



**Shiksha Mandal's
Bajaj College of Science, Wardha
Department of Chemistry**

**Syllabus of M. Sc. Chemistry
(Semester I to IV)**

(Approved in BOS Meeting 13th April, 2022)

Bajaj College of Science, Wardha (Autonomous College)

SUBJECT: CHEMISTRY

Syllabus of M.Sc. I Semester I

PG- CHE (02)- S1-T1: Paper I (Inorganic Chemistry) [L-T-P = 4-0-0]

60 h (4 h per week): 15 h per unit

80 Marks

Unit-I

a) Stereochemistry and Bonding in Main Group Compound: 5L

VSEPR-Shape of simple inorganic molecules and ions containing lone pairs, various stereochemical rules and resultant geometry of the compounds of non-transitional elements, short coming of VSEPR model, bent rule and energetic of hybridization.

b) Crystal Field Theory: 5L

Splitting of d-orbital in tetragonal, square planar and trigonal bipyramidal complexes. Jahn teller effect, spectrochemical series, nephelauxetic effect. Limitations of crystal field theory.

c) Molecular Orbital Theory: 5L

Molecular orbital theory for octahedral, tetrahedral and square planar complexes with and without π -bonding.

Unit-II

a) Electronic spectra: 10L

Spin-orbit (L-S) coupling scheme, calculation of spectral term symbols for ground state and excited states, selection rules, vibronic coupling, electronic spectra of transition metal complexes, charge transfer spectra, band intensities, band energies, band width & shapes, construction and application of Orgel diagrams, Tanabe-Sugano diagrams, spectra of octahedral, tetrahedral and square planar complexes with examples, Jahn teller effect, calculation of crystal field parameters ($10Dq$, B and β) for octahedral Ni(II) and Co(II) complexes from electronic spectra. Spectrochemical series, nephelauxetic effect and nephelauxetic series of ligands. Magnetic moment, electronic spectra and structure of complexes.

b) Magnetochemistry: 5L

Concept of magnetic susceptibility, types of magnetic bodies, magnetic properties of free ions and transition metal complexes of different geometries, factors affecting the magnetic properties, orbital splitting and magnetic properties, quenching of orbital angular momentum, and effect of ligand field on spin-orbit coupling. Temperature dependence of paramagnetism, high spin-low spin crossover, spin crossover in coordination compounds, spin equilibria, magnetic interactions, ferromagnetism and antiferromagnetism. Anomalous magnetic moments and magnetic exchange coupling.

Unit-III

a) Boron hydride: 10L

Classification, nomenclature, structure, bonding and topology of boranes, 4 digit coding (STYX) number for higher borane and their utility, study of metalloborane, carborane and metallocarborane with reference to preparation and structure.

b) Metal ligand equilibria in solution: 5L

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

Unit-IV

Bioinorganic Chemistry:

15L

a) Role of metals in bioinorganic chemistry

i) Classification as enzymatic and non-enzymatic metals, enzymatic redox metals such as Cu

(SOD) and enzymatic non redox metals such as Zn (Hydrolase).

ii) Role of metal ions in non-enzymatic process, Na, K, Ca, Mg (one example of each and brief discussion).

iii) Role of metals in enzymatic processes, transition metals, catalase, peroxidase and nitrogenase (Redox active).

b) Metalloproteins: Iron proteins, introduction of Fe-S proteins, electron transfer proteins (Fe-S, Fe₂S₂, Fe₃S₄, Fe₄S₄). Transport protein (transferrin) and storage protein (ferritin).

c) Bioinorganic Chemistry of Fe: Hemoglobin and myoglobin, its structure and functions.

d) Bioinorganic Chemistry of Co: Vitamin-B12, its structure and function.

Reference books:

- 1] S. F. A. Kettle, J. N. Murrell & S. T. Teddler: Valency Theory
- 2] C. A. Coulson: Valency
- 3] J. E. Huheey : Inorganic Chemistry
- 4] F. A. Cotton & G. Wilkinson: Advanced Inorganic Chemistry 3rd, 5th& 6th Editions.
- 5] A. F. Williams: Theoretical Approach in inorganic chemistry.
- 6] A. Mannas Chanda: Atomic Structure and chemical Bonding
- 7] L. E. Orgel: An introduction to transition metal chemistry, Ligand field theory, 2nd Edition.
- 8] J. J. Logowski: Modern Inorganic Chemistry
- 9] B. Durrant and P. J. Durrant: Advanced Inorganic Chemistry
- 10] J. C. Bailar: Chemistry of co-ordination compounds.
- 11] W. L. Jolly: Modern Inorganic Chemistry
- 12] R. S. Drago: Physical methods in inorganic chemistry.
- 13] Waddington: Nonaqueous solvents.
- 14] Sisler: Chemistry of non-aqueous solvents.
- 15] A. K. Barnard: Theoretical Inorganic Chemistry
- 16] Emeleus and Sharpe: Modern Aspect of Inorganic Chemistry.
- 17] F. A. Cotton: Chemical Applications of Group theory.
- 18] Jones: Elementary Co-ordination chemistry.
- 19] B. N. Figgis: Introduction to Ligand field.
- 20] S. F. A. Kettle: Co-ordination chemistry.
- 21] M. C. Day and J. Selbin: Theoretical Inorganic Chemistry.
- 22] J. Lewin and Wilkins: Modern Co-ordination chemistry.
- 23] Gowariker, Vishwanathan and Sheedar: Polymer science.
- 24] R. L. Dutta and A. Simal: Elements of magneto chemistry
- 25] P. Atkins: Inorganic Chemistry 4th Edition, Oxford University Press.
- 26] D. M. P. Mingos: Essential Trends in Inorganic Chemistry, Oxford University Press
- 27] Bertini, et al: Bioinorganic Chemistry (Viva)
- 28] Fenton, David E.: Biocoordination chemistry, Oxford

60 h (4 h per week): 15 h per unit

80 Marks

Unit-I

Chemical bonding, Aromaticity and Reactive Intermediates: 15L

a) **Chemical bonding:** Recapitulation of delocalized chemical bonding, conjugation, resonance, hyper-conjugation, tautomerism, Inductive effect.

b) **Bonding other than covalent bonding:** Hydrogen bonding, inclusion compounds, rotaxanes, catenanes, cyclodextrins, cryptands, crown ethers, fullerenes.

c) **Aromaticity:** Benzenoid and non-benzenoid compounds, Huckel's rule, antiaromaticity, homoaromaticity, annulenes, azulenes, cyclopentadienyl anion, tropylium cation, tropone and tropolone.

d) **Reactive intermediates:** Generation, structure, stability and chemical reactions of carbocations, carbanions, free radicals, carbenes and nitrenes.

Unit-II

Stereochemistry: 15L

a) Elements of symmetry, optical activity, chirality, enantiomers, diastereomers, meso compounds, stereochemical nomenclature (R-S, D-L, E-Z, threo-erythro), method of resolution, optical purity.

b) Stereochemical principles: prochirality, enantiotopic and diastereotopic atoms, groups and faces, stereochemistry of addition-elimination reactions, stereospecific and stereoselective synthesis, asymmetric synthesis, optical activity in biphenyls, spiranes, allenes.

c) Conformational analysis of n-butane and cycloalkanes (5-8 membered rings), substituted cyclohexanes, mono substituted, disubstituted cyclohexanes, decalines, effect of conformation on reactivity.

Unit-III

Organic reactions-I: 15L

a) **Reaction mechanism:** Types of mechanism, types of reaction, thermodynamics and kinetics requirements and control, thermodynamics Vs kinetics control, Hammond's postulate, Curtin- Hammett principle, potential energy diagrams, transition states and intermediates, methods of determining mechanisms, Kinetic isotope effects, Hard and soft acids and bases.

b) **Aliphatic nucleophilic substitution:** The SN1, SN2, mixed SN1, SN2 & SET, and SNi mechanisms. Nucleophilicity, effect of leaving group, ambient nucleophiles and ambient substrates regioselectivity, substitution at allylic and vinylic carbon atoms, phase transfer catalysis.

c) **Neighboring group participation:** Concept of NGP, anchimeric assistance with mechanism, neighboring group participation by π and σ bonds, classical and non classical carbonations, phenonium ions. Intramolecular displacement by hydrogen, oxygen, nitrogen, sulphur and halogen. Alkyl, cycloalkyl, aryl participation, participation in bicyclic system, norbornyl system, migratory aptitude, carbocation rearrangement in NGP.

Unit-IV

Organic reactions-II: 15L

a) **Aromatic Nucleophilic Substitution:** Introduction to different mechanisms of aromatic nucleophilic substitution S_NAr , SN1, benzyne and $S_{RN}1$ mechanisms. Arynes as reaction intermediate. Reactivity - effect of substrate structure, leaving group and attacking nucleophile. VonRichter, Sommet-Hauser and Smiles rearrangements.

b) **Aromatic electrophilic substitution:** Brief introduction to arenium ion mechanism, orientation and reactivity, energy profile diagrams, o/p ratio, ipso attack, orientation in benzene ring with more than one substituents, orientation in other ring system. Reactions:

nitration, halogenation, sulphonation, Friedel-Crafts alkylation and acylation, Vilsmeier-Hack reaction, Gatterman-Koch reaction, Pechman reaction, Reimer-Tiemann reaction, Diazonium coupling.

c) Effect of Structure on reactivity:

Resonance and field effects, Steric effect, Quantitative treatment: the Hammett equation and linear free energy relationship, substituent and reaction constants. Taft Equation.

Reference books:

- 1] Advanced Organic Chemistry–Reaction mechanism and structure. Jerry March, John Wiley
- 2] Advanced Organic Chemistry- F.A. Carey and R. J. Sunberg, Plenum
- 3] A Guidebook to Mechanism in Organic Chemistry-Peter Skyes, Longman
- 4] Structure and Mechanism in Organic Chemistry-C.K. Gold, Cornell University Press
- 5] Organic Chemistry, R.T. Morrison Boyd. Prentice Hall
- 6] Modern Organic Chemistry-H.O. House, Benjamin
- 7] Principles of Organic Chemistry-R.O.C. Norman and J.M. Coxon, Blackie Academic and Professional
- 8] Reaction Mechanism in Organic Chemistry-S.M. Mukharji and S.P. Singh, Macmillan
- 9] Stereochemistry of Organic Compounds- D. Nasipuri, New Age International
- 10] Stereochemistry of Organic Compounds- P. S. Kalsi, New Age International
- 11] Reactive Intermediate in Organic Chemistry-N. S. Isaacs
- 12] Stereochemistry of Carbon Compounds- E. L. Eliel
- 13] Physical Organic Chemistry-J. Hine
- 14] Name Reaction in Organic chemistry –Surrey
- 15] Advanced Organic Chemistry – L. F. Fieser and M. Fieser.
- 16] Organic Chemistry Vol. I and II - I. L. Finar
- 17] Modern Organic Chemistry- J.D. Roberts and M. C. Caserio
- 18] Organic Chemistry 5th Edition (McGraw Hill), S. H. Pine
- 19] A Textbook of Organic Chemistry- R. K. Bansal New Age International
- 20] Organic Chemistry, J. Clayden, N. Greeves, S. Warren and P. Wothers, Oxford University Press

60 h (4 h per week): 15 h per unit

80 Marks

Unit-I

Classical Thermodynamics: 15L

a] Recapitulation of Laws of thermodynamics, Exact and inexact differentials, condition of exactness, Pfaff differential expression and equations, Applications of Pfaff differential equations to first and second law of thermodynamics, homogeneous function of degree 0 and 1, extensive and intensive properties, derivation of thermodynamic equations of state, Maxwell's relations,

Applications of Maxwell's Relations

b] Third law of thermodynamics, Nernst Heat Theorem, Evaluation of Absolute Entropy, Entropy of reaction, Concept of residual entropy, Numericals based on absolute entropy.

Unit-II

Systems of Variable Compositions: 15L

a] Importance of Partial Molar Properties, Chemical Potential, Gibbs Duhem Equation, Relationship of Chemical Potential with U, H and A; Effect of Temperature on Chemical Potential and Effect of Pressure on Chemical Potential, Chemical Potential of Pure Ideal Gas, Chemical Potential in an Ideal Gas Mixture, Thermodynamics of a Mixture of Ideal Gases (enthalpy and entropy).

b] Chemical Potential of Real Gases and Fugacity, Raoult's Law and Ideal Solution, Thermodynamics of Binary Solution with i) One Volatile Component ii) Two Volatile Components, Chemical Potential in Non-ideal Solution, Excess function of Non-ideal Solution, Activity Coefficients of Nonelectrolytes, Debye-Huckel Theory, Limited and Extended Law (Derivation Expected)

Unit-III

Phase Equilibrium and Macromolecules: 15L

a] **Phase Equilibrium:** Gibbs Phase rule and its derivation, calculation of degrees of freedom, reduced phase rule, one component systems (Helium, carbon), 1st and 2nd order phase transition, lambda line, two component systems forming solid solutions having congruent and incongruent melting point, partially miscible solid phase, three component systems, graphical presentation, influence of temperature, systems with 1, 2, 3 pairs of partially miscible liquids, transition points.

b) **Macromolecules:** Definitions, Number and mass average molecular weights, molecular mass determination by Osmometry, Viscometry, Sedimentation, Diffusion, light scattering method, Numericals.

Unit-IV

Chemical Kinetics: 15L

Recapitulation, Activation energy, Arrhenius Equation and Numericals. Collision Theory and Transition state theory of bimolecular reactions, Thermodynamic formulation of Transition state theory (Eyring equation), Comparison of Transition state theory with Collision Theory, Bodenstein steady state approximation, Rice-Herzfeld mechanism of chain reaction, Kinetics of photochemical chain reaction between H₂ & Cl₂ and H₂ & Br₂, Kinetics of Enzyme catalyzed reaction (Michaelis- Menten equation)

Reference books:

- 1] R. P. Rastogi and R. R. Mishra, An Introduction to Chemical Thermodynamics, Vikas Publication, Gorakhpur, 2010.
- 2] P. W. Atkins and D. Paula, Physical Chemistry, 8th Edition, Oxford University Press, 2010.

3] E. N. Yenemin, Fundamentals of Chemical Thermodynamics, MIR, Publications.4] G. K. Vemulapalli, Physical Chemistry, Prentice – Hall of India, 1997.

- 5] S. Glasstone and De Van No Strand, Thermodynamics for Chemists, 1965.
- 6] S. M. Blinder, Advanced Physical Chemistry,
- 7] D. Mcquarie and J. Simon, Physical Chemistry – A Molecular Approach, University Press, 2000.
- 8] G. M. Barrow, Physical Chemistry, Tata Mc-Graw Hill, V edition 2003.
- 9] H. K. Moudgil, Text Book of Physical Chemistry, Pretice Hall of India, New Delhi, 2010.
- 10] G.M.Panchenkov and V.P.Labadev, “Chemical Kinetics and catalysis”, MIR Publishing.
- 11] E.A. Moelwyn- Hughes, “Chemical Kinetics and Kinetics of Solutions”, Academic.
- 12] K. J. Laidler, Chemical Kinetics, Third Edition (1987), Harper and Row, New York.
- 13] J. Raja Ram and J. C. Kuriacose, Kinetics and Mechanism of Chemical Transformations MacMillan Indian Ltd., New Delhi (1993).
- 14] C. H. Bamford and C. F. H. Tipper, Comprehensive Chemical Kinetics, Vol 1., Elsevier Publications, New York, 1969.
- 15] C. H. Bamford and C. F. H. Tipper, Comprehensive Chemical Kinetics, Vol 2., Elsevier Publications, New York, 1969.
- 16] S. Glasstone, K. J. Laidler and H. Eyring, The Theory of Rate Processes, Mc-Graw Hill, New York, 1941.
- 17] A. Findley, The Phase Rule and its Applications, Longmans Green and Co., Mumbai.
- 18] Santosh Kumar Upadhyay, Chemical Kinetics and Reaction Dynamics, Springer 2006.
- 19] G. K. Agrawal, Basic Chemical Kinetics, Tata-Mc-Graw Hill, 1990.
- 20] N. B. Singh, N. S. Gajbhiye, S. S. Das, Comprehensive Physical Chemistry, New Age International, 2014.
- 21] K. L. Kapoor, Text Book of Physical Chemistry, Vol – I to Vol-VI, 2011.

60 h (4 h per week): 15 h per unit

80 Marks

Unit-I

Introduction and Statistical Analysis: 15L

a) **Introduction to analytical chemistry:** Types of analysis-qualitative and quantitative. Classification of analytical methods- classical and instrumental, basis of their classification with examples.

b) **Statistical analysis and validation:** Errors in chemical analysis. Classification of errors-systematic and random, additive and proportional, absolute and relative. Accuracy and precision. Mean, median, average deviation and standard deviation. Significant figures and rules to determine significant figures. Calculations involving significant figures. Confidence limit, correlation coefficient and regression analysis. Comparison of methods: F-test and T-test. Rejection of data based on Q-test. Least squares method for deriving calibration graph. Application of Microsoft Excel in statistical analysis (statistical functions and spreadsheets in MS-Excel). Validation of newly developed analytical method. Certified reference materials (CRMs). Numerical problems.

Unit-II

Separation Techniques: 15L

a) **Chromatography:** Definition and Classification. Techniques used in Paper, Thin Layer and Column chromatography. Applications in qualitative and quantitative analysis.

b) **Ion exchange:** Principle and technique. Types of ion exchangers. Ion exchange equilibria. Ion exchange capacity. Effect of complexing ions. Zeolites as ion-exchangers. Applications.

c) **Solvent extraction:** Principle and techniques. Distribution ratio and distribution coefficient. Factors affecting extraction efficiency: Ion association complexes, chelation, synergistic extraction, pH. Numericals based on multiple extractions. Role of chelating ligands, crown ethers, calixarenes and cryptands in solvent extraction. Introduction to Solid phase extraction (SPE) and Microwave assisted extraction (MAE), Applications.

Unit-III

Classical Methods of Analysis: 15L

a) **Volumetric analysis:** General principle. Criteria for reactions used in titrations. Primary standards and secondary standards. Theory of indicators. Types of titrations with examples-Acid- base, precipitation, redox and complexometric. Titration curves for monoprotic and polyprotic acids and bases. Indicators used in various types of titrations. Masking and demasking agents.

b) **Gravimetric analysis:** General principles and conditions of precipitation. Concepts of solubility, solubility product and precipitation equilibria. Steps involved in gravimetric analysis. Purity of precipitate: Co-precipitation and post-precipitation. Fractional precipitation. Precipitation from homogeneous solution. Particle size, crystal growth, colloidal state, aging and peptization phenomena. Ignition of precipitates.

Unit-IV

Optical Methods of Analysis-I: 15L

a) **Spectrophotometry and Colorimetry:** Principle of colorimetry. Beer's law, its verification and deviations. Instrumentation in colorimetry and spectrophotometry (single and double beam). Sensitivity and analytical significance of molar extinction coefficient and λ_{max} . Comparison method, calibration curve method and standard addition method for quantitative estimation. Role of organic ligands in spectrophotometric analysis of metal ions. Ringbom plot and Sandell's sensitivity. Photometric titrations. Determination of pK value of indicator. Simultaneous determination. Composition and stability constant of complex by Job's and mole ratio methods. Derivative spectrophotometry. Numerical problems.

b) Flame photometry: Principle. Instrumentation and types of burners. Factors affecting flame photometric determination. Limitations of flame photometry. Interferences in flame photometry. Applications.

Reference books:

- 1] Quantitative analysis: Day and Underwood (Prentice-Hall of India)
- 2] Vogel's Text Book of Quantitative Inorganic Analysis-Bassett, Denney, Jeffery and Mendham(ELBS)
- 3] Analytical Chemistry: Gary D. Christian (Wiley, India).
- 4] Instrumental Methods of Analysis: Willard, Merrit, Dean, Settle (CBS Publishers, Delhi, 1986)
- 5] Instrumental Methods of Chemical Analysis: Braun (Tata McGraw-Hill)
- 6] Advanced Analytical Chemistry: Meites and Thomas (McGraw-Hill)
- 7] Instrumental Methods of Analysis: G. Chatwal and S. Anand (Himalaya Publishing House)
- 8] Analytical Chemistry: Problems and Solution- S. M. Khopkar (New Age International Publication)
- 9] Basic Concepts in Analytical Chemistry: S. M. Khopkar (New Age International Publication)
- 10] Advance Analytical Chemistry: Meites and Thomas: (Mc Graw Hill)
- 11] An Introduction to Separation Science: L. R. Snyder and C. H. Harvath (Wiley Interscience)
- 12] Fundamentals of Analytical Chemistry: S. A. Skoog and D. W. West
- 13] Instrumental Methods of Chemical Analysis: G. W. Ewing

PG- CHE (02)- S1-P1: Practical-I (Inorganic Chemistry Practical) [L-T-P = 0-0-8]

8 h per week

100 Marks

I. Preparation of Inorganic Complexes and their characterization by:

Elemental analysis and physico-chemical methods (Electronic and IR Spectra, magnetic susceptibility measurements, Thermal analysis and Molar conductance studies).

- | | | |
|------------------------------|------------------------|--------------------------------|
| 1. $K_3[Al(C_2O_4)_3](H_2O)$ | 2. $[VO(acac)_2]$ | 3. $Na[Cr(NH_3)_2(SCN)_4]$ |
| 4. $K_3[Cr(SCN)_6]$ | 5. $[Mn(acac)_3]$ | 6. $K_3[Fe(C_2O_4)_3]$ |
| 7. $Hg[Co(SCN)_4]$ | 8. $[Co(Py)_2Cl_2]$ | 9. $[Cu_2(CH_3COO)_4(H_2O)_2]$ |
| 10. $[Ni(DMG)_2]$ | 11. $[Ni(NH_3)_6]Cl_2$ | 12. $[Cu(NH_3)_4(H_2O)_2]SO_4$ |

II. Quantitative Analysis:

Separation and determination of two metal ions from the following alloys involving:
Volumetric, Gravimetric and Spectrophotometric methods

- Copper (II) and Nickel (II)
- Copper (II) and Zinc (II)
- Nickel (II)—Zinc (II) and
- Copper (II)—Iron (III)

III. Qualitative analysis of radicals:

Semi-micro Analysis of inorganic mixture of containing total of five radicals including interfering radicals (not more than one such radical in a mixture), rare earth (not more than two rare earths in a mixture) and combination of cations (minimum 8 mixtures).

Cations: Mercury (I, II), Pb, Ag, Bi (III), Cu (II), Cd (II), As (IV, V), Sb (IV, V), Sn (II, IV), Fe (III), Al (III), Cr (III), Ni (II), Co (II), Mn (II), Zn (II), Barium, Strontium, Calcium and Magnesium.

Interfering radicals: Phosphate, Oxalate, Fluoride and Borate.

Rare Earth: Tl, Mo, W, Se, Ti, Zr, Th, V, U, Ce. (Spot Test for individual cations should be performed)

Reference books:

- 1] Synthesis and Characterization of Inorganic Compounds, W. L. Jolly, Prentice Hall.
- 2] Inorganic Experiments, J. Derck Woollins, VCH.
- 3] Practical Inorganic Chemistry, G. Mairand, B. W. Rockett, Van Nostrand.
- 4] A Text Book of Quantitative Inorganic Analysis, A. I. Vogel, IIIrd Edition
- 5] EDTA Titrations. F. Laschka
- 6] Instrumental Methods of Analysis, Willard, Merit and Dean (CBS, Delhi).
- 7] Inorganic Synthesis, Jolly
- 8] Instrumental Methods of Chemical Analysis, Yelri Lalikov
- 9] Fundamental of Analytical Chemistry, Skoog D.A. & West D.M Holt Rinehart & Winston Inc.
- 10] Experimental Inorganic Chemistry, W.G. Palmer, Cambridge.
- 11] Quantitative Analysis: Day And Underwood
- 12] Physical Methods In Inorganic Chemistry: R. S. Drago
- 13] General And Inorganic Chemistry: N. Akjmetov

PG- CHE (02)- S1-P2 : Practical-II (Physical Chemistry Practical) [L-T-P = 0-0-8]

8 h per week

100 Marks

It is expected to perform minimum 14 experiments in a semester. In examination one experiment from non-instrumental section and one experiment from instrumental section should be asked.

A] Non-instrumental Experiments:

- 1) To study the variation of volume contraction with mole fraction of alcohol in alcohol - water system
- 2) To determine the activation parameters of viscous flow for a given liquid.
- 3) To determine the critical micelle concentration (CMC) of a given surfactant/ soap/ shampoo by surface tension measurements.
- 4) Determination of molecular mass of a polymer by viscometry method.
- 5) To determine integral heat of KNO_3 , at two different conc. and calculation of heat of dilution.
- 6) Effect of 1% NaCl, 1% succinic acid, 0.5% naphthalene on CST in phenol-water systems.
- 7) Distribution of succinic acid in H_2O - benzene, H_2O -ether and comparison of distribution coefficient.
- 8) To construct the phase diagrams of two components system (phenol- urea, diphenyl-aminebenzophenone; α -naphthyl amine-phenol) forming compounds with congruent melting points.
- 9) To study the mutual solubility of glycerol-*m*-toluidine and to determine congruent points.
- 10) To study kinetics of hydrolysis of an ester by NaOH reaction.
- 11) To determine equilibrium constant of the equation $\text{KI} + \text{I}_2 = \text{KI}_3$ by distribution method.
- 12) To study the kinetics of the reaction between potassium persulphate and potassium iodide.
- 13) Determination of order of reaction of oxidation of ethyl alcohol by acid dichromate.

B] Instrumental Experiments:

- 1) To titrate conductometrically monobasic and dibasic acids with NaOH and determine the strength of given acid.
- 2) To determine equivalent conductance of weak electrolyte at infinite dilution by Kohlrausch's method.
- 3) Determination of heat of reaction, entropy change and equilibrium constant of the reaction between metallic Zn^{+2} and Cu^{+2} ions in solution.
- 4) Determination of thermodynamic constants ΔG , ΔH , ΔS for $\text{Zn}^{+2} + \text{H}_2\text{SO}_4 \rightarrow \text{ZnSO}_4 + 2\text{H}^+$ by emf measurement.
- 5) Titration of ferrous ammonium sulphate against ceric sulphate and hence the formal redox potential of $\text{Fe}^{2+} \rightleftharpoons \text{Fe}^{3+}$ and $\text{Ce}^{3+} \rightleftharpoons \text{Ce}^{4+}$ systems.
- 6) To determine the pH of a buffer solutions using a quinhydrone electrode
- 7) Complexometric titrations (EDTA based)

Reference books:

- 1] J. B. Yadav, Practical Physical Chemistry
- 2] Das and Behra, Practical Physical Chemistry
- 3] Carl W. Garland, Joseph W. Nibler and David P. Shoemaker, Experiments in Physical Chemistry, Mc-Graw Hill, 8th Edition, 2009.
- 4] Farrington Daniels, Joseph Howard Mathews, John Warren Williams, Paul Bender, Robert A. Alberty, Experimental Physical Chemistry, Mc-Graw Hill, Fifth Edition, 1956.
- 6] John W. Shriver and Michael George, Experimental Physical Chemistry, Lab Manual and Data Analysis, The University of Alabama in Huntsville, Fall 2006
- 7] Chondhekar T.K: Systematic Experiments In Physical Chemistry, Rajbog S.W., Aniali Pubn.
- 8] Merits And Thomas: Advanced Analytical Chemistry

9] Ewing, G. W. : Instrumental Methods Of Chemical Analysis, Mcgraw-Hill
10] Khopkar S.M.:Basic Concept of Analytical Chemistry

- 11] Wlehov G. J: Standard Methods Of Chemical analysis 6th Ed
- 12] Braun:Instrumental Methods of Chemical Analysis

**Bajaj College of Science, Wardha (Autonomous
College) SUBJECT: CHEMISTRY
Syllabus of M.Sc. I/Semester II**

PG- CHE (02)- S2-T1: Paper V (Inorganic Chemistry) [L-T-P = 4-0-0]

60 h (4 h per week): 15 h per unit

80 Marks

Unit-I

Reaction mechanism of transition metal complexes-I: 15L

Energy profile of reaction, reactivity of metal complexes, inert and labile complexes, kinetics of octahedral substitution: Acid hydrolysis, factors affecting acid hydrolysis, stereochemistry of intermediates in SN1 and SN2, Base hydrolysis, Conjugate base mechanism, Direct and indirect evidences in favor of conjugate mechanism, anation reaction, reaction without metal ligand bond breaking.

Unit-II

Reaction mechanism of transition metal complexes -II: 15L

Substitution reaction in square planar complexes: trans effect, cis effect, steric effect, solvent effect, effect of leaving group, effect of charge, effect of nucleophile, effect of temperature. Trans effect theories, use of trans effect, mechanism of substitution reaction of Pt(II) Complexes, electron transfer reactions. Types of electron transfer reaction, conditions of electron transfer and mechanism of one electron transfer reaction, outer sphere and inner sphere mechanism, two electron transfer reactions, complementary and non-complementary reaction, tunneling effect, cross reactions.

Unit-III

Metal π -Complexes: 15L

a) Metal carbonyls

Structure and bonding, vibrational spectra of metal carbonyls for bonding and structure elucidation, important reaction of metal carbonyls. Metal carbonyl clusters with reference to classification, EAN rule, synthesis and structures.

b) Metal nitrosyls

Nitrosylating agents for synthesis of metal nitrosyls, vibrational spectra and X-ray diffraction studies of transition metal nitrosyls for bonding and structure elucidation, important reactions of transition metal nitrosyls, structure and bonding. Dinitrogen and dioxygen complexes. Wilkinson's catalyst and Vaska's compound.

Unit-IV

Metal cluster: 15L

Occurrence of metal-metal bonds, Classification of metal cluster: binuclear, trinuclear, tetranuclear, pentanuclear and hexanuclear with reference to halide, oxide, alkoxide and acetate clusters. Isopoly, heteropoly acids and their anions.

Reference books:

Books as Suggested in Semester I for Inorganic Chemistry

60 h (4 h per week): 15 h per unit

80 Marks

Unit-I

Addition reactions: 15L

a) Addition to carbon-carbon multiple bond: Mechanistic and stereochemical aspects of addition reaction involving electrophiles, nucleophiles and free radicals, regio and chemoselectivity, **Orientation and stereochemistry**, Addition to cyclopropanes, Hydrogenation of double bond and triple bonds. Hydrogenation of aromatic rings, hydroboration, Michael reaction, Robinson annulations.

b) Addition to carbon-hetero atom multiple bond: Mechanism of metal hydride reduction of saturated and unsaturated carbonyl compounds, acids, esters, and nitriles, Addition of Grignard reagents, organozinc and organolithium reagents to carbonyls and unsaturated carbonyl compounds, Wittig reaction, Mechanisms of condensation reactions involving enolates- **Aldol, Knoevengel, Claisen, Mannich, Benzoin, Perkin, Stobbe reaction**, Hydrolysis of esters and amide.

Unit-II

Molecular rearrangements and free radical reactions: 15L

a) Molecular rearrangements: Classification and General mechanistic treatment of electrophilic, nucleophilic and free radical molecular rearrangement. Mechanism and synthetic applications of **Wagner-Meerwin, Pinacol-Pinacolone, Tiffenev-Demjnov ring expansion, benzil-benzilic acid, Favorski, Baeyer Villiger, Wolff, Arndt-Eistert synthesis, Curtius Lossen, Beckman, Hoffman, Schmidt rearrangement**.

b) Elimination reactions: **E1, E2, E1CB mechanisms**, orientation and stereochemistry in elimination reaction, Saytzeff and Hoffman's rule, Effect of substrate structure, attacking base, leaving group and medium, competition between elimination and substitution, syn eliminations, pyrolytic elimination.

Unit-III

Free radical reactions: 15L

Generation of free radicals, types and mechanism of free radical reactions, free radical substitution mechanism at an aromatic substrate, aliphatic substrate, reactivity at a bridgehead position, Neighbouring group assistance, reactivity for aliphatic and aromatic substrates, reactivity in attacking radicals, effect of solvent on reactivity, Halogenation at an alkyl carbon, allylic carbon (NBS), hydroxylation at an aromatic carbon by means of Fenton's reagent. Auto-oxidation, chlorosulphonation (Reed Reaction) Coupling of alkynes and arylation of aromatic compounds by diazonium salts, Sandmeyer reaction, **Free radical rearrangement: Hunsdiecker reaction, Iododecarboxylation, Barton reaction, Hoffmann-Loefler-Freytag reaction.**

Unit-IV

Green chemistry: 15L

Basic principles of green chemistry, calculation of atom economy of rearrangements, addition, substitution and elimination reaction with suitable examples, Case study of Bhopal gas tragedy and Seveso disaster, **Synthesis involving basic principles of green chemistry- paracetamol, Ibuprofen, hydroquinone, adipic acid, ϵ -caprolactum, styrene, urethanes**, Free radical bromination, Multi- component reactions (Biginelli, Ugi and Passerini reaction), Prevention or minimization of hazardous products, choice of solvents. Sonochemistry, microwave induced reactions, polymer supported reagents, reactions in aqueous medium, zeolites and ionic liquid supported reaction, Solvent free reactions, electrochemical reactions, Biocatalysts in Organic synthesis.

Reference books:

- 1] Books as Suggested in Semester I for Organic Chemistry
- 2] A Textbook of organic chemistry- R.K. Bansal
- 3] Some Modern Methods of Organic Synthesis-W. Carruthers
- 4] Advance Organic Chemistry Part-B-F. A. Caray and R. J. Sundberg Plenum Press
- 1] Principle of Organic Synthesis R. O. C. Norman and J. M. Coxon
- 2] Modern Synthetic Reaction. H. O. House and W. A. Benjamin
- 4] Designing Organic Synthesis-S. Warren
- 5] Some Modern Methods of Organic Synthesis-W. Carruthers
- 7] Advance Organic Chemistry Part-B-F. A. Caray and R. J. Sundberg Plenum Press
- 8] Organic Reaction and their Mechanism-P. S. Kalsi
- 9] New trends in green chemistry -V.K. Ahluwalia and M. Kidwai, Anamaya publishers New Delhi

60 h (4 h per week): 15 h per unit

80 Marks

Unit-I

Quantum Chemistry: 15L

Recapitulation, Postulates of Quantum Mechanics, Operator algebra, Commutator of operators and Numericals. Eigen values, Eigen functions and Numericals. Normalized, orthogonal wave functions and Numericals. Particle in three dimensional box, degeneracy of energy levels, Quantum mechanical principles of Hybridization, Construction of wave functions for sp, sp² and sp³ hybrid orbitals.

Unit-II

a) Electrochemistry and Nuclear Chemistry: 15L

Introduction and over view of Electrochemical Processes, Electrochemical Cell and Reactions, Faradic and Nonfaradiac Processes, Basic Electrochemical Thermodynamics, Free Energy and cell EMF, Half Reaction and Reduction Potentials, Formal Potentials, Reference Electrodes, Measurements of Potential Differences, Electrochemical Potentials, Fermi Level and Absolute Potentials, Liquid Junction Potential. Electrochemical devices: Alkaline fuel cells, Phosphoric acid fuel cells, High temperature fuel cells, **General development of a fuel cell based technology**

b) Nuclear Chemistry: General characteristics of radioactive decay, decay kinetics, parent-daughter decay growth relationship, nuclear deexcitation, secular and transient equilibrium, alpha particle energy spectrum, Geiger-Nutta law, theory of band g decay process, Fission energy natural Ur reactor, classifications of reactors, reactor power, critical size of thermal reactor, excess reactivity and control, breeder reactor, **reprocessing of spent fuel, recovery of Ur and plutonium nuclear waste management.**

Unit-III

Solid State Chemistry: 15L

a) Introduction to crystals, Unit Cell and lattice parameters, Symmetry elements in crystals, Absence of fivefold axis, Space groups, The Bravais Lattices, Miller Indices, Bragg's Equation, seven crystal system, Packing in crystals, Hexagonal Closest Packing (HCP) Cubic Closest Packing (CCP), Voids, packing fraction, **Numericals.**

b) Crystal Defects and Non-stoichiometry: Perfect and imperfect crystals, point defects, line and plane defects. Thermodynamics of Schottky and Frenkel defect formation, colour centers, nonstoichiometry and defects.

Unit-IV

Statistical Thermodynamics and Surface Chemistry: 15L

a) Statistical thermodynamics: Lagrange's Method of Undetermined Multipliers (Conditional Maximization), Stirling Approximation, Concept of Distribution, Thermodynamic Probability and most probable distribution, Maxwell Boltzmann, Bose Einstein, Fermi Dirac statistics, comparison between three statistics.

b) Surface Chemistry: Adsorption definition, Thermodynamics of adsorption, Langmuir adsorption isotherm, Langmuir constant and Gibbs energy of adsorption, Langmuir adsorption with lateral interaction, BET adsorption isotherm, adsorption on heterogeneous surface, the potential theory of Polanyi.

Micelles: micellization, hydrophobic interaction, critical micellar concentration (CMC),

factors affecting CMC of surfactants, counter ion binding to micelles, thermodynamics of micellization- phase separation and mass models, solubilization, micro emulsion, reverse micelles, Numericals.

Reference books:

- 1] Ira .N. Levine, Quantum Chemistry, 5th edition(2000), Pearson educ., Inc.New Delhi
- 2] A.K.Chandra, Introductory Quantum Chemistry, 4th edition (1994), Tata Mcgraw Hill, NewDelhi.
- 3] M.W.Hanna, "Quantum Mechanics in Chemistry", Benjamin
- 4] L. Pualing and E. B. Wilson, Introduction to Quantum Mechanics with Applications to Chemistry, McGraw Hill, New York (1935).
- 5] R. K. Prasad, Quantum Chemistry, New Age International, Delhi.
- 6] R. K. Prasad, Quantum Chemistry through problems and solutions, New Age International, NewDelhi, 2009.
- 7] B. C. Reed, Quantum Mechanics, Jones and Bartlett, New Delhi, 2010.
- 8] S. Glasstone, An Introduction to Electrochemistry, East-West Press Pvt. Ltd., New Delhi, 2004.9] H. K. Moudgil, Text Book of Physical Chemistry, Pretice Hall of India, New Delhi, 2010.
- 10] S. O. Pillai, Solid State Physics, New Age International, New Delhi, 2102.
- 11] N. B. Hanny, Treaties in Solid State Chemistry,
- 12] M. C. Day and J Selbin, Theoretical Inorganic Chemistry, Reinhold Pub. Corp., New York,
- 13] M. C. Gupta, Statistical Thermodynamics, New Age International.14] K. Huang, Statistical Mechanics, Wiley, New Delhi, 2003.
- 15] Andrew Maczek, *Statistical Thermodynamics*, Oxford University Press Inc., New York (1998).16] C.Kittel, "Introduction to solid state Physics",Wiley
- 17] L.V.Azaroff, "Introduction to solids", McGraw Hill
- 18] L. E. Smart and E. A. Moore, Solid State Chemistry-An Introduction, CRC Tylor and Fransis,2005.
- 19] C. N. R. Rao and Gopalakrishnan, "New Directions in Solid State Chemistry" Second Edition,Cambridge University Press.
- 20] Anthony R. West, "Solid State Chemistry and its Applications" Wiley India Edition21] D. K. Chakravorty, Solid State, New Age International.
- 22] Modern Electrochemistry, Volume 1 and 2, J.O.M Bokris and A.K.N, Reddy Plenum Press N.Y. (1970)
- 23] Electrochemical Methods second edition, A.J. Bard and L.R. Faulkner, John Wiley and Son(2001).
24. Physics and Chemistry of Interface, second edition, Hans-Jurgen Butt, Karlheunz Graf, MicaelKappl, Willey VCH (2006), ISBN-13 978-3-527-40629-6
- 25] Physical Chemistry of Surface, A.W. Admson, fifth edition, Wiley Interscience Publiation(1990)
- 26] Surfactant Science and Technology, second edition, Drew Myers, VCH Publishers (1992)
- 27] Principles of Colloids and Surface Chemistry, P.C. Hiemenz Marcel and Dekker, N.Y. (1977)

60 h (4 h per week): 15 h per unit

80 Marks

Unit-I

Sampling and Quantification: 15L

a) **Sampling and sample treatment:** Criteria for representative sample. Techniques of sampling of gases (ambient air and exhaust gases), liquids (water and milk samples), solids (soil and coal samples) and particulates. Hazards in sampling. Safety aspects in handling hazardous chemicals. Sample dissolution methods for elemental analysis: Dry and wet ashing, acid digestion, fusion processes and dissolution of organic samples.

b) **Detection and quantification:** Concepts and difference between sensitivity, limit of detection and limit of quantification, role of noise in determination of detection limit of analytical techniques. Units in chemical analysis and their interconversion.

c) **Stoichiometry:** Stoichiometric and sub-stoichiometric reactions and calculations.

Unit-II

Modern separation techniques: 15L

a) **Gas Chromatography:** Principle including concept of theoretical plates and van-Deemter equation. Instrumental set up- carrier gas, sampling system, column and detector. Types of columns, their advantages and limitations. Detectors in GC analysis. Temperature programmed GC. Factors affecting retention, peak resolution and peak broadening.

b) **Liquid chromatography:** Principle, Instrumentation, Advantages and applications of HPLC. Types of columns and detectors. Principle and applications of size exclusion, gel permeation, ion retardation, normal phase and reverse phase chromatography.

c) **Supercritical fluid chromatography:** Introduction and applications.

Unit-III

Optical methods of analysis-II: 15L

Atomic absorption spectroscopy: Principle. Atomic energy levels. Grotrian diagrams. Population of energy levels. Instrumentation. Sources: Hollow cathode lamp and electrodeless discharge lamp, factors affecting spectral width. Atomizers: Flame atomizers, graphite rod and graphite furnace. Cold vapour and hydride generation techniques. Factors affecting atomization efficiency, flame profile. Monochromators and detectors. Beam modulation. Detection limit and sensitivity. Interferences and their removal. Comparison of AAS and flame emission spectrometry. Applications of AAS.

Unit-IV

Electrochemical methods of analysis-II: 15L

a) **Polarography:** Principle of DC polarography. Instrumentation in polarography. Advantages and limitations of DME. Types of currents- residual current, migration current, diffusion current, limiting current, adsorption current, kinetic current and catalytic current. Ilkovic equation-diffusion current constant and capillary characteristics. Derivation of equation of polarographic wave and halfwave potential. Experimental determination of half wave potential. Reversible, quasi reversible and irreversible electrode reactions. Polarographic maxima and maximum suppressor. Oxygen interference and deaeration. Introduction to pulse, a.c. and oscillographic techniques and their advantages. Applications of polarography in determination of dissolved oxygen, metal ion quantification and speciation, simultaneous determination of metal ions, analysis of organic compounds. Limitations of polarography.

b) **Amperometric titrations:** Principle, types and applications in analytical chemistry.

Reference books:

1] Quantitative analysis: Day and Underwood (Prentice-Hall of India)

2] Vogel's Text Book of Quantitative Inorganic Analysis-Bassett, Denney, Jeffery and Mendham(ELBS)

- 3] Analytical Chemistry: Gary D. Christian (Wiley India).
- 4] Instrumental Methods of Analysis: Willard, Merrit, Dean, Settle (CBS Publishers, Delhi, 1986)
- 5] Sample Pre-treatment and Separation: R. Anderson (John Wiley and Sons)
- 6] Stoichiometry: B.I.Bhatt and S.M. Vora, 2nd Edition (Tata Mc-Graw Hill publication)
- 7] Instrumental Methods of Chemical Analysis: Braun (Tata McGraw-Hill)
- 8] Advanced Analytical Chemistry: Meites and Thomas (McGraw-Hill)
- 9] Instrumental Methods of Analysis: G. Chatwal and S. Anand (Himalaya Publishing House)
- 10] Analytical Chemistry: Problems and Solution, S. M. Khopkar (New Age International Publication)
- 11] Basic Concepts in Analytical Chemistry: S. M. Khopkar (New Age International Publication)
- 12] Advance Analytical Chemistry: Meites and Thomas: (Mc Graw Hill)
- 13] An Introduction to Separation Science: L. R. Shyder and C. H. Harvath (Wiley Interscience)
- 14] Fundamental of Analytical Chemistry: S. A. Skoog and D. W. West
- 15] Instrumental Methods of Chemical Analysis: G. W. Ewing
- 16] Polarography: Koltoff and Ligane
- 17] Electroanalytical Chemistry: Sane and Joshi (Quest Publications)

8 h per week

100 Marks

I. Purification techniques (Demonstrations):

- a) Purification of solvents and reagents using techniques like crystallization, distillation, steamdistillation, vacuum distillation etc.
- b) Chromatography: TLC, Column, paper
- c) Solvent extraction using soxhlet extractor

II. Qualitative Analysis:

Two component mixture separation using chemical and physical techniques and using solvents. (8mixtures minimum)

III. Organic Preparations (minimum 8 preparations):

Spectral characterization of prepared compounds wherever possible:

1. Single step preparation

- a) Aldol condensation: Benzaldehyde → Dibenzal acetone (chalcone)
- b) Benzophenone → benzhydrol
- c) Nitrobenzene → m-di-nitrobenzene
- d) m-di-nitrobenzene → m-nitroaniline
- e) Methyl acetoacetate → 5-methyl-isoxazol-3-ol
- f) Ethyl acetoacetate → 4-aryl-6-methyl-3,4-dihydro-2(1H)-pyrimidinone ester
- g) Ethyl acetoacetate → Diethyl 1,4-dihydro-2,6-dimethyl-4-phenylpyridine-3,5-dicarboxylate
- h) Sulphanilic acid → Methyl orange
- i) p-nitroaniline → p-red

2. Two step preparation

- a) Acetanilide → p-nitroacetanilide → p-nitroaniline
- b) Aniline → 2,4,6-tribromo aniline → 2,4,6-tribromoacetanilide
- c) Nitrobenzene → m-dinitrobenzene → m-nitroaniline
- d) benzophenone → benzophenoneoxime → Benzanilide
- e) Chlorobenzene → 2,4-dinitrochlorobenzene → 2,4-dinitrophenylhydrazine
- f) Glycine → Benzoyl glycine(hippuric acid) → 4-benzilidene-2-phenyl oxazole

8 h per week

100 Marks

Section (A):

I. Classical methods and separation techniques: Calibration, validation and computers

- 1) Calibration of pipette and burette.
- 2) Statistical analysis of data.
- 3) Use of MS-Excel in statistical analysis of data and curve fitting.

II. Volumetry

- 1) Determination of Na_2CO_3 in washing soda.
- 2) Determination of NaOH and Na_2CO_3 in a mixture.
- 3) Estimation of nickel in given solution by direct complexometric titration with EDTA using bromopyrogallol red.
- 4) Estimation of nickel in given solution by complexometric back-titration with EDTA.
- 5) Estimation of chloride in given solution by Mohr's titration.
- 6) Estimation of chloride in given solution by Volhard's titration.
- 7) Determination of volume strength of commercial hydrogen peroxide by redox titration with KMnO_4 .
- 8) Estimation of phenol/ aniline by bromination method.
- 9) Estimation of glucose.
- 10) Estimation of acetone.
- 11) Estimation of formaldehyde.
- 12) Estimation of Mn in the presence of Fe using masking phenomenon (ferromanganese alloy).

III. Gravimetry

- 1) Estimation of barium as barium sulphate.
- 2) Estimation of calcium as calcium oxalate/ calcium carbonate/ calcium oxide.

IV. Separation techniques

- 1) Qualitative separation of metal ions by paper chromatography for 2/3 components.
- 2) Determination of ion-exchange capacity of resin.
- 3) Separation of ions by ion exchange.

Section (B): Instrumental techniques

I. Electroanalytical techniques

- 1) Analysis of commercial vinegar by conductometric titration.
- 2) Estimation of phenol by conductometric titration with NaOH .
- 3) Determination of strength of HCl and CH_3COOH in a mixture conductometrically.
- 4) Determination of strength of HCl and oxalic acid in a mixture conductometrically.
- 5) Determination of strength of oxalic acid and CH_3COOH in a mixture conductometrically.
- 6) Determination of degree of dissociation and dissociation constant of acetic acid conductometrically.
- 7) Estimation of phenol in dilute solution by conductometric titration with NaOH .
- 8) Determination of strength of HCl and CH_3COOH individually and in a mixture potentiometrically.
- 9) Determination of Fe(II) by potentiometric titration with $\text{K}_2\text{Cr}_2\text{O}_7$.
- 10) Determination of three dissociation constants of H_3PO_4 by pH-metric/potentiometric titration

II. Optical methods

- 1) Determination of pK of indicator by colorimetry.
- 2) To estimate the amount of NH_4Cl colorimetrically using Nessler's Reagent.
- 3) To study the complex formation between Fe(III) and salicylic acid and find the formula and stability constant of the complex colorimetrically (Job's method).
- 4) To determine the dissociation constant of phenolphthalein colorimetrically.
- 5) Estimation of iron in wastewater sample using 1,10-phenanthroline.

(Note: One experiment from each section should be performed in the examination.)

Reference Books:-

- Svehla, G. *Vogel's Qualitative Inorganic Analysis*, Pearson Education, 2012.
- Mendham, J. *Vogel's Quantitative Chemical Analysis*, Pearson, 2009.
- Willard, H. H., *Instrumental methods of analysis*, Wiley, 1988
- Khosla, B. D.; Garg, V. C. & Gulati, A. *Senior Practical Physical Chemistry*, R. Chand & Co.: NewDelhi (2011)
- Das R. C., Behra B., *Experimental Physical Chemistry*, Tata McGraw Hill.
- Yadav J. B., *Advanced Practical Physical Chemistry*, Goel Publishing House.
- Alexander Findlay, Levitt B. P., *Findlay's Practical Physical Chemistry*, Longman, London
- <http://nsdl.niscair.res.in>
- <http://ocw.mit.edu>

Bajaj College of Science, Wardha (Autonomous College)

SUBJECT: CHEMISTRY

Syllabus of M.Sc. II/Semester III (WEF 2022-23)

Course Code: PG-CHEM(02)-S3-T1-SP1

Paper-IX : Special I-Organic Chemistry [L-T-P = 4-0-0]

60 h (4 h per week): 15 h per unit

80 Marks

Unit-I

Photochemistry: 15L

Interaction of radiation with matter, types of excitation, rate of excited molecules, quenching, Quantum efficiency, quantum yield, transfer of excitation energy, singlet and triplet states, experimental methods in photochemistry of carbonyl compounds, and transition, **Norrish type I and Norrish type II reactions Paterno-Buchi reaction, Photoreduction**, Photochemistry of enones, Hydrogen abstraction rearrangement of unsaturated ketones and cyclohexadienones, Photochemistry of parabenzoquinones, photochemistry of Aromatic compounds with reference to isomerisation addition and substitution Photochemical isomerization of cis and trans alkenes, Photochemical cyclization of reaction, **Photo-Fries rearrangement, di-pi methane rearrangement**, Photo theory reaction of anilides, photochemistry of vision, Applications of photochemical methods in synthesis: Isocomene, Cedrene, Hirsutene

Unit-II

Pericyclic Reactions: 15L

Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene, allyl system, classification of pericyclic reaction. FMO approach, Woodward-Hoffman correlation diagram method and Perturbation of Molecular Orbital (PMO) approach of pericyclic reaction under thermal and photochemical conditions Electrocyclic reactions, conrotatory and disrotatory motion $4n$ and $(4n+2)$ systems, Cycloaddition reaction with more emphasis on $[2+2]$ and $[4+2]$, Cycloaddition of ketones Secondary effects in $[4+2]$ cycloaddition. Stereochemical effects and effect of substituents on rate of cycloaddition reaction, Diels-Alder reaction, 1,3-dipolar cycloaddition and chelotropic reaction. Sigmatropic rearrangement, suprafacial, and antarafacial shift involving carbon moieties, retention and inversion of configuration, $[3,3]$ and $[3,5]$ sigmatropic rearrangements, **Claisen, Cope, Sommelet-Hauser rearrangements, Ene reaction.**

Unit-III

Oxidation and Reduction: 15L

a) Oxidation:

i) Oxidation of alkanes, aromatic hydrocarbons and alkenes, Dehydrogenation with S, Se, Fremy's salt, **DDQ**, chloranil and $\text{PhI}(\text{OAc})_2$, Oxidation with SeO_2 , Epoxidation of olefins, Sharpless asymmetric epoxidation, Dihydroxylation of olefins using **KMnO_4** , OsO_4 , Woodward and Prevost dihydroxylation, Oxidative cleavage of olefins, Ozonolysis.

ii) Oxidation of alcohols: Chromium reagents, pyridinium chlorochromate (PCC), pyridinium dichromate (PDC), Collins and Jones reagent, Combination of DMSO with DCC, $(\text{COCl})_2$, NCS and $(\text{CH}_3\text{CO})_2\text{O}$ for oxidation of alcohols, Oxidation with MnO_2 , Oppenauer oxidation

iii) Oxidation of aldehydes and ketones, Conversion of ketones to α , β -unsaturated ketones and α -hydroxy ketones, Baeyer-Villiger oxidation, Chemistry and synthetic applications of $\text{Pb}(\text{OAc})_4$, Dess-Martin periodinane, IBX.

(Advantages and limitations of reagents should be covered during teaching)

b) Reduction:

i) Catalytic heterogeneous and homogeneous hydrogenation, Hydrogenation of alkenes, alkynes and arenes, Selectivity of reduction, Mechanism and stereochemistry of reduction of Raney Ni-catalyst, Adam catalyst, Lindlar catalyst, Wilkinson catalyst.

ii) Reduction by dissolving metals, Reduction of carbonyl compounds, conjugated systems, aromatic compounds and alkynes. Birch reduction, Hydrogenolysis

iii) Reduction by hydride transfer reagents: Meerwein-Ponndorf-Verley reduction, Reduction with LiAlH_4 and NaBH_4 , stereochemical aspects of hydride addition, Derivatives of LiAlH_4 and NaBH_4 , Selectivity issues, Diisobutylaluminium hydride (DIBAL-H), Sodium cyanoborohydride, Reduction with boranes and derivatives, Reduction with Bu_3SnH , Reduction of carbonyl group to methylene, Reduction with diimide and trialkylsilanes
(Advantages and limitations of reagents should be covered during teaching)

Unit-IV

Chemistry of P, S, Si, and Boron compounds: 15L

a) **Phosphours and sulphur ylide:** Preparation and their synthetic application along with stereochemistry.

b) **Umpolung concept:** Dipole inversion, generation of acyl anion, use of 1,3-dithiane, ethylmethylthiomethylsulphoxide, bis-phenylthiomethane, metallated enol ethers, alkylidene dithiane, ketone thioacetals, 2-propenethiobismethyl thioallyl anion, thiamine hydrochloride based generation of acyl anion.

c) **Organoboranes:** preparation and properties of organoborane reagents e.g. RBH_2 , R_2BH , R_3B , 9-BBN, catechol borane, Thexyl borane, cyclohexyl borane, ICPBH_2 , IPC_2BH , Hydrboration- mechanism, stereo and regeoselectivity, uses in synthesis of primary, secondary tertiary alcohols, aldehydes, ketones, alkenes, Synthesis of EE, EZ, ZZ dienes and alkyenes. Mechanism of addition of IPC_2BH . Allyl boranes- synthesis, mechanism and uses.

d) **Organo silicon compounds in organic synthesis:** Me_3SiCl , Me_3SiH and Paterson synthesis

Reference books:

- 1] Books as suggested in Semester I for organic chemistry
- 2] Organic Synthesis, The disconnection approach-S. Warren
- 3] Designing Organic Synthesis-S. Warren
- 4] Some Modern Methods of Organic Synthesis-W. Carruthers
- 5] Advance Organic Chemistry Part-B-F. A. Caray and R. J. Sundberg Plenum Press
- 6] Protective Group in Organic Synthesis-T. W. Greene and PGM
- 7] The Chemistry of Organo Phosphorous-A. J. Kirby and S.G. Warren
- 8] Organo Silicon Compound-C. Eabon
- 9] Organic Synthesis via Boranes-H. C. Brown
- 10] Organo Borane Chemistry-T. P. Onak
- 11] Organic Chemistry of Boron-W. Gerrard
- 12] Fundamentals of Photochemistry-K. K. Rohatgi-Mukharji, Wiley Eastern Limited
- 13] Photochemistry-Cundau and Gilbert
- 14] Aspects of Organic Photochemistry-W. M. Horspoot
- 15] Photochemistry-J. D. Calvert
- 16] Photochemistry-R. P. Wayne

Course Code: PG-CHEM(02)-S3-T2-SP2

Paper-X Special II-Organic Chemistry [L-T-P = 4-0-0]

60 h (4 h per week): 15 h per unit

80 Marks

Unit-I

Terpenoids and Porphyrins: 15L

A] Terpenoids: Classification, nomenclature, occurrence, isolation, general methods of structure determination, isoprene rule. **Structure determination**, stereochemistry, and synthesis of the following representative molecules: Citral, Geraniol, α -terpeneol, Menthol, Farnesol, Zingiberene, Santonin, Phytol, Abietic acid and β -carotene, Vitamin A Genesis of biological isoprene unit, Biosynthesis (ONLY) of the following terpenoids: α & β -myrecene, linalool, geraniol, α -terpeneol, limonene, camphor, α -pinene, β -pinene, farnesol, β -bisabolene and squalene.

B] Porphyrins: Structure and synthesis of Haemoglobin and Chlorophyll.

Unit-II

Alkaloids and Prostaglandins: 15L

A] 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, Reserpine and Morphine. Biosynthesis (ONLY) of the followings: Hygrine, Tropinone, Nicotine, Pelletierine, Conine.

B] Prostaglandins: Occurrence, nomenclature, classification, biogenesis and physiological effects. Synthesis of PGE₂ and PGF_{2 α} .

Unit-III

Steroids and Plant Pigments: 15L

A] Steroids: Occurrence, nomenclature, basic skeleton, Diel's hydrocarbon and stereochemistry. Isolation, **structure determination and synthesis** of Cholesterol, Bile acids, Androsterone, Testosterone, Estrone, Progesterone and Aldosterone. Biosynthesis of steroids (lanosterol)

B] Plant Pigments: Occurrence, nomenclature and general methods of structure determination, isolation and synthesis of Apigenin, Luteolin, Quercetin, Myrcetin, Quercetin-3-glucoside, Vitexin, Diadzein, Butein, Cyanidin-7-arabinoside, Cyanidin, Hirsutidin. Biosynthesis of flavonoids: Acetate pathway and Shikimic acid pathway

Unit-IV

Carbohydrates, amino acids, proteins and peptides: 15L

A] Carbohydrate: Types of naturally occurring sugars, deoxy sugars, amino sugars, branched chain sugars, methyl ethers and acid derivatives of sugars, general methods of structure and ring size determination with reference to maltose, lactose, sucrose. Chemistry of starch and cellulose.

B] Amino acids, protein and peptides: Amino acids, structural characteristics, acid-base property, stereochemistry of amino acids, optical resolution, Strecker synthesis, peptide and proteins structure of peptide and protein, primary, secondary, tertiary and quaternary

structure. Reaction of polypeptide, structure determination of polypeptide, Solid phase peptide synthesis, end group analysis.

Reference books:

- 1] Chemistry of Alkaloids-S. W. Pelletier
- 2] Chemistry of Steroids-L. F. Fisher and M. Fisher
- 3] The Molecules of Nature-J. B. Hendrickson
- 4] Biogenesis of Natural Compound - Benfield
- 5] Natural Product Chemistry and Biological Significance- J. Mann, R. S. Devison, J. B. Hobbs, D. V. Banthripde and J. B. Horborne
- 6] Introduction to Flavonoids-B. A. Bohm, Harwood
- 7] Chemistry of Naturally Occurring Quinines-R. H. Thomson
- 8] The Systematic Identification of Flavonoids- Marby, Markham, and Thomos
- 9] Text Book of Organic Medicinal Chemistry-Wilson, Geswold
- 10] Medicinal Chemistry Vol I and II-Burger
- 11] Synthetic Organic Chemistry -Gurudeep Chatwal.
- 12] Organic Chemistry of Natural Products Vol I and II-O. P. Agrawal
- 13] Organic Chemistry of Natural Products -Gurudeep Chatwal
- 14] A Textbook of Pharmaceutical Chemistry-Jayshree Ghosh
- 15] Synthetic Dyes Series -Venkatraman
- 16] Chemistry Process Industries-Shreve and Brink
- 17] Principal of Modern Heterocyclic Chemistry-L. A. Paquelte
- 18] Heterocyclic Chemistry-J. Joule and G. Smith
- 19] Heterocyclic Chemistry-Morton
- 20] An Introduction to Chemistry of Heterocyclic Compound-J. B. Acheson
- 21] Introduction to Medicinal Chemistry-A. Gringuadge
- 22] Wilson and Gisvold Text Book of Organic Medicinal and Pharmaceutical Chemistry-Ed. Robert F Dorge
- 23] An Introduction to Drug Design-S. S. Pandey and J. R. Demmock
- 24] Polymer Science-V. Govarikar
- 25] Principle of Polymer Chemistry-P. J. Flory
- 26] An Outline of Polymer Chemistry-James Q. Allen
- 27] Organic Polymer Chemistry-K. J. Saunders

Course Code: PG –CHEM(02)-S3-P1
Practical –V Special Organic Chemistry Practical I [L-T-P = 0-0-8]

8 h per week

100 Marks

[A] Quantitative Analysis

Student is expected to carry out following estimations (minimum 6 estimations)

1. Estimation of Vitamin "C" Iodometry.
2. Estimation of Phenol by $\text{KBrO}_3\text{-KBr}$.
3. Estimation of Aniline by Bromate/ Bromide solution.
4. Estimation of Formaldehyde by Iodometry.
5. Estimation of Glucose by Benedict's solution.
6. Estimation of given carbonyl compound by hydrazone formation.
7. Estimation of Aldehyde by Oxidation method.
8. Determination of percentage of number of hydroxyl group in an organic compound by acetylation method.

[B] Isolation of Organic Compounds from Natural Source (Any Six)

- a) Isolation of caffeine from tea leaves.
- b) Isolation of casein from milk (the students are required to try some typical colour reactions of proteins)
- c) Isolation of lactose from milk (purity of sugar should be checked by TLC and PC and R_f value reported.)
- d) Isolation of nicotine dipicrate from tobacco
- e) Isolation of cinchonine from cinchona bark
- f) Isolation of piperine from black pepper
- g) Isolation of lycopene from tomatoes
- h) Isolation of β -carotene from carrots
- i) Isolation of cysteine from hair
- j) Isolation of oleic acid from olive oil (involving the preparation of complex with urea and separation of linoleic acid)
- k) Isolation of eugenol from cloves
- l) Isolation of (+) limonine from citrus rinds

[C] QUALITATIVE ANALYSIS

Separation of the components of a mixture of three organic compounds.

Three solids, two solids and one liquid, two liquids and one solid, all three liquids and identification of any two components using chemical methods or physical techniques. (Minimum 10-12 mixtures to be analyzed)

Course Code: PG -CHEM(02)-S3-T3-EL1

Paper-XI Elective I - Environmental Chemistry I [L-T-P = 4-0-0]

60 h (4 h per week): 15 h per unit

80 Marks

Unit -I: Concept and scope of Environmental Chemistry: 15 h

Biosphere, Lithosphere, Hydrosphere and Atmosphere, Ecological principles- aspects of ecology, classification, and types of ecosystems.

Atmospheric chemistry: Composition of atmosphere; photochemical reactions in atmosphere; smog formation, types of smog (sulphur smog and photochemical smog), aerosols; chemistry of acid rain, reactions of NO_x and SO_x ; free radicals and ozone layer depletion, role of CFCs in ozone depletion.

Toxic elements & their hazards: Essential & non-essential elements, Impact of toxic chemicals on enzymes, Biochemical effects of As, Cd, Pb and Hg, their metabolism, toxicity and treatment.

Unit-II: Water 15 h

Origin, physico-chemical properties of water, sources of water, hydrological cycle, criteria of water quality. Types and sources of water pollution. Impact on humans, plants and animals. Measurement of water quality parameters: sampling and analysis for pH, EC, turbidity, TDS, hardness, chlorides, salinity, DO, BOD, COD, nitrates, phosphates, sulphates, heavy metals and organic contaminants. Microbiological analysis MPN. Indian standards for drinking water (IS:10500, 2012).

Unit-III: Soil 15 h

Chemical and mineralogical composition of soil, classification of soil, types of soil- saline and alkaline, Types and sources of soil pollution, classification of soil pollutants, impact of soil pollution on air quality, Specifications for disposal of sewage and effluent on land for irrigation and ground water recharge.

Soil Pollution control: Methodology of waste water disposal on land in India. Management of saline and alkaline soil, soil indicator plants.

Unit IV: Air 15 h

Major regions of the atmosphere, composition of the atmosphere, temperature inversion and air pollution episodes, photochemistry of the atmosphere, depletion of the stratospheric ozone, green house effect, green house gases, remedial measures for reversion of green house effect, acid rain, photochemical smog, particulate matter. Natural versus polluted air, air quality standards.

Air pollution control: Control of automobile emission and control measures in thermal power stations.

Course Code: PG -CHEM(02)-S3-P2

Practical -VI : Elective-Environmental Chemistry Practical [L-T-P = 0-0-8]

8h per week

Marks-100

WATER ANALYSIS

- 1 Sampling of water-tap water, overhead storage tank water, pond water and lake water
- 2 Physico -chemical and organoleptic characteristics of the above water sample
- 3 Statistical evolution of the data obtained for optimization of result
- 4 Determination of total solids, total dissolved solids and total suspended solids and its significance
- 5 Determination and comparison of chlorine content in tap water, storage tank and swimmingpool

- 6 Determination of acidity and alkalinity in water samples
- 7 Determination of total, permanent and temporary hardness of water sample
- 8 Determination of DO, COD, and BOD of water sample
- 9 Analysis of chemicals used in water and waste water treatment-alum, bleaching powder, activated carbon
- 10 Analysis of iron and manganese in water sample by visual titrimetry
- 11 Analysis of copper and nickel in water sample by Spectrophotometry
- 12 Analysis of phenol in water sample by Spectrophotometry
- 13 Analysis of nitrite in water sample by Spectrophotometry
- 14 Analysis of chromium in water sample
- 15 Analysis of chloride in water sample
- 16 Analysis of sulphate in water sample
- 17 Determination of turbidity of a given water sample
- 18 Estimation of Na, K, by flame photometry in given water

AIR ANALYSIS

- 1 Determination of SO_x and NO_x and TSPM (total suspended particulate matter) and RSPM in ambient air

SOIL ANALYSIS

- 1 Analysis of different parameters of soil like pH, conductivity, alkalinity etc.
- 2 Determination of N, K, P of soil by flame photometry
- 3 Analysis of nutrients-nitrogen (total, ammonia, nitrite & nitrate), phosphate total
- 4 Determination of macro & micro nutrients in soil

Reference books:

1. Water analysis : J. Rodier
2. A Text book of Inorganic Analysis : A.I.Vogel
3. Colorimetric Determination of metals : E.B.Sandell
4. Environmental Chemistry : Moore J W and Moore E A. Academic Press, New York, 1976.
5. Environment and Man Vol VII: The Chemical Environment Edited by J Lenihar and W Fleecher Vlackie Publication, 1977.
6. The Chemistry of Environment: R A Horne, Wiley Interscience Publication 1978.
7. Fundamentals of Air Pollution: A C Stern
8. Instrumental Methods of Analysis: Willard, Merrit and Dean
9. Analytical Chemistry: Meites and Thomas
10. Standard Methods for Examination of water and waste water: A E Greenberg, A D Eaton, APHA, AWWA, WEF
11. Chemistry for Environmental Engineering and Science: C N Sawyer, P L McCarty and G F Parkin
12. Laboratory Manual for the Examination of Water, waste water and soil: H H Rupa and H Krist, V C H Publication
13. Manual on Water and Waste water analysis: D S Ramteke and C A Moghe, NEERI
14. Environmental Chemistry: B K Sharma and H Kaur
15. Environmental Chemistry: A K De
16. Environmental Pollution- Management and control for sustainable Development: R K Khatoliya
17. Environmental Chemistry: A K Bhagi and G R Chatwal
18. Environmental Chemistry : P.S. Sindhu

Course Code: PG –CHEM(02)-S3-T3-EL1

Paper–XI Elective I - Polymer Chemistry I [L-T-P = 4-0-0]

60 h (4 h per week): 15 h per unit

80 Marks

Unit-I: Introduction to polymers

15h

Basic Concept, raw materials for polymers. Nomenclature and classification of polymers, Polymerization: condensation, addition, radical chain- ionic and co-ordination and co-polymerization and their mechanisms, Types of polymers- linear, branched, crosslinked, ladder, thermoplastic, thermosetting, fibres, elastomers, natural polymers, addition and condensation polymers. Stereoregular polymers- atactic, syndiotactic and isotactic.

Unit-II: Molar mass and its determination

15h

Molecular mass and molar distribution. Number average, mass average, viscosity, average molecular mass and relation between them. Molecular mass distribution. Determination of molecular mass- Osmometry (membrane and vapour phase), light scattering, gel permeation chromatography, sedimentation and ultracentrifuge, viscosity method and end-group analysis.

Unit III: Physical characteristics of polymers

15h

Morphology and order in crystalline polymers. Configuration of polymer chains, crystal structure of polymers. Morphology of crystalline polymers, strain-induced morphology, crystallization and melting. The glass transition temperature (T_g), relationship between T_g and T_T , Effect of molecular weight, diluents, chemical structure, chain topology, branching and cross linking. Methods of determination of glass transition and crystallinity of polymers.

Unit IV: Commercial polymers

15h

A) Organic polymers: Commercial polymers, synthesis and application of polyethylene, Cellulose Acetate, PMMA, polyamides, polyesters, Urea resins and epoxy resins.

B) Functional Polymers: Conducting polymers, polymeric reagents, polymer supports and catalysts, Photoresponsive Polymers, polymers in lithography Immobilization of Enzymes.

Course Code: PG –CHEM(02)-S3-P2

Practical –VI: Elective- Polymer Chemistry Practical [L-T-P = 0-0-8]

8h per week

Marks-100

1. Synthesis of polymers:

- a) Synthesis of Thiokol rubber (condensation)
- b) Urea-formaldehyde (condensation)
- c) Glyptal resin: glycerine phthalic acid (crosslinked Polymer Chemistry)
- d) Polyacrylonitril (bulk polymerization)
- e) Polyacrylonitril (emulsion polymerization)
- f) Polymethylmethacrylate (emulsion of suspension Polymer Chemistry)
- g) Nylon-66 (interfacial polycondensation)
- h) Coordination polymers
- i) Conducting polymer (electro- or peroxodisulphate oxidation)

2. Characterization of polymers:

- a) End-group analysis
- b) Viscosity and molecular mass

- c) Density of polymer by flotation methods
- d) IR spectra.
- 3. Purification and fractionation of polymer, polystyrene, Nylon 66, PMMA.
- 4. Magnetic and electrical properties of polymers, magnetic susceptibility and electrical conductivity of coordination and conducting polymers.
- 5. Thermal analysis and degradation of polymers:
 - i. TGA: Isothermal and non-isothermal;
 - ii. DTA: Glass transition temperature and melting point
- 6. Crystallinity of polymers by density measurement.
- 7. Swelling and solubility parameters of polymers.
- 8. Synthesis of Graft-Polymers and its characterization by density and IR spectra.
- 9. Dielectric behavior of polymers.
- 10. Kinetics of polymerization:
 - a) Polycondensation
 - b) Peroxide initiation polymerization.

Reference books:

1. Textbook of polymer science: F.W. Billmeyer Jr. Wiley.
2. Polymer science: V.R. Gowarikar, N. V. Viswanathan and J. Sreedhar, Wiley-Eastern.
3. Fractional monomers and polymers: K Takemoto, Y. Inaki, and R.M. Ottam Brite.
4. Contemporary polymer chemistry: H.R. Alcock and F. W. Lambe, Prentice Hall.
5. Principles of polymer Chemistry: Flory, Cornell Univ. press.
6. Introduction to polymer chemistry: R. B. Seymour, McGraw Hill.
7. Principles of polymerization: Odian.
8. A first course in polymer chemistry: A. Strepikheyew, V. Derevistkay and G. Slonimasky, Mir Publishers, Moscow.
9. Laboratory preparation of macro chemistry: EMM effery, McGraw Hill Co.
10. A practical course in polymer chemistry: S. J. Punea , Pergamon Press.

Course Code: PG-CHEM(02)-S3-T3-EL1

Paper-XI Elective I - Medicinal Chemistry I [L-T-P = 4-0-0]

60 h (4 h per week): 15 h per unit

80 Marks

UNIT-I:

15 h

Drug Design

Development of new drugs, factors affecting development of new drugs, sources of lead compounds, serendipity and drug development. Concept of QSAR, QSAR methods and parameters, procedure followed in drug design, structure activity relationship (SAR) method, Free and Wilson analysis, Hansch analysis, concept of prodrugs and softdrugs, SOFT DRUGS, isosterism, bioisosterism, drug receptors, theories of drug action, types of reversible enzyme inhibitors, some special inhibitors and design of inhibitors.

UNIT-II:

15 h

A] Pharmacokinetics and pharmacodynamics: Introduction drugs absorption, distribution and disposition of drugs, excretion and elimination, Pharmacokinetics of elimination and Pharmacokinetics in drug development process.

Pharmacodynamics: Introduction, enzyme stimulation, enzyme inhibition, membrane active drugs, drugs metabolism, biotransformation and significance of drug metabolism

B] Diuretics: Introduction, mode of action, loop diuretics. Synthesis of Bumetanide,

Frusemide, Ethacrynic acid, clorexolone Quinethazone.

C] Analgesics and Antipyretics: Introduction, mode of action, evaluation of analgetic agents. Synthesis of: Aspirin, salsalate, phenacetin, phenylbutazone, Indomethacin, Analgin.

UNIT-III:

15 h

A] Cardiovascular Drugs: Introduction, cardiovascular diseases, Synthesis and uses of cardiovascular drugs; amyl nitrate, diltiazem, varapamil, methyldopa, atenolol, sorbitrate, quinidine, oxyproprenolol.

B] Antineoplastic Agent: Introduction, mechanism of tumor formation, treatment of cancer, types of cancer chemotherapy, role of alkylating agents and antimetabolites in treatment of cancer, carcinolytic antibiotics, mitotic inhibitors, hormones, natural products. Synthesis of melphalan, thiotepa, lomustine.

UNIT-IV:

15 h

A] Psychoactive drugs: Introduction, neurotransmitters, structure of nerve cell, chemical transmitters, CNS depressants, sedative and hypnotics, Synthesis of Barbiturates, Phenobarbital, thiopental sodium, diazepam, lorazepam, bromazepam, ethosuximide, general anaesthetic: Antianxiety drugs, synthesis of oxazepam, alprazolam, puspiron, antipsychotic drugs and antidepressant drugs, MAO inhibitors, antimanic drugs, synthesis of thiopental sodium, ethiosuximide, glutethimide, trimethadione, phenytoin.

B] Coagulant and Anticoagulants: Introduction, factors affecting coagulant and anti-coagulant. Mechanism of Blood coagulation and Anticoagulation. Structure of Vitamin K1, Vitamin K2 and heparin. Synthesis of Coumarins and indanediones.

Course Code: PG –CHEM(02)-S3-P2

Practical –VI: Elective- Medicinal Chemistry Practical [L-T-P = 0-0-8]

8 h per week

Marks-100

1. Volumetric estimation of Ibuprofen.
2. Estimation of aspirin by volumetric and instrumental methods.
3. Analysis of ascorbic acid in biological/tablet sample.
4. Determination of paracetamol by colorimetry.
5. Analysis of ampicillin trihydrate.
6. Determination of vitamin B12 in commercial sample by spectrophotometry.
7. Determination of phenobarbitone in given cough syrup.
8. Determination of tetracycline in given capsule.
9. Determination of iron, calcium and phosphorus from milk or drug sample.
10. To perform I.P. monograph of tablet.
11. Estimation of chloride in serum and Urine.
12. Separation and determination of sulpha drugs in tablets or ointments.

Preparation of Drugs: Synthesis, purification and identification of (8-10) of the following drugs.

- | | |
|--|---|
| 1. Benzocaine from p-nitrobenzoic acid. | 16. 1,5 diphenyl-1,3-pentadiene-2-one from benzaldehyde |
| 2. Dapsone from diphenyl sulphone. | 17. 1,3-diphenyl-prop-2-ene-1-one |
| 3. Paracetamol from p-nitro phenol. | 18. 3-methy pyrazol-5-one from ethylacetoacetate |
| 4. Uracil from sulphanil amide. | 19. 6-methyl uracil from ethylacetoacetate |
| 5. Diphenyl hydantion from benzoin. | 20. Sulphanilamide from acetanilide |
| 6. Aluminium aspirin from salicylic acid. | 21. Barbituric acid (4-hydroxyuracil) from diethylmalonate. |
| 7. 4,6-diphenyl-thiazine from chalcone. | 22. 2,3-dimethyl-1-Phenylpyrazol-5-one(Antipyrin)from ethylacetoacetate |
| 8. 6/8 nitro coumarin from resorcinol. | 23. Fenbufen |
| 9. Copper aspirin from salicylic acid. | 24. 2-Phenylbenzo-4-pyrone (falvone)from o-hydroxyacetophenone |
| 10. N-acetyl parabanic acid. | 25. Chlorobutanol from acetone |
| 11. Nerolin from 2-naphthol | 26. 2,4-dioxypiperazine from glycine |
| 12. Phenothiazine from diphenylamine | |
| 13. Umbelliferon from resorcinol | |
| 14. Benzylidene from benzaldehyde and aniline | |
| 15. 1-phenyl-1,2-pentadine-3-one from benzaldehyde | |

Reference books:

1. Text book of organic medicinal chemistry-Wilson,Geswold
2. Medicinal chemistry Vol I and II-Burger
3. A textbook of pharmaceutical chemistry-Jayshree Ghosh
4. Introduction to medicinal chemistry-A Gringuadje
5. Wilson andGisvold text book of organic medicinal and pharmaceutical chemistry-Ed.Robert F Dorge
6. An introduction to drug design-S S Pandey,and JR Demmock
7. Goodman and Gilmans pharmacological basis of therapeutics- Strategies for organic drug sythesis and design-D Lednicer
8. Textbook of Medicinal Chemistry- A. Kar
9. Medicinal Chemistry – D Sriram and P. Yogeewari

Course Code: PG –CHEM(02)-S3-T4
Paper–XII : Spectroscopy – I (Core Subject Centric) [L-T-P = 4-0-0]

60 h (4 h per week): 15 h per unit

80 Marks

Unit-I

Symmetry properties of molecules and group theory: 15L

Symmetry elements and symmetry operations. Properties of group. Point groups and Schoenflies symbols. Symmetry operations as a group. Matrix representations of groups. Multiplication table for C_{2v} and C_{3v} . Reducible and irreducible representations. Similarity transformation. Classes of symmetry operations. Great Orthogonality Theorem. Derivation of character tables for H_2O and NH_3 using Great Orthogonality Theorem. Application of character tables in selection rules of IR, Raman and Electronic spectroscopy.

Unit-II

Microwave and Mössbauer Spectroscopy: 15L

A] Microwave spectroscopy: Classification of molecules on the basis of M. I., rigid and non rigid rotor, effect of isotopic substitution on transition frequencies, stark effect, microwave spectrometer, application in deriving: molecular structure, dipole moment, atomic mass. Width and intensity of spectral transitions, Fourier transform microwave spectroscopy, rotation spectra of poly atomic molecules. Numericals.

B] Mössbauer spectroscopy:

Basic principle, experimental techniques, recoil emission and absorption, source, absorber, isomer shift, quadrupole interaction, magnetic hyperfine interaction, applications in determining electronic structure, molecular structure, crystal symmetry, magnetic structure, surface studies, biological applications.

Unit-III

Infrared and Raman Spectroscopy: 15L

A] Infrared spectroscopy: Diatomic molecules: Molecules as harmonic oscillator, zero point energy, Anharmonic oscillator, Morse potential energy function, vibrational spectrum, fundamental vibrational frequencies. Force constant, the interactions of rotations and vibrations. P, Q, R branches, vibration of polyatomic molecules, selection rules, normal modes of vibration, IR spectra, regions of IR, Characteristic vibrational frequencies of functional groups, overtone and combination frequencies. Numericals. Structural information from IR spectroscopy, Structural determination of organic molecules by IR spectroscopy, problems based on IR spectral data.

B] Raman Spectroscopy: Rayleigh scattering, Raman Scattering, classical and quantum theories of Raman effect. Rotational Raman Spectra for linear and symmetric top molecules. Vibrational Raman Spectra, rotational fine structure. Selection rules, coherent anti-Stokes Raman spectroscopy, Structure determination from Raman and Infra-red spectroscopy, Surface enhanced raman spectroscopy(SERS), Numericals.

Unit-IV

Diffraction techniques: 15L

A] X ray diffraction: Braggs condition, Miller indices, Laue method, Bragg method, Debye Scherrer method, identification of unit cells from systematic absences in diffraction pattern, structure of simple lattices and x-ray intensity, structure factor and its relation to intensity and electron density, absolute configuration of molecules.

B] Electron diffraction: scattering intensity vs scattering angle, Wierl equation, measurement techniques, elucidation of structure of simple gas phase molecules, low energy electron diffraction and structure of surfaces.

C] Neutron diffraction: Scattering of neutrons by solids and liquids, magnetic scattering, measurement techniques, elucidation of structure of magnetically ordered unit cell.

Reference books:

- 1] Spectroscopic identification of organic compound-RM Silverstein,GC Bassler and TC Morrill, John Wiley
- 2] Introduction to NMR spectroscopy-R. J. Abraham, J. Fisher and P Loftus Wiely
- 3] Application of Spectroscopy to Organic Compound-J. R. Dyer, Printice Hall
- 4] Organic Spectroscopy-William Kemp, ELBS with McMillan
- 5] Spectroscopy of Organic Molecule-PS Kalsi, Wiley, Esterna, New Delhi
- 6] Organic Spectroscopy-RT Morrison and RN Boyd
- 7] Practical NMR Spectroscopy-ML Martin, JJ Delpenck, and DJ Martyin
- 8] Spectroscopic Methods in Organic Chemistry-DH Willson, I Fleming
- 9] Fundamentals of Molecular Spectroscopy-CN Banwell
- 10] Spectroscopy in Organic Chemistry-CNR Rao and JR Ferraro
- 11] Photoelectron Spectroscopy-Baber and Betteridge
- 12] Electron Spin Resonance Spectroscopy-J Wertz and JR Bolten
- 13] NMR –Basic Principle and Application-H Guntur
- 14] Interpretation of NMR spectra-Roy H Bible
- 15] Interpretation of IR spectra-NB Coulthop
- 16] Electron Spin Resonance Theory and Applications-W gordy
- 17] Mass Spectrometry Organic Chemical Applications, JH Banyon

OR

Course Code: PG –CHEM(02)-S3-T4

Paper–XII : (Foundation Course-I) Applied Analytical Chemistry-I [L-T-P = 4-0-0]

60 h (4 h per week): 15 h per unit

80 Marks

Unit-I: Analysis of Pesticides and Fertilizers

15h

Pesticides: General introduction, analysis of pesticides in general with reference to DDT, Dieldrin, Malathion, Parathion, BHC by different analytical methods such as titrimetric, colorimetric, chromatography and electroanalytical methods.

Fertilizers: Sampling and sample preparation, determination of water, total nitrogen, urea, total phosphates, potassium, acid or base forming quality.

Unit-II: Forensic chemistry

15h

Introduction: Classification of poisons on the basis of physical states, mode of action and chemical properties with examples of each type. Methods of administration. Action of poisons in body. Factors affecting poisoning. Study of some common poisons used for suicide. Signs and symptoms of As, Pb, Hg and cyanide poisoning. Poisonous effects of kerosene and cooking gas.

Unit-III: Analysis of petroleum and petroleum products

15h

Introduction, determination of flash and fire point, Pensky Marten's apparatus, cloud and pour point, aniline point, drop point, viscosity and viscosity index, Redwood and Saybolt viscometer, API specific gravity, water and sulphur in petroleum products, carbon residue, corrosion stability, decomposition stability, emulsification, neutralization and saponification number.

Unit-IV: Analysis of alloys

15h

Definition of alloy. phase diagrams of Fe-C, Pb-Sn, Pb-Ag systems and their applications. Types of steel: hypoeutectic, hypereutectic steels, mild steel, and stainless steel. Uses of steel. Composition and uses of brass, bronze and soldering alloy. Analysis of iron, nickel, chromium and manganese in steel. Analysis of copper and zinc in brass, lead and tin in soldering alloy.

Industrial applications of alloys.

Reference books:

- 1] Quantitative analysis: Day and Underwood (Prentice-Hall of India)
- 2] Vogel's Text Book of Quantitative Inorganic Analysis-Bassett, Denney, Jeffery and Mendham (ELBS)
- 3] Analytical Chemistry: Gary D. Christian (Wiley, India).
- 4] Instrumental Methods of Analysis: Willard, Merrit, Dean, Settle (CBS Publishers, Delhi, 1986)
- 5] Instrumental Methods of Chemical Analysis: Braun (Tata McGraw-Hill)
- 6] Advanced Analytical Chemistry: Meites and Thomas (McGraw-Hill)
- 7] Instrumental Methods of Analysis: G. Chatwal and S. Anand (Himalaya Publishing House)
- 8] Analytical Chemistry: Problems and Solution- S. M. Khopkar (New Age International Publication)
- 9] Basic Concepts in Analytical Chemistry: S. M. Khopkar (New Age International Publication)
- 10] Advance Analytical Chemistry: Meites and Thomas: (Mc Graw Hill)
- 11] An Introduction to Separation Science: L. R. Shyder and C. H. Harvath (Wiley Interscience)
- 12] Fundamentals of Analytical Chemistry: S. A. Skoog and D. W. West
- 13] Instrumental Methods of Chemical Analysis: G. W. Ewing

Bajaj College of Science, Wardha (Autonomous College)

SUBJECT: CHEMISTRY

Syllabus of M.Sc. II/Semester IV (WEF 2022-23)

Course Code: PG-CHEM(02)-S4-T1-SP1

Paper-XIII: Special I-Organic Chemistry [L-T-P = 4-0-0]

60 h (4 h per week): 15 h per unit

80 Marks

Unit-I

15L

A] Carbanions in organic Chemistry

Ionization of carbon hydrogen bond and prototopy, Base and acid catalysed halogenation of ketones, keto-enol equilibria, structure and rate in enolisation, concerted and carbanion mechanism for tautomerism, geometry of carbanions, kinetic and thermodynamic control in the generation of enolates, LDA, hydrolysis of haloforms, use of malonic and acetoacetic esters, Aldol, Mannich, Cannizzaro, Darzens, Dieckmann, Claisen Baylis-Hillman reactions, Knoevenagel, benzoin condensation, Julia olefination, alkylation of enolates and stereochemistry thereof, Conjugate additions, enamines in organic synthesis

B] Organometallic reagents -I

Synthesis and applications of organo Li and Mg reagents, nucleophilic addition to aldehyde, ketones, ester, epoxide, CO₂, CS₂, isocyanates, ketenes, imines, amides, lactones, Stereochemistry of Grignard addition to carbonyl compounds, *o*-metallation of arenes using organolithium compounds.

Unit-II

15L

A] Organometallic reagents-II

Organozinc reagents: Preparation and applications, Reformatsky reaction, Simon-Smith reaction. Organocopper reagents: Preparation and applications in C-C bond forming reaction, mixed organocuprates, Gilman's reagent. Organo Hg and Cd reagents in organic synthesis.

B] Transition metals in organic synthesis: Transition metal complexes in organic synthesis- Introduction-oxidation states of transition metals, 16-18 rule, dissociation, association, insertion, oxidative addition, reductive elimination of transition metal.

Organopalladium in organic synthesis-Heck reaction, carbonylation, Wacker oxidation, coupling reactions: Kumada Reaction, Stille coupling, Sonogashira, Negishi and Suzuki coupling reactions and their importance

Applications of Co₂(CO)₈, Ni(CO)₄, Fe(CO)₅ in organic synthesis. Wilkinson catalyst of Ruthenium and Rhodium – synthesis and uses its use in hydrogenation reactions-deallylation, C-C, C-O, C-N bond cleavages. Olefin metathesis by 1st and 2nd generation catalyst, reaction mechanism and application in the synthesis of homo and heterocyclic compounds.

Unit-III

15L

A] Advanced Stereochemistry: Conformation of sugars, monosaccharides, disaccharides, mutarotation, Recapitulation of Stereochemical concepts- enantiomers, diastereomers, homotopic and heterotopic ligands, Chemo-, regio-, diastereo- and enantio-controlled approaches; Chirality transfer, Stereoselective addition of nucleophiles to carbonyl group: Re-Si face concepts, Cram's rule, Felkin Anh rule, Houk model, Cram's chelate model. Asymmetric synthesis use of chiral auxiliaries, asymmetric hydrogenation, asymmetric epoxidation and asymmetric dihydroxylation.

B] Protection and Deprotection of functional groups: Protection and deprotection of

functional groups like, hydroxyl, amino, carbonyl and carboxylic acids groups, Solid phase peptide synthesis.

Unit-IV: Designing the synthesis based on retrosynthetic analysis **15L**

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

B) One Group C-C Disconnections: Alcohols and carbonyl compounds, regioselectivity, alkene synthesis, use of acetylenes and aliphatic nitro compounds in organic synthesis.

Two Group C-C Disconnections: Diels-Alder reaction, 1,3-difunctionalised compounds, α,β -unsaturated carbonyl compounds, control in carbonyl condensations, 1,5-difunctionalised compounds, Michael addition and Robinson annulation, Methods of ring synthesis, Linear and convergent synthesis.

Reference books:

- 1] Principle of Organic Synthesis R. O. C. Norman and J. M. Coxon
- 2] Modern Synthetic Reaction. H. O. House and W. A. Benjamin
- 3] Organic Synthesis: The Disconnection Approach-S. Warren
- 4] Designing Organic Synthesis-S. Warren
- 5] Some Modern Methods of Organic Synthesis-W. Carruthers
- 6] Advance Organic Reaction. Mechanism and Structure-Jerry March
- 7] Advance Organic Chemistry Part-B-F. A. Caray and R. J. Sundberg Plenum Press
- 8] Organic Reaction and their Mechanism-P. S. Kalsi
- 9] Protective Groups in Organic Synthesis-T. W. Greene
- 10] The Chemistry of Organo Phosphorous-A. J. Kirby and S. G. Warren
- 11] Organo Silicon Compound-C. Eabon
- 12] Organic Synthesis via Boranes-H. C. Brown 13] Organo Borane Chemistry-T. P. Onak
- 14] Organic Chemistry of Boron-W. Gerrard

Course Code: PG-CHEM(02)-S4-T2-SP2

._Paper-XIV: Special II-Organic Chemistry [L-T-P = 4-0-0]

60 h (4 h per week): 15 h per unit

80 Marks

Unit-I: Enzyme chemistry

15L

A) Enzymes: Introduction, chemical and biological catalysis, remarkable properties of enzymes like catalytic power, specificity and regulation. Cofactors as derived from vitamins, coenzymes, prosthetic groups, apoenzymes. Nomenclature and classification, Fischer's lock and key and Koshland's induced fit hypothesis, concept and identification of active site by the use of inhibitors, affinity labeling and enzyme modification by site-directed mutagenesis. Baker's yeast catalyzed reactions

B) Mechanism of Enzyme Action: Transition-state theory, orientation and steric effect, acid-base catalysis, covalent catalysis, strain or distortion. Enzyme mechanisms for chymotrypsin, ribonuclease, lysozyme and carboxypeptidase A.

C) Co-Enzyme Chemistry: Structure and biological functions of coenzyme A, thiamine pyrophosphate, pyridoxal phosphate, NAD^+ , NADP^+ , FMN, FAD, lipoic acid, biotin as CO_2 carrier. Mechanisms of reactions catalyzed by the above cofactors.

Unit-II: Heterocycles

15L

A) Azoles: Structural and chemical properties; **Synthesis of pyrazole, isothiazole and**

isoxazole; Synthesis of imidazoles, thiazoles and oxazoles; Nucleophilic and electrophilic substitutions; Ring cleavages, Carbonyldiimidazole as coupling agent

B] Benzofused heterocycles: Synthesis of indole, benzofuran and benzo-thiophene, quinoline and isoquinoline Nucleophilic, electrophilic and radical substitutions; Addition reactions; Indole rings in biology.

C] Diazines: Structural and chemical properties; Synthesis of pyridazines, pyrimidines, pyrazines; Nucleophilic and electrophilic substitutions.

D] Synthesis of following bioactive compounds: Vitamin B₆, Ondansetron, Serotonin, Indometacin, Cyanamid, fentiazac, trimethoprim, papaverine

Unit-III

15L

A] Nucleic Acids: Primary, secondary and tertiary structure of DNA; DNA replication and heredity; Structure and function of m-RNA, t-RNA and r-RNA. Purines and pyrimidine bases of nucleic acids and their preparation.

B] Lipids: Fatty acids, essential fatty acids, structures and functions of triglycerols, glycerophospho lipids, spingolipids, lipoproteins, composition and function, role in atherosclerosis.

Properties of lipid aggregates, micells, bilayers, liposomes and their biological functions, biological membranes, fluid mosaic model of membrane structure, Lipid metabolism, β -Oxidation of fatty acids

C] Vitamins: Structure determination, and synthesis of vitamin A, E and H.

Unit-IV

15L

A] Dyes: General Introduction, classification on the basis of structure and methods of application dying mechanism, methods of dying, such as direct dying, vat dying, dispersive dying, formation of dye in fibre, dying with reactive dyes, study of quinoline yellow, cyamine dye, ethyl red, methylene blue, Alizarin, cyamine-green, fluorescein, cosin, erythrosine, Rhodomines and Indigo.

B] Pharmaceutical chemistry:

History, medical terms in pharmaceutical chemistry, classification of drugs, antibacterial and antifungal drugs, specific clinical applications, Synthesis and applications of: Benzocaine,

C] Polymer chemistry: Importance of polymers, Basic concepts: monomers, repeat units, degree of polymerization. Linear, branched and network polymers. Classification of polymers. **Polymerization:** condensation, addition, radical chain-ionic and co-ordination and co-polymerization and their mechanisms, Polymerization in homogeneous and heterogeneous systems. Ziegler-Natta polymerization with mechanism, Stereo regulated polymers, syndiotactic, isotactic and atactic polymers

Reference books:

- 1] Textbook of Polymer Science, F. W. Billmeyer Jr, Wiley
- 2] Polymer Science, V. R. Gowarikar, N. V. Viswanathan and J. Sreedhar, Wiley-Eastern
- 3] Functional Monomers and Polymers, K. Takemoto, Y. Inaki and R. M. Ottanbrite
- 4] Bioorganic Chemistry: A Chemical Approach to Enzyme Action, Hermann Dugas and C. Penny, Springer-Verlag
- 5] Understanding Enzymes, Trevor Palmer, Prentice Hall
- 6] Enzyme Chemistry: Impact and Applications, Ed. Collin J. Suckling, Chapman and Hall
- 7] Enzyme Structure and Mechanism, A. Fersht, W. H. Freeman
- 8] Introduction to Medicinal Chemistry, A. Gringuage, Wiley-VCH
- 9] Wilson and Gisvold's Text Book of Organic Medical and Pharmaceutical Chemistry, Ed Robert F. Dorge
- 10] Burger's Medicinal Chemistry and Drug Discovery, Vol-1, Ed. M. E. Wolff, John Wiley
- 11] Strategies for Organic Drug Synthesis and Design, D. Lednicer, John Wiley
- 12] The Organic Chemistry of Drug Design and Drug Action, R. B. Silverman, Academic Press

Course Code: PG -CHEM(02)-S4-P1

Practical -VII: Special Organic Chemistry Practical II [L-T-P = 0-0-8]

8 h per week

100 Marks

A] Quantitative Analysis based on classical and instrumental technique (any 9-10)

- 1] Estimation of nitrogen.
- 2] Estimation of halogen.
- 3] Estimation of sulphur.

Spectrophotometric/calorimetric and other instrumental methods of estimation

- 1] Estimation of streptomycin sulphate.
- 2] Estimation of vitamin B-12.
- 3] Estimation of amino acids.
- 4] Estimation of proteins.
- 5] Estimation of carbohydrates.
- 6] Estimation of Ascorbic acid.
- 7] Estimation of Aspirin.
- 8] Solvent extraction of oil from oil seeds and determination of saponification value, iodine value of the same oil.

B] Organic multi-step preparations (Two/Three steps): Minimum 10-12 preparations

- [1] Aniline → Diaminoazobenzene → *p*-aminoazobenzene
- [2] Benzoin → Benzyl → Dibenzyl
- [3] Aniline → acetanilide → *p*-bromoacetanilide → *p*-bromoaniline
- [4] Aniline → Acetanilide → *p*-nitroacetanilide → *p*-nitroaniline
- [5] Benzaldehyde (thiamine hydrochloride) → benzoin → benzil → benzilic acid

- [6] *p*-Nitrotoluene → *p*-nitrobenzoic acid → PABA → *p*-iodobenzoic acid
- [7] *p*-Cresol → *p*-cresylacetate → 2-hydroxy-5-methyl acetophenone → 2-hydroxy chalcone
- [8] Benzaldehyde → benzilidene acetophenone → 4,5-dihydro-1,3,5-triphenyl-1*H*-pyrazole
- [9] Aniline → phenylthiocarbamide → 2-aminobenzthiazole (Microwave in step I)
- [10] Chlorobenzene → 2,4- Dinitrochlorobenzene → 2,4- Dinitrophenylhydrazine.
- [11] Acetophenone → acetophenone phenyl hydrazone → 2-phenylindole
- [12] Benzoin → benzoin benzoate → 2,4,5-triphenyl oxazole
- [13] Benzophenone → benzpinacol → benzopinacolone (Photochemical preparation)
- [14] Benzophenone → Benzophenone oxime → Benzanilide → Benzoic acid + aniline
- [15] Aniline → aniline hydrogen sulphate → sulphanilic acid → Orange II
- [16] Aniline → N-arylglycine → indoxyl → indigo
- [17] Phthalimide → Anthranilic acid → Phenyl glycine-*o*-carboxylic acid → Indigo
- [18] Phalic anhydride → Phthalimide → Anthranilic acid → *o*-chlorobenzoic acid
- [19] Phalic anhydride → Phthalimide → Anthranilic acid → Diphenic acid
- [20] Ethyl acetoacetate → 3-methyl-pyrazol-5-one → 4,4-dibromo-3-methyl-pyrazol-5-one
Butanoic acid
- [21] Biosynthesis of ethanol from sucrose
- [22] Enzyme catalyzed reactions

[C] SPECTRAL INTERPRETATION

Structure Elucidation of organic compounds on the basis of spectral data (UV, IR, ¹H and ¹³CNMR and Mass) (Minimum 12 compounds are to be analysed during regular practicals).

Course Code: PG -CHEM(02)-S4-T3-EL2

Paper-XV: Elective II - Environmental Chemistry II [L-T-P = 4-0-0]

60 h (4 h per week): 15 h per unit

80 Marks

Unit-I:

15 h

Thermal pollution-sources, harmful effects and prevention of thermal pollution.

Noise pollution- sources, effects and control of noise pollution.

Radioactive Pollution- Introduction to radiation chemistry, sources of radioactive pollution, effects of radioactive pollution, nuclear disasters in the two decades, protection from radiation, control of radiation.

Unit-II: Solid waste pollution

15 h

Sources, types and consequences, classification of wastes- domestic, industrial, municipal, hospital, nuclear and agricultural. Impact of solid waste on environment, human and plant health; effect of solid waste and industrial effluent discharge on water quality and aquatic life.

Solid waste Management: Different techniques used in collection, storage, transportation and disposal of solid waste (domestic, industrial and agricultural).

Unit-III:

15 h

Waste water treatment & management: Wastewater Treatment: Primary, Secondary and Advanced treatment methods. Common effluent treatment plant. Drinking water treatment, Coagulation and flocculation, Sedimentation and Filtration, Disinfection and Softening. Removal of hardness by lime-soda process, Zeolite process and synthetic ion-exchange resins. Principle, instrumentation and comparison of these three processes. Numericals based on hardness removal. Desalination of sea- water.

Unit-IV:

15 h

Soil analysis: Physical properties – texture, bulk density, permeability chemical properties—Ion exchange capacity, soil pH and micro and macro nutrient availability.

Analysis of constituents such as nitrogen, phosphorous, potassium and microconstituents (Zn and Cu)

Air pollution analysis— Sampling of aerosols and gaseous pollutants and their effects, SO₂, NO₂, CO, CO₂, particulates-SPM, RSPM, High Volume Sampler, Fabric Filters, Cyclones (direct and Reverse), ESP, ozone layer.

Reference books:

1. Water analysis : J. Rodier
2. A Text book of Inorganic Analysis : A.I.Vogel
3. Colorimetric Determination of metals : E.B.Sandell
4. Environmental Chemistry : Moore J W and Moore E A. Academic Press, New York, 1976.
5. Environment and Man Vol VII: The Chemical Environment Edited by J Lenihar and W Fleecher Vlackie Publication, 1977.
6. The Chemistry of Environment: R A Horne, Wiley Interscience Publication 1978.
7. Fundamentals of Air Pollution: A C Stern
8. Instrumental Methods of Analysis: Willard, Merrit and Dean
9. Analytical Chemistry: Meites and Thomas

10. Standard Methods for Examination of water and waste water: A E Greenberg, A D Eaton, APHA, AWWA, WEF
11. Chemistry for Environmental Engineering and Science: C N Sawyer, P L McCarty and G F Parkin
12. Laboratory Manual for the Examination of Water, waste water and soil: H H Rupa and H Krist, V C H Publication
13. Manual on Water and Waste water analysis: D S Ramteke and C A Moghe, NEERI
14. Environmental Chemistry: B K Sharma and H Kaur
15. Environmental Chemistry: A K De
16. Environmental Pollution- Management and control for sustainable Development: R K Khatoliya
17. Environmental Chemistry: A K Bhagi and G R Chatwal
18. Environmental Chemistry : P.S. Sindhu

Course Code: PG -CHEM(02)-S4-T3-EL2

Paper-XV: Elective II - Polymer Chemistry II [L-T-P = 4-0-0]

60 h (4 h per week): 15 h per unit

80 Marks

Unit-I: Polymerization

15h

Importance, basic concepts, raw materials for polymers, concept of functionality, comparison of chain and step-growth, examples of polymerization reactions (polyadditions, polycondensations) constitution of polymers, homopolymers and copolymers, polymer architectures (graft copolymers, star-branched, hyperbranched and dendrimers), configuration and conformation of polymers, coil formation, mobility in polymers, glass transition temperature, rubber elasticity, molecular weight distribution.

Unit-II: Techniques of polymerization

15h

Techniques of polymerization-suspension, emulsion and bulk polymerization, coordination, polymerization mechanism of Ziegler Natta polymerization, stereospecific polymerization, interfacial polycondensation, mechanism of polymerization.

Unit III: Characterization of polymers

15h

Spectroscopic techniques: Fundamentals, experimental and applications to polymers of the following techniques: UV-visible spectroscopy, IR and Raman spectroscopy, Nuclear Magnetic (proton, carbon), resonance spectroscopy, NMR of polymers in the solid state, two dimensional NMR spectroscopy, pyrolysis GC-MS.

Thermal methods-TGA, DTA, DSC,

Thermomechanical and X-ray diffraction study, Block and Graft copolymers, random, block, graft co-polymers, methods of copolymerization.

Unit IV: Specific polymers

15h

A) Biomedical polymers: Contact lens, dental polymers, artificial heart, kidney and skin.

B) Inorganic polymers: Synthesis and application of silicon, phosphorous and sulphur containing polymers.

C) Coordination polymers: Synthesis and applications of coordination polymers.

D) Diene-based polymers: Polyisoprene, polybutadiene.

Reference books:

1. Textbook of polymer science: F.W. Billmayer Jr. Wiley.
2. Polymer science: V.R. Gowarikar, N. V. Viswanathan and J. Sreedhar, Wiley-Eastern.
3. Fractional monomers and polymers: K Takemoto, Y. Inaki, and R.M. Ottam Brite.
4. Contemporaty polymer chemistry: H.R. Alcock and F. W. Lambe, Prentice Hall.
5. Principles of polymer Chemistry: Flory, Cornell Univ. press.
6. Introduction to polymer chemistry: R. B. Seymour, McGraw Hill.
7. Principles of polymerization: Odian.
8. A first course in polymer chemistry: A. Strepikheyew, V. Derevistkay and G. Slonimasky, Mir Publishers, Moscow.
9. Laboratory preparation of macro chemistry: EMM effery, McGraw Hill Co.
10. A practical course in polymer chemistry: S. J. Punea , Pergamon Press.

60 h (4 h per week): 15 h per unit

80 Marks

UNIT-I:

15 h

A] Drug rules and drug acts, Overview of Intellectual property right, Indian and International framework for patent protection.

B] Statistical method: For sampling and interpretation of results, Statistic in quality control, T-Test, F-Test, Validation of analytical methods as defined proceeding USP Radio immune analysis, Investigational drugs.

C] Antidiabetic Agents- Type-I and Type-II diabetes, Insulin, thiazolidinediones, Synthesis of ciglitazone.

UNIT-II:

15 h

A] Anti-Viral agents: Introduction, viral diseases, viral replication, and transformation of cells, investigation of antiviral agents,. Chemotherapy for HIV. Synthesis of: Idoxuridine, acyclovir, amantadine and cytarabine.

B] Anti-malarial agents: Introduction, malarial parasite, and its life cycle, development of antimalarials, chemotherapy of malaria. Synthesis of: Chloroquin, primaquin, proguanil, and Quinacrine

C] Local Anti-infective drug: Introduction and general mode of action. Synthesis of sulphonamides, ciprofloxacin, norfloxacin, dapsone ,amino salicylic acid, isoniazid, ethionamide, ethambutal, econazole, griseofulvin.

UNIT-III:

15 h

A] Histamines and Antihistamic agents: Introduction, histamine H1-receptor antagonists. Inhibitors of histamine release. Synthesis of: alkyl amines, phenothiazines, piperzines derivatives.

B] Antibiotics: Introduction, β -lactam antibiotics, classification, SAR and chemical degradation of penicillin, cephalosporins-classification, tetracycline antibiotics-SAR, miscellaneous antibiotics. Synthesis of ampicillin, cephadrine, methacycline, chloramphenicol.

UNIT-IV:

15 h

A]Anthelminitics and antiamebic drugs: Introduction to Helminthiasis, Anthelminitics, drugs used in cestode infection, drugs used in trematode infection, origin of antiamebic drug, drugs used in nematode infection. Synthesis of: Clioquinol, Iodoquinol, Haloquinol, Dichlorphen, Niclosamide.

Anti-inflammatory drugs: Introduction, etiology of inflammatory diseases. The inflammatory response, biochemical response. Synthesis of: Phenyl butazone and its derivatives, pyrazolone derivatives, pyrole and indole acetic acid derivatives.

Reference books:

1. Text book of organic medicinal chemistry-Wilson,Geswold
2. Medicinal chemistry Vol I and II-Burger
3. A textbook of pharmaceutical chemistry-Jayshree Ghosh
4. Introduction to medicinal chemistry-A Gringuadje
5. Wilson andGisvold text book of organic medicinal and pharmaceutical chemistry-Ed.Robert F Dorge
6. An introduction to drug design-S S Pandey,and JR Demmock
7. Goodman and Gilmans pharmacological basis of therapeutics- Strategies for organic drug

- synthesis and design-D Lednicer
8. Textbook of Medicinal Chemistry- A. Kar
9. Medicinal Chemistry – D Sriram and P. Yogeeswari

Course Code: PG –CHEM(02)-S4-T4

Paper–XVI: Spectroscopy – II (Core Subject Centric) [L-T-P = 4-0-0]

60 h (4 h per week): 15 h per unit

80 Marks

Unit I:

15 h

A] Ultraviolet and visible spectroscopy: Natural line width, line broadening, transition probability, Born-Oppenheimer approximation, rotational, vibrational and electronic energy levels. General nature of band spectra. Beer- Lambert Law, limitations, Frank-Condon principle, various electronic transitions, effect of solvent and conjugation on electronic transitions, Fiesher Woodward rules for dienes, aldehydes and ketones. **Structure differentiation of organic molecules by UV Spectroscopy**

B] Photoelectron spectroscopy: Basic principles, photoelectric effect, ionization process, Koopman theorem, PES and XPS, PES of simple molecules, ESCA, chemical information from ESCA, Auger electron spectroscopy.

Unit II:

A] ESR spectroscopy: Introduction, principle of ESR, ESR spectrometer, hyperfine coupling, zero field splitting, factors affecting g values, Kramer's degeneracy, application of ESR spectra to study free radicals like hydrogen, methyl radical, 1,4-semibenzoquinone, naphthalene, transition metal complexes, biological systems.

B] Mass spectrometry:

Theory, ion production (EI, CI, FD, FAB), ion analysis, ion abundance, isotopic contribution, N-rule, types of fission processes, high resolution mass spectrometry, metastable peak, molecular ion peak, McLafferty rearrangement, mass spectral fragmentation of organic compounds alkanes, alkenes, alkynes, alcohols, amines, amides, acids, aldehydes, ketones, halides, Structure determination of organic molecules by mass spectrometry, **problem based on mass spectral data.**

Unit III:

15 h

Nuclear magnetic Resonance Spectroscopy

15 h

Magnetic properties of nuclei, resonance condition, NMR instrumentation, chemical shift, spin spin interaction, shielding mechanism, factors affecting chemical shift, PMR spectra for different types of organic molecules, effect of deuteration, complex spin spin interaction (1st order spectra), stereochemistry, variations of coupling constant with dihedral angle, electronegativity, Karplus equation etc., classification of molecules as AX, AX₂, AMX, A₂B₂, Shift reagents. NMR studies of ¹³C, chemical shift in aliphatic, olefinic, alkyne, aromatic, heteroatomic and carbonyl compounds, ¹⁹F, ³¹P. **Structure determination of organic molecules by NMR spectroscopy**

Unit IV:

15 h

A] Application of NMR spectroscopy: FT-NMR, advantages of FT-NMR, two dimensional NMR spectroscopy-COSY, HETCOR, NOSEY, DEPT, INEPT, APT, INADEQUATE techniques, Nuclear overhauser effect, use of NMR in medical diagnosis

B] Problems based on structure determination of organic molecules by using NMR (^1H and ^{13}C nuclei) data, Structure elucidation using combined techniques including UV, IR, NMR and mass spectrometry (based on data and copies of the spectra)

Reference books:

- 1] Spectroscopic identification of organic compound-RM Silverstein,GC Bassler and TC Morrill, John Wally
- 2] Introduction to NMR spectroscopy-R. J. Abraham, J. Fisher and P Loftus Wiely
- 3] Application of Spectroscopy to Organic Compound-J. R. Dyer, Printice Hall
- 4] Organic Spectroscopy-William Kemp, ELBS with McMillan
- 5] Spectroscopy of Organic Molecule-PS Kalsi, Wiley, Esterna, New Delhi
- 6] Practical NMR Spectroscopy-ML Martin, JJ Delpenck, and DJ Martyin
- 7] Spectroscopic Methods in Organic Chemistry-DH Willson, I Fleming
- 8] Fundamentals of Molecular Spectroscopy-CN Banwell
- 9] Spectroscopy in Organic Chemistry-CNR Rao and JR Ferraro
- 10]Photoelectron Spectroscopy-Baber and Betteridge
- 11]Electron Spin Resonance Spectroscopy-J Wertz and JR Bolten
- 12]NMR –Basic Principle and Application-H Guntur
- 13]Interpretation of NMR spectra-Roy H Bible
- 14]Interpretation of IR spectra-NB Coulthop
- 15]Electron Spin Resonance Theory and Applications-W gordy
- 16]Mass Spectrometry Organic Chemical Applications, JH Banyon
- 17]Spectroscopy- H. Kaur

OR

Course Code: PG –CHEM(02)-S4-T4

Paper–XVI: (Foundation Course-II) Applied Analytical Chemistry–II [L-T-P = 4-0-0]

60 h (4 h per week): 15 h per unit

80 Marks

Unit-I: Water treatment

15h

Hardness of water and types of hardness. Problems due to hardness. Removal of hardness by lime- soda process, Zeolite process and synthetic ion-exchange resins. Principle, instrumentation and comparison of these three processes. Numericals based on hardness removal. Desalination of sea- water.

Unit-II: Polymer chemistry and leather analysis

15h

Polymer chemistry: Definition, classification, co-polymers, conducting polymers, determination of acid value, saponification value, iodine value, molar mass by end group analysis- amide and hydroxyl, molecular weight by viscosity method, glass transition temperature of polymers, TGA and DTA studies of polymers.

Analysis of leather: Determination of moisture, acid, free sulphur, total ash, chromic oxide in leather, tensile strength and stretch of leather.

Unit-III: Metallurgy

15h

Ores and minerals, General principles of extraction of metals from ores. Steps involved in metallurgical extraction. Purification and concentration of ores. Extraction of crude metal from concentrated ore-pyrometallurgy, hydrometallurgy and electrolytic processes. Refining of metal. Thermodynamic aspects of metallurgical processes and Ellingham diagram. Furnaces in metallurgy. Metallurgy of Cu, Ag, Au, Al and Fe.

Unit-IV: Clinical analysis**15h**

General composition of blood, Collection and storage of blood samples, Estimation of chloride, calcium, sodium, potassium and bicarbonate in blood sample. Qualitative tests for reducing sugar. Estimation of blood glucose, urea, uric acid, blood urea-nitrogen, total serum protein, serum albumin, serum creatinine, serum phosphate, serum bilirubin, serum cholesterol. Radioimmunoassay (RIA).

Reference books:

1. Textbook of polymer science: F.W. Billmayer Jr. Wiley.
2. Polymer science: V.R. Gowarikar, N. V. Viswanathan and J. Sreedhar, Wiley-Eastern.
3. Fractional monomers and polymers: K Takemoto, Y. Inaki, and R.M. Ottam Brite.
4. Chemistry for Environmental Engineering and Science: C N Sawyer, P L McCarty and G F Parkin
5. Vogel's Text Book of Quantitative Inorganic Analysis-Bassett, Denney, Jeffery and Mendham (ELBS)
6. Analytical Chemistry: Gary D. Christian (Wiley India).
7. Instrumental Methods of Analysis: Willard, Merrit, Dean, Settle (CBS Publishers, Delhi, 1986)
8. Water analysis : J. Rodier
9. A Text book of Inorganic Analysis : A.I.Vogel