Shiksha Mandal's
Bajaj College of Science, Wardha
(An Autonomous Institution)

Department of Chemistry

Proposed Syllabus for Two Year M.Sc. Chemistry

Department Specific Course (DSC)

Semester I courses

Syllabus under Autonomy

(Draft discussed and approved in BOS Meeting 08-July-2023 to be implemented from Academic Session 2023-24)

Shiksha Mandal's

Bajaj College of Science, Wardha

Programme Objectives M.Sc. Chemistry

- The main aim of the programme M.Sc. Chemistry is to make students abreast with sound knowledge about the fundamentals and applications of chemical and scientific theories.
- The important objectives of this programme are to enable students to
    1) become familiar with the different branches of chemistry like analytical, organic, inorganic, physical, environmental chemistry.
    2) be able to easily assess the properties of different elements.
    3) learn to apply appropriate techniques for the qualitative and quantitative analysis of chemicals in laboratories and in industries.
    4) develop analytical skills and problem solving skills requiring application of chemical principles.
    5) acquire the ability to synthesize, separate and characterize compounds using laboratory and instrumentation techniques.
- The students should be applying the scientific knowledge to design, carry out, record and analyze the results of chemical reactions.
- The students may acquire some of the skills required to work efficiently in laboratory of any academic/research institution or industrial unit.
- They should become capable of solving a problem by thinking methodically, independently to draw a logical conclusion.

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Programme Outcomes M.Sc. Chemistry

- After successful completion of the programme the students will have sound knowledge about the fundamentals and applications of chemical and scientific theories.
- They will become familiar with the different branches of chemistry like analytical, organic, inorganic, physical, environmental chemistry.
- They will be able to easily assess the properties of different elements.
- Students can apply appropriate techniques for the qualitative and quantitative analysis of chemicals in laboratories and in industries.
- Students will develop analytical skills and problem solving skills requiring application of chemical principles.
- They acquire the ability to synthesize, separate and characterize compounds using laboratory and instrumentation techniques.
- The graduates achieve the skills required to work efficiently in the **chemical industry like cement industries, agro product, paint industries, rubber industries, petrochemical industries, food processing industries, fertilizer industries** etc.
- They acquire the laboratory skills to transfer and interpret knowledge entirely in the working environment.
- They can understand the causes of environmental pollution and can open up new methods for environmental pollution control.
- Students can find out the green route for chemical reaction for sustainable development.
- They will be able to solve the problem and also think methodically, independently and draw a logical conclusion.
- Students will learn to employ critical thinking and the scientific knowledge to design, carry out, record and analyze the results of chemical reactions.

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Syllabus of M.Sc. I Semester I

DSC I (Theory)

PGCH1T1: Inorganic Chemistry

[60 Hrs] **[4 Credits]**

Course Objectives

1. Understand the stereochemistry and bonding of various molecules on the basis of various theories viz. VSEPR theory, Crystal field theory and Molecular orbital theory.
2. Determine the structure of complex using electronic spectra and magnetic susceptibility measurement studies.
3. Understand the structure, bonding and topology of boron hydrides and its application.
4. Determine the classification of metal clusters containing metal-metal bonds and learn about the factors affecting the stability of metal complexes.
5. Learn about the isopolyacids and heteropolyacids and their structures.
6. Describe the role of metal in biological system and their function.
7. Describe the structural and functional relationships, mechanisms and importance of metalloenzymes.

Course Outcomes

This will equip the learners to gain understanding of:

1. Importance of various theories in determining the stereochemistry and bonding of various molecules.
2. Magnetic and electronic properties of complexes for structure elucidation.
3. Structure and reactivity of boranes, stability of metal clusters and structures of iso and heteropolyacids.
4. Validate the role of bioinorganic chemistry in every day action.

Contents:-

Unit-I

a) Stereochemistry and Bonding in Main Group Compound:

VSEPER-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:

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:

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

Unit-II

a) Electronic spectra:

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:

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:

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

b) Metal ligand equilibria in solution:

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 by:

(1) spectrophotometric method (Job's and Mole ratio method)

(2) Potentiometric method (Irving-Rossotti Method)

Unit-IV BIOINORGANIC CHEMISTRY:

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, Fe_2S_2, Fe_3S_4, Fe_4S_4). 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-B_{12}, its structure and function.

References -

- S. F. A. Kettle, J. N. Murral & S. T. Teddler: Valency Theory
- C. A. Coulson: Valency
- J. E. Huheey: Inorganic Chemistry

- F .A. Cotton & G. Wilkinson: Advanced Inorganic Chemistry 3rd, 5th& 6th Editions.
    - F. Willims: Theoretical Approach in inorganic chemistry.
- Mannas Chanda: Atomic Structure and chemical Bonding
- L. E. Orgel: An introduction to transition metal chemistry, Ligand field theory, 2nd Edition.
- J. J. Logowski: Modern Inorganic Chemistry
- Durrant and P. J. Durrant: Advanced Inorganic Chemistry
- J. C. Bailar: Chemistry of co-ordination compounds.
- W. L. Jolly: Modern Inorganic Chemistry
- R. S. Drago: Physical methods in inorganic chemistry.
- K. Barnard: Theoretical Inorganic Chemistry
- F. A. Cotton: Chemical Applications of Group theory.
- N. Figgis: Introduction to Ligand field.
- S. F. A. Kettle: Co-ordination chemistry.
- M. C. Day and J. Selbin: Theoretical Inorganic Chemistry.
- J. Lewin and Wilkins: Modern Co-ordination chemistry.
- Gowarikar, Vishwanathan and Sheedar: Polymer science.
- R. L. Dutta and A. Symal: Elements of magneto chemistry
- P. Atkins: Inorganic Chemistry 4th Edition, Oxford University Press.
- Bertini, et al: Bioinorganic Chemistry (Viva)
- Fenton, David E.: Bio coordination chemistry, Oxford
- Selected Topics in Inorganic Chemistry by Wahid U Malik, Tuli, Madan.
- A Logical Approach to Modern Inorganic Chemistry by Jagdamba Singh
- Essentials of Bio Inorganic Chemistry by Monal Singh Neerja Gupta
- Concise Coordination Chemistry by R. Gopalan , V. Ramalingam
- Advanced inorganic chemistry Volume I by Madan malik Tuli Prakash S.Chand publication
- Advanced inorganic chemistry Volume II Madan malik Tuli Prakash S.Chand publication

DSC II (Theory)

PGCH1T2: Physical Chemistry

[60 Hrs] **[4 Credits]**

Course Objectives

1. To recapitulate fundamentals of chemical thermodynamics and extending the study to Maxwell's relations and third law of thermodynamics.
2. To learn advanced concepts and theories of chemical kinetics.
3. To understand fundamentals of quantum mechanics and its applications.
4. To study theories of electrolytes and fundamentals of conductometry, potentiometry and their applications.

Course Outcomes

On successful completion of this Course the students should be able to-

1. Derive the Maxwell's relations and understand third law of thermodynamics and related concepts.
2. Learn modern concepts and theories of reaction dynamics.
3. Understand and execute quantum mechanical problems and their applications
4. Understand the theories of electrolytes, apply conductometric and potentiometric titrations for analysis

Contents:-

Unit-I CLASSICAL THERMODYNAMICS:

a) Recapitulation of Laws of thermodynamics, Exact and inexact differentials, condition of exactness, Ptaff differential expression and equations, Applications of Ptaff 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 CHEMICAL KINETICS

a) 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.

b) Bodenstein steady state approximation, Rice-Herzfeld mechanism of chain reaction, Kinetics of photochemical chain reaction between H_2 & Cl_2 and H_2 & Br_2, Kinetics of Enzyme catalyzed reaction (Michaelis-Menten equation), salt effect.

Unit-III FORMULATION OF QUANTUM MECHANICS

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, Numericals 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-IV ELECTROCHEMISTRY

a) 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.

b) Principle of potentiometry, Indicator electrodes: hydrogen electrode, quinhydrone electrode, antimony electrode and glass electrode. Reference electrodes: Calomel electrode and Ag/AgCl electrode. potentiometric titrations, Basic Electrochemical Thermodynamics, Nernst equation, standard electrode potential, Determination of cell potential.

List of books

- R. P. Rastogi and R. R. Mishra, An Introduction to Chemical Thermodynamics, Vikas Publication,
- Gorakhpur, 2010.
- P. W. Atkins and D .Paula, Physical Chemistry, 8th Edition, Oxford University Press, 2010.
- E. N. Yenemin, Fundamentals of Chemical Thermodynamics, MIR, Publications.
- S. M. Blinder, Advanced Physical Chemistry,
- D. Mcquarie and J .Simon, Physical Chemistry –A Molecular Approach, University Press, 2000
- G. M. Barrow, Physical Chemistry, Tata Mc-Graw Hill, V edition 2003.
- H. K. Moudgil, Text Book of Physical Chemistry, Pretice Hall of India, New Delhi, 2010.
- G. M. Panchenkov and V. P. Labadev, "Chemical Kinetics and catalysis", MIR Publishing
- E. A. Moelwyn - Hughes, "Chemical Kinetics and Kinetics of Solutions", Academic
- K. J. Laidler, Chemical Kinetics, Third Edition) 1987(Harper and Row, New York.
- J. Raja Ram and J. C. Kuriacose, Kinetics and Mechanism of Chemical Transformations MacMilllan IndianLtd., New Delhi, 1993
- C. H. Bamford and C. F. H. Tipper, Comprehensive Chemical Kinetics, Vol 1., Elsevier Publications, New York, 1969.
- C. H. Bamford and C. F. H. Tipper, Comprehensive Chemical Kinetics, Vol 2., Elsevier Publications, New York, 1969.

- S. Glasstone, K. J. Laidler and H. Eyring, The Theory of Rate Processes, Mc -Graw Hill, New
  York, 1941.
- Santosh Kumar Upadhyay, Chemical Kinetics and Reaction Dynamics, Springer 2006.
- G. K .Agrawal, Basic Chemical Kinetics, Tata-Mc-Graw Hill, 1990.
- Ira .N. Levine, Quantum Chemistry, 5th edition (2000), Pearson educ., Inc.New Delhi
- A.K.Chandra, Introductory Quantum Chemistry, 4th edition (1994), Tata Mcgraw Hill, New Delhi.
- M.W.Hanna, "Quantum Mechanics in Chemistry", Benjamin
- L. Pualing and E. B. Wilson, Introduction to Quantum Mechanics with Applications to Chemistry, McGraw Hill, New York (1935).
- R. K. Prasad, Quantum Chemistry, New Age International, Delhi.
- R. K. Prasad, Quantum Chemistry through problems and solutions, New Age International, New Delhi, 2009.
- B. C. Reed, Quantum Mechanics, Jones and Bartlett, New Delhi, 2010.
- S. Glasstone, An Introduction to Electrochemistry, East-West Press Pvt. Ltd., New Delhi, 2004.
- K. L. Kapoor, Text Book of Physical Chemistry, Vol – I to Vol -VI, 2011.

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 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=uep2XeLCGkc

For electrochemistry

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

DSC III (Practical)

PGCH1P1: Inorganic Chemistry Practical

[60 Hrs] **[2 Credits]**

Course Objectives

1. To conduct the experiments for the preparation and characterization of metal complexes.
2. To conduct separation and determination of two metal ions from different alloys using Volumetric, Gravimetric and Spectrophotometric methods.
3. To conduct qualitative analysis of inorganic mixture containing total of five radicals including interfering radicals.

Course Outcomes

1. Students will learn to synthesize various inorganic compounds, purify and characterize them.
2. Students will also be able to perform qualitative and quantitative analysis of different compounds and mixtures.

Contents:-

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

i) Copper (II) and Nickel (II)
ii) Copper (II) and Zinc (II)
iii) Nickel (II)—Zinc (II) and
iv) 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:

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

DSC IV (Practical)

PGCH1P2: Physical Chemistry Practical

[60 Hrs] **[2 Credits]**

Course Objectives

The most important objective of this course is to apply theoretical principles to conduct various physic-chemical studies of some systems. The students should learn to apply non-instrumental and instrumental techniques for better understanding of physical chemistry concepts.

Course Outcomes

After completing this course, the students will-

1) Learn the determination of important quantities of liquids such as volume contraction on mixing and activation parameters of viscous flow.
2) Understand the determination of the critical micelle concentration (CMC) of a given surfactant and molecular mass of a polymer.
3) Know how to determine heat of dilution and also study effect of impurity on CST in phenol-water systems.
4) Understand determination of distribution coefficient, know how to construct the phase diagrams of two components system, find the mutual solubility of glycerol-*m*-toluidine.
5) Be able to determine rate constant, equilibrium constant and order of various reactions.
6) Learn to employ conductometry, potentiometry and pH metry for different studies.

Contents:-

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-naphtyl 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 $KI+I_2=KI_3$ 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) To determine the heat of reaction, equilibrium constant and other thermodynamic functions for the reaction $Zn + Cu^{2+} \rightarrow Zn^{2+} + Cu$ potentiometrically.
4) To determine the formal redox potential of $Fe^{2+} \rightleftharpoons Fe^{3+}$ and $Ce^{3+} \rightleftharpoons Ce^{4+}$ systems by titrating ferrous ammonium sulphate against ceric sulphate.
5) To determine the pH of a buffer solutions using a quinhydrone electrode.
6) To determine the strength of given $Cu^{2=}$ solution by potentiometrically titrating against EDTA (Complexometric titrations).

Reference books:

- J. B. Yadav, Practical Physical Chemistry
- Das and Behra, Practical Physical Chemistry
- Carl W. Garland, Joseph W. Nibler and David P. Shoemaker, Experiments in Physical Chemistry, Mc-Graw Hill, 8th Edition, 2009.
- Farrington Daniels, Joseph Howard Mathews, John Warren Williams, Paul Bender, Robert A. Alberty, Experimental Physical Chemistry, Mc-Graw Hill, Fifth Edition, 1956.
- John W. Shriver and Michael George, Experimental Physical Chemistry, Lab Manual and Data Analysis, the University of Alabama in Huntsville, Fall 2006
- Chondhekar T.K: Systematic Experiments In Physical Chemistry, Rajbog S.W., Aniali Pubn.
- Merits And Thomas: Advanced Analytical Chemistry
- Ewing, G. W. : Instrumental Methods Of Chemical Analysis, Mcgraw-Hill
- Khopkar S.M.:Basic Concept of Analytical Chemistry
- Wlehov G. J: Standard Methods Of Chemical analysis 6th Ed
- Braun:Instrumental Methods of Chemical Analysis

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Department of Chemistry

Proposed Syllabus for Two Year M.Sc. Chemistry

ELECTIVE

Semester I courses

Syllabus under Autonomy

(Draft to be discussed and approved in BOS Meeting 08-July-2023 to be implemented from Academic Session 2023-24)

Shiksha Mandal's

Bajaj College of Science, Wardha

Syllabus of M.Sc. I Semester I

ELECTIVE - I

PGCH1E1: Bonding, Stereochemistry and Nucleophilic Substitutions

[60 Hrs] **[4 Credits]**

Course Objectives

To learn

1. Basic idea about important electronic effects in organic chemistry, reactive intermediate, aromaticity.
2. 3-D aspect of organic molecules such as optical activity of asymmetric and dissymmetric molecules.
3. aliphatic nucleophilic substitution reaction.
4. aromatic nucleophilic and electrophilic substitution reactions.

Course Outcomes

Students will gain an understanding of:

1. fundamental knowledge of reactive intermediate, chemical bonding & aromaticity.
2. 3-D aspects of organic molecules.
3. aliphatic nucleophilic substitution reaction.
4. aromatic nucleophilic and electrophilic substitution reactions.

Contents:-

Unit-I

Chemical bonding, Aromaticity and Reactive Intermediates:

Chemical bonding: Recapitulation of delocalized chemical bonding, conjugation, resonance, hyperconjugation, cross conjugation, alternant and non-alternant hydrocarbons, tautomerism, Inductive effect.

A. **Bonding other than covalent bonding:** Hydrogen bonding, inclusion compounds, rotaxanes, catenanes, cyclodextrins, cryptands, crown ethers, Phase transfer catalyst, fullerenes.
B. **Aromaticity**: Benzenoid and non-benzenoid compounds, Huckel's rule, antiaromaticity, homoaromaticity, annulenes, azulenes, cyclopentadienyl anion, tropylium cation, tropone and tropolone.
C. **Reactive intermediates:** Generation, structure, stability and chemical reactions of carbocations, carbanions, free radicals, carbenes, nitrenes and benzyne / arynes.

Unit-II

A. **Stereochemistry:** 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:** 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

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. Nucleophilicty, effect of leaving group, ambient nucleophiles and ambient substrates regiospecificity, substitution at allylic and vinylic carbon atoms

C. Neighbouring Group Participation: Concept of NGP, anchimetric assistance with mechanism, neighboring group participation by π and σ bonds, classical and non-classical carbocations, phenonium ions. Intramolecular displacement by hydrogen, oxygen, nitrogen, sulphur and halogen. Alkyl, cycloalkyl, aryl participation, participation in bicyclic system, migratory aptitude, carbocation rearrangement in NGP.

Unit IV

A. 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, Sommlet-Hauser and Smiles rearrangements

B. Aromatic electrophilic substitution The arenium ion mechanism, orientation and reactivity, energy profile diagrams. The o/p ratio, ipso attack, orientation in benzene ring with more than one substituents, orientation in benzene ring with more than one substituents, orientation in other ring system. Reactions: nitration, halogenation, sulphonation, Friedel-Crafts alkylation and acylation, Vilsmeir-Hack reaction, Gatterman-Koch reaction, Pechman reaction, Reimer-Tieman 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

List of books

- Advanced Organic Chemistry –Reaction mechanism and structure. Jerry March, John Wiley
- Advanced Organic Chemistry- F.A. Carey and R. J. Sunberg, Plenum
- A Guidebook to Mechanism in Organic Chemistry-Peter Skyes, Longman
- Structure and Mechanism in Organic Chemistry-C.K. Gold, Cornell University Press

- Organic Chemistry, R.T. Morrison Boyd. Prentice Hall
- Modern Organic Chemistry-H.O. House, Benjamin
- Principal of Organic Chemistry-R.O.C. Norman and J.M. Coxon, Blackie Academic and Professional
- Reaction Mechanism in Organic Chemistry-S.M. Mukharji and S.P. Singh, Macmilan
- Stereochemistry of Organic Compounds- D. Nasipuri, New Age International
- Stereochemistry of Organic Compounds- P. S. Kalsi, New Age International
- Frontier Orbitals and Organic Chemical Reactions-I. Fleming
- Orbital Symmetry – R. E. Lehr and A. P. Marchand
- Reactive Intermediate in Organic Chemistry-N. S. Isaacs
- Stereochemistry of Carbon Compounds- E. L. Eliel
- Physical Organic Chemistry-J. Hine
- Name Reaction in Organic chemistry –Surrey
- Advanced Organic Chemistry – L. F. Fieser and M. Fieser

ELECTIVE - II

PGCH1E2: Polymer Chemistry I

[60 Hrs] **[4 Credits]**

Course Objectives

The main objectives of this course are

- To study basic concept, raw materials, nomenclature and classification of polymers along with types of polymerization with their mechanisms
- To understand concepts of polymer molar mass and important methods of determination.
- To realize important physical characteristics of polymers
- To learn about synthesis and application of some commercial and functional polymers

Course Outcomes

At the end of this course, students will-

- Be abreast with basic concept, raw materials, nomenclature and classification of polymers. of polymers.
- Understand types of polymerization with their mechanisms
- Realize concepts of polymer molar mass and important methods of determination.
- Gain an understanding of important physical characteristics of polymers
- Have the knowledge about synthesis and application of some commercial and functional polymers

Unit-I: Introduction to Polymer

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

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

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 (Tg), relationship between T_g and T_T, Effect of molecular weight, dilments, chemical structure, chain topology, branching and cross linking. Methods of determination of glass transition and crystallinity of polymers.

Unit IV: Commercial polymers

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

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

Reference books:

- Textbook of polymer science: F.W. Billmayer Jr. Wiley.
- Polymer science: V.R. Gowarikar, N. V. Viswanathan and J. Sreedhar, Wiley-Eastern.
- Fractional monomers and polymers: K Takemoto, Y. Inaki, and R.M. Ottam Brite.
- Contemporaty polymer chemistry: H.R. Alcock and F. W. Lambe, Prentice Hall.
- Principles of polymer Chemistry: Flory, Cornell Univ. press.
- Introduction to polymer chemistry: R. B. Seymour, McGraw Hill.
- Principles of polymerization: Odian.
- A first course in polymer chemistry: A. Strepikheyew, V. Derevistkay and G. Slonimasky, Mir Publishers, Moscow.

Shiksha Mandal's
Bajaj College of Science, Wardha
(An Autonomous Institution)

Department of Chemistry

Proposed Syllabus for Two Year M.Sc. Chemistry

Research Methodology (RM)

Semester I Course

Syllabus under Autonomy

(Draft discussed and approved in BOS Meeting 08-July-2023 to be implemented from Academic Session 2023-24)

Shiksha Mandal's

Bajaj College of Science, Wardha (Autonomous)

Department of Chemistry

M.Sc. I Semester I, NEP-2023-24

PGCH1RM: Research methodology

[4 Credits]

Course Objectives

1. Gain a comprehensive understanding of research methodology and its fundamental concepts.
2. Acquire skills in data collection, analysis, and interpretation using various statistical techniques.
3. Develop the ability to critically evaluate and select appropriate research methods for different types of research.
4. Enhance proficiency in technical writing, research reporting, and adherence to research ethics and academic integrity.

Course Outcomes

After learning research methodology course, students will be able to:

1. Identify and describe the characteristics of different types of research, including basic, applied, and patent-oriented research.
2. Apply descriptive and inferential statistical analysis techniques to analyze and interpret research data and its importance in research, and apply appropriate research methods.
3. Apply scientific thinking and problem identification techniques in the research process.
4. Develop skills in technical writing, research reporting, and the proper structure and organization of research documents and gain awareness of research ethics, academic integrity, and the importance of avoiding plagiarism and academic malpractice

Syllabus:

Module 1: Research basics and perception of research

1.1 Definition, General and specific characteristics of research, types of research (basic, applied and patent oriented).
1.2 Steps of Action (basic) research, objectives of basic research, characteristics of investigators.
1.3 Scientific thinking- characters, steps in process of scientific thinking, Steps in problem identification, criteria for selecting problem, and sources of scientific problems.
1.4 Review of literature- meaning, need, and objectives, structure of review of literature, sources of literature collection, Simple rules of structuring (writing) literature review.

Module 2: Statistical analysis for Chemists

2.1 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.
2.2 Significant figures and rules to determine significant figures. Calculations involving significant figures.
2.3 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.
2.4 Application of Microsoft Excel in statistical analysis (statistical functions and spreadsheets in MS-Excel). Certified reference materials (CRMs). Numerical problems.

Module 3: Scientific Writing and Presentation

3.1 Scientific writing. Types of scientific publications- magazines, journals, reviews, news-letters, structure of scientific paper.
3.2 Report Writing, different steps in report writing, types of reports, layout of research paper.
3.3 Research indicators & Metrics: Impact Factor, CiteScore, h-Index, i10-Index, Citation Index, references/bibliography, structuring the thesis, use of software in thesis writing.
3.4 Intellectual Property Rights (IPR): Introduction to IPR (Patents, Trademarks, Geographical indicators, Copyright, and neighboring rights), concept and theories, kinds of IPR, Advantages and disadvantages of IPR.

Module 4: Use of tools / techniques for Research

4.1 Methods to search required information effectively, Various reference styles, Reference Management Software like Zotero/Mendeley, preparation of bibliography database.
4.2 Software/tools: MS Word, MS Excel, Graph and chart preparation, MS Power Point, OriginLab (For plotting graph), ChemSketch, ChemDraw.
4.3 Research ethics, Academic integrity, Plagiarism, types, detection of plagiarism using software.

Reference/ Books:

1) Shanti Mishra, & Alok, S. (2011). Handbook of Research Methodology: A Compendium for Scholars & Researchers. Educreation Publishing.
2) Singh, Y. kumar. (2006). Fundamentals of Research Methodology and Statistics. New Age International Publishers.
3) Walliman, N. (2010). Research Methods The Basics. Routledge Taylor and Francis Group.
4) Research Methodology- C. R. Kothari
5) Best and Kahn, Research Methodology, PHI Limited
6) Design of Experience: Statistical Principles of Research Design and Analysis, by Robert O. Kuehl Brooks/cole.

7) Patrick Carey, Katherine T. Pinard, Ann Shaffer, Mark Shellman, New Perspectives Microsoft Office 365 and Office 2019 Introductory, 2020.

Assignments based on Research Methodology course

Instructions:

These assignments can enhance the professional skills needed to pursue a career in research/teaching. Therefore, each PG department should identify 10 assignments from the list below. Continuous evaluation will occur throughout the semester. Performance on the assignment will be graded for 40 marks.

1. **Navigate and use Google, Google Scholar, SciHub, PubMed, Web of Science, Elicit and ScienceDirect effectively to search for research papers, perform searches and retrieve relevant research papers.**
   [Suggestion/Working hours:- Dedicate a few hours each week to practice searching on these databases to continually refine your skills.]

2. **Write accurately references in APA format for various types of sources, including books, journal articles, websites, and conference papers and gain a comprehensive understanding of the Zotero platform, including its interface, features, and capabilities for managing bibliographic information.**
   [Suggestion/Working hours- Invest time in exploring and understanding the features of Zotero(https://www.zotero.org/) through guided tutorials and hands-on experience and gain proficiency in using Zotero to input, organize, and format references, and effectively manage bibliographic data]

3. **How to read research paper and develop a thorough understanding of the three-pass approach for effective note-taking from research readings.**

4. **Review and analyze collected references systematically to identify at least three prospective research problems or gaps in your domain.**
   [Suggestion/Working hours:- Review a minimum of 20 relevant references in your domain to gain a comprehensive understanding of current research trends and gaps. Dedicate focused time each week to systematically review references and refine your problem identification skill]

5. **Write at least three research objectives and three hypotheses that are well-defined, focused, and aligned with the research problem.**
   [Suggestion/Working hours:-Within one month, be able to formulate clear and relevant research objectives or hypotheses for the given research problem. Seek feedback from mentors or advisors to refine your research objectives or hypotheses and ensure their relevance and clarity.]

6. **Create a graph (line/bar/pie) using Microsoft Excel. Prepare publication ready graph and write legend for the graph and table.**

7. **Understand structure of scientific poster. Write well-structured scientific poster that effectively communicates research findings, adheres to design principles, and captures audience attention.**

8. **Understand structure of oral presentation and demonstrate the ability to deliver a clear and engaging oral presentation, incorporating effective communication techniques, and supporting visual aids.**

9. **Find out how to use the chosen plagiarism detection tool step by step to check a paper for possible instances of plagiarism. Attain the ability to use the chosen plagiarism detection tool proficiently, including uploading documents, interpreting plagiarism reports, and understanding similarity scores.**

10. **Write one page research proposal. Write research proposal in the format of any funding agency.**

11. **Write minireview article.**

12. **Write short communication with one table and one figure.**

13. **Write scientific blog.**