ST ALOYSIUS

(DEEMED TO BE **UNIVERSITY**)

MANGALURU 575003 – INDIA

Re-accredited by NAAC "A++" Grade

Course Structure and Syllabus of First Year UG and PG

CHEMISTRY

The Academic Advisory Meeting in Chemistry was held on April 19, 2024

Following members were present for the meeting:

Chairperson

1. Dr Rachael Natasha Mary, Assistant Professor, St Aloysius Deemed to be University, Mangaluru

External Advisory Members

2. Dr Suchetan P A, Assistant Professor, Department of Chemistry, Tumkur University, Tumkur.
3. Dr Manoj Mathews, Associate Professor, Research and PG Department of Chemistry, St Joseph's College, Kozikode, Kerala.

Internal Members

4. Dr Ronald Nazareth, Registrar, St Aloysius Deemed to be University, Mangaluru.
5. Dr Chandrashekar Shetty, Associate Dean, School of Physical Sciences, St Aloysius Deemed to be University, Mangaluru.
6. Dr Vinola Rodrigues, Assistant Dean, School of Physical Sciences, St Aloysius Deemed to be University, Mangaluru.
7. Dr Ashwini, Associate Professor, St Aloysius Deemed to be University, Mangaluru
8. Ms Sahana, Assistant Professor, St Aloysius Deemed to be University, Mangaluru
9. Ms Divya Deepthi Monteiro, Teaching Staff Assistant, St Aloysius Deemed to be University, Mangaluru
10. Dr Roshan Fredrick DSouza, Assistant Professor, St Aloysius Deemed to be University, Mangaluru
11. Ms Meghana, Teaching Staff Assistant, St Aloysius Deemed to be University, Mangaluru
12. Ms Hencil Clita Pinto, Teaching Staff Assistant, St Aloysius Deemed to be University, Mangaluru
13. Ms Shreya Bhakta K, Teaching Staff Assistant, St Aloysius Deemed to be University, Mangaluru
14. Dr Jyothi N Rao, Assistant Professor, St Aloysius Deemed to be University, Mangaluru
15. Dr Divya N Shetty, Assistant Professor, St Aloysius Deemed to be University, Mangaluru
16. Dr John Deepak Shetty, Assistant Professor, St Aloysius Deemed to be University, Mangaluru
17. Ms Preema Cealla Pais, Assistant Professor, St Aloysius Deemed to be University, Mangaluru
18. Ms Jyothi Simav Vaz, Assistant Professor, St Aloysius Deemed to be University, Mangaluru
19. Mr Jeesu George, Assistant Professor, St Aloysius Deemed to be University, Mangaluru

20. Dr Akshatha R Salian, Assistant Professor, St Aloysius Deemed to be University, Mangaluru
21. Dr Joseline Neetha DSouza, Assistant Professor, St Aloysius Deemed to be University, Mangaluru

AGENDA:

1. Discussion and approval of semester I and II syllabus of UG and PG.
2. Discussion and approval of syllabus of Certificate courses.
3. Discussion and approval of PhD course work syllabus.
4. Any other matter.

Program Outcomes:

By the end of the program the students will be able to:

PO 1: Develop enthusiasm for Chemistry and its application in various fields of life.

PO 2: Have a broad and balanced knowledge and understanding of key concepts in Chemistry.

PO 3: Develop a range of practical skills to understand and assess risks and work safely measures to be followed in the laboratory.

PO. 4: Develop the ability to apply standard methodology to the solution of problems in Chemistry.

PO. 5: Use evidence based comparative chemistry approach to explain chemical synthesis and analysis.

PO 6: Gain knowledge and skill towards employment or higher education in Chemistry or multi-disciplinary areas involving Chemistry.

PO 7: Employ critical thinking and the scientific knowledge to design, carry out, record and analyze the results of chemical reactions.

SUMMARY OF DISCIPLINE SPECIFIC CORE (DSC)

Course Code	Title of the course	Category of course	Teaching hours per week	ESE	CIA	Total Marks	Credits
SEMESTER I							
G 502 DC1.1	ANALYTICAL AND ORGANIC CHEMISTRY- I	DSC	4	60	40	100	4
G 502 DC2.1P	ANALYTICAL AND ORGANIC CHEMISTRY PRACTICALS-I	DSC	4	25	25	50	2
G 502 OE1.1	CHEMISTRY IN DAILY LIFE	-	3	60	40	100	3
SEMESTER II							
G 502 DC1.2	INORGANIC AND PHYSICAL CHEMISTRY-I	DSC	4	60	40	100	4
G 502 DC2.2P	INORGANIC AND PHYSICAL CHEMISTRY PRACTICALS-I	DSC	4	25	25	50	2
G 502 OE1.2	ESSENTIALS OF PRACTICAL CHEMISTRY	-	3	60	40	100	3

BSc Chemistry (Discipline Specific Core)

FIRST SEMESTER

Course Title: **DSC-1: Analytical and Organic Chemistry - I**	
Course Code: G 502 DC1.1	
Total Contact Hours: 56	Course Credits: 4
Formative Assessment Marks: 40	Duration of ESA/Exam: 2.5 hrs
Summative Assessment Marks: 60	

Course Outcomes (COs): At the end of the course the student should be able to understand,

CO 1: The concepts of chemical analysis, accuracy, precision and statistical data treatment.

CO 2: The concept of volumetric and gravimetric analysis and deducing the conversion factor for determination.

CO 3: The concepts of organic reactions and techniques of writing the movement of electrons, bond breaking, bond forming and reactive intermediates involved.

CO 4: Understand the types of organic reactions with examples.

Unit – I

Introduction to Analytical Chemistry **2 Hrs**

Language of analytical chemistry: Definitions of analysis, determination, measurement, techniques and methods. Classification of analytical techniques. Qualitative analysis; Sample size and techniques - macro, semi-micro and micro. Type of tests - wet, dry and spot tests (terms, definition and examples); Quantitative analysis - Volumetry, Gravimetry and Instrumental analytical methods.

Gravimetric Analysis **3 Hrs**

Requisites of precipitation, mechanism of precipitation; Factors influencing precipitation, co-precipitation, post-precipitation; Advantages of organic reagents over inorganic reagents, reagents used in gravimetry (8-hydroxyquinoline and dimethylglyoxime).

Errors in Quantitative Analysis **4 Hrs**

Types of errors - determinate and indeterminate, methods of minimizing errors. Accuracy - absolute error, relative error. Precision – mean deviation, relative mean deviation, standard deviation, t-test, F-test and Q-test. Significant figures - Rules for computation of results; Problems.

General Purification Techniques **5 Hrs**

Principle, procedure and examples of sublimation, distillation (fractional, steam, distillation under reduced pressure) and crystallization.

Chromatography – Introduction, Types with examples (partition and adsorption), Rf value. Solvent extraction - basic principles and applications.

Nernst distribution law - definition; Partition coefficient; Distribution constant - factors affecting distribution constant, validity of Distribution Law, Modification of distribution law when molecules undergo (a) association (b) dissociation.

Unit – II

Titrimetric Analysis **14 Hrs**

Basic principle of titrimetric analysis. Classification, Preparation and dilution of reagents and solutions. Normality, Molarity and Mole fraction. Use of $N_1V_1 = N_2V_2$ formula, Preparation of ppm level solutions from source materials (salts). Standard solutions – primary and secondary standards. Problems.

Acid-base Titrimetry: Titration curves for strong acid *vs* strong base, weak acid *vs* strong base and weak base *vs* strong acid titrations; Indicators.

Complexometric Titrimetry: Indicators for EDTA titrations - theory of metal ion indicators, titration methods employing EDTA - direct, back, displacement and indirect determinations; Application - determination of hardness of water.

Redox Titrimetry: Balancing redox equations ($KMnO_4$ *vs* oxalic acid; $K_2Cr_2O_7$ *vs* Mohr's salt), calculation of the equilibrium constant of redox reactions, titration curves; Redox indicators; calculation of standard potentials using Nernst equation. Applications.

Precipitation Titrimetry: Titration curves, titrants and standards, indicators for precipitation titrations involving silver nitrate - Volhard's and Mohr's methods and their differences.

Unit – III

Classification and nomenclature of organic compounds, Hybridization (sp^3, sp^2 and sp); Shapes of organic molecules, Influence of hybridization on bond properties.

Nature of Bonding in Organic Molecules **10 Hrs**

Formation of Covalent bond, Types of chemical bonding, localized and delocalized, conjugation and cross conjugation, concept of resonance, electronic displacements: Inductive effect, Electromeric effect, Resonance effect and Hyperconjugation - explanation with examples. Concept of aromaticity, Huckel rule, anti-aromaticity explanation with examples.

Notations used to represent electron movements and directions of reactions – Types of arrows (curved, fish-hook, double headed), formal charges. Types of bonds breaking - homolytic and heterolytic. Types of reagents - Electrophiles, nucleophiles, nucleophilicity and basicity. Types of organic reactions - substitution, addition, elimination, rearrangement reactions; explanation with examples.

Reactive Intermediates - Carbocations, carbanion, free radicals, formation and their order of stability. Rearrangement of carbocations, 1,2-hydride and 1,2-methyl shift (by taking dehydration of 2-methylbutan-1-ol and 3,3-dimethyl-2-butanol as examples). Preparation of carbenes, concept of singlet and triplet carbene. Addition reactions of singlet and triplet carbenes. Concept of nitrenes and benzyne.

Carbon-Carbon pi bonds **4 Hrs**

Formation of alkenes by elimination reaction. Mechanism of E1, E2 reactions. Saytzeff and Hofmann eliminations. Addition of HBr to propene (Markovnikov's rule), Free radical addition of HBr to propene (anti-Markovnikov's rule). Addition of halogens to alkenes - carbocation and halonium ion mechanism.

Unit – IV

Dienes **4 Hrs**

Nomenclature, classification - isolated, conjugated and cumulated; Structure - hybridization; methods of preparation of 1,3-butadiene – dehydration and dehydrohalogenation. Addition reactions of 1,3-butadiene - polymerization; Mechanism of 1,2- and 1,4- addition of bromine and hydrogen bromide, effect of temperature, free radical addition to 1,3-butadiene; Diels-Alder reaction and its importance.

Nucleophilic Substitution at Saturated Carbon **4 Hrs**

Mechanism of S_N1 and S_N2 reactions with suitable examples (hydrolysis of *t*-butyl bromide and methyl bromide, respectively). Energy profile diagrams, and factors effecting S_N1 and S_N2 reactions.

Aromatic Electrophilic Substitution Reactions **3 Hrs**

Mechanisms, σ and π complexes, Halogenation, Nitration, Sulphonation, Friedel Crafts alkylation and acylation with their mechanism. Activating and deactivating groups. Orientation influence, *ortho-para* ratio.

Aromatic Nucleophilic Substitution Reactions **3 Hrs**

S_NAr and Benzyne mechanism with suitable examples. Relative reactivities of alkyl halides *vs* allyl, vinyl and aryl halide.

References:

1. A. Bahl and B. S. Bahl (2019), A Textbook of Organic Chemistry, S. Chand Publications, 22nd Edition.
2. B. K Sharma (2014), Instrumental Methods of Chemical Analysis, 30th Edition.
3. D. A. Skoog, D. M. West, Holler and Crouch (2005), Fundamentals of Analytical Chemistry, 8th edition, Saunders College Publishing, New York.
4. H. Kaur (2012), Instrumental methods of Chemical Analysis, Pragathi Prakashan, 10th

Edition.

5. J. Mendham, R. C. Denney, J. D. Barnes and M. J. K. Thomas (2007), Vogel's Textbook of Quantitative Chemical Analysis, Third Indian Reprint, Pearson Education Pvt. Ltd 6th edition.
6. J. Singh and L. D. S. Yadav (2016), Advanced Organic Chemistry, Pragati Prakashan.
7. P. Y. Bruice (2018), Organic Chemistry, 3rd Edition.
8. S. M. Mukherji, S. P. Singh and R. K. Kapoor (2017), Organic Chemistry, New Age International Publishers, 2nd Edition.
9. V. K. AhIuwalia and K. Parashar (2006), Organic Reaction Mechanisms, Narosa Publishers, 3rd Edition.

DSC LAB-1: ANALYTICAL AND ORGANIC CHEMISTRY PRACTICALS

Course Title: **DSC LAB-1: Analytical and Organic Chemistry Practicals - I**	
Course Code: **G 502 DC2.1P**	
Total Contact Hours: 4 hrs /week	Course Credits: 2
Formative Assessment Marks: 25	Duration of ESA/Exam: 4 hrs
Summative Assessment Marks: 25	

PART – A: Analytical Chemistry

1. Basic Laboratory Practices: Calibration of glassware (pipette, burette and volumetric flask), sampling, weighing and drying. Safety in Chemical laboratory, Rules of fire prevention and accidents, First aid.
2. Preparation of standard decinormal solution of sodium carbonate and standardization of hydrochloric acid and estimation of sodium hydroxide in solution.
3. Preparation of standard decinormal solution of potassium biphthalate and standardization of sodium hydroxide solution and estimation of hydrochloric acid in solution.
4. Determination of oxalic acid and sodium oxalate / sulfuric acid in a given mixture using standard $KMnO_4$/NaOH solution.
5. Preparation of standard decinormal solution oxalic acid and standardization of potassium permanganate solution and estimation of Mohr's salt in solution.
6. Preparation of standard decinormal solution of ferrous ammonium sulphate (Mohr's salt) and standardization of potassium dichromate solution and estimation of ferric chloride in solution.
7. Estimation of ferrous and ferric in a mixture.
8. Determination of sodium carbonate and sodium bicarbonate in a mixture.
9. Standardization of EDTA solution and determination of hardness of water.

PART – B: Organic Chemistry

1. Preparation of acetanilide from aniline using Zn/acetic acid (Green method).
2. Synthesis of p-nitro acetanilide from acetanilide using nitrating mixture.

3. Bromination of acetanilide (i) Conventional method and/or (ii) with ceric ammonium nitrate and potassium bromide (Green method).
4. Hydrolysis of methyl *m*-nitrobenzoate to *m*-nitrobenzoic acid (Conventional method)
5. Synthesis of diazoaminobenzene from aniline (conventional method).
6. Preparation of dibenzalacetone (Green method).
7. Diels Alder reaction between furan and maleic acid (Green method).

(Experiments for projects)

1. Determination of alkali content in antacid tablet using HCl.
2. Determination of alkali present in soaps/detergents.
3. Standardization of silver nitrate and determination of chloride in a water sample
4. Determination of chlorine in bleaching powder using iodometric method.

References:

1. G. H. Jeffery, J. Bassett, J. Mendham, R. C. Denney, John Wiley & Sons (1989) Vogel's textbook of Quantitative Chemical Analysis, 5th Ed.

2. O. P. Pandey, D. N. Bajpai, S. Giri (2000), Practical Chemistry for B.Sc. - I, II, III Year Students, S. Chand & Company.

3. V. K. Ahluwalia, and Renu Aggarwal (2000), Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis, University Press.

BSc Semester 1

Title of the Course: OE-1: CHEMISTRY IN DAILY LIFE Course Code: G 502 OE1.1

Number of Theory Credits	Number of lecture hours / semester	Number of practical credits	Number of practical hours/semester
3	42	-	-

Course Outcomes (COs): At the end of the course the student should be able to understand,

CO 1: Chemistry involved in dairy products and food additives

CO 2: Adulterants in food

CO 3: Structure and importance of vitamins

CO 4: Composition and applications of polymers

Unit – I 14 Hrs

Dairy Products: Composition of milk and milk products. Analysis of fat content, minerals in milk and butter. Estimation of added water in milk. Beverages: Analysis of caffeine in coffee and tea, detection of chicory in coffee, chloral hydrate in toddy, determination of methyl alcohol in alcoholic beverages.

Food additives, adulterants, and contaminants- Food preservatives like benzoates, propionates, sorbates, disulphites. Artificial sweeteners: Aspartame, saccharin, dulcin, sucralose, and sodium cyclamate. Flavors: Vanillin, alkyl esters (fruit flavors), and monosodium glutamate.

Artificial food colorants: Coal tar dyes and non-permitted colors and metallic salts. Analysis of pesticide residues in food.

Unit – II 14 Hrs

Vitamins: Classification and Nomenclature. Sources, deficiency diseases, and structures of Vitamin A1, Vitamin B1, Vitamin C, Vitamin D, Vitamin E & Vitamin K1.

Oils and fats: Composition of edible oils, detection of purity, rancidity of fats and oil. Tests for adulterants like argemone oil and mineral oils. Halphen test.

Soaps & Detergents: Definition, classification, manufacturing of soaps and detergents, composition and uses.

Unit – III 14 Hrs

Chemical and Renewable Energy Sources: Principles and applications of primary & secondary batteries and fuel cells. Basics of solar energy, future energy storer.

Polymers: Basic concept of polymers, examples for polymers with their monomers, Classification of polymers according to mechanical properties, General classification (thermosetting and thermoplastic; condensation and addition polymers), organic polymers, inorganic polymers, copolymers (definition with examples) Applications of polymers– plastics, elastomers, fibres medical fields. Problems of plastic waste management. Strategies for the development of environment-friendly polymers.

References:

1. B. K. Sharma (2006), Industrial Chemistry, Goel Publishing, Meerut, 15th Edition.
2. B. Swaminathan and M. Goswamy (2001), Handbook on Fertilizer Technology, Fertilizer Association of India, 6th Edition.
3. H.E. Cox and D. Pearson (1962), The Chemical Analysis of Foods, 5th Edition.
4. I. L. Finar (2000), Organic Chemistry, Vol. 2, Pearson, 5th Edition.
5. I. L. Finar (2002), Organic Chemistry, Vol. 1, Pearson, 6th Edition.
6. J. R. Fried (2014), Polymer Science and Technology, Prentice Hall, 3rd Edition.
7. N. S. Manay and M. Shadaksharaswamy (2020), Foods: Facts and Principles, , New Age International Publishers, 4th Edition.
8. P. Atkins and J. D. Paula (2002), Physical Chemistry, Oxford University Press, 7th Edition.

SECOND SEMESTER

Course Title: **DSC-2: Inorganic and Physical Chemistry - I**	
Course Code: G 502 DC1.2	
Total Contact Hours: 56	Course Credits: 4
Formative Assessment Marks: 40	Duration of ESA/Exam: 2.5 hrs
Summative Assessment Marks: 60	

Course Outcomes (COs): At the end of the course the student should be able to understand,

CO 1: Basics of Quantum mechanics, quantum numbers and its significance.

CO 2: Variation in properties of s and p block elements.

CO 3: Molecular velocities associated with gases.

CO 4: Different types of crystal systems, structure of liquid crystals and its applications.

Unit – I

Quantum Mechanics-I **14 Hrs**

Bohr's theory, its limitations and atomic spectrum of hydrogen atom. Wave mechanics: de Broglie equation, Heisenberg's Uncertainty Principle and its significance, Schrödinger's wave equation, significance of ψ and ψ^2. Quantum numbers and their significance.

Normalized and orthogonal wave functions. Sign of wave functions. Radial and angular wave functions for hydrogen atom. Radial and angular distribution curves. Shapes of *s*, *p*, *d* and *f* orbitals.

Pauli's Exclusion Principle, Hund's rule of maximum multiplicity, Aufbau's principle and its limitations- Electronic configurations of the elements (Z=1-30), effective nuclear charge, shielding/screening effect, Slater's rules. Variation of effective nuclear charge in Periodic Table.

Unit - II

s and *p* block elements 4 Hrs

Variation of the following properties with reference to *s* and *p*-block elements: atomic radii (van der Waals); ionic and crystal radii; covalent radii; ionization enthalpy - successive ionization enthalpies and factors affecting ionization energy - applications of ionization enthalpy; electron gain enthalpy – trends; electronegativity - Pauling's, Mulliken's, Allred Rachow's and Mulliken-Jaffé's electronegativity scales - variation of electronegativity with bond order, partial charge, hybridization.

Chemistry of *s*-Block Elements 5 Hrs

Hydrogen - isotopes; hydrides – types (ionic, covalent, interstitial, polymeric, complex), preparation and properties; structure of NaH and BeH_2; applications of complex hydrides ($LiAlH_4$, $NaBH_4$). Comparison of standard reduction potentials and reducing properties of alkali metals and alkaline earth metals. Complexation tendencies of alkali metals with crown ether, cryptates. Diagonal relationship - reasons for diagonal relationship, comparison of the properties of Li with Mg and Be with Al.

Chemistry of *p*-Block Elements 5 Hrs

Comparative study of *p*-Block elements and their compounds. Boranes – Diborane (Preparation, properties, structure and bonding), B_4H_{10}, B_5H_9 - structure; Styx number, Wade's rule – closo-, nido- and arachno-boranes. Silicates - types, basic units, structure and applications of zeolites. Noble gases - structure and bonding in Clathrates, XeF_2, XeF_4, XeF_6 and XeO_3.

Unit – III

Gaseous State 8 Hrs

Elementary aspects of kinetic theory of gases, Ideal and real gases. Boyle temperature (no derivation), Molecular velocity, collision frequency, collision diameter, Collision cross section, collision number and mean free path and coefficient of viscosity, calculation of σ and η, variation of viscosity with temperature and pressure.

Maxwell's Boltzmann distribution law of molecular velocities (Most probable, average and root mean square velocities). Relation between RMS, average and most probable velocity and average kinetic energies. (Mathematical derivation not required).

Behaviour of real gases: Deviation from ideal gas behaviour. Compressibility factor (Z) and its variation with pressure for different gases. Causes of deviation from ideal behaviour, vander Waals equation of state (no derivation) and application in explaining real gas behaviour. Critical phenomena - Andrews isotherms of CO_2, critical constants and their calculation from Van der Waals equation, Continuity of states, Law of corresponding states. Numerical problems.

Liquid State **6 Hrs**

Surface Tension: Definition and its determination using stalagmometer, effect of temperature on surface tension.

Viscosity: Definition, Coefficient of viscosity. Determination of viscosity of a liquid using Oswald viscometer. Effect of temperature, size, weight, shape of molecules and intermolecular forces.

Refraction: Specific and molar refraction - definition and advantages. Determination of refractive index by Abbes Refractometer. Additive and constitutive properties.

Parachor: Definition, Atomic and structure parachor; Elucidation of structure of benzene and benzoquinone. Viscosity and molecular structure. Molar refraction and chemical constitution**.**

Unit – IV

Liquid Crystals **4 Hrs**

Explanation, classification with examples - Smetic, nematic, cholesteric, discotic shaped and polymeric. Structures of nematic and cholesteric phases - molecular arrangements in nematic and cholesteric liquid crystals. Applications of liquid crystals.

Solid State **10 Hrs**

Forms of solids: Unit cell and space lattice, anisotropy of crystals, size and shape of crystals, Laws of Crystallography: Law of constancy of interfacial angles, Law of rational indices, Law of symmetry; Symmetry elements – Types: (a) axis of symmetry (b) plane of symmetry (c) centre of symmetry - definition and explanation taking cubic crystal system as an example. Crystal systems, Bravais lattice types and identification of lattice planes. Miller indices and its calculation, X–Ray diffraction by crystals: Bragg's law and derivation of Bragg's equation, Single crystal and powder diffraction methods. Cesium Chloride, Zinc

blende structures. Defects in crystals (Schottky and Frenkel), glasses and liquid crystals. Numerical problems.

References:

1. A. K. Das (2013), Fundamentals Concepts of Inorganic Chemistry, Vol. 1 and 2, CBS Publishers and Distributors, 2nd Edition.
2. A. S. Negi & S. C. Anand (2007), A Textbook of Physical Chemistry, New Age International Publishers, 2nd Edition.
3. B. R. Puri, L. R. Sharma and M. S. Pathania (1962), Principles of Physical Chemistry, Vishal Publishing Co., 46th Edition..
4. F. A. Cotton, G. Wilkinson and P. L. Gaus, (2007), Basic Inorganic Chemistry, Wiley, 3rd Edition
5. G. Raj (2016), Advanced Physical Chemistry, Goel Publishing House, 4th Edition.
6. J. D. Lee (2021), Concise Inorganic Chemistry, Wiley, 4th Edition.
7. P. Atkins and J. D. Paula (2006), Atkins Physical Chemistry, Oxford University Press, 8th Edition.
8. P. J. Collings and M. Hird (1997), Introduction to Liquid Crystals, CRC Press, 1st Edition.
9. P. L. Soni, O.P. Dharmarha and U. N. Dash (2011), A Textbook of Physical Chemistry, Sultan Chand and Sons.
10. S. Glasstone (1996), Textbook of Physical Chemistry, Macmillan.

DSC LAB-2: INORGANIC AND PHYSICAL CHEMISTRY PRACTICALS

Course Title: **DSC LAB-2: Inorganic and Physical Chemistry Practicals-I**	
Course Code: **G 502 DC2.2P**	
Total Contact Hours: 4 hrs /week	Course Credits: 2
Formative Assessment Marks: 25	Duration of ESA/Exam: 4 hrs
Summative Assessment Marks: 25	

PART-A Inorganic Chemistry

Gravimetry

1. Determination of Ba^{2+} as $BaSO_4$
2. Determination of Cu^{2+} as CuSCN
3. Determination of Fe^{2+} as Fe_2O_3
4. Determination of Ni^{2+} as $Ni(DMG)_2$ complex.
5. Determination of Chloride/Silver as AgCl.
6. Determination of Magnesium as oxinate.

PART-B Physical Chemistry

1. Determination of density using specific gravity bottle and viscosity of liquids using Ostwald's viscometer (Ethyl acetate, Toluene, Chloroform, Chlorobenzene or any other non-hazardous liquids)
2. Study of the variation of viscosity of sucrose solution / Glycerol-water mixture with the concentration of solute / mixture.
3. Determination of the density using specific gravity bottle and surface tension of liquids using Stalagmometer (Ethyl acetate, Toluene, Chlorobenzene, any other non-hazardous liquids
4. Study of variation of surface tension of detergent solution with concentration.
5. Determination of the composition of liquid mixture by refractometry (Toluene & Alcohol, Water & Sucrose).
6. Determination of partition/distribution coefficient - i) Acetic acid in water and cyclohexane. ii) Acetic acid in Water and Butanol. iii) Benzoic acid in water and toluene.

(Experiments for projects)

1. Determination of vitamin C content in food.
2. Effluent water analysis: determination of DO, COD, Conductivity, pH.

References:

1. G. H. Jeffery, J. Bassett, J. Mendham, R. C. Denney (1989) Vogel's textbook of Quantitative Chemical Analysis, John Wiley & Sons, 5th Ed.

2. O. P. Pandey, D. N. Bajpai, S. Giri, S (2000), Practical Chemistry for B.Sc. - I, II, III Year Students, Chand & Company.

BSc Semester 2

Title of the Course: OE – 2: Essentials of Practical Chemistry

Course Code: G 502 OE1.2

Number of Theory Credits	Number of lecture hours/semester	Number of Practical Credits	Number of practical hours/ semester
3	42	-	-

Course Outcomes (COs): At the end of the course the student should be able to understand,

CO 1: Laboratory safety measures and use of glassware

CO 2: Qualitative analysis of inorganic ions

CO 3: Basic laboratory techniques

CO 4: Applications of nanotechnology and characterization techniques.

Unit – I

Apparatus Handling and Lab Safety **2 Hrs**

Use of balance, glasswares, burette, pipette, dessicator, filtration apparatus.

Safe use of chemicals, Laboratory precautions.

Qualitative Organic Analysis **6 Hrs**

Determination of melting point and boiling point, detection of elements - N, S and halogen (Lassaigne's Test), detection of unsaturation, reactions of functional groups, preparation of derivatives, recrystallization.

Semi-micro Qualitative Inorganic Analysis **6 Hrs**

Advantages of Semi-micro analysis, wet and dry tests, flame test, centrifugation, reactions of anions, classification of cations into groups, Reactions of cations. Preparation of Nessler's Reagent, Tollen's Reagent, lime water, Bromine water, H_2S.

Unit - II

Quantitative Analysis

Basic Techniques **4 Hrs**

Calibration, washing precipitates, Drying and igniting precipitates, Preparation of common reagents (dilute acids, dilute bases, indicator solutions), problems.

Reactions in Solutions **7 Hrs**

Solubility Product, Common ion effect, Fractional precipitation, Factors affecting solubility (Acid concentration, Temperature, Solvent), Ionic product of water, pH and pOH, Buffer solutions, Solubility and complexation, problems on pH, pOH, buffers, solubility.

Estimation of Elements **3 Hrs**

Principle and calculation involved in the estimation of Nitrogen by Kjeldahl's method, Sulphur and Halogen by Carius method, Carbon and Hydrogen by Leibig's method.

Unit - III **14 Hrs**

Nano Chemistry

Introduction, nanostructures, types with examples, quantum structures, synthesis – electrodeposition, chemical vapour deposition, coprecipitation, hydrothermal synthesis, sol gel method, properties of carbon nano structures.

Physicochemical properties, redox properties, magnetic property of nanomaterials. Inorganic nanotubes and nano wires. Nanocomposites and nanofibers. Applications of nanotechnology in catalysis, biology, nano filters, nano switches, nanomedicines. Characterisation techniques - SEM, XRD, IR.

References:

1. B. Vishwanathan (2013), Nanomaterials, Narosa Publishing house.

2. C.N R Rao (2016), An introduction to Nanoscience and Technology.

3. F. G. Mann and B. C. Saunders (2009), Practical Organic Chemistry, 4th Ed.

4. G. Svehla, B. Sivasankar (2012), Vogel's Qualitative Inorganic Analysis, Pearson Education India, 7th Ed.

4. J. Singh, R.K.P. Singh, J. Singh, L.D.S. Yadav, I. R. Siddiqui, J. Srivastava (2018), Advanced Practical Chemistry.

5. V. K. Ahluwalia, Renu Aggarwal (2000), Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis, University Press.

6. V.K. Ahluwalia, S. Dhingra (2001), Comprehensive Practical Organic Chemistry: Qualitative Analysis, Sangam Books.

Formative Assessment for theory

Assessment Type	**Marks**
Two Internal Tests	10 x 2 = 20
Assignment	5
MCQs	5
Group project	5
Attendance	5
Total	**40**

Formative Assessment for practical

Assessment Type	**Marks**
Continuous assessment	15
Class records	5
Model Practical test	20
Attendance	5
Viva	5
Total	**50 (Converted to 25)**

PATTERN OF THEORY QUESTION PAPER

- Question Papers shall consist of Parts A, B and C

- The Syllabus of each paper shall be grouped into four (4) units.

- The question papers shall consist of Parts A, B and C containing questions drawn from each unit.

- Part A shall contain ten short answer type questions carrying 1 mark each drawn from each unit of the syllabus. Eight questions are to be answered.

  (8 x 1) = 8

- Part B shall contain ten questions carrying 3 marks each drawn from each unit of the syllabus. Eight questions are to be answered.

  (8 x 3) = 24

- Part C shall contain nine questions carrying 4 marks each drawn from each unit. Seven questions are to be answered.

  (7 x 4) = 28

St Aloysius

(Deemed to be University)

Mangalore

Course structure and Syllabus

M.Sc. CHEMISTRY

CHOICE BASED CREDIT SYSTEM

(CBCS)

(2024 –25 BATCH ONWARDS)

PREAMBLE:

St. Aloysius (Deemed to be University) established in 1880 as a minority institution is managed by the Jesuit Fathers of Mangalore Educational Society (MJES). The Department of Chemistry, a pioneer in Chemistry education in the district, aims at building total personality of the student transforming young boys and girls into men and women for others, having compassion concern and commitment to the society. The M.Sc Course in analytical chemistry is an added commitment to the cause of higher education with an aim of serving the community. The course was started under the affiliation of Mangalore University and now is brought under Autonomy. Hence though the same syllabus has been retained with minor modifications, structural changes are incorporated to suit the credit system under autonomy.

OBJECTIVES:

- To provide knowledge and skills in the field of analytical chemistry
- To generate manpower trained in analytical chemistry to meet the need of industry and academia.
- To train students to pursue research in the field of chemistry.
- To impart training in laboratory skills.
- To develop the personality of an individual by giving them the necessary skills.
- To offer 100% placement assistance.

SCOPE OF THE COURSE:

M.Sc in General chemistry is a post graduate course with job opportunities in industry, teaching and research. The Research and Development section of every industry requires personnel who are trained in and handling various instruments. The course structure and curriculum is designed to enable the students to develop analytical and creative abilities which are very much needed by the industry and enable them to face national level competitive exams. The Course is definitely at par with M.Sc Organic Chemistry, M.Sc Analytical chemistry, M.Sc Medicinal Chemistry etc.

COURSE INTAKE:

The maximum number of students to be admitted to the course is 30 each year.

ELIGIBILITY

- Candidates would have studied any branch of Physical or biological science with chemistry as one of the major / optional subject in the under graduate level
- Not less than 45%(40% in case of SC/ST students) marks in the aggregate excluding languages in the under graduate level.
- The students should have studied physics and Mathematics at the higher secondary level.

SYLLABUS

- The course will be conducted in accordance to the semester system
- Each semester consists of 20 weeks inclusive of examinations.
- All examinations including practical/ project/viva will conclude by the end of the 20th week.
- A candidate should secure overall a minimum 40% marks in each paper, including both internal assessment and end semester examination.
- A minimum of 35 % in each paper of end semester examination
- 75% attendance is the minimum requirement for appearing for the semester examinations

EVALUATION SYSTEM

- The evaluation system of the course is based on two components. (i) Continuous evaluation (ii) End semester Examination.
- Continuous Evaluation: Based on this Internal assessment marks are allotted. It includes the following criterion-
- 50% marks for two internal assessment examination- Two examinations of 1 hour 30 minutes duration each carrying 50 marks in each semester are conducted. Total marks secured are reduced to 25.
- 3 marks are given for class participation.

- 7 marks are allotted for class seminar and 5 marks for quiz
- Ten marks for writing assignments and reviews.
- In the practicals of the first and second semester, one model examination is conducted for 40 marks and 10 marks for the viva. The marks are reduced to 25, continuous evaluation is done for 12 marks, 10 marks for class records and 3 marks for class participation. These marks are reduced to 15.
- In the practicals of the third and fourth semester, one model examination is conducted for 40 marks and 10 marks for viva. The marks are reduced to 25, continuous evaluation is done for 12 marks, 10 marks for class records and 3 marks for class participation. These marks are reduced to 30

END SEMESTER EXAMINATION

- Each end semester examination is conducted out of 70 marks. End semester examination question paper consists of questions to assess the conceptual, comprehensive and analytical abilities of the students.
- In all four semesters end semester practical exam is conducted in 50 marks

(40 marks for practical proper and 10 marks for the viva) and the marks are reduced to 35.

PROJECT WORK

- The project work shall be carried out in the last semester for 75 Hours.
- Can be carried out either in the institution or in an Approved Industry or in both.
- To be carried out under the supervision of a teacher and submit a project report.
- Experts from the industries may also be involved in the project work as co-guides and in the evaluation of project reports.

Evaluation

Project will be evaluated for hundred marks which includes presentation of the project.

Program Outcomes:

By the end of the program the students will be able to:

PO1: Inculcate critical thinking to carry out scientific investigation objectively in industry and academia by following scientific approach to knowledge development

PO2: Equip the student with necessary skills to analyse scientific problems, formulate hypothesis, evaluate and validate results, and draw conclusions from the data obtained

PO3: Equip the student with the knowledge for clear understanding of the subject related concepts to lead them for interdisciplinary and trans disciplinary research

PO4: Induce the sense of professional and ethical responsibility and enhance the cross cultural competency

PO5: Demonstrate an understanding of major concepts in all disciplines of chemistry

PO6: Get an awareness of the impact of chemistry on the environment, society, and other cultures outside the scientific community

Structure, Credits and Scheme of Examination of the Postgraduate Courses under Choice Based Credit System

M.Sc. Chemistry 2024							
I Semester = 3 Hard core and 1+5 soft core paper							
Code	**Papers**	**Hours / Week**	**Duration of Exam**	**Marks**		**Total**	**Credits**
				IA	**End Sem**		
PH 581.1	Inorganic Chemistry	4	3	30	70	100	4
PH 582.1	Organic Chemistry	4	3	30	70	100	4
PH 583.1	Physical Chemistry	4	3	30	70	100	4
PS 584.1 PS 585.1	Principles of Analytical Chemistry & Separation Techniques **or** Bioorganic Chemistry	3	3	30	70	100	3
PS 586.1	Research Methodology	3	3	30	70	100	3
PS 587.1P	Inorganic Chemistry - Practicals – I	4	4	15	35	50	2
PS 588.1P	Organic Chemistry Practicals – I	4	4	15	35	50	2
PS 589.1P	Physical Chemistry Practicals – I	4	4	15	35	50	2
						650	**24**
II Semester = 3 Hard core and 1+4 soft core paper and open elective 1 paper							
PH 581.2	Advanced Inorganic Chemistry	4	3	30	70	100	4
PH 582.2	Advanced Organic Chemistry	4	3	30	70	100	4
PH 583.2	Advanced Physical Chemistry	4	3	30	70	100	4
PS 584.2 PS 585.2	Molecular Symmetry and Molecular Spectroscopy **Or** Chemistry of Biomolecules	3	3	30	70	100	3
PS 586.2P	Inorganic Chemistry Practicals – II	4	4	15	35	50	2
PS 587.2P	Organic Chemistry Practicals – II	4	4	15	35	50	2

PS 588.2P	Physical Chemistry Practicals – II	4	4	15	35	50	2
PO 589.2	**Spectral Methods Of Analysis**	3	3	30	70	100	3
						650	**24**

FIRST SEMESTER

PH 581.1: INORGANIC CHEMISTRY

Course Outcome:

Student will be able to:

- **Explain the chemistry of acids, bases, non-aqueous solvents and** the concepts of hard and soft acids and bases
- Describe the types of bonds and molecular shape of compounds with emphasis on VSEPR, VB and MO theory of complexes.
- **Discuss the properties of the non-transition elements like C, B and Si and the**ir **frameworks**
- Illustrate the properties and justify the anomalies of Nitrogen, Phosphorus, Sulphur and noble gas compounds.

FIRST SEMESTER

PH 581.1: INORGANIC CHEMISTRY

UNIT I: **14 hours**

Electronic configuration of atoms, Auf Bau principle, Pauli's exclusion principle, Hunds rule, Slaters rule of the determination of screening constants. Trends in atomic & ionic radii, variation of IP, EA.

Hydrogen bond: types and detection. Intermolecular Forces: Ion-dipole, dipole dipole, ion-induced dipole, dipole-induced dipole interactions, London forces.

Ionic bond: Properties of ionic substances, coordination number of an ion, structures of crystal lattices- NaCl, CsCl, ZnS and Rutile. Lattice energy- Born Lande equation, Born-Haber cycle, Uses of Born-Haber type of calculations. Ionic radii, methods of determining ionic radii, factors affecting ionic radii, radius ratio rule, covalent character in ionic bonds.

Covalent bond: valence bond theory, formal charge, Concept of resonance & resonance energy, hybridization, Dipole moment and percentage ionic character, Deduction of molecular shapes – VSEPR theory, MO theory: application to homo (F_2 and N_2) and hetero diatomic (CO) and triatomic molecules (BeH_2 and nitrite ion).

UNIT II: **14 hours**

Review of acid- base concepts: Arrhenius theory, Bronsted-Lowry theory, Lewis theory, General properties of solvents. Classification of solvents. Factors justifying the need of Non Aqueous solution Chemistry and failure of water as a Solvent.

Acids and Bases: Measures of acid-base strength, Factors affecting strengths of hydracids, oxoacids and Lewis acids and bases, Drago - Wayland equation for Lewis acid - base interactions. Hard & soft acid-bases, Lux-Flood, Usanovich & solvent system

definition of acids and bases, solvent levelling effect, HSAB concepts, Symbiosis. Super acids - Hammet acidity function, Superacids based on arsenic and antimony

Non-aqueous solvents: Molten salts as solvents, ionic liquids, reactions in ionic liquids and applications of ionic liquid media, reactions in liq NH_3, liq SO_2, anhydrous HF as solvents. Supercritical fluids: Properties of supercritical fluids and their uses as solvents.

UNIT III: 14 hours

Diagonal relationship between Boron & Silicon. Similarities in properties of Boron and Silicon.

Chemistry of higher boranes: Classification, types of bonds in higher boranes- the styx number, structures and M.O. description of bonding, framework electron counting, Wade's rules, chemistry of B_6H_{10}, $B_{10}H_{14}$ and $B_nH_n^{2-}$.

Carboranes: Classification, Wade's rules, nomenclature, structures of CB_5H_9, $C_2B_4H_8$, $C_3B_3H_7$ and $C_4B_2H_6$.

Borazine: Structure, preparation, properties. Difference in chemical properties between borazine and benzene, borazine derivatives (N & B substituted). Structure and preparation of boron nitride.

Silicates: Classification, structure, applications – Pyroxenes & amphiboles, Silicones, & zeolites. Aluminosilicates.

UNIT IV: 14 hours

Allotropes of nitrogen and sulphur, electronic configuration of N, P, S. Properties of inert gases, general physical properties and their oxidation states.

Hydrides, oxides and oxyacids of nitrogen, phosphorous, sulphur & halogens.

Phosphazenes- Classification, Cyclophosphazenes-$(NPCl_2)_3$ and $(NPCl_2)_4$ -preparation and structure, Linear polyphosphazenes- preparation and applications, phosphazene polymers. Sulphur-nitrogen compounds- Preparation and structures of S_4N_4 and S_2N_2, $(SN)_x$

Condensed phosphates – linear polyphosphates, long chain polyphosphates and metaphosphates

Inter halogens, pseudohalogens, polyhalide ions, oxyhalogen species.

Noble gas compounds: Xenon oxides and fluorides-Preparation, properties and structures.

REFERENCES:

1. B. E. Douglas, D. McDaniel and A. Alexander (2001), Concepts and Models of Inorganic Chemistry, Wiley.
2. D.F. Shriver, P.W. Atkins and C.H. Langford (1994), Inorganic Chemistry, Oxford Univ. Press, 2nd Edition
3. F.A. Cotton, G. Wilkinson and P. L. Gaus (1995), Basic Inorganic Chemistry, John-Wiley and Sons, 3rd Edition.
4. J. Barrett and M.A. Malati (1998), Fundamentals of Inorganic Chemistry, Harwood.
5. J. D. Lee (2000), Concise Inorganic Chemistry (2000), Blackwell Science, 5th Edition.
6. J.E. Huheey, E.A. Keiter and R.L. Keiter (2000), Inorganic Chemistry – Principles of Structure and Reactivity, Pearson Education Asia Pvt. Ltd., 4th Edition.
7. Madan and Tuli (2010), Selected Topics in Inorganic Chemistry, S Chand, 17th Edition.
8. Manku (2008), Inorganic Chemistry, Tata- McGraw Hill, 1st Edition.
9. Meissler and Tarr (2013), Inorganic Chemistry, Pearson, 5th Edition.
10. N.N. Greenwood and A.E. Earnshaw (1997), Chemistry of Elements, Butterworth Heinemann.
11. Puri, Sharma and Kalia (2016), Principles of Inorganic chemistry, Vishal Publishing House, 33rd Edition.
12. W. W. Porterfield (2005), Inorganic Chemistry-A Unified Approach, Elsevier.

PH 582.1 : ORGANIC CHEMISTRY

Course Outcome:

Student will be able to:

- Explain the basic concepts of organic chemistry and the forces of attraction between different molecules.
- Explain the reaction intermediates and mechanisms.
- Demonstrate the importance of conformation and stereochemistry in understanding the reactivity and stability of organic molecules
- Detail the synthesis and stereochemistry of carbohydrates

UNIT I **14 Hours**

Types of bonding, reactions (specify types), Bonds weaker than covalent: Hydrogen bonds types and applications, intermolecular forces; ion-dipole, dipole-dipole ion induced dipole, dipole-induced dipole interactions and London forces.

Nature of Bonding in Organic Molecules: Localized and delocalized bonding, Conjugation, cross conjugation, resonance, hyper-conjugation and

tautomerism and inductive effects. Aromaticity in benzenoid and non-benzenoid molecules, Huckel rule, alternant and non-alternant hydrocarbons, Homo-aromatic and anti-aromatic systems. Annulenes and hetero-annulenes. Physical methods to study aromaticity-UV, IR & ^{1}H NMR. Addition compounds, Crown ether complexes and Cryptands inclusion compounds, cyclodextrins, Catenanes, rotaxanes and bonding in Fullerences

Acids and Bases : organic acids and bases, pKa and pH, effect of solvent on acid and base strength, effect of structure of organic compound on acid and base strength, relative strengths of acids and bases based on inductive, mesomeric and steric effects.

UNIT II **14 Hours**

Homolytic and heterolytic fission, carbanions and carbocations free radicals, relative stability.

Reaction Intermediates: Generation, structure, stability, reactivity and detection of classical and non-classical, carbenes, nitrenes and arynes(with at least two reactions for each type of intermediates).

Methods of Determining Reaction Mechanism: Identification of products, detection of intermediates, isotopic labeling, stereochemical evidences, cross-over experiments, kinetic evidences and kinetic isotopic effects. Hammett and Taft equations

UNIT III: **14 Hours**

Stereochemistry *Elements of symmetry, Chiral centres, chirality,Chiral molecules, Optical isomerism of lactic acid and tartaric acids.*

Optical Isomerism: Conformation and configuration of molecules, projection formulae, Ball & Stick and Barton Models, Fischer, Saw-horse, Newmann and Flying wedge representations. Absolute configuration (D,L) and (R,S) systems. Molecules with more than one chiral centre, threo and erythro isomers, methods of resolution, stereo specific and stereo selective synthesis, Cram's and Prelog's rules. Optical activity in the absence of chiral carbon-biphenyls, allenes and spiranes. Stereochemistry of compounds containing nitrogen, sulphur and phosphorus. Conformational analysis of cycloalkanes and decalins. Effect of conformation on reactivity.

Asymmetric synthesis, Sharpless reaction.

Geometrical Isomerism: Cis-trans isomerism resulting from double bonds, monocyclic compounds and fused ring systems. E Z-notations, determination of configuration of geometrical isomers, syn and anti-isomers

UNIT IV: **14 Hours**

Carbohydrates: Structural elucidation of fructose, Configuration and conformation of monosaccharide, Chemistry of important derivatives of monosaccharide-ethers, esters, acetals, ketals, deoxysugars, amino sugars. Structures of cellulose, chitin, starch, glycogen, heparin and chondritin.

Organic Name Reactions: Reactions, Mechanisms and synthetic uses of the following: Stobbe condensation, Darzen condensation, Gattermann-Koch reaction, Cannizzaro reaction,Duff reaction Chichibabin reaction, Benzoin condensation, Claisen-Schmidt condensation, Claisen reaction, Simon-Smith reaction, Stork Enamine reactions, Sharpless asymmetric epoxidation, Hofmann-Loffler-Freytag reaction, Woodward and Prevost Hydroxylation, Bucherer reaction, Ullmann reaction. Wittig reaction-Mitsunobu reaction, Stephen reaction.

REFERENCES:

1. Chatwal (2008), The Reaction Mechanism and Reagents in Organic Chemistry, Himalaya, 5th Edition.

2. Claydon and Greaves (2014), Organic Chemistry, Oxford University Press, 2nd Edition.

3. E. L. Eliel (1994), Stereochemistry of Carbon Compounds, Tata McGraw Hill, New Delhi.

4. I. L. Finar (Vol I and II) (1997), Organic Chemistry, ELBS, England.

5. J. Singh and L.D.S Yadav, Advanced Organic Chemistry.

6. P. S. Kalsi (2010), Stereochemistry, Conformation and Mechanism, Wiley Eastern, New Delhi, 6th Edition.

7. P. Y. Bruice (2002), Organic Chemistry, Pearson Education Pvt. Ltd., New Delhi.

8. R.A. Carey and R.J. Sundberg (2008), Advanced Organic Chemistry, Plenum, New York, 5th Edition.

9. R. K. Bansal (2006), A Text book of Organic Chemistry, New Age, New Delhi, 5th Edition

10. R.T. Morrison and R.N. Boyd (2005), Organic Chemistry, Prentice Hall, New Delhi, 7th Edition.

11. V. K. Ahluwalia and Rakesh Kumar Parashar, Organic Reaction Mechanisms, 4th Edition.

PH 583.1: PHYSICAL CHEMISTRY

Course Outcome:

Student will be able to:

- Understand the basic concepts of thermodynamics and its applications.
- Recollect the basics and understand fundamental ideas of chemical kinetics and its applications
- Familiarize with the various concepts in heterogeneous catalysis.
- Study and apply the principle and applications of electrochemistry

UNIT – I : 14 hours

Concept of Entropy, Enthalpy and Free energy (Gibb's and Helmholtz).A brief resume of laws of thermodynamics (combined form of 1st and 2nd laws), entropy as a measure of unavailable energy.

Chemical Thermodynamics: Concept of fugacity and free energy, entropy and free energy changes and spontaneity of processes. Variation of free energy with T & P, Maxwell's relations, thermodynamics equations of state, limitations of Van't Hoff's equation, Nernst heat theorem & its applications. Third Law of Thermodynamics, determination of third law of entropies, Thermochemical equations, Significance of thermochemical equations.

Application of thermodynamics: Entropy and free energy of mixing, partial molar quantities, partial molar volume and free energy (chemical potential), their significance and determinations. Gibbs-Duhem and Duhem-Margules equations.

Thermodynamics of non-ideal solutions -Activity, activity coefficient-standard states.

Thermodynamics of ideal solutions - deductions of laws of Raoult's ebullioscopy, cryoscopy and osmotic pressure.

UNIT - II: 14 hours

Rate of a reaction – definition, rate equations of simple chemical reactions, order of a reaction, Differential and integrated form of rate expressions up to second order reactions

Chemical kinetics: Complex reactions- parallel, consecutive and reversible reactions. Branched chain reactions-general rate expression, explosion limits. Photochemical (hydrogen-halogen reactions- derivation of rate equation for H_2-Br_2) and oscillatory reactions.

Reactions in solution: Ionic reactions- salt and solvent effects. Substituent effects on the rates of reactions-Hammett and Taft equations, linear free energy relations.

Transition state theory: Derivation of rate constant, equilibrium hypothesis, Concept of tunnelling. Applications of TST to reactions in solution & reaction between atoms,

Thermodynamic formulation of transition–state theory, limitations of TST. Extension of TST. Potential energy surfaces: Features & construction. Theoretical calculation of Ea.

UNIT-III **14 hours**

Homogeneous and heterogeneous catalysis, review of adsorption terms, Industrial application of catalysts.

Catalysis: Homogeneous catalysis-equilibrium and steady state treatments, activation energies of catalysed reactions. Acid-base catalysis (general and specific), protolytic and prototropic mechanisms, catalytic activity and acid strength measurements. Kinetics of enzyme catalysed reactions-Michaelis-Menten equation. Effect of pH, temperature & inhibitors

Surface reaction kinetics: A review of adsorption isotherms, Langmuir and Freundlich isotherm (only equations). Uni- and bi-molecular reactions. Multilayer adsorption-BET equation-its derivation and application in surface area determination. Harkin`s–Jura equation and its application. Adsorption from solution, Gibbs adsorption, Mechanism of surface reactions: Langmuir-Hinshelwood & Langmuir Rideal mechanisms. Semiconductor catalysis, n- & p- type.

UNIT-IV **14 hours**

Conductivity, equivalent and molar conductivity and their variation with dilution for weak and strong electrolytes

Electrochemistry of solutions: Nernst equation, Kohlrausch law of independent migration of ions. Activities in electrolytic solutions, mean activity coefficient Ionic atmosphere, Debye – Huckel - Onsager equation of conductivity and its validity. Walden`s rule and its application. Conductance minima, Concept of Ionic strength, Debye - Huckel limiting law (DHL), modifications to DHL-Types, qualitative tests and verification of DHL. Bjerrum theory of ion association-triple ion and significance.

Phase Rule: Basic concepts of phase rule, Three component systems, water-chloroform-acetic acid system, triangular plots. The Nernst distribution law, thermodynamic derivation of the distribution law, limitations of Nernst distribution law, Applications.

REFERENCES :

1. A. W. Atkins (2009), Physical Chemistry, ELBS, 9th Edition.

2. Bockris and Reddy (1998), Modern electrochemistry - vol I 2A &2B, Plenum, New York, 2nd Edition

3. Crow & Crow (2004), Principles and Applications of Electrochemistry, Chapman Hall, London, 4th Edition.

4. G. Raj (2009), Advanced Physical Chemistry, Goel Publishing House, 35th Edition.

5. G. M. Barrow (2002), Physical chemistry, McGraw Hill, Int. St. Ed, 5th Edition.

6. K. J. Laidler (2003), Chemical Kinetics, Harper and Row, 3rd Edition.

7. Maron and Lando (1974), Fundamentals of Physical Chemistry, Collier Macmillan.

8. Puri and Sharma (2016), Principles of Physical Chemistry, Vishal Publishing House 47th Edition.

9. S. Glasstone (2007), Thermodynamics for Chemists, East-west.

10. S. Glasstone (2006), Electrochemistry, Affiliated to East-west press, 1st Edition.

11. S. Upadhyay (2010), Chemical Kinetics and Reaction Dynamics, Springer, 1st Edition.

PS 584.1: PRINCIPLES OF ANALYTICAL CHEMISTRY & SEPARATION TECHNIQUES

Course Outcome:

Student will be able to:

- Imbibe knowledge about various sampling techniques and errors.
- Evoke the fundamental concepts of different titration techniques
- Understand the principle of different chromatography techniques and apply that knowledge for the separation and purification of various samples

UNIT- I: 14 hours

Types of errors- Determinate and indeterminate errors. Accuracy and precision. Introduction to gravimetric analysis

Distribution of random errors- frequency distribution, the normal error curve. Statistical treatment of finite samples. Measures of central tendency- mean, median, mode, range, average deviation, relative average deviation, standard deviation and variance. Student's t test, confidence interval of the mean. Testing for significance, comparison of two means and two standard deviations. Criteria for rejection of an observation-Q test. Principles of sampling- The sampling steps. Methods for sampling solid, liquid and gaseous samples. Effects of sampling uncertainties. Sampling hazards.

Gravimetry: Precipitation methods, the colloidal state, Super saturation and precipitate formation., purity of the precipitate: co-precipitation, post-precipitation, Conditions for precipitation, precipitation from homogeneous solution, washing the precipitate. Fractional precipitation, organic precipitants.

UNIT-II 14 hours

Stability of complexes, stepwise and overall stability constant

Redox titrations: Equilibrium constants for redox reactions - electrode potentials in equilibrium systems, calculation of equilibrium constants. Redox titration curves- formal potentials, derivation of titration curves. Factors affecting the shape of titration curves- concentration, completeness of reaction. Titration of mixtures- feasibility of redox titrations. Detections of end point -redox indicators, theory, specific and non specific indicators, choice of indicator, potentiometric end point detection. Karl Fischer reagent for water determination. Applications

Complexometric titrations: Complex formation reactions, chelating agents. EDTA-acidic properties, complexes with metal ions, equilibrium calculations involving EDTA, conditional formation constants, derivation of EDTA titration curves, effect of other complexing agents, factors affecting the shape of titration curves. Completeness of reaction, indicators for EDTA titrations, theory of common indicators. Titration methods employing EDTA-direct, back and displacement titrations, indirect determinations. Titration of mixtures, selectivity, masking and demasking agents, Typical applications of EDTA titrations- magnesium, manganese and zinc in a mixture. Titrations involving unidenate ligands-titration of chloride with Hg^{2+} and cyanide with Ag^{+}.

Analytical Techniques in Forensic Science - basic principles and significance, finger printing classification, conventional methods of development of fingerprints-fluorescent and chemical methods, application of laser and other radiations for the development of latent finger print. Forensic toxicology: Classification of poisons, estimation of poisons. Treatment in case of poisoning- use of antidotes for common poison.

UNIT III: 14 hours

Basic Concepts - General description, Classification of chromatographic methods. Rf value and factors affecting Rf values.

Exclusion Chromatography: Theory and principle of size exclusion chromatography, experimental techniques for gel-filtration chromatography (GFC) and gel-permeation chromatography (GPC), materials for packing-factors governing column efficiency, methodology and applications.

High Pressure Liquid Chromatography (HPLC): Principle, instrumentation Apparatus, pumps, types of columns, packing and characteristics of liquid chromatographic detectors-UV, IR detectors. Advantages and applications, LC-MS.

Gas Chromatography (GC): Principle, comparison of GSC and GLC. Instrumentation, Columns-packed and tubular. Study of detectors- thermal conductivity, flame ionization, electron capture, GC-MS. Factors affecting separation, applications.

REFERENCES:

1. Bessett, Denney, Jeffery & Mendham (1989), Vogel's Text book of Quantitative Inorganic Analysis, 5thEdition.
2. B. K. Sharma (2012), Instrumental Methods of Chemical Analysis, Goel, 1st Edition.
3. E. Heftman (Ed), Part A and Part B (2004), Chromatography, Elsevier, 5th Edition.
4. G. D. Christian (2007), Analytical Chemistry, Wiley, 6th Edition.
5. Gray Calvin and Bhatia (2009), Instrumental methods of analysis,1stEdition.
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7. H Kaur (2012), Instrumental Methods of Analysis, Pragathi Prakashan.
8. Lobinski and Marczenko (1996), Vol.30, Comprehensive Analytical Chemistry, Elsevier.
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12. Skoog, Holler and Nieman (2006), Principles of Instrumental Analysis, Saunders, 6th Edition.
13. Waiter Huber (1987), Non-aqueous titrations, Academic Press.
14. Willard, Merritt and Dean Settle (2012), Instrumental Methods of Analysis, 7thEdition.

PS 585.1 BIO-ORGANIC CHEMISTRY

Course Outcome:

Student will be able to:

- Understand the chemical principles of living cells, the biomolecules and biocatalytic reactions.
- Study the basic principles underlying the chemistry of nucleic acids.
- Explain the structure determination, synthesis and classification of biomolecules like vitamins and lipids

UNIT I : **14 Hours**

Classification of amino acids based on structure, nature and biological importance. Properties such as isoelectric point, zwitter ion nature and amphoteric nature.

Amino acids and peptides: Introduction and synthesis of amino acids, structure and conformation of peptide bond, N-terminal, C-terminal. Determination of peptides, enzymic cleavage of peptides, reagents for selective cleavage of polypeptide bonds.

Peptide synthesis: Solution phase and Merrifield's solid phase synthesis, solution phase synthesis of oxytocin and vasopressin.

Proteins: Classification, structural detrmination: Primary, secondary, tertiary and quarternary. Stereochemistry of peptide chains, chemical bond involved in protein structure. Protein confuguration: α-helix, amino acids effecting α-helix, rigid and planar peptide bond, Ramachandran plot, β pleated sheets, structure of silk fibroin, random coil structure of proteins, triple helical structure of collagen, similarity in 3D structure of haemoglobin and Myoglobin.

UNIT II : 14 Hours

Types of nucleic acids, differences between DNA & RNA both in structure and biological functions

Nucleic acids : Introduction, nucleosides and nucleotides, structure of nucleoside, chemical synthesis of nucleoside- Adenosine, Guanosine(purine nucleosides), structure of nucleotide, synthesis of nucleotide(AMP). DNA(Watson-Crick model of double stranded DNA) and RNA. Functions of nucleic acids : Replication, transcription, translation, protein synthesis, flow of genetic information, genetic code.

UNIT III : 14 Hours

Introduction, classification and nomenclature- source and deficiency diseases-biological functions of vitamins

Vitamins:. Study of following vitamins: Vitamin A_1& A_2, Vitamin B_1, B_2, B_6&B_{12}, Vitamin C, Vitamin D_2& D_3, Vitamin K_1& K_2, pantothenic acid, folic acid.

Lipids : Introduction, classification of lipids, synthesis of fatty acids. Compound lipids-Phospholipids, Glyco, spingo lipids and derivatives.

REFERENCES :

1. Bender, Kennelly &Rodwell (2015), Harper's Illustrated Biochemistry, McGraw Hill, 30thEdition
2. Chatterjea & Shinde (2011), Text Book of Medical Biochemistry, JayPee Brothers Medical Publications, 8th Edition.
3. G. C. Barret and D. T. Elmore (1998), Amino acids and Peptides, Cambridge University Press.
4. Hermann Dugas (1999), Bioorganic Chemistry, Springer New York, 3rd Edition.
5. J. L. Jain, Vol 1&2 (2005), Fundamentals of Biochemistry, S Chand & Company Ltd.
6. Nelson & David (2013), Lehninger's Principles of Biochemistry, MacMillan, 6th Edition.
7. W. Pigman and D Horton-Vol. IA, IB, IIA and IIB (1970), The Carbohydrates, Academic Press.

PS 586.1 RESEARCH METHODOLOGY

Course Outcome

Student will be able to:

Evaluate Research output with philosophical base and greater relevance to the society

Identify the parameters of Quality research with scientific methodology

Understand the concepts involved in Original Research, ethical guidelines and practices in conducting the research and publication of papers.

Create awareness on Intellectual property Rights and Patents.

Unit 1: Foundation of Research and Research Methodology 14 Hours

Research – Definition, characteristics, objectives, motivation in research, scientific research, need and importance of research. Types of Research, Philosophy and Research Philosophy. Concept of Theory and Theory Building – deduction, induction and abduction. Research Strategies - meaning and types.

Research Problem – meaning, selecting the problem, sources of problem, statement of a problem, research design and report writing.

Review of Literature – meaning and need for literature review, sources of literature review, reporting the review of literature, identification of research gap, Print Sources of information – Primary, Secondary, Tertiary sources. Journals: Journal abbreviations, Abstracts, Current titles, Reviews, Monographs, Dictionaries, Textbooks, Current contents, Introduction to Chemical Abstracts and Beilstein. Subject Index, Substance Index, Author Index, Formula Index and other Indices with examples.

Digital sources: Web resources, E–Journal, Journal access, TOC alerts, hot articles, Citation index: Impact factor. H–Index, i10 index, E–Consortium, UGC infonet, E–Books, Internet discussion groups and communities, Blogs, Preprint server, Search engines, Scirus, Google Scholar, Chem Industry, Wiki – Databases, Chem Spider, ScienceDirect, SciFinder and Scopus.

Unit 2: Chemical Safety and Ethical Handling of Chemicals 14 hours

Safe working procedure and protective environment, protective apparel, emergency procedure and first aid, laboratory ventilation.

Safe storage and use of hazardous chemicals, procedures for working with substances that pose hazards, flammable or explosive hazards, procedures for working with gases at above or below atmospheric pressures, 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 sewage system, incineration and transportation of hazardous chemicals.

Unit 3: Research Ethics and Intellectual Property Rights (IPR): 14 Hours

Ethics – meaning and definition, Ethics vs moral philosophy, Ethical issues, ethical committees. Rights and obligations of Research Participants. Scientific conduct – ethics with respect to science and research, intellectual honesty and research integrity. Scientific misconduct – falsification,
fabrication and plagiarism. Publication ethics – meaning and importance, plagiarism and Self-plagiarism.

IPR – Concept of IPR, nature and characteristics of IPR, origin and development of IPR, justification and rationale for protecting IPR, IPR and sustainable development, IPR and human rights. Forms of IPR – copyrights, trademarks, patents, industrial designs, trade secrets, geographical indications – meaning, features and application of different forms of IPRs. Filing and Registration process of IPRs.

References:

1. A K Singh, Tests, Measurements and Research Methods in Behavioral Sciences, Bharathi Bhawan (Publishers & Distributors), New Delhi.

2. Barbara H., Stanley J., Joan E. Sieber, Gary B. Melton, Research Ethics: A Psychological Approach, University of Nebraska Press.

3. Chemical safety matters (1992)–IUPAC –IPCS, Cambridge Univ. Press.

4. David I Bainbridge (2012), Intellectual Property Rights, Long man Publication.

4. Indian National Science Academy (INSA) (2019), Ethics in Science Education, Research & Governance

4. Jayashree Watal, Intellectual Property Rights in the WTO and Developing Countries, Oxford University Press.

5. Kothari C R., Research methodology: Research & Techniques, New Age International Publishers, New Delhi.

6. Leedy P D., Practical Research: Planning & Design, Washington: Mc Millan Publishing Co., INC.

7. Wallinman N., Your Research Project: A Step-by-Step Guide for the first time Researcher, Sage Publications, London

8. Y. K Singh., Fundamentals of Research Methodology and Statistics, New International (P) Ltd., New Delhi.

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PS 587.1P : INORGANIC CHEMISTRY PRACTICALS – I

Course Outcome:

Student will be able to:

- Estimate the quantity and quality of different compounds and metal ions using gravimetry, volumetry and complexometric techniques.

Any 10 experiments are to be carried out

1. Analysis of Hematite-insoluble residue by gravimetry and Iron by volumetry using Ce^{4+}.
2. Complexometric determination of Mn, Cu.
3. Complexometric determination of Ni and Fe-Cr mixture
4. Analysis of Halide Mixture - Iodide by KIO_3 and total halide by gravimetry.
5. Colorimetric Determination of Iron by thiocyanate and Cu by aqueous ammonia.
6. Analysis of solder - Pb and Sn by EDTA method.
7. Gravimetric Determinations of Mo, Pb/Cr, sulphide, thiocyanate.
8. Estimation of Cr(III) & Fe(III) in a mixture using EDTA.
9. Estimation of Ni(II) & Fe(III) in a mixture using EDTA.
10. Determination of free Chlorine in the given water sample
11. Synthesis and Characterization of Potassium tri-oxalato aluminate
12. Synthesis of MnO_2 /ZnO nanoparticle and its application.
13. Any other experiment of interest

REFERENCES:

1. G. H. Jeffrey, J. Bassette, J. Mendham and R. C. Denny (2009), Vogel's Text Book of Quantitative Chemical Analysis, Longman, 6th Edition.

PS 588.1P: ORGANIC CHEMISTRY PRACTICALS - I

Course Outcome:

Student will be able to:

- Carry out multi-step organic synthesis
- Purify the synthesized organic compounds

Any 10 experiments are to be carried out

1. Electrophilic substitution reactions–Preparations of p-bromoaniline, p-nitroaniline and picric acid
2. Alkylations–Preparations of nerolin and N-methyl anthranilic acid.
3. Acetylations–Preparations of β-D-glucose penta-acetate and 2-naphthyl acetate.
4. Reactions with ring formation–Preparations of 1,2,3,4–tetrahydrocarbazole and 7–hydroxy-4-methyl-coumarin.
5. Diazotisation reactions–Preparations of iodo, chloro and azo compounds.
6. Dehydration reactions–Preparations of cyclohexene and succinic anhydride
7. Condensation reactions–Condensations involving diethylmalonate and ethyl acetoacetate. Aldol condensation and Perkin reactions.
8. Oxidation reactions-Preparation of p-nitrobenzoic acid and adipic acid.
9. Halogenation reactions-Preparation of n-butylbromide &α,β-dibromocinnamic acid.
10. Oxidation reactions–Preparation of adipic & p-nitrobenzoic acids and p-benzoquinone.
11. Reduction reactions–Reductions of nitro compounds and carbonyl compounds.
12. Preparation of Dibenzal Acetone.
13. Preparation of Cinnamic Acid from Benzaldehyde.
14. Preparation of Ethyl Aceto Acetate from Ethyl acetate.
15. Any other experiment of interest

REFERENCES :

1. B. S. Furniss et al (1989), Vogel's Text Book of Practical Organic Chemistry including Qualitative Organic Analysis, Longman-ELBS, London, 2nd Edition.

2. F. G. Mann (2009), Practical Organic Chemistry, Pearson Education, 4th Edition.

3. P. R. Singh et al, Vol. I & II, (2013), Experimental Organic Chemistry, TMH New Delhi.

4. R. K. Bansal (2008), Laboratory Manual in Organic Chemistry, New Age, New Delhi, 5th Edition.

PS 589.1P : PHYSICAL CHEMISTRY PRACTICALS – I

Course Outcome:

Student will be able to:

- Carry out experiments related to chemical kinetics, viscometry, Polarimetry, Refractometry, Conductometry and Potentiometry

Any 10 experiments are to be carried out

1. Potentiometric titration of halides in mixtures (Cl^-, Br^- and I^-) with silver nitrate
2. Potentiometric determination of redox potentials.
3. Potentiometric determination of dissociation constants of weak acids
4. Potentiometric and conductometric acid–base titrations in partial & non-aqueous media.
5. Conductometric titrations of displacement and precipitation reactions
6. Heat of solution by solubility method
7. Determination of solubility of lead iodide at different T & hence molar heat of solution
8. Determination of pH of buffer solutions with a pH meter & evaluation of pKa of acids
9. Analysis of a binary mixture of two miscible liquids by viscometry and the relation between viscosity of a solution and the electrical conductivity
10. Determination of parachor value for CH_2 group by S.T method, the composition of a solution by S.T measurement and the CMC of a soap solution by S.T measurement.
11. Potentiometric determination of solubility of insoluble silver halide and the standard electrode potential using quinhydrone electrode
12. Determination of degree of hydrolysis of CH_3COONa and NH_4Cl.
13. Determination of hydrolysis constant of aniline hydrochloride.
14. Verification of Nernst equation for Ag^+, $Cu^{2+}$and Zn^{2+} species.
15. Determination of transport number of ions by emf method (Ag^+, Cd^{2+}, NO^-_3, SO_4^{2-} etc.)
16. Analysis of the binary mixture by surface tension method
17. Any other experiment of interest

REFERENCES :

1. B. P. Levitt (2010), Findlay's Practical Physical Chemistry, Longman, London.

2. Carl, Joseph, David (2008), Experiments in Physical Chemistry, Tata-McGraw Hill, 8th Edition.

3. Daniels et al (2011), Experimental Physical Chemistry, Nabu Press.
4. Das & Behera (1984), Experimental Physical Chemistry, Tata-McGraw Hill, New Delhi.
5. Yadav (2013), Advanced Practical Physical Chemistry, Krishna Prakashan, 33rd Edition.

SECOND SEMESTER

PH 581.2: ADVANCED INORGANIC CHEMISTRY

Course Outcome:

Student will be able to:

- Understand the Chemistry of d block elements, Lanthanides and Actinides and explain their magnetic and electronic properties
- Describe the VB and MO theory of complexes and electronic and bonding reactivities of transition metals
- Explain the spectral and magnetic properties of metal complexes
- Describe the basic concepts of organometallic chemistry and their bonding patterns especially with unsaturated ligands

PH 581.2: ADVANCED INORGANIC CHEMISTRY

Course Outcome:

Student will be able to:

- Understand the Chemistry of d block elements, Lanthanides and Actinides and explain their magnetic and electronic properties
- Describe the VB and MO theory of complexes and electronic and bonding reactivities of transition metals
- Explain the spectral and magnetic properties of metal complexes
- Describe the basic concepts of organometallic chemistry and their bonding patterns especially with unsaturated ligands

UNIT I: 14 Hours

Definition of metallurgy - roasting and calcination, reduction of mineral to metal (electrolytic reduction, chemical reduction and auto reduction), General characteristics of d and f block elements, lanthanide and actinide contraction.

Reduction of Ores: Methods of reduction of oxide ores Ellingham diagram, chemical and electrolytic reductions, reduction potentials, Latimer and Frost diagrams, Pourbaix diagram, effect of complexation on potential.

d block elements: Comparison of 3d, 4d and 5d series by taking Titanium subgroup as example.

Lanthanides and actinides: Electronic structure and oxidation states, spectral and magnetic properties of lanthanide and actinide complexes, lanthanide and actinide contraction. Extraction and separation of lanthanides. Comparison of spectral and magnetic properties of lanthanides and actinides with d-block ions.

UNIT II: 14 Hours

Review of basic concepts of Co-ordination chemistry, Valence bond theory, Concept of hybridization, coordination number and geometry in coordination compounds.

Coordination numbers 2-10 and their geometry, Crystal Field Theory- Salient features, d-orbital splitting in octahedral, tetrahedral, square planar and tetragonal complexes, spectrochemical series, Jahn-Teller distortions. Preparation of coordination compounds - Simple addition reactions, substitution reactions, oxidation-reduction reactions, thermal dissociation reactions.

Evidence for ligand field splitting: Hydration, ligation and lattice energies, site preference energies. Metal – ligand orbital overlap from ESR, NMR, electronic spectra and antiferromagnetic coupling, nephelauxetic effect and nephelauxetic series, MO theory of coordination compounds- MO energy level diagrams for octahedral, tetrahedral and square planar complexes.

Stability of Metal Complexes - Stepwise and overall formation constants, factors affecting stability of metal complexes, determination of stability constants of metal complexes by spectrophotometry (Job's method), stepwise stability constants by Bjerrum's pH-titration method and polarographic methods.

UNIT III: 14 Hours

Concept of pi acceptor ligands, back bonding, bonding in metal carbonyls, 18 electron rule

Metal Pi-acceptor complexes: Metal carbonyls – preparative methods, structure and bonding, reactions, vibrational spectra of metal carbonyls for bonding and structural elucidation, magnetic and X-ray evidence of structures.

Metal carbonylates and carbonyl halides – preparation and important reactions with Applications.

Metal Nitrosyls – preparation, structure and bonding. Preparation and reactions of dinitrogen and tertiary phosphine complexes, ligand cone angle in phosphine complexes, Metal dioxygen complexes: Preparation, bonding and Importance of O_2 ligand, complexes containing SO_2 and CO_2.

Metal Clusters: Metal-metal bonding in carbonyls and halides, Evidences for M-M bonding, factors favoring M-M bond formation.

UNIT IV: 14 Hours

Quantum numbers and their significance. Brief review of different types of magnetic behaviour

Electronic spectra of transition metal complexes: Spectroscopic term symbols for d^n ions, ground states, microstates, microstate table for p^2 and d^2 system. Selection rules, Racah parameters, Orgel, Tanabe-Sugano diagrams - applications to electronic spectra of

transition metal complexes (V^{3+}, Cr^{3+}, Mn^{2+}, Co^{2+} Ni^{2+} and $[CoCl_4]^{2-}$), charge transfer spectra-types and characteristics.

Magnetic properties of metal complexes: Origin and types of magnetic behaviour-diamagnetism, paramagnetism, ferro and antiferromagnetism, magnetic susceptibility and its measurement by the Guoy and Faraday method, temperature dependence of magnetism – Curie and Curie-Weiss laws, Curie Temperature and Neil temperature, types of paramagnetic behaviour, spin only behaviour, spin orbit coupling, quenching of orbital contribution and spin only behaviour (explanation based on A, E and T terms), application of magnetic data.

REFERENCES:

1. B. E. Douglas, D. McDaniel and A Alexander (2010), Concepts and Models of Inorganic Chemistry, Wiley, 3rd Edition.
2. J. D. Lee (2014), Concise Inorganic Chemistry, Blackwell Science, 5th Edition.
3. J. E. Huheey, E. A. Keiter, R. L. Keiter and O K Medhi (2006), Inorganic Chemistry, Pearson Education, 4th Edition.
4. Madan, Malik and Tuli (2010), Selected Topics in Inorganic Chemistry, S Chand, 17th Edition.
5. Meissler and Tarr (2013), Inorganic Chemistry, Pearson Prentice Hall, 5th Edition.
6. Puri, Sharma and Kalia (2016), Principles of Inorganic Chemistry, Vishal Publishing House, 33rd Edition.
7. Shriver, Atkins and Langford (2009), Inorganic Chemistry, Oxford, 5th Edition.
8. W.W. Porterfield (2009), Inorganic Chemistry, A Unified Approach, Elsevier, 2nd Edition.

PH 582.2: ADVANCED ORGANIC CHEMISTRY

Course Outcome:

Student will be able to:

- Describe the mechanisms of different types organic reactions.
- Understand the chemistry of radical reactions and its applications.
- Understand the mechanism of additions to various Carbon-based multiple bonds
- Achieve skills in constructing homo/heterocyclic rings of significant molecules

UNIT I **14 hours**

Generation of Nucleophiles and electrophiles, electrophilic and Nucleophilic substitution reactions.

Aliphatic Nucleophilic Substitution Reactions: Mechanism and scope of aliphatic nucleophilic substitution reactions - S_N1, S_N2 and S_Ni. Stereochemistry of nucleophilic

substitution reactions, allylic, vinylic and benzylic nucleophilic substitution reactions, neighbouring group participation and anchimeric assistance.Factors influencing the rates of nucleophilic substitution reactions.

Aliphatic Electrophilic Substitution Reactions: Bimolecular mechanisms - S_E1, S_E2 and S_Ei mechanism. Electrophilic substitution reactions accompanied by double bond shifts.

Aromatic Electrophilic and Nucleophilic Substitution Reactions: Mechanism of aromatic electrophilic substitution reaction pathway, Arenium ion mechanism, orientation and reactivity, energy profile diagram. The ortho/para ratio, ipso attack, orientation in other ring systems.

Mechanisms of aromatic nucleophilic substitution reactions:SNAr, SN1 and aryne mechanism. Von-Richter rearrangement, Sommelet-Houser rearrangement, Smiles rearrangement.

UNIT II **14 hours**

Elimination reactions, dehydration, dehydrohalogentation and dehalogenation

Free Radical Reactions: Types of radical reactions, mechanisms of free radical substitution reactions and neighbouring group assistance. Reactivity for the aliphatic and aromatic substances at a bridgehead. Reactivity of the attacking radical. The effect of solvent on reactivity. Auto-oxidation, coupling of alkynes. Arylation of aromatic compounds by diazonium salts. Sandmeyer, Ullmann and Hunsdiecker reaction

Elimination Reactions: Discussions of E1, E2, E1cB and E2cB mechanisms. Orientation during elimination reactions. Saytzeff and Hofmann rules. Reactivity-effects of substrate structures, attacking base, leaving group and solvent medium.

Pyrolytic Eliminations: Mechanisms of pyrolysis of esters of carboxylic acids, (acetate pyrolysis), Chugaev reaction, Hofmann degradation and Cope elimination

UNIT III **14 hours**

Addition and condensation reactions, aldol condensation and Perkin reaction

Formation and Hydrolysis of Esters: Plurality of mechanism. Mechanism of esterification reactions. Ester hydrolysis-$A_{AC}2$, $B_{AC}2$, $A_{AC}1$ & $A_{AL}1$ mechanism. Transesterification – acetyl and benzoyl migrations.

Addition to Carbon-Carbon Multiple Bonds: Addition reactions involving electrophiles, nucleophiles and free radicals. Cyclic mechanisms. Orientation and stereochemistry. Addition of halogens, hydrogen halides, carboxylic acids and amines. Addition to cyclopropanes, hydroboration, Michael addition. Addition of oxygen across double bonds.

Addition to Carbon-Hetero Multiple Bonds: Electrophilic, nucleophilic and free radical additions to C=O and C=N systems. Addition of Grignard reagents. Reformatsky reaction, Knoevenagel condensation and Wittig reactions.

UNIT IV **14 hours**

Introduction and classification of heterocycles

Chemistry of Heterocyclic Compounds: Nomenclature of 3,4, 5, 6 membered heterocyclic and fused heterocycles, synthesis and reactions of oxiranes, thiranes, aziridenes, azirenes. Synthesis and reactions of pyridine, quinoline, isoquinoline, indole,coumarin. Synthesis and reactivity(Nucleophilic reactions) of heterocycles containing two hetero atoms ex:pyrazole, imidazole, thiazole.

Organic Photochemistry:

Norrish Type-I, Type-II reactions and Yang cyclisation. Barton reaction and Photo Fries rearrangement, Paterno-Buchi reaction,Photochemistry of alkenes, benzenes, Di-pi methane rearrangement..

REFERENCES:

1. Acheson (2008), An Introduction to the Chemistry of Heterocyclic Compounds, Wiley –Eastern, 3rd Edition.
2. Bansal (2012), Organic Reaction Mechanisms, Tata McGraw Hill, New Delhi, 4th Edition.
3. Carey and Sundberg (1990), Advanced Organic Chemistry, 3rd Edition.
4. Chatwal (2010), The reaction mechanism and reagents in Organic Chemistry, Himalaya, Bombay, 5th Edition.
5. Claydon and Greaves (2012), Organic Chemistry, 2ndEdition.
6. David Gutsche (1988), The Chemistry of Carbonyl Compounds, Prentice-Hall, New Delhi.
7. I.L. Finar, Vol. –I & II (2002), Organic Chemistry, Longman-ELBS, England, 6th Edition.
8. J. A. Joule & K. Mills (2010), Heterocyclic Chemistry, Wiley-Blackwell, 5th Edition
9. J. Joule & G. Smith (1995), Heterocyclic Chemistry, Van-Nostrand, ELBS, 3rd Edition.
10. Mukherji, Singh and Kapoor, Vol. –I & II (2012), Organic Chemistry, Wiley Eastern, New Delhi, 2nd Edition.
11. Mukherji, Singh and Kapoor (1984), Reaction Mechanisms in Organic Chemistry, McMillan, 3r Edition.
12. P.S. Kalsi (2010), Organic Reactions and Their Mechanisms, New Age, New Delhi, 3rd Edition.
13. P.Y. Bruice (2014), Organic Chemistry, Pearson Education, New Delhi, 7th Edition.

14. R. K. Bansal (2010), Text Book of Heterocyclic Chemistry, 5thEdition.

15. Smith (2012), March's Advanced Organic Chemistry, Wiley, NY, 6th Edition.

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PH 583.2: ADVANCED PHYSICAL CHEMISTRY

Course Outcome:

Student will be able to:

- Gather knowledge of Quantum Chemistry and its application
- Explain the approximation methods in quantum mechanics
- Explain the relationship between microscopic properties of molecules with macroscopic thermodynamic observables
- Describe the quantum mechanical explanation of chemical bonding

UNIT - I : 14 hours

Bohr's theory of hydrogen atom. Comparison of classical and quantum mechanical particles. Cartesian, Polar and spherical polar coordinates and their interrelations. Operators, matrix representation and commutation relationships, Angular momenta (commutations, relations, operators). Schrödinger equation, significance and characteristics of wave function, eigen functions and eigen values. Probabilities, normalisation and orthogonality. Postulates of quantum mechanics φ, θ Solution of Schrödinger wave equation for exactly solvable problems such as particle in a box (1D and 3D), particle in a ring, harmonic oscillator, rigid rotor and hydrogen atom **(**separation of r,φ, θ equations and their solutions).

UNIT–II: 14 hours

Pauli exclusion principle, Term symbols, Russell-Saunders terms and coupling schemes

Approximate methods in quantum chemistry: Approximate methods of solving Schroedinger equation for problems of chemical interest - variation and perturbation methods. Application of variation method to H & He atoms, the structure of many electron systems/atoms (secular equations & determinants). Spin-orbit interaction, antisymmetry, Slater orbitals and SCF method for many electron systems.

Molecular wave functions: Born-Oppenheimer approximations. Covalent bond – valence bond and molecular orbital approaches with comparisons. Hydrogen molecule – Heitler-London (VB) treatment. Energy level diagram. MO theory applied to homonuclear and heteronuclear diatomics by LCAO methods, correlation diagrams, non-crossing rule.

UNIT -III : 14 hours

Hybridization and Valence Bond Theory (VBT), Molecular Orbital Theory(MOT).

Theory of directed valence - Geometry of molecules in terms of molecular orbitals (bond angle, dihedral angle), localised and delocalised molecular orbitals.

Conjugated and aromatic molecules: Huckel molecular orbital (HMO) theory of linear conjugated systems (ethene, allyl & butadiene systems) and aromatic molecules (benzene as an example). Calculation of delocalization energies, bond order & charge density. An introduction to Extended Huckel Theory.

UNIT - IV : 14 hours

Concept of molecular energy levels. Maxwell`s distribution of molecular velocities

Statistical Thermodynamics : Micro and macrostates, phase space and ensembles. Concept of distribution - thermodynamic probability and most probable distribution - Maxwell-Boltzmann distribution law. Maxwell-Boltzmann statistics and applications, Bose-Einstein and Fermi-Dirac statistics. Partition functions - definitions and separations, evaluation of translational, rotational, vibrational and electronic partition functions for monoatomic, diatomic and polyatomic gaseous molecules. Calculations of thermodynamic functions and equilibrium constant in terms of partition functions, entropy of monoatomic gas - Sackur-Tetrode equation, comparison of 3rd law and statistical entropies. Heat capacity behaviour of solids – Einstein and Debye theories. Introduction to Irreversible Thermodynamics

REFERENCES :

1. A. K. Chandra (2009), Introductory Quantum Chemistry, Tata McGraw Hill, 4th Edition.
2. Donald Mcquarrie (2011), Quantum Chemistry, Tata McGraw Hill, 2nd Edition.
3. F. L. Pilar (1990), Elementary Quantum Chemistry, McGraw Hill, 2nd Edition.
4. M. C. Gupta (1991), Statistical Thermodynamics, Wiley Eastern Ltd, 2nd Edition.
5. P. Atkins (2009), Physical Chemistry, ELBS, 9th Edition.
6. Puri, Sharma and Pathania (2008), Principles of Physical Chemistry,1st Edition.
7. P. W. Atkins & R. S. Friedman (2012), Molecular Quantum Mechanics, Oxford University Press, 5th Edition.
8. R. K. Prasad (2020), Quantum Chemistry, New Age, 4th Edition.
9. T. Engel and P. Reid (2006), Physical Chemistry, Pearson Education, 1st Edition.

PS 584.2: MOLECULAR SYMMETRY AND MOLECULAR SPECTROSCOPY

Course Outcome:

Student will be able to:

- Apply the principles of group theory in chemical bonding.
- Define aspects of specific spectroscopic techniques, applications of molecular symmetry in Microwave and Vibrational spectroscopy
- Define aspects of specific spectroscopic techniques, applications of molecular symmetry in Rotational and Raman spectroscopy

UNIT – I : 14 hours

Elements of Symmetry, Definitions of groups and sub groups, symmetry operations

Symmetry and Group Theory: Relation between orders of a finite group and its subgroup and group multiplication tables, Conjugate relationships and classes, Schoenflies symbols, Matrix representations of symmetry operations, products of symmetry operations, some properties of matrices and vectors, classification of molecules into point groups. Reducible and irreducible representations. Mulliken's symbols for IR's The Great Orthogonality theorem (without proof), character tables for C_{2v}, C_{3v}, and C_2 point groups, the direct product. Transformation properties of atomic orbitals. Applications of group theory to molecular vibrations and chemical bonding (IR &Raman).

UNIT – II : 14 hours

Rigid rotator definition & derive $I=\mu r^2$. Electromagnetic radiation, dual nature, regions of the spectrum.

Unifying Principles: Interaction of electromagnetic radiation with matter - absorption, emission, transmission, reflection, refraction, dispersion, polarization and scattering. Natural line width and broadening, intensity of spectral lines

Microwave Spectroscopy: The rotation and classification of molecules, selection rules, rotation spectra of diatomic and polyatomic molecules. Rigid and non-rigid rotator models. of molecules, rotation spectra of diatomic molecules. Rigid and non-rigid rotator models. Derivation of the expression for moment of inertia of diatomic molecule, Determination of bond lengths, isotope effect on rotation spectra. Moment of inertia expression for linear polyatomic molecules. Stark effect, nuclear and electron spin interaction. Microwave Spectrometer.

Vibrational Spectroscopy: Vibration spectra of diatomic molecules - linear harmonic oscillator, vibrational energies, zero point energy, force constants and bond strengths, energy curves for simple harmonic oscillator. Anharmonicity of molecular vibrations - Morse potential energy diagram, selection rules, fundamental, overtones and hot bands. Vibrations of polyatomic molecules - normal modes of vibrations and nature of molecular vibrations (Ex - CO_2 and H_2O).

UNIT –III: 14 hours

Introduction to Raman Spectroscopy, Stokes and Anti Stokes lines.

Vibration-rotation spectra of diatomic and polyatomic molecules, selection rules, PQR branches.

Raman Spectroscopy: Classical and quantum theories of Raman effect, concept of polarizability and polarizability ellipsoid. Rotational and vibrational Raman spectra, selection rules, Raman activity of vibrations, mutual exclusion principle, polarization of Raman lines. An introduction to Laser Raman Spectroscopy. Raman Spectrometer – instrumentation. Applications of IR and Raman spectroscopy in elucidation of molecular structure (Ex - H_2O, N_2O & CO_2 molecules). An introduction to Resonance Raman Spectroscopy. Advantages of Raman spectroscopy over IR spectroscopy.

REFERENCES:

1. Banwell & McCash (2015), Fundamentals of Molecular Spectroscopy, Tata McGraw Hill, 5th Edition.

2.Donald L. Pavia, Gary M. Lampman, George S. Kriz, James A. Vyvyan (2008), Introduction to Spectroscopy, 42ndEdition.

3. K. Veera Reddy (2010), Symmetry and Spectroscopy of molecules, 2ndEdition.

4. L. D. field (2013), Organic Structures from Spectra, 5thEdition.

5. P. S. Kalsi (2004), Spectroscopy of Organic Compounds, , 6thEdition.

6. Silverstein, Bassler & Monnill (2010), Spectrometric Identification of Organic Compounds, Wiley, 6th Edition.

7. W. Kemp (2011), Organic Spectroscopy, Mac, 3rd Edition.

8. Y. R. Sharma (2013), Elementary organic spectroscopy, S. Chand, 5th Edition.

PS 585.2 : CHEMISTRY OF BIOMOLECULES

Course Outcome:

Student will be able to:

- Explain the structure and role of biomolecules like peptide, proteins and lipids
- Understand the chemical principles of living cells, their biomolecules and biocatalytic reactions.
- Detail the synthesis and stereochemistry of carbohydrates

UNIT I : **14 Hours**

Cell Structure and Functions: Structure of prokaryotic and eukaryotic cells, intra cellular organelles and anabolism, comparison of animal and plant cells

Overview of metabolic processes- catabolism and anabolism. ATP- the biological energy currency. Origin of life - unique properties of carbon, chemical evolution and rise of living systems.

Lipids: Fatty acids, essential fatty acids, structure and function of triglycerides, glycerophospholipids, sphingolipids, cholesterol, bile acids, prostaglandins.

Lipoprotiens: Composition and function, role in atherosclerosis, properties of lipid aggregates, micelles, bilayers, liposomes and their biological functions. Biological membranes-Fluid mosiac model of membrane structure. Lipid metabolism (oxidation of fatty acids).

UNIT II : **14 Hours**

General structure, classification, D and L Notation.

Amino Acids : Specific rotation, distribution in proteins, location in proteins, physical properties, non-standard protein aminoacids and non-protein aminoacids. General methods of synthesis of synthesis of aminoacids with specific examples.

Steriods and Hormones: Classification of steriods, Biological importance, Cholesterol, Occurance, properties, test and physiological activities of cholesterol. Sex hormones, thyroid gland hormones and adrenal gland hormones.

Enzymes: Enzymes in organic synthesis, α-carboxy peptidase-A and Ribonuclease. Enzymatic synthesis of α-amino acids and peptides. Transformations of lipases and esterases. Kinetic resolutions of carboxylic acids, esters and alcohols-Trans esterification. Enzymatic synthesis of α-amino acids and peptides.

UNIT III : **14 Hours**

Introduction, Definition, classification, reducing and non reducing sugars.

Carbohydrates : Configuration and conformation of monosaccharides, Chemistry of important derivatives of monosaccharides - ethers, esters, acetals, ketals, deoxysugars, aminosugars, structure of disaccharides - maltose, cellobiose and sucrose. Structure of tri and tetra saccharides.

General methods of structural degradation of polysaccharides-methylation, partial hydrolysis, per iodate oxidation, Smith degradation and alkaline degradation techniques. Structures of cellulose, chitin, starch(Amylose and amylopectin), glycogen, heparin and chondroitin. Hemicelluloses, regenerated cellulose and cellulose derivatives.

REFERENCES :

1. Bender, Kennelly & Rodwell (2015), Harper's Illustrated Biochemistry, Mc Graw Hill, 30th Edition.

2. Chatterjea & Shinde (2011), Text Book of Medical Biochemistry, JayPee Brothers Medical Publications, 8th Edition.

3. G. C. Barret and D. T. Elmore (1998), Amino acids and Peptides- Cambridge University Press.

4. H. Dugas (1999), Biorganic Chemistry, Springer New York, 3rd Edition.

5. J. L. Jain, Vol 1&2 (2005), Fundamentals of Biochemistry, S Chand & Company Ltd.

6. Nelson & David (2013), Lehninger's Principles of Biochemistry, MacMillan, 6th Edition.

7. W. Pigman and D. Horton, Vol. IA, IB, IIA and IIB (1970), The Carbohydrates, Academic Press.

PS 586.2P : INORGANIC CHEMISTRY PRACTICALS – II

Course Outcome:

Student will be able to:

- Estimate binary mixtures of metallic ions in solution
- Analyse the presence of inorganic salts qualitatively

Qualitative Analysis of mixtures of Inorganic Salts containing 3 metal ions and 2 anions (1 less common metal ions like Tl, W, Mo, V, Zr, Th, U, Ce, Ti and Li to be included among anions organic acid radicals, phosphate, borate and fluoride separation included).

REFERENCES

1. G. H. Jeffrey, J. Bassette, J. Mendham and R. C. Denny (2009), Vogel's Text Book of Quantitative Chemical Analysis, Longman, 6th Edition.

2. G. Svehla (2006), Vogel's Qualitative Inorganic Analysis, Longman, 7th Edition.

PS 587.2P : ORGANIC CHEMISTRY PRACTICALS – II

Course Outcome:

Student will be able to:

- Separate and analyse the binary mixture of Organic Compounds

Separation and Systematic Qualitative Analysis of Binary Mixtures of Organic Compounds

REFERENCES :

1. A. I. Vogel (2005), Practical Organic Chemistry, Pearson India, 5th Edition.
2. F. G. Mann and B. C. Saunders (2009), Practical Organic Chemistry, ELBS, England, 4th Edition.
3. Furniss (2005), Vogel's Text Book of Practical Organic Chemistry, Pearson India, 5th Edition.
4. R.K. Bansal (2008), Laboratory Manual in Organic Chemistry, New Age Intl, 5th Edition.
5. R. L. Shriner (1980), The Systematic Identification of Organic Compounds– A Lab Manual, John Wiley & Sons, 6th Edition.
6. Singh et al, Vol. I &II (2005), Experimental Organic Chemistry, Campus Books Intl, 5th Edition.

PS 588.2P : PHYSICAL CHEMISTRY PRACTICALS – II

Course Outcome:

Student will be able to:

- Determine cryoscopic constants, dissociation constants and various other physical properties of compounds

At least 10 experiments are to be carried out

1. Determination of cryoscopic constants of solvents and molecular weight of non volatile substances using water and benzene as solvents.
2. Determination of degree of dissociation & Vant Hoff factor of an electrolyte by cryoscopic method.
3. Phase diagram of two component systems by thermal analysis- determination of eutectic point.
4. Phase diagram of two component systems by thermal analysis- determination of molecular weight.
5. Determination of association constants carboxylic acids in organic solvents by distribution method.
6. Preparation of colloidal solutions.
7. Kinetics of the reaction between potassium persulphate and potassium iodide- Temperature variation
8. Kinetics of the reaction between potassium persulphate and potassium iodide- Dielectric constant variation.
9. To study the adsorption of iodine on charcoal from alcoholic solution.
10. Kinetics of the reaction between sodium formate and iodine.
11. To study the effects of gelatin solution on the precipitation values.
12. Adsorption of oxalic acid
13. Determination of partial molar volume : NaCl- water system
14. Determination of partial molar volume: ethanol-water system
15. Decomposition of diacetone alcohol-Dilatometry.
16. Any other relevant experiments of interest.

REFERENCES:

1. B. P. Levitt (2010), Findlay's Practical Physical Chemistry, Nabu Press.

2. Das & Behera (1984), Experimental Physical Chemistry, Tata McGraw Hill, New Delhi.

3. Daniels (2011), Experimental Physical Chemistry, Nabu Press.

4. James and Prichard (2008), Experiments in Physical Chemistry, Tata-McGraw Hill, 8th Edition.

5. J. C. Ghosh (2008), Experiments in Physical Chemistry, Tata-Mcgraw Hill, 8th Edition.

6. Yadav (2013), Advanced Practical Physical Chemistry, Krishna Prakashan, 33rd Edition.

PO 589.2- SPECTRAL METHODS OF ANALYSIS

Course Outcome:

Student will be able to:

- Understand theory and application to mass spectrometry, ultraviolet and visible spectroscopy
- Understand the concept of infrared spectroscopy, X-Rays
- Gain a basic understanding of nuclear magnetic resonance spectroscopy

UNIT I

ULTRAVIOLET AND INFRARED SPECTROSCOPY 14 Hours

Beer-Lambert law, instrumentation, molecular vibrations – modes of vibrations

UV absorption spectroscopy: Molar absorptivity, theory of electronic spectra, formation of bands, effect of conjugation with examples; Concept and effect of addition of chromophore and auxochrome. Absorption and intensity shifts- Bathochromic, hypsochromic, hyperchromic and hypochromic shifts. Application of UV spectroscopy in the structural study of organic molecules.

IR spectroscopy: Principle dipole moment, expression to obtain vibrational frequency, force constant, determination of force constant and qualitative relation of force constant and bond energies. Fingerprint region and functional group region. Effect of delocalisation and conjugation. Structural elucidation of simple organic compounds with amino, amide, carbonyl, carboxylic, ester functional groups.

UNIT II

NMR AND MASS SPECTROMETRY 14 Hours

Shielding and deshielding in NMR, Instrumentation of mass spectrometry

Nuclear magnetic resonance (^{1}H and ^{13}C) Spectroscopy- Chemical shift, factors affecting chemical shift values, spin-spin splitting-predicting the multiplicity of protons. Pascal's triangle. Interpretation of ^{1}H and ^{13}C spectra of simple organic molecules.

Mass Spectrometry: Basic principles, ionization technique MALDI, interpretation of mass spectra, molecular ions, meta-stable ions and isotope ions. Fragmentation processes-representation of fragmentation, basic fragmentation types and rules. Factors influencing fragmentations and reaction pathways. McLafferty rearrangement, retro Diels-Alder fragmentation. Nitrogen rule. Mass spectra of alcohols and aldehydes

UNIT III **14 Hours**

DIFFRACTION TECHNIQUES : X-ray diffraction and electron diffraction basic principles X-ray diffraction: Bragg condition, Miller indices, Laue method, Bragg method, Debye-Scherrer method, method of x-ray structural analysis, film method (Weissenberg method). X-ray diffractometers. Systematic absences. Intensities of diffracted X-rays and structural analysis, X-ray scattering by atoms and molecules, Factors affecting X-ray intensities.

Electron Diffraction: Introduction, theory of electron diffraction, Wierl equation and its significance. Structure of surfaces - Low and high energy electron diffraction, TEM, SEM.

REFERENCES:

1. Banwell & McCash (2007), Fundamentals of Molecular Spectroscopy, Tata McGraw Hill, New Delhi.
2. B. K. Sharma (2013), Spectroscopy, Goel Prakashan, Meerut.
3. C. Whiston, J. Wiley & Sons (1987), X-ray methods, New York.
4. D. L. Pavia (2007), Spectroscopy, Cengage Learning India Pvt. Ltd., Delhi
5. G. Aruldhas (2009), Molecular Structure and Spectroscopy, Prentice Hall, 2nd Edition.
6. H. Kaur (2012), Spectroscopy, Pragathi Prakashana, Meerut.
7. J. A. K. Tareen and T. R. N. Kutty (2001), A Basic Course in Crystallography, University Press, Hyderabad.
8. M. A. Waheb (2009), Essentials of Crystallography, Narosa Publishing House, New Delhi.
9. P. S. Kalsi (2004), Spectroscopy of Organic Compounds, New Age Intl., 6th Edition.
10. Silverstein, Bassler & Monnil (2011), Spectrometric Identification of Organic Compounds, John Wiley & Sons.
11. W. Kemp (2011), Organic Spectroscopy, Macmillan, 3rd Edition.
12. Williams (2004), Spectroscopic Methods in Organic Chemistry, TMH, 5th Edition.

PO 549.2- ANALYTICAL TECHNIQUES

Course Outcome:

Student will be able to:

- Gain a domain knowledge about biomolecules and the chemistry related to it
- Understand different electro-analytical techniques
- Understand the chemistry of Polymers

UNIT I: BIOMOLECULES AND ANALYSIS 14 HOURS

Dairy products- composition of milk and milk products; Carbohydrates- sources and classification; Vitamins: Classification and Nomenclature

Carbohydrates : Structure of monosaccharides - Glucose and Fructose, Disaccharides – Sucrose and Maltose. Polysaccharides – Starch and Cellulose

Vitamins: Source and deficiency diseases, biological functions of Vitamins- Vitamin A2 , Vitamin B, Vitamin C & Vitamin K.

Food Analysis: Analysis of fat content, minerals in milk and butter, Estimation of added water in milk. Analysis of caffeine in coffee and tea, detection of chicory in coffee, chloral hydrate in toddy, estimation of methyl alcohol in alcoholic beverages.

Food additives, adulterants, and contaminants- Food preservatives like benzoates, propionates, sorbates, disulphites. Artificial sweeteners: Aspartame, saccharin, dulcin and sodium cyclamate. Flavors: Vanillin, alkyl esters (fruit flavors) and monosodium glutamate.

Artificial food colorants: Coal tar dyes and non-permitted colors and metallic salts. Analysis of pesticide residues in food.

UNIT II: ELECTROANALYTICAL TECHNIQUES 14 HOURS

Electrochemical cells- types, Electrode Potential, Cell Potential, salt bridge representation of cell, Electrolytes and types of electrolytes.

Introduction to electrochemistry: liquid junctions, salt bridge representation, Faradaic and non-Faradaic currents. Reversible and irreversible cells. Indicator Electrodes, Reference electrodes.

Potentiometric: Principle, Potentiometric titrations, Applications.

Conductometry: Definitions, conductance measurement, Conductometric titrations and applications

Voltammetric Techniques: Polarization, Theory of classical polarography, polarographic measurements, polarographic currents, cyclic voltammetry.

UNIT III- ANALYTICAL CHEMISTRY OF POLYMERS 14 Hours

Monomers, general structure and naming of polymers
Basic concepts: Classification of Polymers.
Determination of molecular weights - Number average molecular weight and weight average molecular weight concept; Viscosity, light scattering, osmometry and sedimentation method, GPC techniques.

Thermal Characterization: Glass transition temperature and melting point correlation with structure - Factors affecting Tg and Tm. Characterization of polymers using DSC, DTA, DTG and TGA techniques.

REFERENCES:

1. A.Bahl and B. S. Bahl (2012), Textbook of Organic Chemistry, S. Chand.
2. B. H. Vassos and G. W. Ewing (1983), Electroanalytical Chemistry, Wiley, N.Y.
3. B.K. Sharma (2007), Instrumental Methods of Chemical Analysis, Krishna Prakashan, 19th Edition.
4. D.A. Skoog (2007), Principles of Instrumental Analysis, Thomson Learning, 6th Edition.
5. F. W. Billmeyer (1994), Text book of Polymer Science, John Wiley, 3rd Edition.
6. G. R Chatwal (2007), Instrumental Methods of Chemical Analysis, Himalaya Publishing House, 5th Edition.
7. H.R. Allcock and F.W. Lampe (1990), Contemporary Polymer Chemistry, Prentice Hall, 2nd Edition.
8. J.R. Fried (2014), Polymer Science and Technology, Pearson Prentice Hall, 2nd Edition.
9. M. K. Jain, W. H. Freeman (1968), Principles of Organic Chemistry.
10. N. Shakuntala O. Manay and S. Swamy (2009), Foods – Facts and Principles, New Age International, 4th Edition.
11. P. Bahadur and N. V. Sastry (2002), Principles of Polymer Science, Narosa Publishers.
12. R.A. Day and A. L. Underwood (2008), Quantitative Analysis, PHI, 6th Edition
13. R. J. Young and P. A. Lovell (2002), Introduction to Polymers, Chapman & Hall, 2nd Edition.
14. T. Riley and C. Tomlinson (2011), Principles of Electroanalytical Methods, Wiley India
15. V. R. Gowariker, N. V. Viswanathan & T. Sreedhar (2006), Polymer Science, New Age, 1st Edition.
16. Y. Pomeranz (2008), Food Analysis: Theory and Practice, Springer.

THEORY QUESTION PAPERS PATTERN

- The Syllabus of each paper shall be grouped into units of 14 teaching Hours.
- All hard core papers will have 4 units. Soft core and open elective papers will have 3 units.
- Question Papers in all the four semesters shall consist of Parts A and B.
- For hard core papers - Part A shall contain eight (8) very short answer objective type questions carrying 2 marks each drawn from all the four units of the syllabus (2 questions per unit). Five (5) questions are to be answered.
- Part B shall contain eight (8) brief and/or long answer questions carrying 12 marks each drawn from all the four units of the syllabus (2 questions per unit).
- For soft core and open electives Part A shall contain 9 very short answer objective type questions carrying 2 marks each drawn from all the three units of the syllabus (3 questions per unit). Seven (7) questions are to be answered.
- Part B shall contain six (6) brief and/or long answer questions carrying 14 marks each drawn from all the three units of the syllabus (2 questions per unit).
- There may be a maximum of four sub-divisions per question, carrying 3 or more marks per sub-division. Five (5) out of eight (8) questions for hard core while 4 out of 6 questions for soft core and Open electives are to be answered choosing at least one question from each unit.

CERTIFICATE COURSES IN CHEMISTRY

1. Forensic Chemistry – Scientific Approach to Crime Investigations

Objectives:

This 30-hour online course aims to explain the scientific ideas and methodologies that underpin forensic scientists' work, particularly in the field of chemical science. Various topics will be supported by illustrations with numerous case studies from in and around the region. Students will be able to understand different methodology involved in forensic sciences in particular focus on the chemical analysis.

Learning outcomes:

After successful completion of this course candidate will be able to relate some of the basic facts, concepts and principles relevant to chemical analysis involved in forensic sciences

Contents:

Introduction to Forensic Chemistry, branches of and cases involved in Forensic chemistry, Crime scene investigation. Separation of complex mixtures using chromatography and extraction methods, Spectroscopic techniques – UV, IR and Mass spectroscopy and elemental analysis, Fingerprint analysis – Chemical methods, Narcotics and Drugs, Forensic toxicology, Analysis of fibers, paints and polymers, chemical analysis of glass and soil, Chemistry of fire and explosives. Each chapter will be followed by a case study.

Evaluation Pattern:

3 Assignments; 3 MCQ tests after 3 Modules (15 Marks);1 Final test (25 Marks)

2. Chemistry Drawings using Chemsketch Software

Objectives:

Chemistry Drawings using ChemSketch software is a 30 hours Certificate online course in training of basic chemistry software Chemsketch. This course aimed at imparting skills on use of open-source chemistry tools that are essential for any student or researcher with chemistry. At the end of course, the participants will be able to use this software for drawing chemical structures, generation of their names, retrieve information about physical properties calculations, three-dimensional molecular structure calculations, spectroscopic signatures and other parameters efficiently.

Learning outcomes:

After successful completion of this course candidate will be able to use ACD ChemSketch for generation and processing of simple and complex chemical structures.

Contents:

Introduction of ACD ChemSketch software, download and installation process, Drawing various chemical structures (acyclic, cyclic, polycyclic, heterocyclic), name generation from structures, conversion of name of molecule into its structure, calculation of physical properties such as density, molecular weight, molecular formula, refractive index from structural formula, bond angles, bond lengths, dihedral angles..

Evaluation Pattern:

3 Assignments (25 Marks each); 3 Tests (25 Marks);1 Final Exam (100 Marks)

3. Advanced Characterisation Techniques.

Objectives:

Provide hands-on training in the operation and handling of advanced characterization instruments, Familiarize participants with the principles and applications of Photocatalytic reactor, X-ray diffractometer, BET Surface area analyser, Gas Chromatography, FTIR, and Thermogravimetric analyser, Enhance participants' skills in interpreting data obtained from advanced instruments for the characterization of various organic and inorganic compounds, Prepare participants for research and industrial roles requiring proficiency in advanced characterization techniques, Foster a deeper understanding of the significance of advanced characterization in the context of global advancements in science and technology.

Learning outcomes:

Operate and handle Photocatalytic reactor, X-ray diffractometer, BET Surface area analyser, Gas Chromatography, FTIR, and Thermogravimetric analyser proficiently, Understand the underlying principles behind each characterization technique and its applications, Analyze and interpret data obtained from advanced instruments to characterize organic and inorganic compounds effectively, Apply advanced characterization techniques in research and industrial settings to enhance the quality of work, Appreciate the importance of staying updated with global advancements in advanced characterization techniques.

Contents:

Session 1: Introduction to Advanced Characterization Techniques

Overview of advanced characterization instruments

Importance of advanced characterization in research and industry

Session 2: Hands-on Training with Photocatalytic Reactor

Principles and operation of Photocatalytic reactor

Practical demonstration and hands-on exercises

Session 3: X-ray Diffractometer

Principles of X-ray diffraction analysis
Data interpretation and applications in material characterization
Session 4: BET Surface Area Analyser
Theory of BET analysis
Practical demonstration and interpretation of surface area data
Session 5: Gas Chromatography
Fundamentals of gas chromatography
Sample preparation, injection techniques, and data analysis
Session 6: Fourier Transform Infrared Spectroscopy (FTIR)
Introduction to FTIR spectroscopy
Spectral interpretation and applications in compound identification
Session 7: Thermogravimetric Analyser
Basics of thermogravimetric analysis
Interpretation of thermal degradation profiles and applications
Session 8: Data Analysis and Interpretation
Statistical analysis of characterization data
Case studies and real-world applications
Session 9: Applications of Advanced Characterization Techniques
Case studies showcasing the use of advanced techniques in various fields
Future trends and advancements in advanced characterization techniques
Session 10: Hands-on Practice and Assessment
Recap of learned techniques
Practical exercises and assessment of participants' proficiency
Evaluation Pattern:
2 Assignments (10 Marks each); 3 MCQs (10 Marks);1 Final Exam (100 Marks)

4. Chemistry and Kitchen – Introduction to Culinary Science

Objectives:

Culinary Chemistry-Everyday chemistry of cooking is a 30 hours Certificate online course aims to explore basic chemical concepts of everyday used materials in kitchen. Students will be able to relate food and related topics to various chemistry concepts and understand the Chemical reactions, processes of cooking. This is an interesting and applicable course which encourages the students to explore science, specially Chemistry in everyday life.

Learning outcomes:

After successful completion of this course candidate will be able understand the chemistry of food products, chemical reactions involved in cooking and understand the right use of various gadgets and utensils used in kitchen.

Contents:

Taste and Flavor : Sense of taste and smell, Chemical reactions in cooking, Maillard reactions. Foams: Egg Foam, Fat foam, Gluten foam, Sugar foam, Gelatin foam – bread recipe, leavening alternatives. Protein Chemistry: Amino acids, Denaturing proteins, milk, egg, meat, enzymes, glutamate and cheese. Emulsions: Emulsifying agents, Gum stabilizers. Colloids, Gel and suspensions: Water based colloids, Starches, Agar and agarose, pectin and protein gels. Oils and Fats: Saturated fats, Monosaturated fats, polysaturated fats, Omega-3 and Omega-6 fats, trans fats. Solutions: Syrups and broth, candy and liquors. Crystallization: Sugar crystals and controlling the size of the crystals. Heating: Browning reactions, Protein denaturing, volume reducing and drying, flavour producing, carcinogens, colour changes, nutrition changes and leavening. Acids and bases: Cooking with acids and cooking with bases. Oxidation and Reduction: Apples, Avacados and lemon juice, Vinegar from wine, antioxidants. Boiling and Freezing: Raising the boiling point, Pressure cookers; Lowering the freezing point, making ice cream. Chemistry of yeast, yogurt, buttermilk, wine and beer. Cooking utensils: Methods and gadgets

Evaluation Pattern:

Assignments – 3 of 10 M (30M total); Quiz – 3 of 10 M (30M total); Final test – 25M

5. Spectral Interpretation of Organic Compounds

Objectives:

To learn problem solving skills in spectral analysis and To analyse the patterns in spectroscopy

Learning outcomes:

After successful completion of this course candidate will acquire skills required to elucidate any complex organic structure from spectra.
Completion of the course can make the candidate prepared to attend any related problems in national level competitive examinations and interviews.

Contents:

Introduction to Spectroscopy, Introduction to NMR, Chemical Equivalency, Shielding Effect, Chemical Shift, Spin Coupling, Problem Solving, Anisotropy, Problem Solving

Evaluation Pattern:

Assignment: 2 ; Quiz: 2

6. Cosmetic Chemistry

Objectives:

Post graduate department of chemistry offers 20 hours Certificate course in training of basic chemistry employed in cosmetics. This course is aimed at understanding the principles underlying cosmetic technology, analytical techniques in cosmetic products, Good manufacturing practices and quality assurance in cosmetic technology. At the end of course, the participants will be able to have a better outlook on cosmetic formulations and their usage.

Learning outcomes:

After successful completion of this course candidate will be able to understand the theory and tricks employed behind marketing of cosmetics.

Contents:

Introduction to the principles of cosmetic technology, Analytical techniques in cosmetic products, Good manufacturing practices and quality assurance in cosmetic technology, Product development and cosmetic formulations, approach to cosmetic research and development, Global regulatory and IPR guidelines for Cosmetics. color cosmetics.

MODULE 1:
Introduction to cosmetic chemistry, Learning objectives and outcomes, Origin and History of cosmetics

MODULE 2:
Classification of cosmetics, Advancement of Cosmetics, Ingredients in cosmetic Formulations

MODULE 3:
Nail care cosmetics (Chemistry of Nail cosmetics), Face care cosmetics (Formulations of Face powders, creams, Shaving creams etc)

MODULE 4:
Lip care cosmetics (Chemistry of Lipsticks), Oral care cosmetics (Chemistry of Dentifrices, toothpastes), Body care cosmetics (Chemistry of moisturizing lotions, Perfumes, Deodorants and Antiperspirants)

MODULE 5:
Herbal cosmetics, Cosmetic Packaging, Global Regulatory and IPR Guidelines for the manufacture of Cosmetics

Evaluation Pattern/Task	Marks Allotted/task	No of tasks	Total
quizzes	25	3	75
Assignment	25	3	75
Final Quiz	50	1	50

			200

7. Separation Techniques in Chemical Analysis

Objectives:

Separation techniques in chemical analysis is a 30 hours online course aims at exploring the different separation processes applied in chemical analysis.

Learning outcomes:

After successful completion of this course candidate will be able to account for the application of chromatographic methods in component analysis.

Contents:

Introduction, history, classification, principle & basic theory of chromatography, Column adsorption chromatography, Partition chromatography, Band broadening & column efficiency, factors affecting, Plate theory, Rate theory of chromatography. Column Chromatography - High pressure liquid chromatography (HPLC): Principle, instrumentation Apparatus, pumps, types of columns, packing and characteristics of liquid chromatographic detectors-UV, IR detectors. Advantages and applications of liquid chromatography.

Solvent Extraction: Definition, types, principle and efficiency of extraction. Sequence of extraction process. Factors affecting extraction - pH, oxidation state, modifiers, synergistic, masking and salting out agents. Techniques-batch and continuous extraction, applications.

Ion-exchange Chromatography (IEC): Synthesis and types of ion-exchange resins. Principle, factors affecting ion-exchange equilibria. Resin properties- ion-exchange capacity, applications of IEC in preparative, purification and recovery processes.

Gas Chromatography (GC): Principle, comparison of GSC and GLC. Instrumentation, Columns - packed and tubular. Study of detectors - thermal conductivity, flame ionization, electron capture, GC-MS. Factors affecting separation, applications.

TLC and HPLC: Introduction, preparation of TLC plate, Basic principles, instrumentation of HPTLC, application of HPTLC.

Evaluation Pattern:

Assignments – 3 of 10 M (30M total); Quiz – 3 of 10 M (30M total); Final test – 25M

8. Molecular Spectroscopy: A Theoretical Approach

Objectives:

Understand the fundamentals of the electromagnetic spectrum and explore the interaction of electromagnetic radiation with matter; Analyze the factors influencing the width and intensity of spectral lines in molecular spectra; Interpret the rotational spectrum of a rigid diatomic molecule and its significance and solve related numerical problems; Comprehend the concepts of vibrational and Raman spectroscopy.

Learning outcomes:

Students will be able to apply the principles learned to analyze and interpret various spectroscopic techniques, enabling them to understand molecular structures and properties more deeply.

Contents:

Introduction: Electromagnetic spectrum, interaction of electromagnetic radiation with matter, types of molecular spectra, factors contributing width and intensity of spectral lines.

Rotational spectroscopy: Classification of molecules, rotational spectrum of rigid diatomic molecule, isotope effect on rotational spectra and numericals.

Vibrational spectroscopy: simple harmonic oscillator, vibrational motion of a diatomic molecule, force constants and bond strengths, zero point energy, anharmonicity of molecular vibrations and its consequences, Morse potential energy diagram, normal modes of molecular vibrations and numericals.

Raman spectroscopy: theories of Raman effect, Rule of mutual exclusion.

Evaluation Pattern:

3 Tests of 25 marks each (multiple choice or descriptive); 3 Assignments of 25 marks each.

A Final exam for 100 marks (multiple choice or descriptive).

9. Role of Reagents in Organic Synthesis

Objectives:

Reagents in organic synthesis is a 30 hours certificate online course aims to explore the structural feature, property and role of various reagents used in organic synthesis. To select a suitable reagent for a given organic transformation. To explain role of the reagent in a given transformation and explain the mechanism

Learning outcomes:

On successful completion of this course students will be able to analyze a given target molecule, identify simple reactants and reagents to make various bonds to synthesize a given target molecule.

Contents:

Structure, properties and synthetic applications of Gilman reagent, aluminium isopropoxide, NBS, DDQ, DCC, LTA, lithium aluminium hydride, sodium borohydride, selenium dioxide, perbenzoic acid, wittig reagent, osmium tetroxide, PCC , organoboranes and organosilicon compounds.

Evaluation Pattern:

3 Tests of 25 marks each (multiple choice or descriptive), 3 Assignments of 25 marks each, A final exam for 100 marks (multiple choice or descriptive)

ST ALOYSIUS

(DEEMED TO BE UNIVERSITY)

MANGALURU 575003 - INDIA

DEPARTMENT OF POSTGRADUATE STUDIES & RESEARCH IN CHEMISTRY
SYLLABUS FOR Ph.D. COURSE WORK

SCHEME OF EXAMINATION FOR Ph.D. COURSE WORK IN CHEMISTRY

Course	Particulars	Hours per week	Duration of exam (hrs.)	Marks			
				IA	Theory	Total	Credits
Course-1	Research Methodology	4	3	50	50	100	4
Course-2	Research and Publication Ethics	2	3	50	50	100	2
Course-3	Review of Literature	14	-	-	-	150	6
	Review report Viva					50	2
					Total	400	14

Note: The IA will be based on internal tests/Assignments/Seminars/Group Discussion.

Learning objectives of Ph.D. Programme

The department offers PhD programme in Physics in Condensed Matter Physics, Nuclear and Radiation Physics, Theoretical High Energy Physics and related areas. Candidates applying for the programme will have to undergo admission procedure as per the PhD regulations of St Aloysius (Deemed to be University). The candidate will have to undergo a mandatory course work for 6 months in areas like research methodology, ethics of research and publications and also topics related to various areas of research.

Programme Outcome (PO)

PO1. Application of knowledge acquired in physics to address and propose various problems.

PO2. Use research based knowledge in solving the problems also to use experimental and theoretical techniques to solve problems.

PO3. Use methodologies in research to investigate and solve problems in physics.

PO4. To create, select and apply appropriate techniques of physics to predict and model advanced problems in physics.

PO5. Apply the assessed knowledge to understand the health, safety, and cultural issues of the society relevant to the professional knowledge of physics.

PO6. Apply the professional knowledge of physics to society and environment and demonstrate the knowledge for sustainable development.

PO7. Apply and commit to professional ethics of research in physics.

PO8. To communicate effectively on physics research to the physics community and society.

PO9. To demonstrate the research knowledge of physics to multidisciplinary environments.

PO10. Recognise the need to engage in independent and life-long research in the broadest context of scientific/ technological change.

Ph.D. Programme Specific Outcome (PSO)

PSO1. The Ph.D. programme in physics aims to equip researchers with techniques in contemporary research fields.

PSO2. Achieve an understanding of the physics related to the chosen field of research.

PSO3. Imparting the research findings to the scientific community upholding scientific ethics.

PSO4. Update the progress of the selected research work

COURSE 1: Research Methodology (52 hrs.)

Course objective

- To understand literature review and identification of a research problem.
- To discuss experimental setup, data collection and interpretation of the results.
- To learn various statistical theories and models used in scientific research.
- To understand how to write and publish a scientific research article.
- To learn error analysis and mathematical techniques in scientific research.
- To learn advanced nuclear techniques such as nuclear cross section, Neutron activation analysis, Gamma spectrometry, Proton induced X-ray emission.
- To discuss experimental Techniques and material preparation.

o To discuss principle and working of instruments such as XRD, SEM, TEM, AFM and STM.

Course outcome

CO1. Knowledge to the research student to do the literature review and to identify a research problem.

CO2. Understanding of the experimental setup, data collection and interpretation of the results. CO3. Knowledge of various statistical theories and models used in scientific research.

CO4. Capability to write and publish scientific papers.

CO5. Knowledge of error analysis and mathematical techniques in scientific research.

CO6. Understanding of advanced nuclear techniques such as Neutron activation analysis, Gamma spectrometry, Proton induced X-ray emission.

CO7. Knowledge of experimental techniques and material preparation.

CO8. Understanding of the principle and working of instruments such as XRD, SEM, TEM, AFM and STM.

UNIT I (13 hrs.)

Introduction to Research Methods: Identification of a problem and literature survey. Collection of data and analysis, experimental findings and interpretations. Sources of Research

problems. Outcome of research. Introduction to probability - kinds of probability. Random variables; Definition, probability distribution function, probability density function, continuous, discrete and mixed random variables. Functions of random variables. Solving problems, expectation and introduction to estimation. Paper writing and publishing a scientific paper.

UNIT II :Ultraviolet and Infrared Spectroscopy: (13 hrs.)

UV absorption spectroscopy: Molar absorptivity, theory of electronic spectra, formation of ands, effect of conjugation with examples; Concept and effect of addition of chromophore and auxochrome. Absorption and intensity shifts-Bathochromic, hypsochromic, hyperchromic and hypochromic shifts. Application of UV spectroscopy in the structural study of organic molecules.

IR spectroscopy: Principle dipole moment, expression to obtain vibrational frequency, force constant, determination of force constant and qualitative relation of force constant and bond energies. Fingerprint region and functional group region. Structural elucidation of simple organic compounds with amino, amide, carbonyl, carboxylic, ester functional groups.

UNIT III :NMR, Error Analysis and Software Tools: (13 hrs.)

Nuclear magnetic resonance (1H and 13C) Spectroscopy: Basic Principle, Chemical shift, factors affecting chemical shift values, spin-spin splitting-predicting the multiplicity

of protons. Pascal's triangle. Interpretation of 1H and 13C spectra of simple organic molecules. Basic introduction to 2D NMR.

Error Analysis: Least Square Fitting. Newton's Interpolation, Chi- Square fit, Standard Deviation, error propagation, Eigen value problem, diagonalization (applications to quantum mechanics), Basics of programming using MATLAB and use of software for plotting.

UNIT IV: Vacuum Techniques, Synthesis and Characterization (13 hrs.)

Vacuum Techniques – rotary pump, turbo-molecular pump, ion pump, gas transfer pumps and pressure gauges. Cryogenics -Production, storage and measurement of low temperature.

Synthesis and Characterization

Physical and chemical methods of thin films and nanomaterials synthesis.

X-ray production, X -ray diffraction: Bragg condition, Miller indices, Laue method, Bragg method, Debye-Scherrer method, method of x-ray structural analysis, Interpretation of powder patterns, film method (Weissenberg method). X-ray diffractometers. Systematic absences. Intensities of diffracted X-rays and structural analysis, X-ray scattering by atoms and molecules, Factors affecting X-ray intensities. Electron Diffraction: Introduction, theory of electron diffraction, Wierl equation and its significance. Structure of surfaces - Low and high energy electron diffraction, TEM, SEM, AFM, STM, Resistivity and dielectric measurements.

Reference Books

1. Arfken G B, Weber H J, Harris F E, 'Mathematical Methods for Physicists', (VII Edn. Academic Press, 2013)
2. Ashcroft N W, Mermin N D, 'Solid State Physics', (Harcourt Asia, 1974)
3. Barron R F: Cryogenics Systems (2nd Edition (Oxford university Press 1985)
4. Cullity B D, Stock S R, 'Elements of X-ray Diffraction', (Prentice Hall, 2001)
5. Goswami A, 'Thin film fundamentals', (New Age International, 1996)
6. Harper C, 'Introduction to Mathematical Physics', (PHI, 1978)
7. Henry Stark & John Woods: Probability and random processes with applications to Signal Processing (3rd Edition, Pearson Education Asia, 2002).
8. Ibach H, Luth H, 'Solid State Physics', (Narosa, 1991)
9. Kittel C, 'Introduction to Solid State Physics', (VIII Edn. Wiley India, 2005)
10. Kothari C R. Research methodology: Research & Techniques. New Age International Publishers, New Delhi.
11. Mary L Boas, 'Mathematical Methods in the Physical Sciences', (John Wiley, 1983)
12. Ohring M, 'The Materials Science of Thin films', (Academic Press, 1992)
13. Omar A, 'Elementary Solid State Physics', (Pearson India, 1999)
14. Roth A: Vacuum Technology (2nd Edition North Holland, 1982)

COURSE 2: Research and Publication Ethics (30 Hrs)

Modules	Unit Title	Teaching Hours
Theory		
RPE 01	**PHILOSOPHY AND ETHICS**	**4**
RPE 02	**SCIENTIFIC CONDUCT**	**4**
RPE 03	**PUBLICATION ETHICS**	**7**
Practice		
RPE 04	**OPEN ACCESS PUBLISHING**	**4**
RPE 05	**PUBLICATION MISCONDUCT**	**4**
RPE 06	**DATABASES AND RESEARCH METRICS**	**7**
		30

Course objective

o To introduce the basics of philosophy of science and ethics.
o To inculcate research integrity.
o To discuss publication ethics.
o To educate on how to identify research misconduct and predatory publications.
o To discuss Indexing and citation databases.
o To provide information on open access publications and research metrics.
o To introduce various plagiarism tools.

Course Outcome

CO1.Understanding of basics of philosophy of science and ethics.
CO2.Knowledge of research integrity.
CO3.Understanding of publication ethics.
CO4.Knowledge of identifying research misconduct and predatory publications.
CO5.Knowledge of Indexing and citation databases.
CO6.Knowledge of open access publications and research metrics.
CO7.Knowledge of various plagiarism tools.

THEORY (15 hrs.)

RPE 01: PHILOSOPHY AND ETHICS (3 hrs.)

1. Introduction to philosophy: definition, nature and scope, concept, branches
2. Ethics: definition, moral philosophy, nature of moral judgments and reactions

RPE 02: SCIENTIFIC CONDUCT (5 hrs.)

1. Ethics with respect to science and research
2. Intellectual honesty and research integrity
3. Scientific misconducts: Falsification, Fabrication, and Plagiarism (FFP)
4. Redundant publications: duplicate and overlapping publications, salami slicing
5. Selective reporting and misrepresentation of data

RPE 03: PUBLICATION ETHICS (7 hrs.)

1. Publication ethics: definition, introduction and importance
2. Best practices/standards-setting initiatives and guidelines: COPE, WAME, etc.
3. Conflicts of interest
4. Publication misconduct: definition, concept, problems that lead to unethical behavior and vice versa, types
5. Violation of publication ethics, authorship and contributorship
6. Identification of publication misconduct, complaints and appeals
7. Predatory publishers and journals

Practice

RPE 04: OPEN ACCESS PUBLISHING (4 hrs.)

1. Open access publications and initiatives
2. SHERPN/ RoMEO online resource to check publisher copyright & self-archiving policies
3. A software tool to identify predatory publications developed by SPPU
4. Journal finder/ journal suggestion tools viz. JANE, Elsevier Journal Finder, Springer
5. Journal Suggester, etc.

RPE 05: PUBLICATION MISCONDUCT (4 hrs.)

A. Group Discussions (2 hrs.)

1. Subject-specific ethical issues, FFP, authorship

2. Conflicts of interest

3. Complaints and appeals: examples and fraud from India and abroad

B. Software tools (2 hrs.)

1. Use of plagiarism software like Turnitin, Urkund and other open-source software

tools

RPE 06: DATABASES AND RESEARCH METRICS (7 hrs.)

A. Databases (4 hrs.)

1. Indexing databases

2. Citation databases: Web of Science, Scopus, etc.

B. Research Metrics (3 hrs.)

1. Impact Factor of a journal as per Journal Citation Report, SNIP, SJR, IPP, Cite Score

2. Metrics: h-index, g-index, i10-index, Altmetrics

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2. Bird, A. (2006). Philosophy of science. Routledge.
3. Chaddah. P. (2018). Ethics in Competitive Research: Do not get scooped; do not get plagiarized, ISBN:978-9387480865
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5. MacIntyre, Alasdair. (1967). A Short History of Ethics. London.
6. National Academy of Sciences, National Academy of Engineering and Institute of Medicine. (2009). On Being a Scientist: A Guide to Responsible Conduct in Research: Third Edition. National Academies Press.
7. Resnik, D. B. (2011). What is ethics in research & why is it important. National Institute of Environmental Health Sciences, 1-10. Retrieved from https://www.niehs.nih.gov/research/resources/bioethics/whatis/index.cfm

COURSE 3: Review of Literature (14 hrs./week)

Course Objective

- To introduce the various methods of review literature.
- To learn how to identify research gaps in the chosen research field based on the review of the literature.
- To understand how to formulate a research hypothesis based on the research gap identified.
- To study the instrumentation and experimental setup.
- To learn the scientific methodology and data collection.
- To learn how to arrive at the novelty of the proposed study and expected outcome.
- To understand how to contribute new scientific information to enhance the domain knowledge.

Course Outcome

CO1.Know-how of review of literature.

CO2.To identify the research gap in the chosen field and to find a research problem.

CO3. To formulate a research hypothesis.

CO4.To familiarize with the of instrumentation and experimental setup needed for the proposed study.

CO5.To learn scientific methodology and data collection.

CO6.To foresee the new scientific information that can enhance the domain knowledge in specific and enhance the quality of living in general.

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