



INSTITUTE OF SCIENCE, NAGPUR
(An Autonomous Institute of Government of Maharashtra)
Civil Lines, R. T. Road, Nagpur 440001
NAAC Accredited "A" Grade

Phone: 0712-2561148

Web: www.iscnagpur.ac.in

Email: ioscnagpur@gmail.com

Syllabus for Master of Science Two Year (Four Semesters) Degree Course

With effect from 2024-25 as per NEP 2020

SUBJECT- CHEMISTRY
M.Sc.- Two Year: Semester-I
Name of the Course Category: DSC
Title of the Paper: Inorganic Chemistry
Course code: M-CH511T
Paper I

Number of Credits: 04

Marks: 60M

Total Number of Hrs: 60 Hrs (4 h per week)

Expected Learning Outcomes: After studying this course the student will be able to:

- 1) Identify shapes and structure of inorganic molecules on the basis of VSEPR theory
- 2) Split the d orbital's on the basis of CFT and understand the molecular orbital theory for different complexes
- 3) Study different types of Stability of complexes and the methods to determine them experimentally.
- 4) Study the kinetics of different types of inorganic reactions and draw their energy profile diagrams
- 5) Understand different types of boron-hydrides their preparations and structures.
- 6) Explain how metal clusters are classified.

Unit I:

15h

A] Stereochemistry and Bonding in Main Group Compound:

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's rule and energetics of hybridization.

B] Metal – Ligand Bonding: Crystal Field Theory: Splitting of d-orbital in tetragonal, square planar and trigonal bipyramid complexes. John teller effect, spectrochemical series, nephelauxetic effect. Limitation of crystal field theory. M.O. theory for octahedral, tetrahedral & square planar complexes with and without π -bonding.

Unit II

15h

A] Metal-Ligand Equilibria in Solution: Stepwise and overall formation constants; trends in stepwise formation constants; factors affecting stability of metal complexes with reference to nature of metal ion, ligand, chelate effect and thermodynamic origin. Determination of formation constant by : (1) spectrophotometric method (Job's and Molar ratio method) (2) Potentiometric method (Irving-Rossotti Method).

B] Reaction Mechanism of Transition metal complexes: Energy Profile of a reaction, reactivity of metal complexes, Inert and Labile complexes, Kinetics of Octahedral substitution: Acid hydrolysis, factors affecting acid hydrolysis, Stereochemistry of intermediates in SN1 & SN2 , Base hydrolysis, Conjugate base mechanism, Direct and indirect evidences in favour of conjugate mechanism, Anation reaction, reaction without metal-ligand bond breaking.

Unit III: Cluster-I

15h

Boron hydrides: Classification, nomenclature, structure, bonding and topology of boranes, 4-digit coding (s, t, y, x) numbers for higher boranes and their utilities. Chemistry of diboranes: Study of Metalloboranes, Carboranes and Metallocarboranes with reference to preparations and structures.

Unit IV: Cluster-2

15h

A] Metal-Metal bonds: Occurrence of metal-metal bond, Classification of metal clusters, Binuclear, trinuclear, tetranuclear, pentanuclear and hexanuclear with reference to halide, oxide, alkoxide and acetate clusters.

B] Isopoly, Heteropoly acids and their anions.

References:

- 1) S. F. A. Kettle, J. N. Murrell and S. T. Teddler: Valency Theory
- 2) C. A. Coulson: Valency
- 3) J. E. Huheey :Inorganic Chemistry
- 4) F. A. Cotton and G. Wilkinson: Advanced Inorganic Chemistry 3rd, 5th and 6th Editions.
- 5) F. Willims: Theoretical Approach in inorganic chemistry.
- 6) 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 coordination 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 nonaqueous solvents.
- 15) K. Barnard: Therotical Inorganic Chemistry
- 16) Emeleus and Sharpe: Modern Aspect of Inorganic Chemistry.
- 17) F. A. Cotton: Chemical Applications of Group theory.
- 18) Jones: Elementary Coordination chemistry.
- 19) B. N. Figgis: Introduction to Ligand field.
- 20) S. F. A. Kettle: Coordination chemistry.
- 21) M.C.Day and J.Selbin: Theoretical Inorganic Chemistry.
- 22) J. Lewin and Wilkins: Modern Coordination Chemistry.
- 23) Gowarikar, Vishwanathan and Sheedar: Polymer science.
- 24) H. H. Jattey and M. Orchin: Symmetry in chemistry.
- 25) D. Schonaland: Molecular Symmetry in chemistry.
- 26) L. H. Hall: Group theory and Symmetry in chemistry
- 27) H. H. Jattey and M. Orchin: Symmetry in chemistry
- 28) R.L.Dutta and A.Symal: Elements of magneto chemistry
- 29) Inorganic Chemistry 4th Edition, P.Atkins, Oxford University Press.
- 30) Essential Trends in Inorganic Chemistry, D.M.P.Mingos, Oxford University Press

A. M. Rahatgaonkar

SUBJECT- CHEMISTRY
M.Sc.- Two Year: Semester-I
Name of the Course Category: DSC
Title of the Paper: Organic Chemistry
Course code: M-CH512T
Paper II
To be implemented from 2024-25

Number of Credits: 04

Marks: 60M

Total Number of Hrs: 60 Hrs (4 h per week)

Expected Learning Outcomes: After studying this course the student will be able to:

- 1) Explain and describe different types of bonding, reactions of organic molecules and the reactive intermediates involved in them and effect of structure on reactivity, mechanisms involved in various types of organic reactions.
- 2) Identify the type of isomerism exhibited by a set of organic compounds.
- 3) Illustrate the possible conformations of simple straight chain hydrocarbons such as ethane and butane and compare the relative stabilities of various conformations;
- 4) Draw the possible conformations of cyclohexane and compare their relative energies and stabilities.

Unit I: Stereochemistry:

15h

Optical activity and chirality, Cahn-Ingold-Prelog System: definition and classification of chiral molecules as asymmetric and dissymmetric carbon. Stereoisomers - definition based on symmetry and energy criteria, rotamers, prochiral carbons. Stereoisomerism due to molecular dissymmetry - allenes, biphenyls, spiro compounds, trans cyclooctene, cyclononene and molecules with helical structures. Configurational and conformational isomers. Absolute configuration - enantiomers - R, S nomenclature. 2 Geometrical isomerism. E, Z nomenclature of olefins, geometrical and optical isomerism (if shown) of disubstituted cyclopropanes, cyclobutanes and cyclopentanes. Identification of topicity -enantiotopic, homotopic and diastereotopic hydrogens in compounds with carbons up to ten only. Stereospecific and stereoselective reactions. Inter conversion of Sawhorse, Newman and Fischer projections. Molecules with two and more asymmetric centers - definition of diastereoisomer-constitutionally symmetrical, unsymmetrical chiral compounds e.g. erythro and threo compounds. Asymmetric synthesis.

Unit II: Conformational Analysis:**15h**

Conformational analysis of acyclic molecules - 1,2 - disubstituted ethane derivatives. Conformation of monocyclic compounds – disubstituted cyclohexanes and their stereochemical features [geometrical and optical isomerism (if shown) by these derivatives]. Conformation and reactivity of substituted cyclohexanols (oxidation and acylation), cyclohexanones and tert-butyl cyclohexanols (reduction involving selectrides) and cyclohexane carboxylic acid derivatives (esterification and hydrolysis). Conformation and stereochemistry of fused bicyclic system - cis and trans decalins and 9-methyldecalin.

Unit III: Reaction mechanism:**15h**

- A] Structure and Reactivity:** Resonance and field effects, Steric effect, Types of mechanism, Types of reaction, Thermodynamics and kinetics requirements, Kinetic and thermodynamic control, Hammond's postulate, Curtin-Hammett principle, Potential energy diagrams, Transition states and Intermediates, Methods of determining mechanisms, Isotope effects, The Hammett equation and Linear free energy relationship, Substituent and reaction constants. Taft Equation.
- B] Reactive Intermediates:** Generation, structure, stability and chemical reactions involving carbocations, carbanions, free radical, carbenes, and nitrenes.
- C] Aromaticity:** Aromaticity in benzenoid and non-benzenoid compounds, alternant and non-alternant hydrocarbons Huckel's rule, energy level of π -molecules orbitals, annulenes, antiaromaticity, homo aromaticity. Aromatic character and chemistry of cyclopentadienyl anion, tropylium cation, tropone and tropolone. Bonds weaker than covalent-addition compounds, crown ether complexes and cryptands, inclusion compounds, cyclodextrins, catenanes and rotaxanes, bonding in fullerenes.

Unit IV: Nucleophilic Substitution Reaction:**15h**

- A] Aliphatic nucleophilic substitution:** The SN1, SN2, mixed SN1, SN2 and 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
- B] Neighboring group participation:** Anchimeric assistance with mechanism, neighboring group participation by π and σ bonds, classical and non-classical carbocations, Intramolecular displacement by hydrogen, oxygen, nitrogen, sulphur and halogen. Alkyl, cycloalkyl, aryl participation, participation in bicyclic system, migratory aptitude, carbocation rearrangements and related rearrangements in neighboring group participation.
- C] Aromatic Nucleophilic Substitution:** A general introduction to different mechanisms of aromatic nucleophilic substitution SNAr, SN1, benzyne and SRN1 mechanisms, arynes as reaction intermediate, Reactivity - effect of substrate structure leaving group and attacking nucleophile.

The Von Richter, Sommet Hauser and Smiles rearrangements.

References:

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. Principal 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. Frontier Orbitals and Organic Chemical Reactions-I. Fleming
12. Orbital Symmetry – R. E. Lehr and A. P. Marchand
13. Reactive Intermediate in Organic Chemistry-N. S. Isaacs
14. Stereochemistry of Carbon Compounds- E. L. Eliel
15. Physical Organic Chemistry-J. Hine
16. Name Reaction in Organic chemistry –Surrey
17. Advanced Organic Chemistry – L. F. Fieser and M. Fieser.
18. Organic Chemistry Vol. I and II - I. L. Finar
19. Modern Organic Chemistry- J.D. Roberts and M. C. Caserio
20. The Search for Organic Reaction Pathways (Longmann), Peter Skyes
21. Organic Chemistry 5th Edition (McGraw Hill), S. H. Pine
22. Organic Chemistry (Willard Grant Press Botcon), John Mcmurry 23) A Textbook of Organic Chemistry- R. K. Bansal New Age International
23. New Trends in Green Chemistry –V. K. Ahluwalia and M. Kidwai, Anamaya publishers New Delhi
24. Organic Chemistry, J. Clayden, N. Greeves, S. Warren and P. Wothers, Oxford University Press
25. Organic Chemistry, 4th Edition, G Marc Loudon, Oxford University Press

A. M. Rahatgaonkar

SUBJECT- CHEMISTRY
M.Sc.- Two Year: Semester-I
Name of the Course Category: DSC
Title of the Practical: Inorganic and Organic Chemistry
Course code: M-CH513P
Practical-III

To be Implemented from 2024-25

Number of Credits: 12

Marks: 180M

Total Number of Hrs: 180 Hrs (12h per week)

Expected Learning Outcomes:

After studying this course and performing the given experiments, the student will be able to:

- 1) Discuss the principle involved in determination of metal ions from the different alloys, by Volumetric, Gravimetric and Spectrophotometric methods.
- 2) Select and use appropriate apparatus and techniques for various types of experiments related to chemistry.
- 3) Detect the rare metal ions in an inorganic mixture by its semi-micro analysis containing four cations.
- 4) Record observations and calculate the results after performing the experiments and to maintain laboratory records for the experiments performed during this course.

SECTION A: INORGANIC CHEMISTRY

Quantitative Analysis: (Minimum 2-3 experiments can be taken)

- I. Separation and determination of two metal ions from the following alloys involving:

Volumetric, Gravimetric and Spectrophotometric methods

- 1) Copper (II) and Nickel (II)
- 2) Copper (II) and Zinc (II)
- 3) Nickel (II) and Zinc (II) and
- 4) Copper (II) and Iron (III)
- 5) Cobalt (III) and Nickel (II)

- II. **Qualitative analysis of radicals: (Minimum 3-4 Mixtures can be taken)**

Semi-micro analysis of inorganic mixture containing four cations out of which two will be rare metal ions such as W, Mo, Ti, Zr, Ce, Th, V and U. (Spot Test for individual cations should be performed)

SECTION B: ORGANIC CHEMISTRY

Expected Learning Outcomes: After studying this course and performing the given experiments, the student will be able to:

- 1) Separate and identify organic compounds from the unknown organic mixture by different physical and chemical transformation reactions.
- 2) Study the different methods of purifications including chromatographic techniques.
- 3) Prepare different organic compounds by following different name reactions.
- 4) Utilize different reagents for the synthesis of organic compounds.
- 5) Record observations and calculate the results after performing the experiments and to maintain laboratory records for the experiments performed during this course.

[A] Qualitative Analysis:

Separation, purification and identification of the mixture of two organic compounds (binary mixture solid-solid, solid-liquid and liquid-liquids) using chemical methods or physical techniques. Minimum **3-4 mixtures** to be analyzed.

[B] Organic preparations:

Student is expected to carry out minimum of **3-4 two stage organic preparations** and **2-3 single stage preparation** from the following lists.

- 1) Oxidation: Adipic acid by chromic acid oxidation of cyclohexanol.
- 2) Benzophenone → benzhydrol
- 3) Aldol condensation: Dibenzal acetone from benzaldehyde.
- 4) Sandmeyer reaction: p-chlorotoluene from p-toluidine
- 5) Cannizzaro reaction
- 6) Friedel Crafts Reaction: β -Benzoyl propionic acid from succinic anhydride and benzene.
- 7) Benzil → 2,4,5-triphenyl imidazole
- 8) Sucrose → Oxalic acid
- 9) Methyl acetoacetate → 5-methyl-isoxazol-3-ol
- 10) Ethyl acetoacetate → 4-aryl-6-methyl-3,4-dihydro-2(1H)-pyrimidinone ester.
- 11) Ethyl acetoacetate → Diethyl 1,4-dihydro-2,6-dimethyl-4-phenylpyridine-3,5-di Carboxylate
- 12) Dye preparation : Sulphanilic acid → Methyl orange
- 13) Dye preparation : p-nitroaniline → p-red.
- 14) Acetanilide → p-nitroacetanilide → p-nitroaniline
- 15) Aniline → 2,4,6-tribromo aniline → 2,4,6-tribromoacetanilide
- 16) Nitrobenzene → m-dinitrobenzene → m-nitroaniline
- 17) Toluene → p-nitrotoluene → p-nitrobenzoic acid
- 18) Glycine → Benzoyl glycine → 4-benzilidene-2-phenyloxazole

A. M. Rahafgaonkar

SUBJECT- CHEMISTRY
M.Sc.- Two Year: Semester-I
Name of the Course Category: DSE
Title of the Paper: Bioinorganic Chemistry
Course code: M-CHIC514T
Paper IV
To be implemented from 2024-25

Number of Credits: 4

Marks: 60M

Total Number of Hrs: 60 Hrs (4h per week)

Course Outcomes: At the end of the course, student would be able to

1. Apply the principles of transition metal coordination complexes in understanding functions of biological systems
2. Identify the medicinal applications of inorganic compounds
3. Understand mechanism of energy transfer processes in biological systems
4. Develop the possible enzymatic pathways in biosystems
5. Explain oxygen transport mechanisms in biosystems

Unit I: Essential and trace metals in biological systems

15h

- A]** Biological functions of inorganic elements, biological ligands for metal ions. Coordination by proteins, Tetrapyrrole ligands and other macrocycle. Influence of excess and deficiency of V, Cr, Mn, Fe, Co, Cu and Zn. Genetic defects in the absorption of trace elements. Regulation and storage of trace elements. Role of minerals. Toxic effects of metals.
- B]** Metal storage, transport and biomineralization with respect to Ferritin, Transferrin and Siderophores, Na⁺ /K⁺ pump. Role of Ca in transport and regulation in living cells.
- C]** Medicinal use of metal complexes as antibacterial, anticancer, use of cis-platin as antitumor drug, antibiotics and related compounds. Metal used for diagnosis and chemotherapy with particular reference to anti-cancer drugs.

Unit II: Bio-energetics, ATP cycle and Electron transfer in Biology

15h

- A]** DNA polymerization, metal complexes in transmission of energy, chlorophylls, photosystem I and photosystem II in cleavage of water, Model systems.
- B]** Structure and functions of metalloproteins in electron transfer proteins, cytochromes and Fe-S proteins, non-heme iron proteins; Rubredoxins, Synthetic models. Biological Nitrogen fixation (in vitro and in vivo)

Unit III: Transport and Storage of Dioxygen

15h

Heme proteins and oxygen uptake, structure and functions of haemoglobin, myoglobin, hemocyanin and

hemerythrin. Perutz mechanism showing structural changes in porphyrin ring system. Oxygenation and deoxygenation. Model compounds. Cyanide poisoning and treatment. Vanadium storage and transport.

Unit IV: Metallo-enzymes

15h

Apoenzymes, Haloenzyme and Coenzyme. The principle involved and role of various metals in i) Zn-enzyme: Carboxyl peptidase and Carbonic anhydrase. ii) Fe-enzyme: Catalase Peroxidase and Cytochrome P-450 iii) Cu-enzyme: Super Oxide dismutase iv) Molybdenum: Oxatransferase enzymes, Xanthine oxidase, Co-enzyme Vit.B12, Structure of vitamin B12, Co-C bond cleavage, Mutase activity of coenzyme B-12, Alkylation reactions of Methyl Cobalamin. Synthetic model of enzyme action, stability and ageing of enzyme.

List of Books:

- 1) Akhmetov, N.: General and Inorganic Chemistry
- 2) Aylett, B. and Smith, B.: Problems in Inorganic Chemistry, (English University Press)
- 3) Bertini, et al: Bioinorganic Chemistry
- 4) Charlot, G and Bezier, D.: Quantitative Inorganic Analysis (John Wiley).
- 5) Douglas, B. E. McDanirl, D. H. et al: Concept and Models of Inorganic Chemistry (4th edt.) J. Wiley
- 6) Dutt P. K.: General and Inorganic Chemistry. (Sarat Books House)
- 7) Fenton, David E.: Biocoordination chemistry, Oxford
- 8) Jolly, W. L. Inorganic Chemistry (4th edn) Addison-Wesley
- 9) Katakis, D. and Gordon, G.: Mechanism of Inorganic Reactions (J.Wiley)

A.M. Rahatgaonkar

SUBJECT- CHEMISTRY
M.Sc.- Two Year: Semester-I
Name of the Course Category: DSE
Title of the Paper: Chemistry of Biomolecules
Course code: M-CHOC514T
Paper IV
To be implemented from 2024-25

Number of Credits: 4

Marks: 60M

Total Number of Hrs: 60 Hrs (4h per week)

Course Outcomes: At the end of the course students would be able to

1. Draw the structures of essential biomolecules
2. Understand the role of biomolecules in various life processes
3. Understand the way how drug can be administrated, absorbed, distributed and metabolized
4. Understand the relation of drug with different types of receptors, chemical messengers, binding site and DNA.

Unit I: Carbohydrates

15h

Types of naturally occurring sugars, deoxy sugars, amino sugars, branched chain sugars, methyl ethers and acid derivatives of sugars, configurations of aldoses and ketoses, general methods of structure and ring size determination with reference to maltose, lactose, sucrose, Structural features and applications of inositol, starch, cellulose, chitin and heparin

Unit II: Amino acids, protein and peptides

15h

Amino acids, structural characteristics, acid base property, stereochemistry of amino acids, optical resolution, Stecker synthesis, peptide and proteins structure of peptide and protein, primary, secondary, tertiary and quaternary structure. Reaction of polypeptide, structure determination of polypeptide, end group analysis, strategy of peptide bond synthesis: NProtection and C-Activation, Solid phase peptide synthesis

Unit III: Nucleic Acids

15h

Primary, secondary and tertiary structure of DNA; DNA replication and heredity; Structure and function of mRNA, tRNA and rRNA. Purines and pyrimidine bases of nucleic acids and their preparation, Biosynthesis of DNA and RNA, Polymerase Chain Reaction (PCR) and RTPCR **Lipids:** Fatty acids, essential fatty acids, structures and functions of triglycerols, glycerophospholipids, 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

Unit IV: Enzyme chemistry

15h

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 catalysed 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) Vitamins and Co-Enzyme Chemistry: Structure and biological functions of coenzyme A, thiamine pyrophosphate, pyridoxal phosphate, NAD⁺, NADP⁺, FMN, FAD, lipoic acid, biotin as CO₂ carrier. Mechanisms of reactions catalyzed by the above cofactors

List of books

1. Bioorganic Chemistry: A Chemical Approach to Enzyme Action, Hermann Dugas and C. Penny, Springer-Verlag
2. Understanding Enzymes, Trevor Palmer, Prentice Hall
3. Enzyme Chemistry: Impact and Applications, Ed. Collin J. Suckling, Chapman and Hall
4. Enzyme Structure and Mechanism, A. Fersht, W. H. Freeman
5. Introduction to Medicinal Chemistry, A. Gringuage, Wiley-VCH
6. Wilson and Gisvold's Text Book of Organic Medical and Pharmaceutical Chemistry, Ed Robert F. Dorge
7. Strategies for Organic Drug Synthesis and Design, D. Lednicer, John Wiley

Weblink to Equivalent MOOC on NPTEL/SWAYAM if relevant:

- Essentials of Biomolecules: Nucleic Acids and Peptides
<https://nptel.ac.in/courses/104/103/104103121/>
- Biocatalysis in Organic Synthesis <https://archive.nptel.ac.in/courses/104/105/104105032/>
- Biochemistry <https://archive.nptel.ac.in/courses/104/105/102105034/>
- Organic Chemistry in Biology and Drug Development
<https://archive.nptel.ac.in/courses/104/105/104105120/>

A.M. Rahafgaonkar

SUBJECT- CHEMISTRY
M.Sc.- Two Year: Semester-I
Name of the Course Category: DSE
Title of the Paper: Thermodynamics and Electrochemistry
Course code: M-CHPC514T
Paper IV
To be implemented from 2024-25

Number of Credits: 04

Marks: 60M

Total Number of Hrs: 60 Hrs (4 h per week)

Expected Learning Outcomes: After studying this course the student will be able to

1. Understand, the mathematical concepts used in chemistry
2. Understand the principle involved in fundamental physical chemistry
3. Understand the concept of ideal and non-ideal solutions
4. Understand the theories of electrolytes

Unit I: Mathematical concepts

15h

Equation of a straight line and calculation of slope and intercepts, Differentiation, Derivative function, various differential formulas, Chain rule, finding minima and maxima, partial differentiation. Integration, methods of integration, integration by parts, integration formulas, permutation combination fundamentals, Vectors, Matrices, Determinants, Complex numbers, series expansions, Stirling approximation, Practice numerical based on these concepts.

Unit II: Thermodynamics and Phase Equilibria

15h

Concept of fugacity, determination of fugacity, The Le-Chatelier's Principle and its quantitative treatment. Ideal solutions and Raoult's law, non-ideal solutions (Henry's Law), Deviation from ideal behavior, Chemical potential in Non-ideal solutions, excess functions for non-ideal solutions, Partial molar quantities: Determination of partial molar quantities, chemical potential, partial molar volume, Gibbs- Duhem equation, Gibbs Duhem Margules equation Entropy of mixing, Enthalpy of mixing, Fractional Distillation, Distillation of Azeotropic Mixtures.

Unit III: The Phase Rule

15h

Recapitulation of Gibbs Phase rule (Without Derivation), degrees of freedom, reduced phase rule, construction of phase diagram, one component systems (Water, Sulphur, carbon), 1st and 2nd order

phase transition, lambda line, Helium, system, Eutectic systems, two component systems forming solid solutions having congruent and incongruent melting point, Construction of a phase diagram, partially miscible solid phase, three component systems, graphical presentation, related Numerical.

Unit IV: Electrochemistry – I

15h

Electrolytic conductance (Specific, Equivalent and molar), Variation of Eq./molar conductance with dilution, Transport number and its determination using Hittorf's method and Moving boundary method, Kohlrausch's law, calculation of molar ionic conductance, conductometric titrations, High frequency titrations, Ostwald dilution law, Determination of ionic mobility, numerical. Principle of potentiometry, Indicator electrodes: hydrogen electrode, quinhydrone electrode, antimony electrode and glass electrode. Reference electrodes: Calomel electrode and Ag/AgCl electrode. potentiometric titrations, Nernst equation, standard electrode potential, Determination of cell potential, n , K_f and K_{sp} . pH titrations.

References:

- 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) Ira N. Levine, Quantum Chemistry, 5th edition(2000), Pearson educ., Inc. New Delhi
 - 9) G. M. Barrow, Physical Chemistry, Tata Mc-Graw Hill, V edition 2003.
 - 10) A. Findley, The Phase Rule and its Applications, Longmans Green and Co., Mumbai.
 - 11) N. B. Singh, N. S. Gajbhiye, S. S. Das, Comprehensive Physical Chemistry, New Age International, 2014.
 - 12) K. L. Kapoor, Text Book of Physical Chemistry, Vol – I to Vol-VI, 2011.
 - 13) Spectroscopic identification of organic compound-RM Silverstein, GC Bassler and TC Morrill, John Wiley
 - 14) Application of Spectroscopy to Organic Compound-J. R. Dyer, Printice Hall
-

NPTEL sources Weblinks

For Classical Thermodynamics:

- <https://archive.nptel.ac.in/courses/104/103/104103112/>
- <https://digimat.in/nptel/courses/video/104106094/L18.html>

For Phase rule:

- <https://www.youtube.com/watch?v=2LywAiZBQW4>
- <https://archive.nptel.ac.in/courses/113/104/113104068/>
- <https://archive.nptel.ac.in/courses/104/103/104103112/>

For electrochemistry

- https://onlinecourses.nptel.ac.in/noc23_cy19/preview
<https://www.youtube.com/watch?v=XTt3gXB0a84>

A. M. Rahafgaonkar

SUBJECT- CHEMISTRY
M.Sc.- Two Year: Semester-I
Name of the Course Category: DSE
Title of the Paper: Analytical Separation Techniques
Course code: M-CHAC514T
Paper-IV
To be implemented from 2024-25

Number of Credits: 04

Marks: 60M

Total Number of Hrs: 60 Hrs (4h per week)

Expected Learning Outcomes: After studying this course the student will be able to:

1. Understand various separation technique based on sample and target analyte
2. Elaborate the working principles of various separation techniques.
3. Apply logic behind working and applicability of each technique.
4. Identify most suitable separation tool resolution of mixtures.
5. Develop separation methods for multicomponent analysis.
6. Evaluate efficiency of separation of mixture based on analysis parameters.

Unit I: Column, paper and thin layer chromatography

15h

A] Chromatography: Definition and general classification of chromatographic techniques. Normal and reverse phase chromatography. Terminology used in separation techniques. Column chromatography: Basic principle, technique and applications in qualitative and quantitative analysis. Properties of good column adsorbents.

B] Paper chromatography: Basic principle, techniques and applications in qualitative and quantitative analysis. Calculations involving R_f values. Paper electrophoresis: Principle and technique. Factors affecting migration of ions. Applications. Thin layer chromatography: Principle and technique. Advantages over paper and column chromatography. Applications.

Unit II: Ion exchange and solvent extraction

15h

A] Ion exchange: Principle and technique. Types of ion exchangers and their structures. Ion exchange equilibria and action of cation and anion exchange resins. Factors affecting ion exchange efficiency. Ion exchange capacity. Experimental determination of ion exchange capacities of cation and anion exchange resins. Effect of complexing ions. Zeolites as ion-exchangers. Applications of ion exchange.

B] 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: Gas Chromatography

15h

- A] Gas Chromatography:** Principle including concept of theoretical plates. Calculations involving number of theoretical plates and height equivalent of theoretical plates. Column resolution, retention factor and selectivity factor. van-Deemter equation. Factors affecting retention, peak resolution and peak broadening. Instrumental set up- carrier gas, sampling system,.
- B] Types of columns and detector in GC:** Packed and open tubular, their advantages and limitations. Detectors in GC analysis. Characteristics of ideal detectors. Construction and working of thermal conductivity, flame ionization, electron capture and mass spectrometric detectors. Temperature programmed GC and its advantages.

Unit IV: Liquid Chromatography

15h

- A] HPLC:** Principle of HPLC. Instrumentation including mobile phase injection system, sample injection system, column and detector. Types of columns and packing materials. Normal and reverse phase systems. Detectors in HPLC: Construction and working of UV detector, fluorescence detector, photodiode array detector. Principle and applications of size exclusion, gel permeation and ion retardation chromatography. Comparison of HPLC with GC
- B] Supercritical fluid chromatography:** Principle, advantages and applications.

List of 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] Fundamentals of Analytical Chemistry: S. A. Skoog and D. W. West
- 5] Instrumental Methods of Analysis: Willard, Merrit, Dean, Settle (CBS Publishers, Delhi, 1986)
- 6] Introduction to Instrumental analysis: Robert Braun (Tata McGraw-Hill)
- 7] Advanced Analytical Chemistry: Meites and Thomas (McGraw-Hill)
- 8] Instrumental Methods of Analysis: G. Chatwal and S. Anand (Himalaya Publishing House)
- 9] Analytical Chemistry: Problems and Solution- S. M. Khopkar (New Age International Publication)
- 10] Basic Concepts in Analytical Chemistry: S. M. Khopkar (New Age International Publication)
- 11] Advance Analytical Chemistry: Meites and Thomas: (Mc Graw Hill)
- 12] An Introduction to Separation Science: L. R. Snyder and C. H. Harvath (Wiley Interscience)
- 13] Instrumental Methods of Chemical Analysis: G. W. Ewing.

- 14] Instrumental Methods of Chemical Analysis: Braun (Tata McGraw-Hill)
- 15] Instrumental Methods of Analysis: G. Chatwal and S. Anand (Himalaya Publishing House)
- 16] Analytical Chemistry: Problems and Solution- S. M. Khopkar (New Age International Publication)
- 17] Basic Concepts in Analytical Chemistry: S. M. Khopkar (New Age International Publication)
- 18] An Introduction to Separation Science: L. R. Snyder and C. H. Harvath (Wiley Inter science)
- 19] Web link for related NPTEL courses: Analytical Chemistry: <https://nptel.ac.in/courses/104105084>

A. M. Rahafgaonkar

SUBJECT- CHEMISTRY
M.Sc.- Two Year: Semester-I
Name of the Course Category: RM
Title of the Paper: Research
Methodology
Course code: M-CH515T
Paper: V
To be implemented from 2024-25

Number of Credits: 04

Marks: 60M

Total Number of Hrs: 60 Hrs (4h per week)

Objectives: To make students

- 1) Acquire knowledge of research design and the types of research.
- 2) Formulate the research problems and connect the research outcomes to society.
- 3) Understand the concept of sampling and data analysis in research.
- 4) Help in gaining the knowledge of safety and ethical handlings of chemicals in the lab and households.

Expected Learning Outcomes: After studying this course the student will be able to:

- 1) Able to interpret the Foundations of Research and identify research problems.
- 2) Able to Demonstrate knowledge of research design and the types of research
- 3) Able to find out the local solution.
- 4) Able to communicate the research at an appropriate level.

Unit I: Literature Survey

15 h

A] Print: Sources of information: Primary, secondary, tertiary sources; Journals: Journal abbreviations, abstracts, current titles, reviews, monographs, dictionaries, text-books, current contents. Introduction to Chemical Abstracts, Subject Index, Substance Index, Author Index, Formula Index, and other Indices with examples.

B] Digital: Web resources, E-journals, Journal access, TOC alerts, Hot articles, Citation index, Impact factor, H-index, E-books, Search engines, Google Scholar, ChemSpider, Science Direct, Scopus. Internet discussion groups and communities, Blogs, Preprint servers, Search engines, Scirus, Google Scholar, ChemIndustry, Wiki- Databases, ChemSpider, Science Direct, SciFinder, Scopus. Information Technology and Library Resources: The Internet and World Wide Web.

C] Internet resources for chemistry. Finding and citing published information. Open source chemistry designing sources, Essentials of Problem formulation and communication with society.

Unit II: Research Methodology for Chemistry

15h

A] Research Design and Types of Research: Concept and Importance in Research, Features of a good research design, Exploratory Research Design & Descriptive Research Designs concept, types and uses. Qualitative and Quantitative research.

B] Methods of Scientific Research and Writing Scientific Papers: Reporting practical and project work. Idea about public funding agencies of research. Writing literature surveys and reviews. Organizing a poster display: Giving an oral presentation. Writing scientific papers – justification for scientific contributions, bibliography, description of methods, conclusions, the need for illustration, style, publications of scientific work. Writing ethics. Avoiding plagiarism. Assessment of locally available resources.

Unit III: Chemical Safety and Ethical Handling of Chemicals:

15h

A] Chemical Safety: Safe working procedure and protective environment, protective apparel, emergency procedure and first aid, laboratory ventilation Safe storage and use of hazardous chemicals, procedure for working with substances that pose hazards, flammable or explosive hazards, procedures for working with gases at pressures above or below atmospheric pressure.

B] Handling of Chemicals: safe storage and disposal of waste chemicals, recovery, recycling and reuse of laboratory chemicals, procedure for laboratory disposal of explosives, identification, verification and segregation of laboratory waste, disposal of chemicals in the sanitary sewer system, incineration and transportation of hazardous chemicals.

Unit IV: Data Analysis

15 h

A] The Investigative Approach: Making and Recording Measurements. SI Units and their use. Scientific method and design of experiments. Analysis and Presentation of Data: Descriptive statistics. Choosing and using statistical tests. Analysis of variance (ANOVA), Correlation and regression, Curve fitting, fitting of linear equations, simple linear cases, weighted linear case, analysis of residuals, General polynomial fitting, linearizing transformations, exponential function fit, r and its abuse. Basic aspects of multiple linear regression analysis. Biostatistics

B] Exposure of chemistry software: Chemistry Students must be given exposure to different software. Hands-on experiments of different software. Assessment Methods: Writing review on an identified research problem, Poster presentation, and examination.

References:

- 1) Dean, J. R., Jones, A. M., Holmes, D., Reed, R., Weyers, J. & Jones, A. Practical skills in chemistry 2ndEd. Prentice-Hall, Harlow, 2011.
- 2) Hibbert, D. B. & Gooding, J. J. Data analysis for chemistry. Oxford University Press. 2006.
- 3) Topping, J. Errors of observation and their treatment. Fourth Ed. Chapman Hall, London. 1984.
- 4) Harris, D. C. Quantitative chemical analysis. 6th Ed., Freeman Chapters 3-5, 2007.
- 5) Levie, R. de, How to use Excel in analytical chemistry and in general scientific data analysis. Cambridge Univ, 2001.
- 6) Chemical safety matters – IUPAC – IPCS, Cambridge University Press, 1992.
- 7) OSU safety manual 1.01.
- 8) Additional Resources: Introductory Biostatistics by Chap T Le.
- 9) Teaching-Learning Process: Lecture with conventional teaching aids, presentations, invited talks on thrusting areas, group discussions.

A. M. Rahatgaonkar



INSTITUTE OF SCIENCE, NAGPUR
(An Autonomous Institute of Government of Maharashtra)
Civil Lines, R. T. Road, Nagpur 440001
NAAC Accredited "A" Grade

Phone: 0712-2561148

Web: www.iscnagpur.ac.in
Email: ioscnagpur@gmail.com

Syllabus for Master of Science Two Year (Four Semesters) Degree course

SUBJECT- CHEMISTRY
M.Sc.- Two Year: Semester-II
Name of the Course Category: DSC
Title of the Paper: Physical Chemistry
Course code: M-CH521T
Paper I
To be implemented from 2024-25

Number of Credits: 04

Marks: 60M

Total Number of Hrs: 60 Hrs (4 h per week)

Expected Learning Outcomes: After studying this course the student will be able to:

- 1) Study about classical thermodynamics, its laws and applications.
- 2) Apply the Gibbs phase rule in calculation of degrees of freedom and partial molar quantities.
- 3) Study different macromolecules and determine their molecular weight by different methods.
- 4) Explain the principle and terms involved w.r.t. adsorption and surface phenomenon.
- 5) Study kinetics of chemical reactions.

Unit I: CLASSICAL THERMODYNAMICS

15h

- 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, Caratheodory's principle and its equivalence to the Kelvin Plank and Clausius statement of the Second law of Thermodynamics, Homogeneous functions of degree 0 and 1, extensive and intensive properties, derivation of thermodynamic equations of state, Maxwell's relations.
- B]** Third law of thermodynamics, Nernst Heat Theorem, unattainability of absolute zero, calculation of entropy based on third law of thermodynamics, residual entropy and its application. Virial equation of state.

UNIT II: FORMULATION OF QUANTUM MECHANICS

15h

- A]** Introduction of Quantum Mechanics, Wave Function, Acceptability of Wave Functions, Normalized and Orthogonal Wave Functions, Operators, Operator Algebra, Eigen Functions and Eigen Values of Quantum Mechanical Properties) e.g .Linear, Angular momentum, etc(., Hermitian Operators, Orbital and generalized Angular Momentum, Postulates of Quantum Mechanics, Problems on Operator algebra, Eigen Values and Average Values of quantities.
- B]** Application of Schrödinger Wave Equation to Simple Systems: Particle in a 3-Dimensional Box, Concept of degeneracy and breakdown in degeneracy, Rigid Rotor, Potential Well of Finite Depth (Tunneling Effect), Simple Harmonic Oscillator, The Hydrogen Atom.

Unit III: SURFACE PHENOMENA AND MACROMOLECULES

15h

- A]** Recapitulation of Surface tension, Adsorption: Freundlich adsorption isotherm, Langmuir theory, Gibbs adsorption isotherm, BET theory and estimation of surface area, enthalpy and entropy of adsorption. Surface film on liquids and catalytic activity, Electro- kinetic phenomena, Surface active agents, hydrophobic interactions, micellization, Critical Micelle Concentration (CMC), mass action model and phase separation model of micelle formation, shape and structure of micelles, factors affecting CMC, micro-emulsion and reverse micelles.
- B]** **Macromolecules:** Definitions, Number and mass average molecular weights, molecular mass determination by Osmometry, Viscometry, Sedimentation, Diffusion, light scattering method, Numerical.

Unit IV: CHEMICAL KINETICS

15h

- A]** Temperature dependence of chemical reaction rates, Arrhenius equation, Energy of activation, pre exponential factor and its limitations, Collision theory and its limitations, steric factors, Transition State theory of gas and liquid phase bimolecular reactions, comparison of three theories of reaction rates
- B]** Bodeinstein steady state approximation and its application in consecutive reactions, Dynamics of unimolecular reactions: Lindeman-Hinshelwood mechanism, RRKM theory, Thermodynamic formulation of transition state theory, Enthalpy, Gibbs free energy and enthalpy of activation.

References:

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 Mac Millan 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) K. S. Birdi, Surface Chemistry Essentials, CRC Press, New York, 2014.
18. Eric Keightley Rideal, An Introduction to Surface Chemistry, Cambridge University Press, 1926.
20. D. M. Ruthven, Principles of Adsorption and Adsorption Processes, John Wiley & Sons, New York, 1984.
19. A. W. Adamson, A. P. Gasi, Physical Chemistry of Surfaces, Wiley, 2007.
20. P. C. Hiemenz and R. Rajagopalan, Principles of Colloid and Surface Chemistry, CRC Taylor and Fransis, 2007.
21. P. D. Hede and S. P. Beier, Inorganic and Applied Chemistry, e-Book, 2007. 23) G. K. Agrawal, Basic Chemical Kinetics, Tata-Mc-Graw Hill, 1990.

22. N. B. Singh, N. S. Gajbhiye, S. S. Das, Comprehensive Physical Chemistry, New Age International, 2014.
23. K. L. Kapoor, Text Book of Physical Chemistry, Vol – I to Vol-VI, 2011.
24. Spectroscopic identification of organic compound-RM Silverstein, GCBassler and TC Morrill, John Wiley
25. Application of Spectroscopy to Organic Compound-J .R .Dyer, Printice Hall
26. Organic Spectroscopy-William Kemp, ELBS with McMillan 39) Spectroscopy of Organic Molecule-PS Kalsi, Wiley, Esterna, New Delhi
27. Organic Spectroscopy-RT Morrison and RN Boyd
28. Spectroscopic Methods in Organic Chemistry-DH Willson, I Fleming
29. Fundamentals of Molecular Spectroscopy, C. N. Banwell

A.M. Rahatgaonkar

SUBJECT- CHEMISTRY
M.Sc.- Two Year: Semester-II
Name of the Course Category: DSC
Title of the Paper: Analytical Chemistry
Course code: M-CH522T
Paper-II
To be implemented from 2024-25

Number of Credits: 04

Marks: 60M

Total Number of Hrs: 60 Hrs (4h per week)

Expected Learning Outcomes: After studying this course the student will be able to:

- 1) Select a specific analytical technique based on sample and target analyte
- 2) Develop analytical ability and critical thinking in selection of statistics and their use in making interpretation meaningful and productive.
- 3) Explain the logic behind working of indicator used in each type of titration
- 4) Elaborate interaction of radiation with matter and its application in chemical analysis.
- 5) Develop spectral methods of analysis for desired analytes.
- 6) Apply electroanalytical techniques based on conductance and emf measurements.

Unit I:

15h

A] Introduction to analytical chemistry: Types of analysis-qualitative and quantitative. Classification of analytical methods- classical and instrumental, basis of their classification with examples. Classification of analysis based on sample size (macro, semimicro, micro and ultramicro) and constituent type (major, minor, trace and ultratrace).

B] Volumetric Calculations: Stoichiometric and substoichiometric volumetric analysis. Concentration units: Unified atomic mass unit and the mole, Molarity, Normality, Weight and volume percent, Mole fraction, Formality, etc and their interrelation. Standard solutions. Primary standards and secondary standards. Numerical problems based on standard solution preparation, titrimetric analysis and gravimetric analysis. Calculations involved in acid-base, precipitation, redox and complexometric reactions.

Unit II: Classical methods of analysis

15h

A] Volumetric analysis: General principle. Criteria for reactions used in titrations. 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 III: Optical methods of analysis-I

15h

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.

Unit IV: Electrochemical methods of analysis-I

15h

A] Conductometry: Concepts of electrical resistance, conductance, resistivity and conductivity. Specific, molar and equivalent conductance and effect of dilution on them. Measurement of conductance. Kohlrausch's law, Applications of conductometry in determination of dissociation constant, solubility product. Conductometric titrations. High frequency titrations. Numerical problems.

B] Potentiometry: Circuit diagram of simple potentiometer. Indicator electrodes: hydrogen electrode, quinhydrone electrode, antimony electrode and glass electrode. Reference electrodes: Calomel electrode and Ag/AgCl electrode. Theory of potentiometric titrations. Nernst equation, standard electrode potential, Determination of cell potential, n , K_f and K_{sp} . pH titrations. Buffers and buffer capacity. pH of buffer mixtures based on Henderson-Hasselbalch equation and calculations.

List of 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

A.M. Rahatgaonkar

SUBJECT- CHEMISTRY
M.Sc.- Two Year: Semester-II
Name of the Course Category: DSC Lab
Title of the Practical: Physical Chemistry and Analytical Chemistry
Course code: M-CH523P
Paper-III
To be implemented from 2024-25

Number of Credits: 12

Marks: 180M

Total Number of Hrs: 180 Hrs (12h per week)

Expected Learning Outcomes: After studying this course and performing the given experiments, the student will be able to:

- 1) Calibrate and handle the instruments independently.
- 2) Study quantitative determination of analyte by using Spectrophotometer / Colorimeter /Turbidity meter/Flame photometer.
- 3) Characterize the functional group of organic compounds using IR spectral data.
- 4) Determine the structure of simple organic compounds using $^1\text{H-NMR}$ Spectrometry.
- 5) Interpret the spectra of unknown compounds for structure determination from the structural information available from different types of spectra such as Mass Spectrum, UV-VIS Spectrum, IR Spectrum and $^1\text{H-NMR}$ Spectrum.
- 6) Solve the problems based on different spectral data.

SECTION A: PHYSICAL CHEMISTRY

Expected Learning Outcomes: After studying this course and performing the given experiments, the student will be able to:

- 1) Apply the theoretical concept of thermodynamics, adsorption, phase rule, molecular weight determination, kinetics, viscosity and surface tension by performing the experiments based on these principles and learn the applicability.
- 2) Conduct various types of titrations such as redox, complexometric, acid-base by using different instruments such as conductivity meter, potentiometer etc.
- 3) How to calibrate instruments and use different electrodes according to the type of instrument.
- 4) Prepare salt bridge.
- 5) Record observations and calculate the results after performing the experiments and to maintain laboratory records for the experiments performed during this course.

It is expected to perform minimum 12 experiments in a semester

- 1) To study the variation of volume contraction with mole fraction of alcohol in alcohol- water system
- 2) To determine the critical micelle concentration (CMC) of a given surfactant / soap /shampoo by surface tension measurements.
- 3) Determination of molecular mass of a polymer by viscometry method.
- 4) To determine integral heat of KNO_3 , at two different conc. and calculation of heat of dilution.
- 5) Effect of 1% NaCl, 1% succinic acid, 0.5% naphthalene on CST in phenol-water systems.
- 6) Distribution of succinic acid in H_2O - benzene, H_2O -ether and comparison of distribution coefficient.

- 7) To construct the phase diagrams of two components system (phenol- urea, diphenyl amine benzophenone; a-naphtyl amine-phenol) forming compounds with congruent melting points.
- 8) To study the mutual solubility of glycerol-m-toluidine and to determine congruent points.
- 9) To study kinetics of hydrolysis of an ester by NaOH reaction.
- 10) To determine equilibrium constant of the equation $KI + I_2 = KI_3$ by distribution method.
- 11) To study the kinetics of the reaction between potassium persulphate and potassium iodide.
- 12) Determination of order of reaction of oxidation of ethyl alcohol by acid dichromate.
- 13) To titrate conductometrically monobasic and dibasic acids with NaOH and determine the strength of given acid.
- 14) To determine equivalent conductance of weak electrolyte at infinite dilution by Kohlrausch's method.
- 15) Determination of heat of reaction, entropy change and equilibrium constant of the reaction between metallic zinc and Cu^{+2} ions in solution.
- 16) Titration of Ferrous Ammonium Sulphate against Ceric sulphate and hence the formal redox potential of Fe^{2+} Fe^{3+} and Ce^{3+} Ce^{4+} systems.

SECTION B: Analytical Chemistry

Expected Learning Outcomes:

1. At the end of the course, student will be able to
2. Carry out calibration of glassware available in the laboratory.
3. Analyze the data obtained through experiments using statistical analysis parameters.
4. Estimate quantitatively analyte present in different samples using classical and instrumental methods of analysis.
5. Design experiments based on classical and instrumental techniques.
6. Understand the principles involved in visual and instrumental volumetric techniques.
7. Formulate experiments based on optical and electroanalytical techniques.

Part I: Classical methods and separation techniques: Calibration of pipette and burette.

1. Statistical analysis of data.
2. Use of MS-Excel in statistical analysis of data and curve fitting.

Part II: Volumetry :

1. Estimation of nickel in given solution by direct complexometric titration with EDTA using bromopyrogallol red.
2. Estimation of nickel in given solution by complexometric back-titration with EDTA.
3. Estimation of chloride in given solution by Mohr's titration.
4. Determination of volume strength of commercial hydrogen peroxide by redox titration with $KMnO_4$.

5. Estimation of phenol/ aniline by bromination method.
6. Estimation of glucose.
7. Estimation of acetone.
8. Estimation of formaldehyde.
9. Estimation of Mn in the presence of Fe using masking phenomenon (ferromanganese alloy)

Part III: Gravimetry

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

Part 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.

Part V: Instrumental techniques and Electroanalytical techniques

1. Determination of strength of HCl and CH₃COOH in a mixture conductometrically.
2. Determination of strength of HCl and oxalic acid in a mixture conductometrically.
3. Determination of strength of oxalic acid and CH₃COOH in a mixture conductometrically.
4. Determination of degree of dissociation and dissociation constant of acetic acid conductometrically.
5. Estimation of phenol in dilute solution by conductometric titration with NaOH.
6. Determination of strength of HCl and CH₃COOH individually and in a mixture potentiometrically.
7. Determination of Fe(II) by potentiometric titration with K₂Cr₂O₇.
8. Determination of three dissociation constants of H₃PO₄ by pH-metric/ potentiometric titration.

Part VI: Optical methods

1. Determination of pK of indicator by colorimetry.
2. To estimate the amount of NH₄Cl 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.

References:

- 1) Vogel A, IIIrd Edition : A Textbook Of Quantitative Inorganic Analysis, Longman
- 2) J. B. Yadav, Practical Physical Chemistry
- 3) Das and Behra, Practical Physical Chemistry
- 4) Carl W. Garland, Joseph W. Nibler and David P. Shoemaker, Experiments in Physical Chemistry, Mc-Graw Hill, 8th Edition, 2009.
- 5) 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) Day And Underwood :Quantitative Analysis
- 8) Merits And Thomas:Advanced Analytical Chemistry
- 9) Ewing, G. W. : Instrumental Methods Of Chemical Analysis, Mcgraw-Hill
- 10) Drago, R.S:Physical Methods In Inorganic Chemistry
- 11) Christain G.D:Analytical Chemistry
- 12) Khopkar S.M.:Basic Concept of Analytical Chemistry
- 13) Koltath And Ligane:Polorography
- 14) Braun:Instrumental Methods of Chemical Analysis
- 15) Willard, Merritt And Dean: Instrumental Methods of Chemical Analysis ,Van Nostrand
- 16) Strouts,Crifi;Llan And Wisin: AnalytiacI Chemistry
- 17) Skoog S.A. And West D. W.:Fundamental Of Analytical Chemistry
- 18) Dilts R.V.: AnalytiacI Chemistry
- 19) Jahgirdar D.V :Experiments In Chemistry
- 20) Chondhekar T.K: Systematic Experiments In Physical Chemistry, Rajbog S.W., Aniali Pubn.
- 21) Wlehov G. J: Standard Methods Of Chemicalanalysis 6th Ed
- 22) Akjmetov, N :General And Inorganic Chemistry
- 23) Practical Physical Chemistry: J. B. Yadav (Goel Publishing House)
- 24) Spectroscopic identification of organic compound-RM Silverstein,GC Bassler and TC Morrill, JohnWally
- 25) Introduction to NMR spectroscopy-R. J. Abraham, J. Fisher and P Loftus Wiely
- 26) Application of Spectroscopy to Organic Compound-J. R. Dyer, Printice Hall
- 27) Organic Spectroscopy-William Kemp, ELBS with McMillan
- 28) Spectroscopy of Organic Molecule-PS Kalsi, Wiley, Esterna, New Delhi
- 29) Organic Spectroscopy-RT Morrison and RN Boyd
- 30) Practical NMR Spectroscopy-ML Martin, JJ Delpenich, and DJ Martyin
- 31) Spectroscopic Methods in Organic Chemistry-DH Willson, I Fleming

- 32) Fundamentals of Molecular Spectroscopy-CN Banwell
- 33) Spectroscopy in Organic Chemistry-CNR Rao and JR Ferraro
- 34) Photoelectron Spectroscopy-Baber and Betteridge
- 35) Electron Spin Resonance Spectroscopy-J Wertz and JR Bolten
- 36) NMR –Basic Principle and Application-H Guntur
- 37) Interpretation of NMR spectra-Roy H Bible
- 38) Interpretation of IR spectra-NB Coulthop
- 39) Electron Spin Resonance Theory and Applications-W gordy
- 40) Mass Spectrometry Organic Chemical Applications, JH Banyon
- 41) Quantitative analysis: Day and Underwood (Prentice-Hall of India)
- 42) Analytical Chemistry: Gary D. Christian (Wiley India).
- 43) Experiments and calculations in Engineering Chemistry- S. S. Dara (S. Chand and Co.)
- 44) Experiments in Chemistry-D. V. Jahagirdar (Himalaya)

A.M. Rahatgaonkar

SUBJECT- CHEMISTRY
M.Sc.- Two Year: Semester-II
Name of the Course Category: DSE
Title of the Paper: Solid state and organometallic chemistry
Course code: M-CHIC524T
Paper IV
To be implemented from 2024-25

Number of Credits: 04

Marks: 60M

Total Number of Hrs: 60 Hrs (4 h per week)

Course Outcomes: At the end of the course, student would be able to

- 1) Understand the structures of various types of solids.
- 2) Establish structure-property correlation in solids.
- 3) Unravel and interpret the structural aspects of metal clusters.
- 4) Explain structures and applications of organotransition compounds,
- 5) Predict the mechanism of complex reactions.
- 6) Establish the thermodynamic and kinetic stability of reactants and products in complex reactions.

Unit I: Solid State Chemistry

15h

Ionic Crystals and their structures, radius ratio rule, effect of polarization on crystals. Covalent structure type: Sphalerite and Wurtzite. Geometry of simple crystal AB type: NaCl, CsCl and NiAs. AB₂ type: Fluorite, antiferrofluorites, Rutile structures. Li₂O, Na₂O, CdCl₂, CdI₂ structures. Ternary Compounds ABO₃ type: Perovskite, Barium titanate, lead titanate, CaTiO₃, Tolerance factor, charge neutrality and deviation structures FeTiO₃. Solids of AB₂O₄ type: Normal and inverse, 2-3 and 4-2 spinel, packing of oxygen in tetrahedral and octahedral sites, sites occupancy number of sites surrounding each oxygen, application of charge neutrality principles, site preferences in spinel, distorted spinel. Hausmannite (Jahn-Teller distortions), Factors causing distortion in spinel.

Unit II: Metal – Ligand Bonding in Transition Metal Complexes

15h

- A]** Recapitulation of Crystal Field Theory, Application of CFT to Tetragonal, square-planer, Trigonal bipyramidal complexes, Jahn-Teller effect, Nephelauxetic effect, Limitations of crystal field theory.
- B]** Magnetic Properties of Transition Metal complexes: Abnormal magnetic properties, orbital contributions and quenching of orbital angular momentum, spin-orbit coupling. Magnetic moment, electronic spectra, and structure of tetrahalocobalt (II) complexes, tetrahedral and octahedral Ni(II) complexes. High spin-low spins crossover.

Unit III: Reaction mechanism of Transition Metal Complexes-II

15h

Substitution reaction in square planar complexes: the trans effect, cis effect, steric effect, solvent effect, effect of leaving group, effect of charge, effect of nucleophile, effect of temperature. Trans effect theories, uses of trans-effect, mechanism of substitution reactions in Pt(II) complexes. Electron transfer reactions. Types of electron transfer reactions, conditions of electron transfer, and mechanism of one-electron transfer reactions, outer sphere, and inner sphere mechanisms, two electron transfer reactions complimentary and noncomplimentary reactions. Tunnelling effect, cross-reaction, Marcus-Hush theory, bridged activated mechanism.

Unit IV: Organ transition Metal Chemistry

15h

Alkyls and Aryls of Transition Metals: Types, routes of synthesis, stability and decomposition pathways of alkyls and aryls of transition metals. Organocopper in Organic synthesis. Compounds of Transition Metal – Carbon Multiple bonds: Alkylidenes, alkylidynes, low valent carbenes and carbynes–synthesis, nature of bond, structural characteristics, nucleophilic and electrophilic reactions on ligands, role inorganic synthesis.

List of Books

- 1) J.E. Huheey: Inorganic Chemistry
- 2) F.A. Cotton and G. Wilkinson: Advanced Inorganic Chemistry 3rd, 5th and 6th Editions.
- 3) A.F. Williams: Theoretical Approach in inorganic chemistry.
- 4) Mannas Chanda: Atomic Structure and chemical Bonding
- 5) L. E. Orgel: An Introduction To transition metal chemistry, Ligand field theory, 2nd Edition.
- 6) J. J. Logowski: Modern Inorganic Chemistry
- 7) B. Durrant and P.J. Durrant: Advanced Inorganic Chemistry
- 8) J C. Bailar: Chemistry of coordination compounds.
- 9) W. L. Jolly: Modern Inorganic Chemistry Jones: Elementry Coordination chemistry.
- 10) B. N. Figgis: Introduction to Ligand field.
- 11) M.C. Day and J. Selbin: Therotical Inorganic Chemistry.
- 12) J. Lewin and Wilkins: Modern Co-ordination chemistry.
- 13) Purcell and Kotz: Inorganic Chemistry.
- 14) D. Banerjea: Co-ordination chemistry, Tata Mc. Graw. Pub.
- 15) A.F. Wells: Structural inorganic chemistry, 5th Edition, Oxford.
- 16) S. G. Davies: Organotransition metal chemistry applications to organic synthesis.
- 17) R. C. Mehrotra: Organometallic chemistry Tata McGraw Hill. Pub.
- 18) G. S. Manku: Thereotical priciples of inorganic chemistry
- 19) A. B. P. Lever: Inorganic electronic spectroscopy.
- 20) R.C. Maurya: Synthesis and charecterisation of novel nitrosyls compounds, Pioneer Pub. Jabalpur 2000.
- 21) R.H. Crabtree: The Organometallic chemistry of Transition metals, John Wiley.
- 22) D.N. Styanaryan: Electronic Absorption Spectroscopy and related techniques, University Press.
- 23) R. S. Drago: Physical methods in inorganic chemistry
- 24) F. Basolo and G. Pearson: Inorganic Reaction Mechanism
- 25) Organometallics II and I complexes with transition metal- carbon bonds: Manfred Bochmann-Oxford Press.
- 26) Advanced Inorganic Chemistry Vol I and II – Satyaprakash, Tuli, Bassu and Madan- S Chand.
- 27) M. Tsusui, M. Nlevy, M. Ichikwa and K. Mori: Introduction to metal pi-complexe chemistry, Plenum press, NY
- 28) A.E. Martel; Coordination Chemistry-Volland II, VNR.

A. M. Rahatgaonkar

SUBJECT- CHEMISTRY
M.Sc.- Two Year: Semester-II
Name of the Course Category: DSE
Title of the Paper: Organic Reaction Mechanism
Course code: M-CHOC524T
Paper IV
To be implemented from 2024-25

Number of Credits: 04

Marks: 60M

Total Number of Hrs: 60 Hrs (4 h per week)

Course Outcomes:

At the end of the course students will be able to:

- 1) Predict the orientation and stereochemistry of the product of addition and elimination reaction
- 2) Apply enolate chemistry to achieve molecular complexity
- 3) Design organic reactions in order to achieve the required product(s)
- 4) Formulate green chemistry synthesis to increase atom economy
- 5) Application of free radicals in functional group transformation

Unit I : Addition to carbon-carbon multiple bond

15h

- A]** Mechanistic and stereochemical aspects of addition reaction involving electrophiles, nucleophiles, and free radicals, regio and chemoselectivity, Orientation and stereochemistry of common reactions, Addition to cyclopropanes, Hydrogenation of double bond and triple bonds. Hydrogenation of aromatic rings, hydroboration-oxidation, epoxidation, Michael addition
- B]** Elimination reactions: The E1, E2 and E1CB mechanisms, Stereochemistry of E2 elimination, Orientation of the double bond, Saytzeff and Hoffman's rule, Effect of substrate structure, attacking base, leaving group and medium, Mechanism and orientation in pyrolytic elimination involving selenium oxide, Cope and Chugaev elimination

Unit II: Addition to carbon-hetero atom multiple bond

15h

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, Mechanism of metal hydride reduction of saturated and unsaturated carbonyl compounds, acids, esters, and nitriles, Wittig reaction, Mechanisms and synthetic applications of condensation reactions involving enolates- Aldol, Knoevenagel, Claisen, Mannich, Benzoin, Perkin, Stobbe reaction, Robinson annulation, Hydrolysis of esters and amide, Baylis-Hillman reactions, Ugi and Passerini reaction.

Unit III: Free radical reactions

15h

Generation of free radicals, Type of free radical reactions, free radical substitution, mechanism at an aromatic and aliphatic substrate, reactivity at a bridgehead position. The reactivity and selectivity principle of

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, Hunsdiecker reaction, Barton reaction, Hoffmann-Loeffer-Freytag reaction, McMurry coupling, Samarium(II) iodide reagents for functional group transformations and C-C bond formation. Applications of tributyltin hydride: Reduction of halides, alcohols and acids, addition to carbon-carbon double bond, cyclization of free radical intermediates, tandem radical cyclization reactions, fragmentation reactions

Unit IV: Molecular rearrangements

15h

Definition and classification. Mechanism, stereochemistry and synthetic applications of Pinacol-Pinacolone, Wagner-Meerwein, Tiffenev-Demjnov ring expansion, Arndt Eistert synthesis, Dienone-phenol rearrangement, rearrangement due to electron deficient nitrogen: Hofmann, Lossen, Curtius, Schmidt and Beckmann rearrangements, Baeyer-Villiger oxidation, Dakin oxidation, [1,2]-Wittig rearrangement, Base catalysed rearrangements: Benzilic acid, Favourski, Neber, Sommelet-Hauser and Smiles rearrangement, Stevens rearrangement Fragmentation reactions: Electron push and pull requirement, Beckmann fragmentation, Eschenmoser fragmentation, Grob Fragmentation

Weblink to Equivalent MOOC on SWAYAM if relevant:

- Essentials of Oxidation, Reduction and C-C Bond Formation. Application in Organic Synthesis- <https://nptel.ac.in/courses/104101127>
- Principles of Organic Synthesis- <https://nptel.ac.in/courses/104103110>
- Introductory Organic Chemistry II- https://onlinecourses.nptel.ac.in/noc21_cy46/preview

A. M. Rahatgaonkar

SUBJECT- CHEMISTRY
M.Sc.- Two Year: Semester-II
Name of the Course Category: DSE
Title of the Paper: Quantum, Statistical and Nuclear Chemistry
Course code: M-CHPC524T
Paper IV
To be implemented from 2024-25

Number of Credits: 04

Marks: 60M

Total Number of Hrs: 60 Hrs (4 h per week)

Course Outcomes: At the end of the course students will be able to

- 1) Understand, the concept of statistical thermodynamics and their uses.
- 2) Understand the quantum mechanical applications in actual practice and in spectroscopy
- 3) Understand the thermodynamics of real processes
- 4) Understand the distribution laws and their applications
- 5) Understand the fundamentals of nuclear sciences

UNIT I: QUANTUM MECHANICS - II

15h

Approximate methods, variation principle, its application in Linear and non-linear functions, MO theory applied to H₂ + molecule and H₂ molecule (calculation of energy), Introduction to perturbation theory (First order correction to wave function and energy), Application to He atom. Electronic structure of atoms: Russel Sanders terms and coupling schemes, term separation energies of the pn configuration, term separation energies for dn configuration, magnetic effects: spin orbit coupling and Zeeman splitting. Hybridization, hybrid orbitals in terms of wave functions of s and p orbitals, sp and sp² hybridizations, Simple Hückel theory applied to: ethylene, butadiene and cyclobutadiene.

UNIT II: STATISTICAL THERMODYNAMICS

15h

Statistical thermodynamics :Lagrange's Method of Undetermined Multipliers) Conditional Maximization(, Stirling Approximation, Concept of Distribution, Thermodynamic Probability and most probable distribution, Maxwell Boltzmann, Bose Einestein, Fermi Dirac statistics, comparison between three statistics. Partition function, Translational partition function, Rotational partition function, Vibrational partition function, electronic partition function, Applications of partition functions, Numerical.

UNIT III: STATISTICAL MECHANICS OF ENSEMBLES AND NON-EQUILIBRIUM THERMODYNAMICS

15h

Atomic and Molecular quantum levels, Significance of Boltzmann Distribution law, partition Functions and ensembles, ensemble averaging, postulates of ensemble averaging, canonical, grand canonical and micro canonical ensembles, corresponding distribution laws using Lagranges method of undetermined multipliers. Ortho and para hydrogen, principle of equipartition of energy, calculation of average energy. Nonequilibrium

Thermodynamics :Conservation of mass and energy in time dependent closed and open systems, Thermodynamic criteria of irreversibility, rate of entropy production and entropy exchange in irreversible processes .The generation of the concept of Chemical Affinity and the extent of advancement of chemical reactions, Thermodynamic constraints on the signs of chemical affinity and the velocity of chemical reaction, application to any one coupled reaction.

UNIT IV: NUCLEAR CHEMISTRY

15h

Introduction, radioactive decay and equilibrium, thermonuclear reactions, photonuclear reactions, Radiometric titration, isotopic dilution analysis, NAA. Nuclear models: Fermi gas model, shell model, liquid drop model, application of liquid drop models semiempirical mass equation. Counters: proportional counter, GM counter, scintillation counter, ionization chamber counter.

List of 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 Mc-graw Hill, New Delhi.
- 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, New Delhi, 2009.
- 7) B .C .Reed, Quantum Mechanics, Jones and Bartlett, New Delhi, 2010.
- 8) R .P .Rastogi and R .R .Mishra, An Introduction to Chemical Thermodynamics, Vikas Publication, Gorakhpur, 2010.
- 9) P .W .Atkins’and D .Paula, Physical Chemistry, 8th Edition, Oxford University Press, 2010.
- 10) G .K .Vemulapalli, Physical Chemistry, Prentice –Hall of India, 1997.
- 11) S .Glasstone, An Introduction to Electrochemistry, East-West Press Pvt .Ltd., New Delhi, 2004.
- 12) H .K .Moudgil, Text Book of Physical Chemistry, Pretice Hall of India, New Delhi, 2010.
- 13) S .O .Pillai, Solid State Physics, New Age International, New Delhi, 2102.
- 14) N .B .Hanny, Treaties in Solid State Chemistry,
- 15) M .C .Day and J Selbin, Theoretical Inorganic Chemistry, Reinhold Pub .Corp., New York,
- 16) I Prigogine and R .Defay, Chemical Thermodynamics, Longmans, London, 1954.
- 17) S .R .DeGroot and P .Mazoor, Non-Equilibrium Thermodynamics, North-Holland Co., Amsterdam, 1969.
- 18) G .Lebon, D .Jou and Casa Vazquez, Understanding Non-equilibrium Thermodynamics, Springer, 2008.
- 19) I.Prigoggine, “An Introduction to Thermodynamics of Irreversible Processes, ”WileyInterscience.
- 20) R .P .Rastogi, Introduction to Non-equilibrium Physical Chemistry, Elsevier, Amsterdam, 2008.
- 21) G .A .Somorjai, Introduction to Surface Chemistry and Catalysis, Wiley, 2010.
- 22) M .C .Gupta, Statistical Thermodynamics, New Age International.
- 23) K .Huang, Statistical Mechanics, Wiley, New Delhi, 2003.
- 24) Andrew Maczek, Statistical Thermodynamics, Oxford University Press Inc., New York)1998.
- 25) C.N. Rao .Nuclear Chemistry
- 26) B .G .Harvey, Introduction to Nuclear Physics and Chemistry, Prentice Hall, Inc) .1969.(27) H.J .Arnikar, Essentials of Nuclear Chemistry, 4th Edition)1995(, Wiely-Eastern Ltd., New Delhi.
- 27) L .E .Smart and E .A .Moore, Solid State Chemistry-An Introduction, CRC Tylor and Fransis, 2005.
- 28) D .D .Sood, A .V .R .Reddy, Fundamentals of Radiochemistry, Indian Association of Nuclear Chemists and Allied Scientists, 2007.

- 29) C .N .R .Rao and Gopalakrishnan, “New Directions in Solid State Chemistry” Second Edition, Cambridge University Press.
- 30) Anthony R .West, “Solid State Chemistry and its Applications ”Wiley India Edition.
- 31) C .Kalidas and M .V .Sangaranarayana, Non-Equilibrium Thermodynamics.

NPTEL sources weblinks:

Quantum Chemistry:

1. <https://archive.nptel.ac.in/courses/104/105/104105128/>
2. <https://www.youtube.com/watch?v=InNx7cYE9DI>
3. https://onlinecourses.nptel.ac.in/noc22_cy02/preview

For statistical Thermodynamics:

https://onlinecourses.nptel.ac.in/noc23_me69/preview

<https://nptel.ac.in/courses/104103112>

For Nuclear Chemistry:

https://onlinecourses.nptel.ac.in/noc23_cy21/preview

<https://www.youtube.com/watch?v=iMhDYarsfII>

<https://archive.nptel.ac.in/courses/112/103/112103243/>

A. M. Rahafgaonkar

SUBJECT- CHEMISTRY
M.Sc.- Two Year: Semester-II
Name of the Course Category: DSE
Title of the Paper: Instrumental Methods of Analysis
Course code: M-CHAC524T
Paper IV
To be implemented from 2024-25

Number of Credits: 04

Marks: 60M

Total Number of Hrs: 60 Hrs (4 h per week)

Course Outcomes: At the end of the course students will be able to -

- 1) Understand the importance of sampling and sample treatment.
- 2) Select appropriate sampling technique based on sample and target analyte.
- 3) Explain principle and instrumentation involved in AAS.
- 4) Deduce the necessity to remove interferences in AAS and methods involved .
- 5) Select proper technique among the available techniques.
- 6) Formulate experiments based on optical and electroanalytical techniques.

Unit I:

15h

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. Methods of quantification: Absolute method, comparison method, calibration curve method, standard addition method and internal standard method.

Unit-II: Atomic absorption spectroscopy

15h

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-III: Polarography and amperometry

15h

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 half wave 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.

Unit IV: Miscellaneous techniques

15h

A] Fluorometry and phosphorimetry: Principles of fluorescence and phosphorescence. Jablonski diagram. Concentration dependence of fluorescence intensity. Fluorescence quenching. Instrumentation. Applications.

B] Nephelometry and turbidimetry: Principle, instrumentation and applications.

C] Photoacoustic spectroscopy: Theory. Instrumentation. Advantages over absorption spectroscopy. Chemical and surface applications of PAS.

List of 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)
- 18) Web link for related NPTEL courses Analytical Chemistry: <https://nptel.ac.in/courses/104105084>

A. M. Rahatgaonkar

SUBJECT- CHEMISTRY
M.Sc.- Two Year: Semester-II
Name of the Course Category: OJT
Title of the Paper: Internship / Apprenticeship
Course code: M-CH525P
Paper: V
To be implemented from 2024-25

Number of Credits: 04

Marks: 200M

Total Number of Hrs: 120 Hrs (8h per week)

On job training or a Field Project is a skill based practical program. It has to be carried out in accordance Government Resolution of dated 16 May 2023 of General Guidelines for M.Sc. program.

1. Every student admitted to M.Sc. Second Semester is compulsorily required to undergo this course bearing 4 credits.
2. During second semester, all students will have to undergo OJT/Internship/FP of 120 Hours.
3. Each student will be required to submit a detailed report to the Department/Institute for the work undertaken during this period within 7 days of completion of the training following which the evaluation and assessment for OJT/Internship/FP will be done by the concerned institute.
4. The Report submitted must be according to the Learning outcomes and in tune with the rubric for evaluation.
5. Institute is required to assign Supervisor/Mentor to students for OJT/Internship/FP who will guide the students in attaining the outcomes of this course.
6. The Internal Examiner and External Examiner shall jointly evaluate the report submitted by the student and her/his seminar and shall immediately submit the evaluation report in the prescribed format provided along with

A.M. Rahatgaonkar

Weblinks to Equivalent MOOC on NPTEL Online Courses

For Quantum Chemistry Introduction:

- ✓ <https://archive.nptel.ac.in/courses/104/108/104108057/>
- ✓ https://onlinecourses.nptel.ac.in/noc20_cy27/preview/
- ✓ <https://nptel.ac.in/courses/104106083/>
- ✓ <https://nptel.ac.in/courses/104108057/>
- ✓ <https://www.digimat.in/nptel/courses/video/104108057/L11.html/>

For Chemical Kinetics

- ✓ <https://archive.nptel.ac.in/courses/104/101/104101128/>
- ✓ <https://www.youtube.com/watch?v=uep2XeLCGk/>

For Essentials of Biomolecules: Nucleic Acids and Peptides

- ✓ <https://nptel.ac.in/courses/104/103/104103121/>
Biocatalysis in Organic Synthesis
- ✓ <https://archive.nptel.ac.in/courses/104/105/104105032/>

Biochemistry

- ✓ <https://archive.nptel.ac.in/courses/104/105/102105034/>

Organic Chemistry in Biology and Drug Development

- ✓ <https://archive.nptel.ac.in/courses/104/105/104105120/>

- ✓ NPTEL sources Weblinks

For Classical Thermodynamics:

- ✓ <https://archive.nptel.ac.in/courses/104/103/104103112/>
- ✓ <https://digimat.in/nptel/courses/video/104106094/L18.html>

For Phase rule:

- ✓ <https://www.youtube.com/watch?v=2LywAiZBQW4>
- ✓ <https://archive.nptel.ac.in/courses/113/104/113104068/>
- ✓ <https://archive.nptel.ac.in/courses/104/103/104103112/>

For electrochemistry

- ✓ https://onlinecourses.nptel.ac.in/noc23_cy19/preview
- ✓ <https://www.youtube.com/watch?v=XTt3gXB0a84>

Analytical Chemistry:

- ✓ <https://nptel.ac.in/courses/104105084>

Introductory Organic Chemistry I-

- ✓ <https://nptel.ac.in/courses/104106119>

Mechanisms in Organic Chemistry-

- ✓ https://onlinecourses.nptel.ac.in/noc22_cy42

Mechanisms in Organic Chemistry:

- ✓ https://onlinecourses.nptel.ac.in/noc20_cy26/preview

Stereochemistry-

- ✓ <https://nptel.ac.in/courses/104105086>

Stereochemistry and Applications-

- ✓ <https://nptel.ac.in/courses/104106127>

Structure, Stereochemistry and Reactivity of Organic Compounds and Intermediates: A

Problem-solving Approach-

- ✓ <https://nptel.ac.in/courses/104105127>

A.M. Rahatgaonkar