DR. BABASAHEB AMBEDKAR MARATHWADA UNIVERSITY, AURANGABAD.

Curriculum under Choice Based Credit &

Grading System

M.Sc. I Year

Chemistry

Semester–I & II

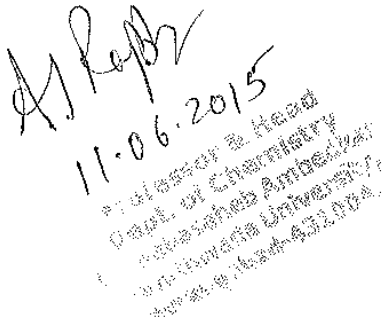
run at college level from the

Academic Year 2015-16 & onwards

DR. BABASAHEB AMBEDKAR MARATHWADA UNIVERSITY, AURANGABAD
DEPARTMENT OF CHEMISTRY

Credit based syllabus

M.Sc. Chemistry I & II Semester



Effective from June 2013

91

DR. BABASAHEB AMBEDKAR MARATHWADA UNIVERSITY, AURANGABAD
DEPARTMENT OF CHEMISTRY

Syllabus Based upon Credit System Effective from –June 2013

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

The M. Sc. Chemistry program of each specialization is divided into Four Semesters with 108 credits, comprising of 16 theory papers and 16 laboratory courses including projects, seminars and tutorials.

A) The 16 theory papers of each specialization include:

Core Courses: 08

Specialized Courses: 08

Elective Courses: 02 not compulsory

Service Courses: 01

B). The 16 laboratory course includes:

Core Courses: 08

Specialized Courses: 08

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 2013

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
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
I& II Semester Laboratory Course	CHE -209	Laboratory course (General & Analytical)	135 hrs	4.5
	CHE- 210	Laboratory course (Inorganic)	135 hrs.	4.5
	CHE- 211	Laboratory course (Organic)	135 hrs.	4.5
	CHE-212	Laboratory course (Physical)	135 hrs.	4.5

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

M. Sc. Chemistry –I Semester

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

M.Sc. Chemistry Semester- I

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

M.Sc. Chemistry Semester- II

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**: Theories 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.

M.Sc. Chemistry Semester-II

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 - Atkin 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 LABORATORY COURSE (INORGANIC)

Laboratory work hours: 135 hrs. **Credit : 4.50**

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.

CHE -209 LABORATORY COURSE (General & Analytical Chemistry)

Laboratory work hours: 135 hrs. **Credit : 4.50**

List of Experiments

1. Determination of saponification value of an oil sample.
2. Determination of active chlorine in the given sample of bleaching powder.
3. Determination of ion exchange capacity of given ion-exchange resin.
4. Determination of Mg^{++} from given sample of talcum powder.
5. Determination of asprin in the given tablet.
6. Determination of molality of given unknown solution by volhard method.
7. Determination of Hardness of the water sample.
8. Determination of pKa value of given substituted Benzoic acid
9. Determination of chemical oxygen demand (COD) of the given water sample.
10. Determination of Cu^{2+} ion in the given solution spectrophotometrically.
11. Determination of dichromate & permanganate ion simultaneously in the given sample spectrophotometrically.
12. Determine the molecular weight of a given polymer by turbidimetry
13. Determine the concentration of sulphuric acid, acetic acid & copper sulphate in the given solution by conductometric titration method.
14. Estimation of Na/ K/ Li/ Ca by Flame photometry
15. Determination of Phosphoric acid cola averages by pH meter
16. Estimation of Vitamin C by 2,6 dichloro-indophenol method
17. Assay sulpha drugs.

Scheme of marking :-

Max. Mark – 50

1) Experiment I - 20
2) Experiment II - 20
3) Record Book - 05
4) Viva - 05

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 LABORATORY COURSE (ORGANIC)

Laboratory work hours: 135 hrs. **Credit : 4.50**

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 LABORATORY COURSE (PHYSICAL)

Laboratory work hours: 135 hrs. **Credit : 4.50**

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.

Curriculum under Choice Based Credit &

Grading System

M.Sc.

Organic Chemistry

Semester–III & Iv

run at college level from the

Academic Year 2015-16 & onwards

Dr. Babasaheb Ambedkar Marathwada University, Aurangabad
Department of chemistry

Revised Syllabus

11.06.2015

Professor & Head
Dept. of Chemistry
Babasaheb Ambedkar
Marathwada University,
Aurangabad-431004.

M. Sc.III & IV semester Organic Chemistry

Effective from June 2014

The following will be the structure for revised syllabus for M. Sc. Organic Chemistry III & IV semester effective from June 2014

Semester	Paper Nos.	Title of Paper	Dura-tions (Hr)	Max. Marks	Credits
III- Semester Theory courses	CHE-313	Structural Elucidation by Spectral methods	60	50	4
	CHEO- 314	Organic Synthesis	60	50	4
	CHEO-315	Asymmetric Synthesis and Bio-Organic Chemistry	60	50	4
	CHEO-316	Photochemistry, Free Radicals And Pericyclic Reactions	60	50	4
IV semester Theory Courses	CHEO: 417	Organic Synthesis: Retrosynthetic Approach	60	50	4
	CHEO: 418	Advanced Organic and Heterocyclic Chemistry	60	50	4
	CHEO: 419	Chemistry of Natural Products	60	50	4
	CHEO: 420	Medicinal Chemistry	60	50	4
III & IV Semester Laboratory Courses	CHEO-421	Laboratory course (Organic)	135	50	4.5
	CHEO - 422	Laboratory course (Organic)	135	50	4.5
	CHEO- 423	Laboratory course (Organic)	135	50	4.5
	CHEO- 424	Project work (Organic)	135	50	4.5

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

Structural Elucidation by Spectral methods

UNIT-I ***Nuclear Magnetic Resonance Spectroscopy (^1H 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, ^1H 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

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

Organic Synthesis

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, Moffatt oxidation

(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.

UNIT-IV *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-V *Formation of Carbon-Carbon bonds via organometallic reagents*

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

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. Organic Chemistry: An Intermediate Text: Robert V. Hoffmann
12. Advanced Organic Chemistry: Jerry March
13. Organic Synthesis: R. O. C. Norman and Coxan
14. Name Reactions: Jie Jack Li

--

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

Asymmetric Synthesis and Bio-Organic 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.

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. 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. Stereochemistry of Organic Compounds (Principle and application): D. Nasipuri
8. Stereochemistry of Organic compounds: Ernest L. Eliel / Samuel H. Wilen
9. Advanced Organic Chemistry; Part A and B: F. A. Carey & R. J. Sundberg
10. Organic Chemistry: Clayden, Greeves, Warren and Wothers
11. Organic Synthesis: W. Carruthers
12. Organic Synthesis: M. B. Smith

Third Semester **CHEO-316** **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 (π cycloadditions. 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-417** **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-418** **Credits: 04**

Advanced Organic and Heterocyclic Chemistry

PART A: *Advanced Organic Chemistry*

UNIT-I *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-II *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, Mannich, Strecker amino acid synthesis. Bamford-Steven, Baylis-Hillmann, Corey-Fuchs Reaction, Julia Olefination, Mukaiyama aldol, Mitsunobu, Peterson olefination, Corey-Winter olefination, Woodward and Prevost dihydroxylation, Shapiro, Ritter, Stille, Heck, Sonogashira, Suzuki, Duff, Chugaev, Petasis, McMurry reaction and Coupling. Ring closing metathesis (Grubb's metathesis), Aldol-Tishchenko reaction (Evans-Tishchenko reaction), Ugi, Passerini, Biginelli, Hantzsch condensation.

Reference Books:

1. Organic Chemistry: Clayden, Greeves, Warren and Wothers
2. Organic Synthesis: W. Carruthers
3. Organic Synthesis: M. B. Smith
4. Advanced Organic Chemistry; Part A and B: F. A. Carey & R. J. Sundberg
5. Modern Organic Synthesis: An Introduction: G. S. Zweifel & M. H. Nantz
6. Organic Synthesis Concepts, Methods, Starting Materials: J. Fuhrhop, G. Penzlin
7. Name Reactions and Reagents in Organic Synthesis: B. P. Mundy, M. G. Ellerd, F. G. Favaloro
8. Organic Chemistry: An Intermediate Text: Robert V. Hoffmann
9. Multicomponent Reactions: J. Zhu, H. Bienayme (Wiley-VCH)
10. Advanced Organic Chemistry: Jerry March
11. Organic Synthesis: R. O. C. Norman and Coxan
12. Name Reactions: Jie Jack Li

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

Fourth Semester **CHEO-419** **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-420** **Credits: 04**

Medicinal Chemistry

UNIT-I Basic consideration of drug activity

Definition and Introduction of following terms-Drug, 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 contents 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) from following classes:

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

II. Anti-hypertensive Drugs: (a) Verapamil (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) Antagonist: 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 COURSES

CHEO-421 **Duration: 4.5 Hrs/Week** **Credits: 4.5**

Qualitative analysis of ternary mixtures.

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

CHEO-422 **Duration: 4.5 Hrs/Week** **Credits: 4.5**

Organic multistep preparations.

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.

CHEO-423 **Duration: 4.5 Hrs/Week** **Credits: 4.5**

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

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

CHEO-424 **Duration: 4.5 Hrs/Week** **Credits: 4.5**

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.