions, importance of order of events in organic synthesis, one and two group C-X disconnections, selective organic transformations: chemoselectivity, regioselectivity, stereoselectivity, enentioselectivity, Reversal of polarity, cyclization reactions, amine synthesis.

UNIT-II *Protecting Groups*

Protection and deprotection of hydroxyl, carbonyls in aldehydes and ketones, amines, carboxylic acids, alkenes and alkynes.

UNIT-III *C-C Disconnections*

(i) One group C-C Disconnections:

Alcohols (including stereoslectivity), carbonyls (including regioselectivity), Alkene synthesis, use of acetylenes and aliphatic nitro compounds in organic synthesis.

(ii) Two group C-C Disconnections:

Diels-Alder reactions, 1,3 difunctionalized compounds and α, β-unsaturated compounds, control in carbonyl condensations, 1,5 difunctionalized compounds, Michael addition and Robbinson annealation.

UNIT-IV *Ring Synthesis*

Introduction to ring synthesis, saturated heterocycles, synthesis of 3, 4, 5 and 6 membered rings, rearrangements and photochemistry in synthesis, aromatic heterocycles.

UNIT-V *Complex molecules*

Synthetic routes based on retrosynthetic analysis for following molecules:

Longifoline, Reserpine, Juvabione, Amphidicoline, Taxol.

Reference Books:

1. Organic Synthesis: The Disconnection Approach: Stuart Warren
2. Designing Organic Synthesis: Stuart Warren
3. Organic Synthesis: Strategy and Control: Paul Wyatt and Stuart Warren
4. The Logic of Chemical Synthesis: E. J. Corey and Xue-Min Chelg
5. Classics in Total Synthesis I, II and III: K. C. Nicolaou and others
6. Organic Synthesis Concepts, Methods, Starting Materials: J. Fuhrhop, G. Penzlin
7. Some Modern Methods of Organic Synthesis: W. Carruthers
8. Organic Synthesis: M. B. Smith
9. Principles of Organic Synthesis: R. Norman and J. M. Coxan.
10. Advanced Organic Chemistry: Jerry March
11. Organic Chemistry: Clayden, Greeves, Warren and Wothers

Fourth Semester **CHEO-419** **Credits: 04**

HETEROCYCLIC AND POLYMER CHEMISTRY

PART A: *Heterocyclic Chemistry*

UNIT-I

Nomenclatures of all types of heterocycles, Classification of heterocycles: as aromatics based upon various membered ring systems.

UNIT-II

General synthetic routes based on name reactions, reactivities, utilities and wherever possible spectral analyses of the following class of heterocycles.

Four membered: Azitidines, including β- lactums.

Five membered: Thiazoles, Oxazoles, Pyrazoles and Imidazoles.

Six membered: Pyridines, Pyrimidines.

Fused heterocycles: Flavones, Chromones, Coumarines, Indoles, Quinolines, Benzodiazepines, and Phenothiazines.

Reference Books:

1. Heterocyclic Chemistry: vol. I, II, III: R. R. Gupta, M. Kumar and M. Gupta
2. Heterocyclic Chemistry: Joules and Mills
3. Modern heterocyclic Chemistry: L. A. Paquette (Benjamin)
4. Organic Chemistry: Jonathan Clayden

PART B: *Polymer Chemistry*

UNIT-I *Introduction*

(i) Introduction to organic polymers and various terms like Monomer, comonomer, mesomer, homopolymer, heteropolymer, co-polymer, degree of polymerization, plastic, resin, fibers etc.

(ii) Mechanism of polymerizations (Chain and condensation) and methods of polymerizations viz. mass, solution, emulsion and suspension.

(iii) Molecular weight of polymers and their determinations by end group analysis, sedimentation, osmometric and viscometric measurements.

UNIT-II *Natural Polymers*

Isolations, characterizations and regenerations/derivatizations of natural polymers like Cellulose, Rubber and natural silk/ wool.

UNIT-III *Synthetic Polymers*

Mechanism of polymerization, reactivity, stability, and applications of following polymers:

Polyethylene, polypropylene, polyvinyl chloride, polyvinyl acetate, and polymethyl methacrylate.

Polyethylene terphthalate, alkyd resin, polycarbonate and nylons.

Phenoplast, urea- formaldehyde resin, melamine-formaldehyde resin, polyurethanes, polysiloxane and epoxy resins

Reference Books:

1. Textbook of Polymer Science: Fred W. Billmeyer. Jr.
2. Polymer Science: V. R. Gowarikar, N. N. Viswanathan, Jaydeep Sreedhar
3. Organic Polymer Chemistry: K. J. Saunder

Fourth Semester **CHEO-420** **Credits: 04**

CHEMISTRY OF NATURAL PRODUCTS

UNIT-I *Terpenoids & Carotenoids*

Classification, Nomenclature, occurrence, isolation, general methods of structure determination, isoprene rule

Structure determination, stereochemistry, and synthesis of the following representative molecules: Citral, Geraniol, α-Terpineol, Menthol, Farnesol, Zingiberene, Phytol, Abietic acid and β- Carotene.

UNIT-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 and synthesis of the following:

Ephedrine, (+)-coniine, nicotine, atropine, Quinine and Morphine.

UNIT-III *Steroids*

Occurrence, nomenclature, basic skeleton, Diel's hydrocarbon and stereochemistry. Isolation, structure determination and synthesis of Bile acids, Androsterone, Testosterone, Estrone, Progestrone.

UNIT-IV *Anthocyanins and Flavones*

Occurrence, nomenclature and general methods of structure determination.

Synthesis of cyanidin chloride, cyanin, Hirsutidin chloride, Flavones (Kostanecki and Baker-Venkataraman approaches), Flavonols, Qurcetin, and Isoflavones.

UNIT-V *Biogenesis*

The building blocks and construction mechanisms of the following

(a) Terpenoids: Mono-, Sesqui-, Di-, Tri-Terpenoids and steroids.

(b) Alkaloids: pyridine alkaloids, Benzyl Isoquinoline alkaloids, morphine alkaloids and Indole alkaloids.

(c) The Shikimic acid pathway.

Reference Books:

1. The Organic Chemistry of Drug Design and Drug Action: R. B. Silverman, Academic press.
2. Natural Products: Chemistry and Biological Significance: J. Mann, R. S. Davidson, J. B. Hobbs, D. V. Banthrope and J. B.Harborne, Longman, Essex.
3. Organic Chemistry: Vol. II, I. L. Finar, ELBS.
4. Introduction to Flavonoids: B. A. Bohm, Harwood Academic Publishers
5. New Trends in Natural Product Chemistry: Atta-ur-Rahman and M. I. Choudhary, Harwood Academic publishers.
6. Biogenesis of Natural Products: Baldev Kumar and Harishkumar Chopra (Narosa Publication)

Fourth Semester **CHEO-421** **Credits: 04**

MEDICINAL CHEMISTRY

UNIT-I

Definition and Introduction of following terms-Durg, Prodrug, Hard and Soft drugs, agonists, antagonists, affinity, efficacy, potency, isosterism, bioisosterism, pharmacophores, lead molecule, lethal dose (LD50) and effective dose (ED50) (i) Factors affecting bioactivity, (ii) Theories of drug activity, (iii) Structure activity relationship (SAR), QSAR (2D and 3D method) and Hantzsch equation (iv) Drug receptor mechanism.

UNIT-II *Pharmacokinetics*

(i) Drug absorption, Distribution and deposition of drugs.

(ii) Excretion and elimination of drugs, Bioavailability.

UNIT-III *Pharmacodynamics*

(i) Mechanism of drug action: Enzyme stimulation and enzyme inhibition, antimetabolites, membrane active drugs, chelation; (ii) Drug metabolism and inactivation: Factors affecting drug metabolism, pathways of drug metabolism [Metabolic
reaction (Phase I) and conjugation reaction (Phase II)].

UNIT-IV *Classification of Drugs*

The detail content of the each class of the drugs.

UNIT-V

Synthesis and Utilities of the following drug molecules at least one convenient synthetic route with possible mechanism (Wherever possible of certain be discussed steps) from various classes:

I. Anti inflammatory Drugs: (a) Naproxen (b) Ibuprofen (c) Oxaprozin (d) Diclofenac Sodium (e) Rofecoxib (f) Celecoxib.

II. Anti-hypertensive Drugs: (a) Vexapamil (b) Captopril (c) d-sotalol (d) Atenolol (e) Diltiazem (f) Semotiadil fumarate.

III. Drugs acting on CNS: (a) CNS Stimulant : Dextro-amphetamine

(b) Respiratory Stimulant : Doxapram

(c) CNS anti-depressant : (i) Chlorpromazine (Antipsychotic) (ii) Diazepam (Anxiolytic)

(iii) Phenobarbitol (Antiepileptic)

IV Anesthetic Drugs:

(a) General : Ketamine (b) Local : (i) Lidocaine (ii) Procaine

V. Antibiotics: (a) Chloramphenicol (b) Ampicillin (c) Amoxycillin (d) Cefepime (e) Cefpirome (f) Antimycobactrial: Ethambutol (g) Antiviral: Acyclovir (h) Antimicrobial: Sulfamethoxazole

VI. Antidiabetics : (a) Troglitazone (b) Chlorpropamide (c) Tolbutamide

VII. Antineopastic Drugs: (a) Antagenists: Fluorouracil (b) Alkylating agents: i) Chlorambucil (ii) Cis-Platin

Reference Books:

1. FOYE'S Principles of Medicinal Chemistry VIth Edition: Thomas L. Lemke, David A. Williams, Victoria F. Roche and S. William Zito.
2. Introduction of Medicinal Chemistry: A. Gringuage, Wiley-VCH.
3. Synthesis of Essential Drugs: R. S. Vardanyan and V. J. Hruby.
4. Volumes of Burger's Medicinal Chemistry: M. E. Wolf, JohnWiley.
5. Medicinal Chemistry: David J. Triggle.
6. Essentials of Medicinal Chemistry IInd: Andrejus Korolkovas, WileyVCH.

ORGANIC CHEMISTRY LABORATORY COURSE

CHEO-422 (a,b) **Duration: 06 Hrs/Week** **Credits: 06**

Qualitative analysis of ternary mixtures.

In a mixture at least one liquid one water soluble compound be given.

CHEO-423 (a,b) **Duration: 06 Hrs/Week** **Credits: 06**

Organic preparations.

(A) Preparations involving at least two stage based on name reactions, condensations, cyclocondensations, reagents and rearrangements (as covered under the theory). Separation purification of the product by column is desired.

(B) Preparations involving one stage based upon the green synthetic protocols (as covered in theory syllabus).

CHEO-424 (a,b) **Duration: 06 Hrs/Week** **Credits: 06**

(A) Structure elucidation of organic compounds by spectral analyses.

(B) Project work: Dissertation be prepared and should contain literature survey, aim, scope of the project, experimental details and concluding discussions.

Reference Books:

1. Textbook of Practical Organic Chemistry: Vogel
2. Organic Synthesis Collective Volumes: Blatt
3. Research Periodicals including internet services.

DR. BABASAHEB AMBEDKAR MARATHWADA UNIVERSITY, AURANGABAD

Department of Chemistry

Revised Syllabus

M.Sc. III & IV Semester Physical Chemistry

Effective from June 2012

Effective from June 2012

The following will be the structure for revised syllabus for M. Sc. Physical Chemistry III & IV semester effective from June 2012.

Semester	Paper Nos.	Title of Paper	Durations (Hr)	Max. Marks	Credits
III- Semester	CHE-313	Structural elucidation by spectral methods	60	50	4
	CHEP- 314	Solid State Chemistry	60	50	4
	CHEP -315	Macromolecules and Biophysical Chemistry	60	50	4
	CHEP -316	Nano Chemistry	60	50	4
	CHEP -317	Advanced Electrochemistry	60	50	4
IV semester	CHEP: 418	Nuclear Chemistry	60	50	4
	CHEP: 419	Thermodynamics	60	50	4
	CHEP: 420	Surface and Magnetochemistry	60	50	4
	CHEP: 421	Chemical Dynamics and Catalysis	60	50	4
	CHEP (PR) - 422	Physical Chemistry Laboratory Course -I	180	50	6
	CHEP (PR) - 423	Physical Chemistry Laboratory Course -II	180	50	6
	CHEP (PR) - 424	Physical Chemistry Laboratory Course -III	180	50	6

Solid State Chemistry : CHEP-314

Duration : 60 hrs **Marks: 50** **Credit : 04**

Unit -1: Solid State Reactions: **12 Hrs.**

General Principles, Classification, Wagner reaction mechanism, Laws governing nucleation, Growth of nuclei, Improving reactivity of solids, coprecipitation as a precursor to solid state reactions, Kinetics of solid state reactions, factors affecting the reactivity of solid state reactions. Growth of single crystals, czochralski method, zone melting, flux method, Epitoxial growth of thin layer, Hydrothermal method.

Unit-2: Imperfections in solids: **12 Hrs.**

Perfect and imperfect crystal, Point defects, Stiochiometric defects, Schottky and Frenkel defects. Thermodynamics of their formation, colour centers.Nonstoichiometric defects. Metal excess and metal deficiency defects. Line imperfections, edge dislocation and screw dislocation, Burger's circuits. Surface imperfection, grain boundries and stacking faults.Numericals.

Unit-3: Semiconductors and their devices: **12 Hrs.**

Intrinsic and extrinsic semiconductors, semiconductors materials and their fabrication, semiconductors devices p-n junctions, properties of p-n junctions, semiconductors diode as rectifier, Filters circuits, Zener diode as avoltage stabilizer, transistors transistor as an amplifier

Super conductivity: conventional super conductors, organic super conductors (organic metals),fullerence,high temperature super conductors, organic charge transfer complexes Applications.

Unit- 4: Theories of solid state and properties of solids: **12 Hrs**

Free electron theory, Counduction by free electrons, Band theory, refinement to simple band theory, band structure of metals. Insulator and semiconductors.

Optical properties, Luminescence and phosphors, Lasers, photoconduction, photoelectric effects. Electrical properties. Thermoelectric effects, Thomson effects, peltier effects, seebeck effects, Thermocouples, Hall effects.

Unit-5: Ceramics: **12 Hrs.**

Introduction, major components of ceramics, clays, silica, feldspar, clay minerals, classification of clay minerals, properties of clay minerals, pillared clays, principal of pillaring, variety of pillaring species, modification of pillared clays, preparation of pillared clays, catalytic applications.

Reference Books

1 Solid State chemistry and its Applications-A.R.West (John Wiley and sons)
2 Principles of Solid State –H.V.Keer (Wiley Eastern Limited)
3 Material science and Engineering-V.Raghavan (prentice Hall of India)
4 Principles of Electronics- V.K.Metha (S.Chand and co.)
5 Engineering chemistry –P.C.Jain and M.Jain (Shanpat Rai and Sons)
6 Industrial chemistry –B.K.Sharma (Goel publishing House)
7 Selected topics in solid state physics vol.12 The growth of crystals from liquids J.C.Brice, North Hollond/American Elesvier(1973)
8 Chemistry of imperfect crystal-F.A.Krogen

Dr. Babasaheb Ambedkar Marathwada University Aurangabad 431 004

Department of Chemistry

Macromolecules and Biophysical Chemistry

CHEP- 315

Lectures: 60 **Marks: 50**

Chapter 1. Fundamentals of Biological Macromolecules.

Chemical bonds in biological systems; Properties of water; Thermodynamic principles in biological systems; Properties and classification of amino acids; Structures of nucleic acids, Protein structure and function, Properties of nucleosides and nucleotides, Composition of nucleic acids, Electrophoresis, Factors affecting on Electrophoretic Mobility; Types of Electrophoresis; Free electrophoresis and Gel electrophoresis; Electrophoresis in genetic analysis; DNA Sequencing and DNA foot Printing.

Chapter 2. Macromolecules.

Introduction, Formation of synthetic high polymers classification, Polymerization reactions: Chain and Step. Average molecular weight, Number average weight, Methods of determination of molar masses of polymers; Viscosity, Osmometry, Molar mass of charged macromolecules, Donnan membrane equilibrium, Ultracentrifugation, light scattering, Diffusion.

Chapter 3. Chemistry of Polymerization.

Chain polymerization: free radical polymerization, ionic polymerization, co-ordination polymerization, Ziegler-Natta catalysts.

Step Polymerization: polycondensation, .polyaddition, ring opening, electro chemical polymerization, group, Transfer polymerization, Polymerization techniques.

Chapter 4. Kinetics of Polymerization:

Free radical chain polymerization, Anionic polymerization, Cationic polymerization, Copolymerization, Free radical copolymerization, Ionic copolymerization, Copolycondensation.

Chapter 5. Electronically Conducting Polymers.

Introduction, Theories of electronic conduction; Band theory of conduction, Hopping conduction, Super conduction, Mechanism of conduction, Doping mechanism, p-type, n-type, auto doping, Stimuli sensitive (smart) polymers, pH and temperature sensitive smart polymers, Applications: Photovoltaic devices, Sensors, LED and Solar cells, Electro chemical devices, Batteries etc.

Recommended Texts:

1. Cantor, C. R. and Schimmel Biophysical Chemistry Vols. 1-3, W. H. Freeman (1980).
2. Lehninger, A.L., Nelson, D. L. and M. M. Lehninger, Principles of Biochemistry 4th Ed., W. H. Freeman (2004).
3. U. Satyanarayana; Biochemistry.
4. Upadhyay; Biophysical Chemistry.
5. L. Stryer, Biochemistry, 5th Edition, (2002) Freeman and Co. New York.
6. D. Voet, J. G. Voet, Biochemistry 3rd Edition (2004), Wiley International Publication.
7. D. L. Nelson and M. M. Cox, Lehninger Principles of Biochemistry 3rd Edition (2002) McMillan North Publication.
8. Polymer Science. By V. R. Gowariker, N. V. Viswnathan, Jayadev Sreedhar.
9. Polymers and Resins. By Brage Golding.
10. Electrical Properties of Polymers. By Tony Blythe and David Bloor.
11. Self doped conducting polymers. By Michael S. Freund and Bhavana Deore.
12. Polymer Science and Technology. By Premamoy Ghosh.

Dr. Babasaheb Ambedkar Marathwada University
Physical Chemistry M.Sc. III[rd] Sem.
Nanochemistry
Paper CHEP- 316 **60 hours**
(4hrs/week)

I) **General introduction & synthesis of nanomaterials by physical methods: [12]**

Objective of study, synthesis of nanoparticles by physical method, mechanical methods- high energy ball milling, melt mixing, method based on evaporation, physical vapour deposition with consolidation. Ionized cluster beam deposition. Laser vaporization, Laser pyrolysis, sputter diposition, electric arc deposition, Chemical Vapour Deposition (CVD).

II) **Synthesis of Nanomaterials by Chemical Methods** **[12]**

Introduction, colloids and colloids in solution, interaction of colloids and medium, colloids in vacuum, colloids in medium, effect of charge on colloids, stearic repulsion, synthesis of colloids, growth of nanoparticles, synthesis of metal and semiconductor nanoparticles by colloidal route, Langmuir-Blodgett (L-B) method, sol gel method, electrochemical method.

III) **Analysis Technique :** **[12]**

Introduction, microscopes, electron microscopes,SEM, TEM, Scanning probe microscope (SPM), Scanning Tunnelling microscope, Atomic force microscope, X-ray diffraction, UV-visible and IR spectroscopy.

IV) **Properties, types and application of Nanomaterials:** **[12]**

i) Properties of nanomaterials – Mechanical, electrical, optical, magnetic, semiconductor.

ii) Some special nanomaterials – Carbon nanotubes, porous silicon, Arogels, Zeolites.

iii) Application – Electronic, energy automobiles, sport and toys, textile, cosmetics, domestic appliances, biotechnology, medical, space, defence & environment.

V) **Thin films:** **[12]**

Introduction, deposition by chemical reactions, deposition by electrochemical reaction, chemical vapor deposition of inorganic Thin films, chemical etching.

Reference Books:

1) Nanotechnology: Principles and practices- Sulabha K. Kulkarni (capital Pub. Co.)
2) NANO- The next revolution –Mohan Surendra Rajan(Natioinal book Trust, India)
3) The British Glass Website- Types of Glass://www.britiglass.org.uk.
4) Fundamental of Nanotechnology – Gabor L. Hornyak, John J. Moore, Harry F. Tibbals, Joydeep Dutta.
5) Recent advances in the liquid phase synthesis of Inorganic Nanoparticles- B. LCushing, V. L. Kolesmichenko & C.J.O".Connor Chemical Review 104, 3893-3946.(2004)
6) Hand book of Thin film technology- H. R. Khan.
7) Thin film phenomenon- K. N. Chopra. Mcgrawa Hill publication
8) Material Science deposition & structure –Milton.

Physical Chemistry :III[rd] Semester

ADVANCED ELECTRO CHEMISTRY : CHEP-317

Duration : 60 hrs *Marks: 50* *Credit : 04*

Unit -1: Oxidation - Reduction Systems: **12 Hrs.**

Oxidation potentials, reversible ox-red systems, determination of standard ox-red potentials, variation of ox-red potential, ox-red equilibria, ox-red systems in analytical chemistry, ox-red indicators, two stage ox-red , semiqinone formation constant. Numericals.

Unit-2: Bio- electrochemistry and Electrocatalysis : **12 Hrs.**

Donnan membrane equilibrium, membrane potential, theories of membrane potential,introduction to electrocatalysis, relative power of electrocatalysts, mechanism of electrocatalysis, bioelectro catalysis, immobilization, application of enzymes on electrodes.

Unit-3: Electrodeposition : **12 Hrs.**

Introduction , the electrogrowth of metals on electrodes , the reaction pathway for electro deposition ,surface diffusion of ions , cathodic deposition of metals from solutions , factors affecting cathodic deposition of metals , electrochemical dissolution and passivity of metals , anodic dissolution of metals , film and adsorption theories of passivity.

Electroplating of metals, mechanism, throwing power of an electroplating bath , factors affecting throwing power , typical electrodeposition processes , applications of electroplating of metals . Numericals.

Unit-4: Polarisation and Overpotentials : **12 Hrs.**

Polarisation , concentration polarization , decomposition potentials ,over voltage ,hydrogen , oxygen and metal overvoltages ,types of overvoltages , factors affecting overvoltages ,experimental determination of decomposition potential and overvoltage, Tafels theory and Tafel equation , simultaneous deposition of metals .Numericals .

Unit -5: Conversion and storage of electrochemical energy: **12 Hrs.**

Introduction of storage cells, fuel cells, solar cells Types of storage cells (batteries) ,measure of cell performance , charging and discharging , introduction of classical batteries , modern batteries –zinc-air , nickel-metal oxide and lithium batteries.

Brief history of fuel cells, efficiency of fuel cells, hydrogen-oxygen fuel cell, phosphoric acid fuel cell, direct methanol and biochemical fuel cells .

Solar cells introduction, intrinsic and extrinsic semiconductors, majority and minority carriers, p-n junctions, principle and working of solar cells, advantages.

Reference Books :

1) Modern Electrochemistry, Vol 1,2A and 2B, John O" M Bokris
2) An Introduction to Electrochemistry, Samuel Glasstone.
3) Theoretical Electrochemistry, L.Antropov.
4) Advanced Physical Chemistry, Gurtu and Gurtu.
5) Principles of Physical Chemistry, Puri,Sharma and Pathania.
6) Text Book of Physical Chemistry, S. Glasstone
7) Physical Chemistry, Robert J. Silbey.
8) Physical Chemistry, G.K.Vemulapalli.
9) Physical Chemistry, Maron and Pruton.
10) Physical Chemistry, P.W. Atkins.D ELECTROCH--

CHEP: 418 Nuclear Chemistry

Period : 60 hrs. **50 Marks** **Credit : 04**

Unit- I Nuclear particles and its properties [12 hrs]

The fundamental particles, roll call of elementary particles, composition of the nucleus, theories of nuclear composition, nuclear properties, mass defect and binding energy, nuclear stability explained by different factors.

Nuclear size and density, mechanical effects due to orbiting and spinning of nucleons, orbital angular momentum of the nucleons, Total angular momentum of the nucleons, magnetic quantum numbers, principal and radial quantum numbers, total angular momentum of nucleus, total magnetic nuclear angular momentum quantum number, magnetic properties of the nucleous, the neutron magnetic moment, the structure of nucleon the net magnetic moments, The spin of odd Z odd N nuclei, The Nordhein rule.

Unit- II Nuclear models : [12 hrs.]

The shell model and its salient features, periodicity in nuclear properties- magic numbers, forces of nuclear potential, energy level in nuclear potential well, the sequence of filling the orbital including models, nuclear configuration. The liquid drop model, and its details and The Fermi gas model.

Unit III Radioactivity: [12 hrs.]

Historical, background, natural radioactive elements, general characteristics of α, β, γ rays, detection and measurement of radioactivity, the theory of radioactive disintegration, decay kinetics, units of radioactivity, parent daughter growth relationship- secular and transient equilibrium, theory of α decay, β decay – energetics of β decay problems of β decay, fermis theory of β decay, nuclear de-excitation – emission, numerical

Unit-IV Nuclear Reactions. [12 hrs.]

Definition and Bethes notation, nuclear reaction energetic, nuclear reaction and threshold energy, characteristics of nuclear reactions, types of nuclear reactions, conservation in nuclear reactions, nuclear reactions cross section, cross section and reaction rate, the compound nucleus theory, general properties of compound nucleus, optical model, direct interaction model, specific nuclear reactions- photonuclear reactions, stripping and pickup reactions evaporation, spallation, fragmentation, direct nuclear reactions, thermonuclear reactions.

Unit - V Radiation chemistry and its applications [12hrs]

A. Introduction of radiation with matter, primary effects due to charged particle/radiation, Linear energy transfer(LET), Bethes equation for LET, Bremsstrahulung, the cerenkov radians, interactions of electron with matter, interaction of neutrons with matter, interaction of heavy charged particles with matter, interaction of rays with matter, units for measuring radiation absorption, absorption in water **B.** Typical reactions involved in the preparations of isotopes: the scillard-chalmers reactions, radiochemical principles in the use of tracers, typical application of radioisotopes as tracers- chemical investigation, physio-chemical research, analytical applications, agricultural applications, industrial applications, use of nuclear radiations, radioisotope as a source of electricity

Reference Books.

1. Source of Atomic energy by s. Glasstance, D. Van Nostrand co. INC
2. Essentials of nuclear chemistry by *H.J. Arnikar 4th Edn, New Age International(p) Ltd.*
3. *Introduction to Nuclear By chemistry* B. G. Harvey,
4. Nuclear chemistry by M. G. Arora & M. Singh Anmol publication, New Delhi
5. Elements of nuclear chemistry by A. K. Srivastav, P. C. Jain, S. Chand & Co.
6. A text book of Nuclear chemistry by C.V. Shekar Deminant publication & distribution, New Delhi.
7. Radiochemistry & nuclear chemistry, 3rd edn G. chappin, Butterwerth-Heinemann.

Dr. Babasaheb Ambedkar Marathwada University Aurangabad 431 004

Department of Chemistry

Physical Chemistry- MSc IVth Semester Paper- CHEP- 419

Thermodynamics

Lectures: 60 **Credits: 04**

Statistical Thermodynamics

Unit I Introduction **12hrs**

Combinatorial problems, Thermodynamics probability and most probable distribution, ensembles-canonical, grand canonical and micro canonical Stirlings approximation, distribution laws, the law of equipartition of energies. Quantum statistics- Max Well-Boltzmann, Bose-Einstein and Fermi-Dirac, limit and applicability of various distribution laws.

Unit II Molecular Partition function **12hrs**

Partition function, Expression for translational, rotational, vibrational and electronic partition functions, Third law of thermodynamics and partition function, Numerical problems.

Unit III Application to chemical systems **12hrs**

Partition function and Thermodynamic functions, Sackur-Tetrode equation (derivation), determination of equation of state of an ideal gas. Internal rotation, residual entropies, heat capacity of solids: Einstein model, Debye modification (model), characteristic temperature, statistical mechanics of solutions ideal and nonideal.

Unit IV Applications to quantum systems **12hrs**

Nuclear spin statistics, ortho and para nuclear states, ortho and para hydrogen.Fermi energy, Fermi energy of electron gas in metals, Plancks distribution law and radiation, Bose-Einstein degenerate gas (He gas).

Unit V Irreversible Thermodynamics **12hrs**

Postulates, entropy production in heat, entropy production in matter flow, entropy production in chemical reactions, Onsager's theory, microscopic reversibility and Onsager's reciprocity, stationary states and entropy production, Prigogine's principle of minimum entropy, application to thermoelectric effects-Seeback and Peltier effect.

Books Suggested:

1) Statistical Thermodynamics, Donaid A. Mc Qurrie, Harper & Row, York 1973.
2) Statistical Thermodynamics, M.C. Gupta, Wiley Eastern Ltd. New Delh
3) Elements of Statistical Thermodynamics, L. K. Nash Addison Wesle Menlo Park, 1972.
4) Physical chemistry, P. W. Atkins, ELBS
5) Non Equilibrium Thermodynamics, Progogine Kalyani Publication.
6) Thermodynamics and Non Equilibrium Thermodynamics, Gurudeep Raj.

Surface and Magetochemistry : Paper CHEP- 420

Duration : 60 hrs **Marks: 50** **Credit : 04**

Unit-1: Surface chemistry : **[12hrs]**

Adsorption ,adsorption isotherms ,Langmuirs unimolecular theory of adsorption statistical derivation of Langmuirs adsorption isotherm , BET theory of multilayer adsorption ,derivation of BET equation, determination of surface area of adsorbent ,heat of adsorption and its determination

Unit-2: Colloidal state of matter : **[12hrs]**

Introduction to colloids, classification, properties, specific properties like,electrical properties, charge on colloidal particals, origin of charge, electrical double layer, electrokinetic properties,electrophoresis, electroosmosis, streaming potential, sedimentation potential, determination of size of colloidal particals, applications of colloids, Numericals.

Unit-3: Introduction to magnetochemistry : **[12hrs]**

Definition of magetic properties, types of magnetic behaviour, sources of paramagnetism, Pascals constants and it's applications, Determination of magnetic susceptibility. Numericals.

Unit-4: Valence theories : **[12hrs]**

Valence bond theory, crystal field theory, octahedral, tetrahedral, square planar, trigonal bipyramidal and square pyramidal stereorio chemistries, John -Teller effect. Magnetic properties based on crystal field model. Limitations of crystal field theory. Molecular orbital theory.

Unit-5: Magnetic Moments and Electronic spectra : [12hrs]

Crystal field strength and its terminology, crystal field diagrams of d1 and d2 configuration. Tanabo – Sugano diagrams, electronic transitions, selection rules, d-d transitions and charge transfer transitions in metal complexes

REFERENCES:

1) K.J.Laidler, J.H.Meiser and B.C. Sanctuary, Physical Chemistry, Houghton Mifflin Company, New York, 2003.
2) A.W.Adamson, Physical Chemistry of Surfaces, 4 th edition, Interscience, New York,1982.
3) G.K.Vemulapalli, Physical Chemistry, Printice Hall of India.
4) Gurtu and Gurtu , Advanced Physical Chemistry.
5) S.Glasstone, Text book of Phycal Chemistry.
6) Gurdeep and Raj, Advanced Physical Chemistry.
7) A.R.West, Solid State Chemistry and its Applications, John Wiley and Sons, 2003(reprint 2009)
8) H.V.Keer, Principles of Solid State.
9) A.Earn Shaw, Introcuction to Magnetochemistry; Academic Press.
10)J.Sharma, Magnetochemistry.
11) R.I.Dutta and Syamal, Elements of magnetochemistry.
12)Oliver Kahn,Molecular Magnetism, VCH Weinheim(1993)
13)S. Pahari, Physical Chemistry ,vol.II.
14) Puri, Shrma, Pathania, Principles of Physical Chemistry.
15)Charles Kittle, Introduction to Solid State Physics 7 th edition, John Wiley and Sons,2004(reprint 2009)

Chemical Dynamics and Catalysis : CHEP-421

Duration : 60 hrs **Marks: 50** **Credit : 04**

Unit-1: Kinetics of Complex Reactions: **12 hr**

Opposing or reversible reactions, parallel and competative reactions, consecutive reactions, chain reactions, branched chain reactions and explosions, hydrogen-oxygen reactions, kinetics of polymerization-step wise and free radical polymerization Effect of temperature on rates of simple and complex reactions. Numericals

Unit-2: Reactions in solution: **12 hrs.**

Diffusion controlled reactions, substitution and correlation effect, Hammet equation, Taft effects, compensation effect. Electron transfer reactions, proton transfer reactions. Ion dipole and dipole-diople interactions. Influence of pressure on rate in solution. Numericals

Unit-3: Photochemical Reactions: **12 hr**

Introduction, photocatalytic reactions, types of photocatalytic reactions, photooxidation, photoreduction, photosensitization, photocatalytic degradation, use of metal ions in photochemical processes. Chemiluminescence, photosynthesis, photoelectrochemistry of excited state, redox reactions. Solar energy conversion and storage. Numericals.

Unit-4: Homogeneous and Hetrogeneous Catalysis: **12 hr**

Introduction, mechanism of catalysis, Acid-base catalysis, effect of pH on rate constant. Micellar catalysis, enzyme catalysis, factors governing rate of enzyme reactions, kinetics of enzyme catalysed reactions.

Unimolecular surface reactions, bimolecular surface reactions, effect of temperature on heterogeneous reactions, transition state theory and the rates of surface reactions, theory of heterogeneous catalysis.

Unit-5: Preparation and characterization of catalyst: **12 hr**

General methods for preparation of catalysts, precipitation, sol-gel, hydrothermal, impregnation, hydrolysis, vapour deposition.methods Activation of catalysts, calcinations, reaction. Catalyst characterization, surface area, pore size distribution, particle size determination, XPS, AES, UV-Vis, FT-IR and thermal methods. Applications.

Reference Books

1 Chemical kinetics — E.S.Laidler pearson Education
2 Chemical kinetics and Reaction dynamics — Bul Houston
3 Chemical kinetics and Reaction Mechanism — F-Wilkinson-VanNostral Reinhdd
4 kinetics and Mechanism Of Chemical Transformations — J. Rajaram Macmillan India Ltd
5 Atkins physical chemistry — J.C.Curiacose.
6 physical chemistry — Atking and Oxford University press D.Paula
7 physical chemistry-principles And Appllication in Biological Sciences — Berry, Rice, Ross Oxford University press
8 physical chemistry — Tinoco, Sauer Pearson Education.
W.J.Moore.

DR. BABASAHEB AMBEDKAR MARATHWADA UNIVERSITY, AURANGABAD

DEPARTMENT OF CHEMISTRY

Physical Chemistry Laboratory Course

M. Sc. III and IV Semester

(Effective from June 2012)

Paper CHEP-422 Laboratory course - I

Duration : 180 Hr **Marks 50** **Credits : 06**

Spectroscopy

1) To determine the indicator constant P^k_{in} of an indicator by using half height method (Bromo cresol purpule)(DVJ-200)
2) To determine the stability constant of metal complex between 5-SSA and Fe^{+3} with help of Job's curve and Bent and French method (for weak complex)(DVJ-204)
3) To determine the concentration of Fe(II) and Cu(II) by spectrophotometric titration with EDTA.
4) To investigate the effect of ionic strength on pKa of bromo cresol green and thus determine pK_{in} (DVJ-211)
5) To investigate the reaction kinetics between $K_2S_2O_8$ and KI by spectrophotometrically (TKC-223)
6) To determine simultaneously the dichromate and permagnate ions in the given solution.

Polarimetry

7) Determine the percentage of two optically active substances in a mixture.(TKC-194)
8) To investigate the complex ion formation between Fe(II) and thiocynate ion.
9) To study Kinetics of hydrolysis of sucrose by Hammett-Zuckerman approach.(DVJ)
10) Investigate the effect of substitution of chloride ions on rate constant of inversion of cane sugar by using mono, di and trichloro acetic acid as catalyst.

Refractometry

11) Determine the refractive indices of series of solution of a salt and determine the concentration of the salt in the given unknown solution.

12) Determine the molar refraction of ethyl, propyl and butyl acetate and show the constant of contribution to the molar refraction made by CH_2 group.

13) Determine the molar refraction of methyl acetate, ethyl acetate, n-hexane and carbon tetrachloride and calculate the atomic refraction of C, H and Cl atoms.

14) Study the variation of refractive indices with composition of mixture of carbon tetrachloride and ethyl acetate and determine the composition and molar refraction of the given unknown mixture.

Viscosity

15) Determine the variation of viscosity with composition of I) ethanol-water, II) methanol-ethylidene chloride, III) nitric acid- chloroform and and conform the formation of compound.(TKC-250)

16) Determine the molecular weight of macromolecules.(TKC-251)

17) Determine the iso-electric point of gelatin and examine the effect of aging by viscometric methods.(DVJ-29)

Flame Photometry

18) Estimation of Na, K, Li & Ca by flame photometry.

Paper CHEP-423 Laboratory course - II

Duration : 180 Hr **Marks 50** **Credits : 06**

Potentiometer

1) Titrate ferrous ammonium sulphate with cerric sulphate and find out formal redox potential of Fe^{+2}/Fe^{+3} and Ce^{+3}/Ce^{+4} system
2) Titrate potentiometrically phosphoric acid solution against NaOH and calculate pK_1, pK_2 and pK_3 of the acid.
3) Titrate potentiometricaly NaCl solution against $AgNO_3$ and find out the concentration of NaCl and hence determine the solubility product of AgCl.
4) To determine the standard free energy changes ΔG° and equilibrium constant for reaction $Cu + 2Ag^+ \longrightarrow Cu^{++} + Ag$ (TKC-167)
5) Determine the activity coefficient of silver ions using a concentration cell without transference.(TKC-154)

pH metry

6) To determine the proton-ligand stability constant of an organic acid and the metal-ligand stability constant of its complex by pH measurements.(TKC-176)
7) Determine the Hammett constant of a given substituted benzoic acid by pH measurements.(TKC-170)
8) Determine the pH values of various mixtures of sodium acetate and acetic acid in aqueous solution and hence find out the dissociation constant of the acid.(TKC-173)
9) To determine the hydrolysis constant of aniline hydrochloride by pH measurements. (TKC-174)

Conductometry

10) To determine the thermodynamic dissociation constant of weak acid conductometrically.
11) Investigate the kinetics of basic hydrolysis of ethyl acetate conductometrically.
12) Conductometric titration of a mixture of strong acid, weak acid and a salt.(DVJ)
13) To determine the degree of hydrolysis and hydrolysis constant of sodium acetate conductometrically.

Magnetochemistry

14) To determine the magnetic susceptibility and number of unpaired electrons in given compound.
15) Verification of Weidemann's law using nickel chloride solution.

Surface Tension

16) Study the effect of surfactant (n-propyl alcohol) at various concentrations on the surface tension of water and hence determine the limiting cross sectional area of alcohol molecule by stalagmometer.
17) Determine the parachor of a solid by stalagmometer.

Thermodynamics

18) Determine the partial molar volume of ethanol and water in a given composition by density measurements.
19) To determine heat of neutralization of strong acid and heat of ionization of weak acid calorimetrically.
20) To determine the integral heat of solution of KNO_3.
21) To determine the heat of dissociation of benzoic acid in water.
22) To determine heat of precipitation of $BaSO_4$.

Paper CHEP-424 Laboratory course - III

Duration : 180 Hr **Marks 50** **Credits : 06**

Section(A):

Chemical Dynamics

1) Investigate the influence of ionic strength on the rate constant of the reaction between $K_2S_2O_8$ and KI.(TKC-335)
2) Determine the order of a reaction by 1) substitution method , (II) fractional change method and (III) differential method.
3) Investigate the reaction between bromic acid and hydrochloric acid.(TKC-335)
4) To investigate the reaction between H_2O_2 and KI kinetically.
5) Investigate the kinetics of iodination of acetone.

Phase equalibria

6) Determine the critical solution temperature of phenol and water in presence of 1) 1% NaCl 2) 0.5% naphthalene 3) succinic acid
7) Construct the phase diagram of three-component system containing ethanol benzene and water.
8) Determine the equilibrium constant of the tri-iodide formation in aqueous solution by distribution method .

Adsorption

9) Investigate the adsorption of acetic / oxalic acid by activated charcoal and test the validity of Freundlich and Langmuir's isotherm.

Section(B): PROJECT WORK.

SCHEME OF MARKING

For paper CHEP(Pr)-422 & CHEP(Pr)-423

Record book & Viva: 05

	Experiment(I)	Experiment II
1) Observation :	10	08
2) Calculation:	05	04
3) Graph:	05	04
4) Accuracy & Result:	05	04
Total:	25	20

Paper CHEP(Pr)-424

Record book & Viva: 05

	Experiment(I)	Experiment II
5) Observation :	10	08
6) Calculation:	05	04
7) Graph:	05	04
8) Accuracy & Result:	05	04
Total:	**25**	**20**

Project evaluation: 25 marks

1) Literature survey, status of problem:	05
2) Presentation of work: (Understanding of problem, development Of problem, conclusion)	05
3) Content and amount of work done Accuracy of experiments	05
4) Result(calculation, graph)	05
5) Dissertation & accuracy/ Answer	05
Total	**25**

NOTE: STUDENT WILL NOT BE ALLOWED FOR PRACTICAL EXAMINATION IF HIS/HER RECORD BOOK IS NOT COMPLETED AND CERTIFIED.

DR. BABASAHEB AMBEDKAR MARATHWADA UNIVERSITY,

AURANGABAD

DEPARTMENT OF CHEMISTRY

PRevised Syllabus

M. Sc. Analytical Chemistry

Effective from June 2013

Third Semester **CHE-313** **Credits: 04**

STRUCTURAL ELUCIDATION BY SPECTRAL METHODS

❖ UNIT-I *Nuclear Magnetic Resonance Spectroscopy (^{1}H NMR)*

Elementary ideas (Recapitulation); Spin-spin couplings, Different types of couplings, factors affecting on coupling constants, Karplus equation, Spin systems (AB, AX, ABX, AMX), Rate processes, spin decoupling, shift reagents, Nuclear Overhauser effect (NOE), INEPT and INADEQUATE.

❖ UNIT-II *^{13}C Nuclear Magnetic Resonance Spectroscopy*

Elementary ideas, instrumental problems, chemical shifts (aliphatic, olefinic, alkyne, aromatic, heteroaromatic and carbonyl carbons); Effect of substituents on chemical shifts.

❖ UNIT-III *Mass Spectroscopy*

Introduction, ion production (EI, CI, FD and FAB), ion analysis, ion abundance, factors affecting on fragmentation, fragmentation of different functional groups, molecular ion peak, isotopic peaks, metastable peak, Nitrogen rule, McLafferty rearrangement, Retro-Diels-Alder reaction.

❖ UNIT-IV

Problems based on joint applications of UV, IR, ^{1}H NMR, ^{13}C NMR and Mass spectroscopy.

❖ UNIT-V

(A) Mossbauer spectroscopy: Principle, factors affecting the line position and shape, isomer effect and Quadrupole splitting iron salt like compounds, complexes, carbonyl compounds (temperature dependence of isomer shift and Quadrupole splitting in simple compound and coordination, polynuclear complexes), Numericals.

(B) Electron Spin Resonance Spectroscopy: Introduction, principle of ESR spectroscopy, presentation of spectrum, hyperfine splitting in various structures, hyperfine splitting digram of representative examples, factors affecting the magnitude of 'g' values, Zero field splitting, Kramer's degeneracy, Anisotropy in the hyperfine coupling constant, electron delocalization, instrumentation and applications.

Reference Books:

1. Introduction to Spectroscopy: D. L. Pavia, G. M. Lampman, G. S. Kriz
2. Spectrometric Identification of Organic Compounds: R. M. Silverstein & F. X. Webster
3. ^{13}C NMR Spectroscopy: G. C. Levy, R. L. Lichter, G. L. Nelson
4. Spectroscopic Methods in Organic Chemistry: D. H. Williams & I. Flemming
5. Absorption Spectroscopy of Organic Compounds: V. M. Parikh
6. Mass Spectrometry: K. G. Das & James
7. Coordination Chemistry by Experimental Methods: K. Barger
8. Coordination Chemistry vol. I: E. Martell
9. Physical Methods for Chemistry: R. S. Drago
10. Structural Methods in Inorganic Chemistry: E. A. V. Ebsworth & D. W. H. Rankin
11. Organic Structure Analysis: Philips Crews

Dr. Babasaheb Ambedkar Marathwada University, Aurangabad.

Department of Chemistry

CHEA: 314-Electroanalytical Techniques

L = 60 **Credits: 04**

❖ Unit-I **12**

a) a)Ion selective electrodes:

Types and construction of electrode:- Glass electrode, Solid state electrode and precipitate electrode, Liquid-liquid membrane electrodes, Enzyme and gas electrode, Applications of ion selective electrodes, numericals.

b) Potentiometry:

Introduction, Instrumentation, Various electrodes in potentiometry:- Ion selective electrode, Liquid membrane electrode, Weston cell.

Potentiometric titrations:- Types of potentiometric titrations, Variations in potentiometric titrations, Limitations, Numericals.

❖ Unit-II Coulometry: **12**

Introduction, Principle, Technique, Coulometry at constant current and coulometry at controlled potential, Coulometric titration, Flowing stream coulometry, Applications, Stripping analysis.

❖ Unit-III Cyclic voltrametry: **12**

Introduction, Beginning of cyclic voltametry, Range of cyclic voltrametric techniques, Limitations. The acceptable sweep rate range, The shape of the peak in potential sweep curves, Quantitative calculations of kinetic parameters from potential sweep curves, The role of non aqueous solution in cyclicvoltametry, Crieteria of reversibility of electrochemical reactions Quasi reversible and irreversible processes, Qualitative and quantitative analysis by cyclic voltametric techniques, Linear sweep voltametry for reactions that include simple adsorbed intermediates and Numericals.

❖ Unit-IV **12**

a) **Polarography:**

Theory, Instrumentation of polarography, Differtial pulse polarography, Factors affecting on polarographic wave, Modified polarographic techniques:- Sinusoidal AC polarography, Chronopotentiometry and their applications in qualitative and quantitative analysis, Numericals.

b) High frequency titration:

Introduction, Theory and instrumentation, High frequency titrimetry, Types of cells, Advantages of high frequency methods and applications.

❖ Unit-V 12

a) Electro-Gravimetry:

Introduction, Theory of electrogravimetry, Terms used in electrogravimetric analysis. Completeness of deposition, Electroanalytical separation of metals, Applications.

b) Electrophoresis:

Introduction, Paper electrophoresis technique, Factors affecting migration of ions, Capillary and zone electrophoresis, Applications, Numericals.

Reference Books:

1. Quantitative analysis -. Alexeyev. V
2. Instrumental methods of analysis – Chatwal and Anand.
3. Introduction to instrumental analysis – R. D. Braun.
4. Instrumental methods of analysis – Willard, Meritt, Dean and Settle.
5. Standard methods of chemical analysis – F. G. Welcher, Vol III, Part A & B.
6. Electroanalytical chemistry – H. W. Neurenberg.
7. Principles of electrochemistry – D. A. Maclines.
8. Ion selective electrodes – (John Wiley) Stulic.
9. Vogel's textbook of quantitative chemical analysis V edition by Jeffery Bassett Mendham Denney.
10. Modern Electrochemistry vol.I - John O'M Bockris
11. Modern Electrochemistry vol.II - John O'M Bockris
12. Analytical Chemistry – Gary D. Christian, 6th edition
13. Priciples of Instrumental Analysis–Skoog, F.J.Holler & J.A.Nieman
14. Instrumental Methods of Chemical Analysis–Galen W. Ewing. 5th edition

Dr. Babasaheb Ambedkar Marathwada University, Aurangabad.

Department of Chemistry

CHEA:-315 Environmental Analysis and Monitoring

L = 60 **Credits: 04**

❖ Unit-I Air Pollution **12**

General considerations: polluted air, Types of pollution and units of measurements. Air quality standards, Sampling, Monitoring, Analysis of CO, Sources and sinks of CO pollution, Effects of CO on plants and humans, Control of CO pollution, Analysis of oxides of nitrogen, NOx sources and sinks of NOx pollution, Control of NOx pollution, Hydrocarbons and photochemical smog and its control, Analysis of hydrocarbon in exhaust gasses, Petrol and air, Sulpher di oxide sources, Analysis and control, Acid rain particulates and their effects on human and climate, Control of particulates.

❖ Unit-II **12**

a. Water Pollution:

Aquatic environment, Water pollutants, Sampling of water and its preservation Trace metals in water, Chemical speciation with special reference to Copper, Lead, Mercury and Arsenic. Water quality standards Water quality parameters.

b. Oxygen Demanding Wastes:

Dissolved oxygen, Biological oxygen demand, Monitoring techniques and methodology with special reference to ammonia, Nitrates, Nitrites, Fluorides, Cyanides, Total hardness, Lead, Cadmium and Mercury. Detection and control of Detergents, oils, Pesticides, Sewage treatment.

❖ Unit-III **12**

a) Chemical toxicology:

Toxic chemicals in environment, Impact of toxic chemicals on enzymes, Biochemical effects of Arsenic, Cadmium, Lead, Mercury, Carbon monoxide, Sulphur dioxide, Pesticides and Carcinogens.

b) Soil analysis:

Sampling of soil, Determination of water holding capacity, Determination of total nitrogen, phosphorous and sulphur in soil.

❖ Unit-IV Industrial pollution: 12

Pollution due to cement industry, Distillery, Pharmaceutical (Drug) industries, Sugar industry, Paper and pulp industries, Thermal power plants, Nuclear power plants, Metallurgical industries, Polymer industries. Recycle, reuse, recovery, disposal,and management of solid industrial waste.

❖ Unit-V GreenChemistry: 12

Principle and concepts of Green Chemistry: Sustainable development and green chemistry, Atom economy,examples of atom economic and atom un-economic reactions,reducing toxicity.

Organic solvents: environmentally benign solutions,solvent free systems,supercritical fluids,ionic liquids as catalysts and solvents.

Emerging green technologies: Photochemical reactions (Advantages and challenges),examples, chemistry using microwaves, sonochemistry,electrochemical synthesis.

Designing greener processes: Inherently safer design (ISD),Process intensification(PI),in-process monitoring.

Reference Books:

1. A. K. De, Environmental Chemistry, Wiley Eastern Ltd. New Delhi.
2. S. L. Chopra and J. S. kanwar, Analytical, Agricultural Chemistry, Kalyani Publishers, New Delhi.
3. R. K. Trivedy and P. K. God, Chemical and biological methods for water pollution studies, Environmental publications, co. New Delhi.
4. L. A. Richards, Diagnosis and improvement of saline and alkali soils. Oxford IBH publications co. New Delhi.
5. S. M. Khopkar, Environmental chemistry, Environmental pollution analysis.
6. M. S. Creos and Morr, Environmental chemical analysis, American publications.
7. M. Sitting, Resources, Recovery and Recycling, Handbook of industrial waste.
8. Standard methods of water and waste water analysis, American public health association Washington D. C.
9. R. Gopalan and Amrutha Anand, "Environmental chemistry laboratory manual Emerald Publication.
10. Standards for water for drinking and other purposes, Beaurau of Indian Standards India.
11. Guideline for drinking water quality recommendations of world health organization, Geneva.
12. B. K. Sharma and H. Kaur, Environmental Chemistry, Guel publishing house Meerut.
13. Thomas G. Spiro and Willian M. Stigliani, Chemistry of environment.
14. Green Chemistry: An Introductory Text, Mike Lancaster, Royal Society of Chemistry,(2002)
15. New Trends in green Chemistry, V.K.Ahluwalia and M. Kidwai, Anamaya Publishers New Delhi, (2004)

Dr. Babasaheb Ambedkar Marathwada University, Aurangabad.

Department of Chemistry

CHEA: 316-Advanced Analytical Techniques-I

L = 60 **Credits: 04**

❖ Unit-I Atomic Spectroscopy 12

Photoacoustic Spectrometry : Principle, Instrumentation, and applications

Atomic Emission Spectroscopy with Plasma and Electrical Discharge Sources.

Principle, Instrumentation, and applications, ICP Atomic Fluorescence Spectroscopy, ICP versus AAS

❖ Unit-II 12

Atomic Mass Spectroscopy: General features, Mass Spectrometers, Inductive Coupled Plasma Mass Spectrometry, Spark Source Mass Spectrometry, Glow Discharge Mass Spectrometry, and other Mass Spectrometric Methods.

❖ Unit-III Atomic X-ray Spectrometry: 12

Principle, X-ray Spectra, Instrumentation, Direct X-ray Methods, X-ray Absorption Methods, X-ray Fluorescence Methods, The Electron Microprobe.

❖ Unit-IV Molecular Luminescence Spectrometry: 12

Theory of fluorescence and phosphorescence-Excited states producing fluorescence and phosphorescence, Rates of absorption and emission, Deactivation processes, Variables affecting fluorescence and phosphorescence, Emission and excitation spectra.,

Instruments for measuring fluorescence and phosphorescence-Components of fluorometers & spectrofluorometers, Instruments designs, & standardization.

Applications and photoluminescence methods-Fluorometric determination of inorganic and organic species.,phosphorimetric methods, Application of fluorometry and phophorimetry for detection in liquid chromatography. Lifetime measurements.

Chemiluminescence- Phenomenon, Measurement & Applications

❖ Unit-V Radiochemical Methods. 12

Introduction, Radioactive isotopes- Radioactive decay products, Decay process,

Decay rates, Counting statistics, Instrumentation: Measurements of alpha , beta particles and gamma radiation.

Neutrons and neutron sources, Interaction of neutrons with matter.

Experimental considerations in activation methods- Destructive and non-destructive methods.

Principle and applications of neutron activation and Isotope dilution method

Application of radionuclide as tracers

Reference Books

1. Instrumental Methods of Analysis–Willard, Merritt, Dean & Settle, 7^{th} edition
2. Priciples of Instrumental Analysis–Skoog, F.J.Holler & J.A.Nieman
3. Instrumental Methods of Chemical Analysis–Galen W. Ewing. 5^{th} edition
4. Analytical Chemistry – Gary D. Christian, 6^{th} edition
5. Handbook of Instrumental Techniques for Analytical Chemistry –Frank Settle,Editor
6. Analytical Chemistry Handbook – John A. Dean.
7. Introduction to Instrumental Analysis-R.D. Braun, McGraw Hill.
8. Fundamental of Analytical Chemistry,-D.A. Skoog, D.M.West and F.J. Holler.
9. Instrumental methods of analysis – Chatwal and Anand
10. Instrumental methods of analysis – B. K. Sharma

Dr. Babasaheb Ambedkar Marathwada University, Aurangabad.

Department of Chemistry

CHEA: 317-Advanced Analytical Techniques-II

L = 60 **Credits: 04**

❖ Unit-I Surface Characterization by Spectroscopy and Microscopy: 12

Introduction to the study of surfaces.

General techniques in surface spectroscopy.

Principle, instrumentation and applications of the followings

Auger Electron spectroscopy.

Ultraviolet Photoelectron Spectroscopy.

Secondary – Ion Mass Spectrometry.

Laser – Microprobe Mass Spectrometry.

The Electron Microprobe.

Scanning Electron Microscopy: Scanning Electron Microscope.

The Scanning Tunneling Microscope, The Atomic Force Microscope

❖ Unit-II Supercritical Fluid Chromatography and Extraction: 12

Properties of Supercritical Fluids, Supercritical Fluid Chromatography, Supercritical Fluid Extraction.

❖ Unit-III 12

High performance thin layer chromatography, Ultra performance liquid chromatography, Advanced flash chromatography.- Principle, Instrumentation and Application.

❖ Unit-IV Hyphenated Techniques. 12

Introduction, Need for hyphenation, Possible hyphenation, Interfacing devices and applications of the following:

GC-MS, GC-IR, MS-MS, HPLC-MS, ICP-MS,

Spectroelectrochemistry and radio-chromatography.

❖ Unit-V Automated Methods of Analysis. 12

Principle of automation, Automated instruments: Process control (continuous analyzers and discrete analyzers).Advantages and disadvantages of automatic analyzers.

Flow – injection Analysis: Principle, instrumentation and applications. Sequential injection Analysis. Concept of online analyzer.

Reference Books

1. Instrumental Methods of Analysis–Willard, Merritt, Dean & Settle, 7th edition
2. Principles of Instrumental Analysis–Skoog, F.J.Holler & J.A.Nieman
3. Instrumental Methods of Chemical Analysis–Galen W. Ewing. 5th edition
4. Analytical Chemistry – Gary D. Christian, 6th edition
5. Handbook of Instrumental Techniques for Analytical Chemistry –Frank Settle,Editor
6. Analytical Chemistry Handbook – John A. Dean.
7. Introduction to Instrumental Analysis-R.D. Braun, McGraw Hill.
8. Fundamental of Analytical Chemistry,-D.A. Skoog, D.M.West and F.J. Holler.
9. Quality measuring Instruments in on-line process Analysis, D.J. Huskins.
10. Gas Chromatography, P.S. Ramnathan, 4-volumes
11. Wilson and Wilson Compressive Analytical Chemistry. Ed. G. Svehla, A series of volumes.
12. Instrumental methods of analysis – Chatwal and Anand.
13. Instrumental methods of analysis – B. K. Sharma.

Dr. Babasaheb Ambedkar Marathwada University, Aurangabad.

Department of Chemistry

CHEA:418-Analysis of Ores, Alloys & Explosive

L = 60 **Credits: 04**

❖ Unit-I **12**

a. Analysis of ores

Composition and analysis of Dolomite, Galena, Bauxite, Ileminite, Pyrolusite, Zinc blend and calcite for their major constituents using one of the standard methods of analysis.

b. **Analysis of alloys.**

Composition, Properties, uses and analysis of-
1. Brass 2. Bronze 3. Solder 4. Steel 5. Stainless steel
6. Monel-metal 7. Type-metal 8. Silver coin
for their major constituents using one of the standard methods of analysis.

❖ Unit-II Analysis of Paints and Pigments. **12**

Introduction, Determination of non volatile and volatile components, Flash point, Separation of pigments and thinner of solvent type coating, Pigment type, Identification of binders , Analysis of Vehicle and drying oils,
Analysis of pigments: Classification of organic and inorganic pigments, White tinted pigments.

❖ Unit-III **12**

Analysis of Cement and bulding materials.: Types of cement, Sampling, Analysis of- Silicon dioxide, Aluminium oxides, Ferric oxides, Calcium oxide, Magnesium oxide, Sodium and potassium oxide.
Analysis of Glass: Types of glasses, Determination of lead and lead glass.

❖ Unit-IV Explosive : **12**

Explosion, Detonation, Classification of explosives, Propelant, Fulminates, Detonators, Blasting-cap, Thermochemistry, Hygroscopicity of explosives, Moisture by Karl-Fisher titration, Isolation from debris, Qualitatiove test,Cation & anion analysis by capillary electrophoresis, EDXRF, Analysis by TLC,HPLC, IR,GC-TEA method.

❖ Unit-V Cosmetic Analysis. **12**

a) Introduction to cosmetics.
b) Evalution of cosmetic materials-raw materials, additives, colours, perfumes.

c) Legislation and recent amendments with respect to cosmetic materials.
d) Analysis of Physical and chemical constituents of
    a. Skin powder
    b. Creams
    c. Lipsticks
    d. Lotions

Reference books.

1. Hillenbrand Lhundel, Bright and Hoffman, Applied inorganic analysis, John Wiley.
2. Snell and Biffen, Commercial methods of analysis.
3. P. G. Jeffery, Chemical methods of rock analysis, pergamon.
4. Rieche, Outline of industrial organic chemistry, Butter worth.
5. Kent, Rieg's Industrial chemistry, Rain hold
6. P. G. Jeffery and. J. Hatchinsion, Chemical methods of rock analysis.
7. F. J. Welcher Standard methods of chemical analysis, A series of volume Robert and Krigeger Publishing Company.
8. Metallurgical analysis by S. K. Jain and K. K. Jain.
9. www.dghs.gov.in

Dr. Babasaheb Ambedkar Marathwada University, Aurangabad.

Department of Chemistry

CHEA:419- Food, Fertilizer & Pesticides Analysis

L = 60 **Credits: 04**

❖ Unit-I General concepts of food analysis. 12

Nutrient value of food.
Physical characteristics & chemical constituents
Proximate composition of food
Legislation related to food and recent amendments, Standards and public health

a) General idea regarding food processing and preservation
b) Food contamination and spoilage
c) Food safety considerations.
d) Adulteration-Introduction,Types,Tests for adulterants, control

❖ Unit-II Analysis of food- 12

a) Study of followings with their estimation methods
   Food preservatives,
   Food emulsifiers,
   Food stabilizers,
   Food thickener
b) Introduction, Standard composition and Analysis of the following foods.
   Milk and milk products, Tea, Coffee, Cereals & Flour, , Honey, Soft drinks & Alcoholic beverages.

❖ Unit- III Analysis of Oils, Fats Soap and Detergents 12

Introduction to natural oils and fats, Analysis of oils and fats, Softing point, Congent point, Titer point, Cloud point, Iodine, Saponification, acid, Hydroxyl, R-M and polenske values, Elaiden test.

Introduction to soaps, Analysis of soaps, for saponification, Unsaponifiable and unsaponified matter in soaps, Estimation of free alkali and phenol in soap, Classification of detergents (in Brief), Analysis of active ingredients from detergents (methelene blue and hyamine 1622 method), Estimation of CMC, Chlorides, Total phosphates

❖ Unit-IV 12

a. Analysis of fertilizers.

Classification of fertilizer, NPK value, Chemical composition of superphosphate, Lime and Potash fertilizer, Analysis of commercially available fertilizers for N, P & K.

b. **Analysis of pesticides.**

Legislation and recent amendments with respect to pesticides materials.

Names of pesticides and their chemical structures.

Application dosage of different pesticides.
Analysis of specific pesticides.

❖ Unit-V Analysis of Vitamins. 12

Analytical techniques of determination of water and fat soluble vitamins including microbiological techniques.

Human nutrition: Biological values and estimation of enzymes, Carbohydrates, essential amino acids, proteins and lipids.

Reference Books:-

1. Chemical analysis of food By Pearson.
2. Introductions to food science and technology , food science and technology series by G.F.Stewart and M.A.Amerine Academic process.
3. Cosmetics by W.D.Poucher (Three volumes)
4. Applied chemistry .AText book for Engineers and technologists by H.D.Gesser.
5. Food analysis by Nielson.
6. Food additives by S.N.Mahindry (APH) publication
7. Analytical chemistry by Dr.Alka Gupta (pragati prakashan)
8. Jacob(M.B) chemical Analysis of food and food products (Van Nostrand co. New York)
9. Analytical chemistry of foods (C.S.James) Blackie Academic and professional
10. Food Analysis principles and techniques D.W.Gruenwedel and J.R.Whitaker, Mercel Dekker
11. Food analysis Theroy and practice Y.pomeranz and C.E.Meloan,Chapman and Hill
12. Food Analysis ,2nd edition S.S Nelsen, Aspen publishers
13. Chopra S.L and Kanwar:J.S.1991 Analytical agricultural chemistry,Kalyani publishera,New Delhi Ludiana India
14. Food analysis, A. G. Woodman, McGraw Hill

Dr. Babasaheb Ambedkar Marathwada University, Aurangabad.

Department of Chemistry

CHEA:420 (Petrochemical &Polymer Analysis)

L = 60 **Credits: 04**

❖ Unit-I polymer:- 12

Introduction, classification of polymer, condensation polymerization, Addition polymerization. Mechanism, and stereochemistry of addition polymerization, Free redical addition polymerization,Cationic addition polymerization,Anionic addition polymerization Chain transfer reaction, Branching and cross linking in free radical addition polymerization, Ionic copolymerization,co-polycondensation Ring opening polymerization,Group transfer polymerization. .Co-ordination polymerization. Molecular mass, Number and mass average molecular mass, Molecular mass determination by osomometry, Viscometry, light scattering and Sedimentation methods, Kinetics of polymerization Numericals

❖ Unit-II Study of individual polymers:- 12

Preparation and applications of following polymers:- polyethylene, polystyrene polyacrylonitrile polyesters polyparaphenylene polycarbonates polyamides, polyethylene glycol polypropylene alcohol, polyvinyl chloride polytetrafluoethylene, silicone polymers.

❖ Unit-III Polymer degradation:- 12

Introduction, Types of degradation .Thermal degradation, Mechanical degradation, photo degradation, Degradation by high energy radiation .Degradation by ultrasonic wave. Oxidative degradation. Ozone oxidation degradation .oxidative degradation of saturated polumers. Oxidation of phenol, formaldehyde.Antioxidants.

❖ Unit-IV. Fuels:- 12

Introduction, calorific value. Determination of calorific value. Modern concept of fuels. Classifications of fuels ,criterion of selection of fuels , properties of fuels. Method of processing. Solids fuels ,Natural solid fuels, Artificial solid fuels ,Industrial solids fuels .Formation of coal properties of

coal ,Classification of coal., coking and non-coking coals. pulverised coal. .Role of sulphur and ash in coal ,approximate analysis ,Ultimate analysis. .Numerical.

❖ Unit-V Petroleum:- 12

Occurrence, mining of petroleum. Prospecting colour and consistency. Origin composition, classification ,terms related to petroleum. .Distillation of crude petroleum. Treatment of the residual liquid, Determination of flash point. Determination of aniline point .Knocking and Anti-knocking compounds. Octane number .Cetane number,Numericals.

Reference Books:-

1. Text Book of polymer science By F.W.Billmeyer, New York: Wiley
2. Physical polymer science by L.H .Sperling wiley –Interscience New York
3. Fundamentals of polymer science & Engineering By A Kumar & S.K.Gupta,Tata mcgraw Hill
4. Introduction to polymer science ,V.R.Gowarnikar, N.V.Vishwanathan & J.
5. Industrial Chemistry, B. K. Sharma, Goel publishing House Meerut.
6. Kent, Rieg's Industrial chemistry, Rain hold.
7. Handbook of Instrumental Techniques for analytical chemistry. Frank Settle, editor 1st Indian print 2004.
8. Polymer science by Vasant Govarikar, Wiley Earstewen. New York.
9. Principle of polymer science, Behadhar and Sastri, Narosa Publishing house.

Dr. Babasaheb Ambedkar Marathwada University, Aurangabad.

Department of Chemistry

CHEA:421-Pharmaceutical, Clinical & Forensic Analysis

L = 60 **Credits: 04**

❖ Unit-I Pharmaceutical Analysis-I 12

a. General idea regarding pharmaceutical industry, Definition and classification of drugs, types of dosage forms. Introduction to pharmaceutical formulations,
b. Sources of impurities in pharmaceutical chemicals, raw materials & Products,
c. Standardization of finished products& their characteristics,
d. Limit tests of As,Hg,Cu, Pb, Fe, Cl and SO_4, Solubility tests, disintegration tests, stability studies.

❖ Unit-II Pharmaceutical legislation: 12

Introduction to drug acts, drug rules,FDA and ISO standards & their amendments , ISO-9000, an overview, Clauses / requirement of ISO-9000, Significance and scope. Steps for ISO-9000, implementation, Series of ISO, Case studies of ISO. ISI, Agmark and other standard for goods & cosmetics particularly w.r.t. the testing of drugs, and raw material concerned.

Pharmaceutical standards BP/IP/USP/NE/EP.

Documentation, Record Keeping.

Contents of labels ,Types of packaging materials

❖ Unit-III Clinical Analysis. 12

Introduction: Body fluids: Composition, Collection and Preservation of body fluids and detection of abnormal levels of certain constituents leading to diagnosis of diseases and disorders.

Analysis of constituents of physiological fluids, viz.1.Blood -PH, Glucose, Urea. 2.Serum-uric acid, total protein,albumin,globulin&A/G ratio, barbiturates, alkaline phosphatase, acid phosphatase,bilurubin, cholesterol, amylase, creatinine carbohydrates.3.Urine-

Immunological methods: General process of immune response, Antibody-Antigen ratio, Precipitation reactions, Enzyme and fluoro-immune assays radioimmunoassay, ELISA

❖ Unit-IV Forensic Analysis. 12

Introduction, Special features of forensic analysis, Sampling, Sample storage, Sample dissolution

Toxicology: Classification of poisons and poisoning, Lethal Dose, Significance of LD50 and LC50.

Extraction methods in toxicology: Isolation, Identification and determinations of-

Narcotics: Heroin, Morphine, Codeine.

Stimulants: Caffeine, Cocaine, Amphetamines.

Despressant: Benzodiazepines- Diazepam, Oxazepam, Nitrazepam. Barbiturates- Phenobarbitone, Amylobarbitone, Pentobarbitone, Thiopentone.

Hallucinogens: LSC and Cannabis.

Analysis of biological stains and materials including blood, semen and saliva (qualitative and quantitative). Viscera, Stomach wash, Vomit and post mortem blood for poisons like cyanides, As, Hg, Insecticides and Pesticides.

❖ Unit-V Pharmaceutical Analysis-II 12

Assay of main classes of drugs with reference to Introduction, Type, Properties, Mode of action and Methods of Analysis.

Reference Books:

1. General Microbiology- R. V. Stainer 6th edition
2. Principle of microbiology- A. J. Salle
3. Microbiology- Pleczar
4. Isolation and Identification of drug-n E. G. Clarke vol.- I
5. Laboratory procedure manual-Forensic Toxicology- Directorate of forensic science, MHA Govt. of India.
6. Analytical Biochemistry, D. J. Holme and H.Peck, Longman
7. Bioanalytical Chemitry,S.R. Mikkelsen and E. Corton, John Wiley and Sons.
8. Immunoassay – a practical guide Eds,D.W.Chan and M.T.Perlstein, Academic Press.
9. Hawk's Physiological Chemistry, McGraw Hill.
10. Pharmaceutical Analysis Edited by David C. Lee, and Michael Webb.
11. An Introduction to Practical Biochemistry, David Plummer.
12. Biochemical methods, S. Sadasivam, A.Manickam.
13. Standard Methods of Biochemical Analysis, S.R. Thimmaiah