M. Sc. CHEMISTRY SYLLABUS

Under Choice Based Credit System

(Effective from Academic Session: 2021-22)

POST GRADUATE DEPARTMENT OF CHEMISTRY
MAHARAJA SRIRAM CHANDRA BHANJA DEO UNIVERSITY
SRIRAM CHANDRA VIHAR
BARIPADA, ODISHA-757 003

The entire P.G. Syllabus of Chemistry is spread over in four semesters consisting of 100 Credits of which 95 Credits are assigned to the **Core Courses** and the remaining 5 Credits is assigned to open course which is offered in Semester-II for other Departments in the University.

Code	Title	Credit	Marks		Total
			Internal	Semester	
CH-401	Physical Chemistry-I	05	20	80	100
CH-403	Inorganic Chemistry-I	05	20	80	100
CH-405	Organic Chemistry-I	05	20	80	100
CH-407	Polymer Chemistry	05	20	80	100
CH-409	Inorganic General Practical	05		100	100
Total		**25**	**80**	**420**	**500**

SEMESTER - II

Code	Title	Credit	Marks		Total
			Internal	Semester	
CH-402	Analytical Chemistry	05	20	80	100
CH-404	Organic Chemistry-II	05	20	80	100
CH-406	Inorganic Chemistry-II	05	20	80	100
CH-408	Spectroscopy-I	05	20	80	100
CH-410	Physical General Practical	05		100	100
OE-CH-412	General Environmental Chemistry	05	20	80	100
Total		**30**	**80**	**520**	**600**

SEMESTER - III

Code	Title	Credit	Marks		Total
			Internal	Semester	
CH-501	Advanced Environmental Chemistry	05	20	80	100
CH-503	Computer for Chemists	05	20	80	100
CH-505	Physical Chemistry-II	05	20	80	100
CH-507	Elective-1	05	20	80	100
CH-509	Organic General Practical	05		100	100
Total		**25**	**80**	**420**	**500**

SEMESTER - IV

Code	Title	Credit	Marks		Total
			Internal	Semester	
CH-502	Spectroscopy-II	05	20	80	100
CH-504	Elective – II	05	20	80	100
CH-506	Practical (Elective)	05		100	100
CH-508	Project work, Presentation and viva	05		100	100
	Total	**20**	**40**	**360**	**400**
	GRAND TOTAL	**100**			**2000**

Core Elective: The students can opt for any one out of Physical/Organic/ Polymer/Inorganic chemistry groups for Elective-I and Elective-II.

ELECTIVE COURSES

Group - A (Organic Chemistry)

Elective - I : Organic Synthesis – I
Elective - II : Organic Synthesis - II

Group - B (Inorganic Chemistry)

Elective - I : Photoinorganic and Supramolecular Chemistry
Elective - II : Organo-Transition Metal Chemistry

Group - C (Physical Chemistry)

Elective - I : Biophysical chemistry
Elective - II : Surface chemistry

Group - D (Polymer Chemistry)

Elective - I : Macromolecular Synthesis and Characterization
Elective - II : Physical Chemistry of Polymers

OPEN ELECTIVE COURSE

Open Elective : General Environmental Chemistry

M. Sc. Chemistry Examination
SEMESTER SYSTEM
(Choice Based Credit System)
To be effective from the session: 2021-22

1. The course is of two years duration comprising of four semesters of theory and laboratory work.
2. The theory examination shall be held for 80 marks and one Internal Assessment Examination (IAE) of 20 marks per each theory paper having full marks of 100 of 03 hrs duration.
3. All units of each paper of semesters are compulsory.
4. For IAE, question shall be asked at least from any two units of a paper covered and will be of one hour duration. The question shall be of unit pattern with two alternatives from each unit.
5. The duration of the practical examination shall be 06 hrs.
6. Each student has to carry out project work from Semester-IV and submit a dissertation before the commencement of Semester-IV examination.
7. For passing semester examination, a candidate must secure a minimum of 40% marks in practical and 30% marks in theory papers.
8. If candidate passes all the four semester examinations she/he will be declared to have passed the M.Sc. (Semester) Examinations in Chemistry, provided further that in no case a candidate shall be allowed to appear any Semester Examination after twice the duration of course period.
9. In order to be eligible to appear at the University examination, a student has to secure at least 75% of attendance.

PROGRAMME OUTCOMES (POs):

On completion of the programme (M.Sc. Chemistry) the students will be able to:

- Acquire conceptual knowledge and comprehensive understanding of the fundamental principles in respective discipline.
- Apply knowledge, understand and critically evaluate the concepts and scientific developments to take up any challenge towards teaching and research.
- Visualize and gain practical knowledge on multidisciplinary aspects related to current research in the fields of Chemical sciences.
- Acquire various skills so as to get motivated to innovate, design methods and techniques to carry out research.
- Communicate effectively, present and publish scientific ideas in Native and English language.
- Employ innovative and greener methods inculcating novel ideas to solve complex and challenging societal and environmental issues.

PROGRAMME SPECIFIC OUTCOMES (PSOs):

On completion of the specific programme the student will be able to:

- Acquire confidence to face competitive examinations of national level like NET, GATE and capable of doing research independently. Utilize skills in problem solving, critical thinking, and analytical reasoning in chemistry.
- Enhance Skill in planning and conducting advanced level chemical experiments, elucidating the structure of compounds / complexes using chemical characterization techniques.
- Develop a creative scientific mind to communicate effectively in public forum-scientific ideas and their impact on socio-economic issues and also provide value based ethical leadership and sensitize the need for a green environment.
- Apply the knowledge of chemistry to effectively function as an individual / team leader / entrepreneur in academic field, chemical or related industries.
- Opt for two specializations namely Inorganic Chemistry and Organic Chemistry to specialize in their favorite subject.
- Opt for two supportive courses in Sem-II and Sem-III of 10 credits.

SEMESTER-I

CH- 401 **Marks- 80 (5 Credits)**

PHYSICAL CHEMISTRY-I

OBJECTIVES:

Primary objective in Units I & II is to introduce students to formal quantum mechanical theory and concepts, to solve exactly some model as well as realistic systems, learn about the approximate methods in quantum mechanics. The objective of Unit-III is to make students learn about reaction rates, their control and their dependence on catalysts and mechanisms. Unit-IV introduces students to various concepts in electrochemistry and help them in understanding electrochemical cells and batteries.

CONTENTS:

UNIT – I

Quantum Chemistry-I

Introduction to formal theory and applications to exact systems

Operators and commutation relations, setting of operators for observables, The Schrodinger's equation and the postulates of quantum mechanics. Hermitian operators Discussion of solutions of the Schrodinger equation to some model systems viz., practice in a box, the harmonic oscillator, the rigid rotor, the hydrogen atom.

Approximate Methods

The variation theorem, Linear variation principle. Perturbation theory (first order and non-degenerate), Applications of variation method and perturbation theory to the Helium atom.

UNIT-II

Quantum chemistry-II

Angular Momentum: Ordinary angular momentum, generalized angular momentum, eigen functions for angular momentum, eigen values of angular momentum, operator using ladder operators, addition of angular momenta, spin, anti-symmetry and Pauli exclusion principle.

Molecular Orbital Theory

Huckel-Theory of conjugated systems, bond order and charge density calculations, Applications to ethylene, butadiene, cyclopropenyl radical.

UNIT – III

Chemical Dynamics

Theories of reaction rates, collision theory of reaction, steric factor, activated complex theory, Arrhenius equation and the activated complex theory, ionic reactions, kinetic salt effects, steady state kinetics, kinetic and thermodynamic control of reactions, treatment of unimolecular reactions. homogeneous catalysis, kinetics of enzymes reactions, general features of fast reactions, study of fast reactions by flow method, relaxation method, flash photolysis and the nuclear magnetic resonance method.

UNIT – IV

Electrochemistry

Electrochemistry of solutions Debye -Huckel - Onsager treatment and its extension, ion solvent interactions. Deby-Huckel-Jerum mode Thermodynamics of electrified interface equations. Derivation of electro-capillarity, Lippmann equations (surface excess), methods of determination, Structure of electrified interfaces. Guay - Chapman, Stern, model. Over potentials, exchange current density, derivation of Butler Volmer equation, Tafel plot. Introduction to corrosion, Homogenous theory, forms of corrosion, corrosion monitoring and prevention methods. Batteries, primary and secondary fuel cells.

COURSE OUTCOMES:

On completion of the course the student will be able to.

- Realize and appreciate the wave-particle duality at microscopic level and the need of quantum theory, the significance of wave functions, eigenfunctions, eigenvalues and uncertainties
- Learn about the qualitative results from rigid rotor, harmonic oscillator and hydrogen atom problems.
- Learn about theories to approximately calculate eigenvalues and eigenfunctions through the variational and perturbation methods and apply these methods to the helium atom.
- Learn about different types of angular momentums – orbital, spin and total angular momentum of a single particle, rules for vector addition of these angular momentums for multiparticle systems like an atom.
- Learn and apply the semiempirical method of Huckel theory to conjugated molecular systems like ethylene, butadiene, etc and calculate their bond order and charge density.
- Acquire in depth knowledge about theories of chemical kinetics and to calculate specific rate, activation energy and frequency factor
- Acquire knowledge on unimolecular reactions, kinetics of enzyme reactions and study of fast reactions by different methods.
- Study of models on electrified interfaces such as Guay Chapman model and Stern model.
- Acquire knowledge on exchange current density, able to derive Butler Volmer equation and Tafel plot.
- Acquire knowledge on corrosion, Batteries and fuel cells

Books Recommended:

1. Physical Chemistry, P.W. Atkins, ELBS
2. Introduction to Quantum Chemistry, A.K. Chandra, Tata McGraw Hill.
3. Quantum Chemistry, Ira N. Levine, Prentice Hall
5. Chemical Kinetics, K.J. Laidler, Mcgraw-Hill.
6. Kinetics and Mechanism of Chemical Transformations, J. Rajaraman & J. Kuriacose, McMillan.
7. Modern Electrochemistry Vol. I and Vol.ll J.O.M. Bockris and A.K.N. Reddy, Plenum.
8. Introduction to Eletrochemistry by Samuel Glasstone

CH - 403 **Marks- 80 (5 Credits)**

INORGANIC CHEMISTRY-I

OBJECTIVE:

This course is aimed to equip the students with knowledge on requirements for the formation of metal complexes and their stability, symmetry elements and their operations, basics on electronic spectra and the chemistry lies on the π acid ligands.

CONTENTS:

UNIT - I

Reactivity of metal complexes

Energy of a reaction, theromodaynamic and kinetic stability of metal complexes, kinetic applications of valence bond and crystal field theories.

Metal-Ligand Equilibria in Solution

Stepwise and overall formation constants and their interrelation, trends in stepwise constants, factors affecting the stability of metal complexes with reference to nature of metal ion and ligand, chelate effect and its thermodynamic origin, determination of binary formation constants by pH-metry, spectrophotometry, Job's method of continuous variation.

UNIT - II

Symmetry and Group Theory in Chemistry

Symmetry elements and symmetry operation, definitions of group, subgroup, relation between orders of a finite group and its subgroup. Conjugacy relation and classes. Point symmetry group. Schonflies symbols, representations of groups by matrices (representation for the C_n, C_{nv}, C_{nh}, D_{nh}, etc.groups to be worked out explicitly). Character of a representation. The great orthogonality theorem (without proof) and its importance. Character tables and their use:

UNIT – III

Electronic Spectra and Magnetic Properties of Transition Metal Complexes

Spectroscopic ground states, correlation, Orgel and Tanabe-Sugano diagrams for transition metals complexes (d^1 to d^9 states), calculations of Dq, B and β parametres, charge transfer spectra, spectroscopic method of assignment of absolute configuration in optically active, metal chelates and their sterochemical information, anomalous magnetic moments, magnetic exchange coupling and spin crossover.

UNIT - IV

(a) Metal - Ligand Bonding

Limitations of crystal field theory, molecular orbital theory: sigma bonding and energy level diagram in octahedral, tetrahedral and square planar complexes; p-bonding and energy level diagram in octahedral complexes, angular overlap model.

(b) Metal Complexes

Metal carbonyls, structure and bonding, vibrational, spectra of metal carbonyls for bonding and structural elucidation, important reactions of metal carbonyls; preparation, bonding, structure and important reactions of transition metal nitrosyl, dinitrogen and dioxygen complexes; tertiary phosphine as ligand.

COURSE OUTCOMES:

On completion of the course the student will be able to

- Discuss the kinetic applications of CFT and valence bond theory; describe the stability of metal complexes in terms of formation constant.
- Able to determine the binary formation constant by pH metry, spectrophotometry and Job;s method of continuous variation.
- Demonstrate detailed functional knowledge about the symmetry, bonding in octahedral and tetrahedral systems, spin orbit coupling and derive term symbols of free ions.
- Understand electronic transitions in metal complexes. interpret the spectra of coordination complexes and learn charge transfer spectra.
- Understand the angular overlap model to estimate amount of interaction takes place between metal d orbitals and ligand orbitals.
- Gain knowledge about the bonding of metal carbonyls, nitrosyls, dinitrogens and metal dioxygen complexes.

Books Recommended:

1. Advanced Inorganic Chemistry, Cotton and Wilkinson, John Wiley
2. Inorganic Chemistry, J.E. Huheey, Ellel A. Keiter, Richard L. Keiter & Okhil K.Medhi
5. Inorganic Chemistry, Gary L. Miessler and Donald A. Tarr
6. Symmetry and Spectroscopy of Molecules, K.V, Reddy
7. Chemical Application of Group Theory, F.A. Cotton

CH - 405 **Marks-80 (5 Credits)**

ORGANIC CHEMISTRY-I

OBJECIVES:

The objective of the course is to understand the concept of Stereochemistry of organic molecules and their effect on reactivity. Also, to learn about different types of reactions and their mechanism and to gain the idea about bioorganic chemistry more specifically the structure and the functions of different co-enzymes

CONTENTS:

UNIT – I

Stereochemistry, Structure and reactivity

Conformational analysis of decalins, effect of conformation on reactivity. Elements of symmetry, chirality, molecules with more than one chiral center, threo and erythro isomers, optical purity, enantioptic and diasterotopic atoms, groups and faces, stereospecific and steroselective synthesis. Asymmetric synthesis. Optical activity in the absence of chiral carbon (biphenyls, allenes and spiranes), chirality due to helical shape. thermodynamic and kinetic requirements, kinetic and thermodynamic control, Curtin-Hammett principle, methods of determining mechanisms, isotope effects.

UNIT – II

(a) Nucleophilic Substitution Reactions

The S_N2, S_N1, mixed S_N1 and S_N2 mechanisms. The neighbouring group mechanism, neighbouring group participation by Pi and sigma bonds, anchimeric assistance. Classical and non-classical carbocations, phenonium ions, norbornyl system, common carbocations rearrangements.

Substitution at an allylic, aliphatic trigonal, vinylic carbon.

Substitution on aromatic substrates. Mechanism, reactivity, effects of substrate structure, attacking nucleophile, leaving group and reaction medium, The von Richter, Sommelet-hauser, and smiles rearrangements.

(b) Electrophilic Substitution Reaction

Bimolecular mechanisms on aliphatic substrates - The S_E1, S_E2 and S_Ei. Mechanism, electrophilic substitution accompanied by double bond shifts. Effect of substrates, leaving group and the solvent polarity on the reactivity.

Substitution on aromatic substrates-the arenium ion mechanism, orientation and reactivity, Quantitative treatment on reactivity in substrates and electrophiles. Diazonium coupling, Vilsmer reaction, Gattermann-Koch reaction.

UNIT - III

Addition and Elimination Reaction

Addition to cyclopropane ring. Hydrogenation of double and triple bonds, hydrogenation of aromatic rings. Hydrocarbonylation. Michael reaction. Sharpless asymmetric epoxidation.

Mechanism of metal Hydride reduction of saturated and unsaturated carbonyl compounds, acids, esters and nitriles. Addition of Grignard reagents, organo zinic and organolithium reagents to carbonyl and unsaturated carbonyl compounds. Witting reaction.

The E_2, E_1 and E_1CB mechanisms and their spectrum, Orientation of the double bond. Reactivity - effect of substrate structures, attacking base, the leaving group and the medium. Mechanism and orientation in pyrolytic elimination.

UNIT - IV

Co-Enzyme Chemistry

Cofactors as derived from coenzymes, prosthetic groups, apoenzymes. Structure and biological functions of coenzyme A, thiamine pyrophosphate, pyridoxal phosphate, NAD^+, $NADP^+$, FMN, FAD, Mechanisms of reactions catalyzed by the above cofactors

COURSE OUTCOMES:

On completion of the course the student will be able to.

- Ensures the students to understand and acquire knowledge on topicity and asymmetric synthesis.
- Demonstrate chirality in organic molecules using units such as center, axial, planar and helicity.
- Illustrate the reaction mechanism aspects in the context of addition, elimination and substitution reaction.
- Assess the structural effects of organic molecules and functional groups on the tendency to participate in various types of organic reactions.
- Describe the methods of asymmetric synthesis which involve chiral substrate, chiral reagents, chiral auxiliary and chiral catalyst.
- Understand the mechanism of enzyme catalyzed reactions
- Get job in Pharmaceutical Sector

Books Recommended:

1. Smith, M. B., March J., (Latest Ed.). March's Advanced Organic Chemistry, John Wiley and Sons, 6th edition, New York.
2. Carey B. F. A., Sundberg R.J., (2007). Advanced Organic Chemistry Part A and Part B, Springer, 5th edition.
3. Kalsi, P.S., (2010). Stereochemistry: Conformation and Mechanism, New Age International (p) Ltd. New Delhi.
4. Morrison, R.T., Boyd, R.N. (2011). Organic Chemistry, Prentice- Hall of India, 6th edition, New Delhi.
5. Sykes, P., (1997). A Guide Book to Mechanism in Organic Chemistry, Prentice Hall, 6^{th} edition.
6. Nasipuri, D. (Latest edition). Stereochemistry of Organic Compounds: Principles & Applications, New Age International Publishers.
7. Structure and Mechanism in Organic Chemistry, C. K. Ingold, Cornell University Press.
8. McMurry J., Organic Chemistry, Asian Book Pvt. Ltd, 8th edition, New Delhi.

9. Bruice Paula, Y., (2015). Organic Chemistry, 7th Edition, Pearson Edition.
10. Lowry, T. H. & Richardson, K. S. Mechanism and Theory in Organic Chemistry Addison-Wesley Educational Publishers, Inc. (1981).
11. Principles of Organic Synthesis, R.O.C., Norman and J.M. Coxon, Blackie Academic & Professional.
12. P.S.Kalsi, Sterochemistry, conformation and mechanism, 7thWiley Eastern Ltd., Chennai
13. Clayden, J.; Greeves, N.; Warren, S., (2012). Organic Chemistry, Oxford University press, 2nd edition.
14. Bioorganic, Bioinorganic & Supramolecular Chemistry (2020), P. S. Kalsi, J. P. Kalsi & A. Chaudhary, New Age International Publishers. 4th Edition.

CH - 407 **Marks- 80 (5 Credits)**

POLYMER CHEMISTRY

OBJECTIVES:

It increases students' knowledge of the structure and behaviours of different polymer materials. The program teaches students about how polymers are made, how they behave, and how modern techniques are used to create new and advanced materials to suit the needs of society and the environment.

CONTENTS:

UNIT - I

Basics

Importance of Polymers. Basic concepts. Monomers, repeat units, degree of polymerization, Linear, branched and network polymers. Classification of Polymers. Polymers. Polymerization: condensation, addition, radical chain-ionic and co-ordination and co-polymerization. Polymerization conditions and polymer reactions. Polymerization in homogeneous and heterogeneous systems.

UNIT - II

Polymer Characterization

Polydispersion-average molecular weight concept. Number, weight and viscocity average molecular weights. Polydispersity and molecular weight distribution. The practical significance of molecular weight. Measurement of molecular weight. End-group, viscosity, light scattering, osmotic and ultracentrifugation methods.

UNIT – III

Structure and Properties.

Morphology and order in crystalline polymers-configurations of polymer chains. Crystal structures of polymers. Morphology of polymers. Morphology of crystalline Polymers, strain-induced morphology, crystallization and melting. Polymer structure and Physical properties-crystalline melting point, Tm-melting points of homogeneous series, effect of chain flexibility and other steric factors, entropy and heat of fusion. The glass transition temperature, Tg-Relationship between Tm and Tg, effects of molecular weight, diluents, chemical structure, branching and cross linking.

UNIT - IV

Properties of Commercial Polymers

Polythylene, polyvinyl chloride, polyamides, polyesters, phenolic resins, epoxy resins, electrically conducting polymers. Biomedical polymers - contact lens, dental polymers, artificial heart kidney, skin and blood cells.

COURSE OUTCOMES:

On completion of the course the student will be able to

- Acquire knowledge on basics of polymers and various polymerization processes.
- Characterize the polymers with respect to their molecular weight, viscosity and disparity.
- Measure molecular weight by different methods.
- Acquire knowledge on crystalline structure and various properties like melting point,chain flexibility of the polymers.
- Acquire knowledge on various applications of commercial polymers, electrically conducting polymers and biomedical polymers.
- Get employability in Polymer and plastic industry

Books Recommended:

1. Text book of Polymer Science, F.W. Billmeyer Jr. Wiley.
2. Polymer Science, V.R. Gowariker, N.V. Viswanathan and J.Sreedhar. Wiley-Eastern.
3. Functional Monomers and Polymers, K.Takemoto.Y.Inaki and R. M. Ottanbrite.
4. Contemporary Polymer Chemistry, H.R.Alcock and F.W.Lambe, Prentice Hall.

CH-409 **Marks-100 (6 Credits)**

INORGANIC GENERAL PRACTICAL

OBJECTIVES:

This course is aimed to gather practical knowledge on synthesis of metal complexes and estimation of metal ions present in mixture solution.

CONTENTS:

1. Qualitative analysis

Analysis of Inorganic salt mixtures containing not more than six radicals (organic acid radicals should be excluded). One of the following rare metal ions like Mo, W, Ti, V and insoluble like TiO_2, $BaSO_4$ etc. may be included.

2. Quantitative Analysis

Separation and determination of two metal ions like Cu-Fe, Zn-Cu, Ni-Zn, Cu-Ni etc. involving volumetric and gravimetric methods.

3. Preparations

Preparation of some selected inorganic compounds and handing of air and moisture sensitive compounds.

(i) $Mn(acac)_3$
(ii) $[Ni(NH_3)_6]Cl_2$
(iii) $K_3[Fe(C_2O4)_3]$
(iv) $Ni(dmg)_2$
(v) *Cis* - $K[Cr(C_2O_4)_2(H_2O)_2]$

COURES OUTCOMES:

On completion of the course the student will be able to

- Prepare coordination complexes.
- Estimate amount of Fe and Cu in a mixture solutions of both.
- Estimate amount of Zn and Cu in a mixture solutions of both.
- Identify the unknown radicals present in a inorganic mixture.

Books recommended:

1. A Text book of Qualitative Analysis, A. I. Vogel
2. A Text book of Quantitative Analysis, A. I. Vogel
3. Inorganic synthesis, Vol. 1-20

SEMESTER - II

CH - 402 **Marks-80 (5 Credits)**

FUNDAMENTALS OF ANALYTICAL CHEMISTRY

OBJECTIVES:

The objective of an analytical chemist is to identify the chemical makeup of various substances. You perform specific procedures to identify and isolate chemical elements and compounds for research or informational purposes.

CONTENTS:

UNIT-I

Introduction

Role of analytical chemistry, classification of analytical methods: classical and instrumental, types of instrumental analysis, selection of analytical methods. Errors in analytical chemistry, classification of errors, source and minimization of errors, absolute and relative error, accuracy and precision, significant figures, mean value and deviation, average and standard deviation, median value, range, confidence intervals. Sampling in analysis: Definition, theory of sampling, technique of sampling, statistical criteria of good sampling, stratified sampling, transmission and storage of samples.

UNIT-II

Thermal analysis and Chromatography

Thermogravimetric analysis (TGA): Instrumentation, derivative thermo gravimetric analysis (DTG), application of theromogravimetry.

Differential Thermal Analysis (DTA): Instrumentation and application of differential thermal analysis simultaneous TG-DTA curves.

Thermogravimetric titration: Principle and applications.

Basic principles and applications of ion chromatography and high performance liquid chromatography

UNIT-III

Electroanalytical methods

Classification of electroanalytical methods, principles and applications of voltammetry, cyclic voltammetry, anodic stripping voltammetry, polarography, amperometry, coulometry, conductometry and ion selective electrodes. (Extensive instrumentations are to be excluded).

UNIT-IV

Spectroscopic methods

Atomic adsorption spectroscopy: Principle and instrumentation, flame atomization, hollow cathode lamps, application of AAS in qualitative and quantitative analysis.

Flame photometric methods: Basic principle and instrumentation, interference in flame photometry, applications in quantitative analysis

Nephelometric method: Principle and instrumentation, application in analysis

COURSE OUTCOMES:

On completion of the course the student will be able to

- Know about classification and selection of analytical methods, errors, accuracy, precision, mean, deviation and sampling.

- Know about Thermo gravimetric analysis (TGA), Differential Thermal analysis (DTA), Ion Chromatography and High performance liquid chromatography (HPLC).
- Know about voltametry, polarography, amperometry, coulometry, conductometry and ion selective electrode.
- Acquire knowledge about Atomic absorption spectroscopy (AAS), Flame photometry and Nephelometric methods.

Books recommended:

1. Analytical Chemistry, Gary D. Christian, 6th Edition, Wiley publication
2. Basic concepts of Analytical Chemistry, S. M. Khoopkar, New Age publication

CH - 404 **Marks-80 (5 Credits)**

ORGANIC CHEMISTRY-II

OBJECIVES:

The objective of the course is to gain the knowledge on symmetry, molecular orbitals and their applications on pericyclic reactions. In addition, to learn in-detail about different categories of pericyclic reactions.

CONTENTS:

UNIT – I

Pericyclic Reactions

Molecular orbital symmetry, frontier orbitals of ethylene, 1,3- butadiene, 1,3,5 - hexatriene. Classification of pericyclic reactions. Woodward - Hoffmann correlation diagrams. FMO approach. Electrocyclic reactions- conrotatory - antrafacial and suprafacial additions, 4n and 4n+2 systems, 2+2 addition of ketenes, 1,3 dipolar cycloadditions. Sigmatropic rearrangements - suprafacial and antrafacial shifts of H, Sigmatropic shifts involving carbon moieties, 3,3 - and 5,5 - Sigmatropic rearrangements, Claisen, Cope and aza- Cope and Ene reaction

UNIT-II

(a) Photochemical Reactions

Interaction of electromagnetic radiation with matter, type of excitations, fate of excited molecule, quantum yield, transfer of excitation energy, actinometry.

(b) Photochemistry of Alkenes

Intramolecular reactions of the olefinic bond - geometrical isomerism, cyclisation reactions, rearrangement of 1,4- and 1.5 - dienes.

(c) Photochemistry of Carbonyl Compounds

Intramolecular reactions of carbonyl compounds - saturated, cyclic and acyclic, b,l unsaturated and a, b- unsaturated compounds. cyclohexadienones.

UNIT - III

Photochemistry of Aromatic Compounds

Isomerisations, additions and substitutions.

Miscellaneous Photochemical Reactions

Photo-Fries reactions of anilides. Photo-Fries rearrangement. Barton reaction. Singlet molecular oxygen reactions. Photochemical formation of smog. Photodegradation of polymers. Photochemistry of vision

UNIT – IV

Host-guest chemistry, chiral recognition and catalysis, molecular recognition, molecular asymmetry and prochirality. Biomimetic chemistry, crownethers, cryptates. Cyclodextrins, cyclodextrin based enzymes models, calixarenes

COURSE OUTCOMES:

On completion of the course the student will be able to

- Predict and formulate the outcomes of pericyclic reactions in terms of orbital interactions and/or the Woodward-Hoffmann Rules & FMO approach of concerted reactions: Electrocyclic reactions, cycloadditions and sigmatropic rearrangements.
- Gain advanced knowledge on interaction of radiation with matter, principles of photochemistry and its applications.
- Understand the basic principles of light-matter interactions and principles of photochemistry.
- Demonstrate the difference between radiative and non-radiative transitions with the help of Jablonski diagram.
- Identify the mechanism of various photochemical reactions of alkenes, carbonyl compounds and aromatic compounds, and able to compare direct photolysis and sensitized photolysis reactions.
- Understand the mechanism of selected photochemical process.
- Understand the principles of molecular recognition and topological aspects of molecular receptors.
- Understand the principles of biomimetic chemistry involving crown ethers, cyclodextrin and calixarenes merged with catalysis.
- Get employability in Pharmaceutical Sector

Book Recommended:

1. Carey B. F. A., Sundberg R.J., (2007). Advanced Organic Chemistry Part A and Part B, Springer, 5th edition.

2. Sankaraman, S. (2005). Pericyclic reactions: Reactions, Applications and Theory, Wiley-VCH.
3. Halton, B.; Coxon J. M. (2011), Organic Photochemistry, Cambridge University Press.
4. Photochemistry & Pericyclic Reactions, Jagdamba Singh & Jaya Singh, New Age International Publishers, Third edition 2012.
5. Dr. Satyajit Dey Dr. Nirmal Kr. Hazra, Through Solved Problems, Techno World Publishers, 2019
6. Fleming, I., Pericyclic Reactions, Oxford Science Publications (1998).
7. Horspool, W. M. Aspects of Organic Photochemistry Academic Press (1976).
8. Fundamentals of Photochemistry, K.K. Rohtagi-Mukherji, Wiley-Eastern limited
9. Essentials of Molecular Photochemistry, A.Gilberi and J.Baggorr, Blackwell Scientific Publication.
10. Molecular Photochemistry, N. J. Turro, W. A. Benjamin.
11. Introductory Photochemistry, A Cox and T.Camp McGraw-Hill.

CH - 406 **Marks- 80 (5 Credits)**

INORGANIC CHEMISTRY-II

OBJECTIVES:

This course is aimed to gather knowledge on chemistry of boranes & metal clusters, inorganic reaction mechanisms, Ion storage and transport proteins, various metalloenzymes, electron transfer proteins and biological nitrogen fixation.

CONTENTS:

UNIT - I

Reaction Mechanism of Transition Complexes

Substitution reactions of octahedral complexes: acid hydrolysis, factors affecting acid hydrolysis; base hydrolysis, conjugate base mechanism, direct and indirect evidences in favour of conjugate mechanism; anation reactions, reactions without metal ligand bond cleavage. Substitution reactions in square planar complexes: the trans effect and its application to synthesis of complexes, theories of trans effect, mechanism of substitution reaction and the factors affecting the substitution reactions.

Redox reactions: Outer-sphere reactions, Marcus theory for outer-sphere reaction, inner sphere reactions.

UNIT – II

Inorganic ring, cage and cluster compounds

Higher boranes, carboranes, metalloboranes and metallocarboranes, Metal carbonyl and halide clusters, compounds with metal-metal multiple bonds.

UNIT – III

(a) Metal ions in Biological Systems

Inophores, Na^+-K^+ Pump, and transport of ions and its mechanism.

Metal ion transport and storage: Ferritin, Transferrin, Siderophores.

(b) **Bioenergetics and ATP Cycle**

Metal complexes in transmission of energy; chloroCHlls, photosystem-I and photosystem-II in cleavage of water. ATP as a energy currency in biological system .

(c) Metalloenzymes:

Carbonic anhydrase, carboxypeptidase and vitamin B_{12}.

UNIT - V

Electron Transfer in Biology

Structure and function of metalloproteins in electron transport processes- cytochromes and ferrodoxin

Nitrogenase

Biological nitrogen fixation, molybdenum nitrogenase, spectroscopic and other evidences.

COURSE OUTCOMES:

On completion of the course the student will be able to

- Learn structure, bonding, stablility and reactivity of simple boranes, carboranes and metallo carboranes.
- Explain structural aspects of metallic clusters and polyanions of important compounds
- Explain different types of electron transfer reactions and factors governing them.
- Evaluate and gain knowledge on various mechanism of substitution reactions in coordination complexes.
- Know about ionophores, metal ion transport and storage protein like ferritine,transferrin and siderophores.
- Aquire knowledge on various metalloenzymes, metalcomplexes in transmission of energy, metalloproteins in electron transport processes and on biological nitrogen fixation.

Books Recommended:

1. Principles of Bioinorganic Chemistry, S. J. Lippard and J. M. Berg, University Science Books.
2. Bioinorganic Chemistry, I Bertini, H.B.Gray, S.J.Lippard and J.S Valentine, University Science Books.
3. Inorganic Chemistry, J.E. Huheey, Ellel A. Keiter, Richard L. Keiter & Okhil K.Medhi.
4. Inorganic Chemistry, Gary L. Miessler and Donald A. Tarr
5. Bioinorganic Chemistry. Asim K. Das
6. Hughes, M. N. The Inorganic Chemistry of Biological Processes, 2nd Ed., Wiley (1981).

7. Lippard, S. J. & Berg, J. M. Principles of Bioinorganic Chemistry Univ. Science Books (1994).
8. Lippard, S. J. Progress in Inorganic Chemistry Vols. 18 and 38, Wiley-Interscience (1991).

CH - 408 **Marks- 80 (5 Credits)**

SPECTROSCOPY-I

Objectives:

This paper introduces the very fundamentals of atomic and molecular spectroscopy from a theoretical point of view. Basic understanding of absorption and emission spectra, the factors affecting the position of signals and their widths and intensities are taught in order to gain insight into the recorded spectrum. This paper deals with fundamentals of all major spectroscopic techniques used; these are microwave, IR, Raman, electronics spectra of both atoms and molecules, NMR and ESR.

UNIT - I

Introduction

Characterization of electromagnetic radiation, quantization of energy, regions of the spectrum, representation of the spectra, basic elements of practical spectroscopy, resolving power, width and intensity of spectral transitions, Fourier transform spectroscopy.

Microwave Spectroscopy

Classification of molecules, rotational energy levels of rigid diatomic molecule, intensities of spectral lines, effect of isotopic substitution, the non-rigid rotator

UNIT-II

Infrared Spectroscopy

Vibrational energies of diatomic molecules: simple harmonic oscillator, force constant and bond strengths, anharmonicity and Morse potential energy function, Vibration-rotation spectroscopy, selection rules, P, Q, R branches, breakdown of Born-Oppenheimer approximation, vibration of polyatomic molecules, normal modes of vibration, group frequencies, overtone and combination frequencies, influence of nuclear spin

Raman Spectroscopy

Classical and quantum theories of Raman effect, polarizability and Raman activity of vibrations, mutual exclusion principle, pure rotational and vibrational Raman spectra, selection rules, rotational fine structure

UNIT - III

Atomic Spectroscopy

Brief discussion of atomic structure, Hydrogen atom spectrum, spin-orbit coupling and fine structure of Hydrogen atom spectrum, spectra of Hydrogen-like species and alkali metals, many electron atoms, Term symbols, spectrum of Helium and alkaline earths.

Molecular Spectroscopy

Born-Oppenheimer approximation, Intensities of vibronic transitions, Frank-Condon principle, dissociation and predissociation of molecules, molecular orbitals, molecular term symbols, selection rules, spectrum of Hydrogen molecule, re-emission of energy by excited molecule: radiative and non-radiative decay

UNIT – IV

Photoelectron Spectroscopy

Basic principles; photo-electric effect, ionization proces, Koopman's theorem. Photoelectron spectra ofsimple molecules, ESCA, chemical information from ESCA Auger electron spectroscopy- basic idea.

Introduction to Spin Resonance Spectroscopy

Nuclear and electronic spin, interaction between spin and magnetic field, Larmor precession and resonance, population of energy levels, relaxation time and width of signal, ESR spectroscopy: the g factor, electron-nucleus coupling and hyperfine structure of ESR, McConnel equation and electron density distribution, application to methyl and benzene radical

COURSE OUTCOMES:

On completion of the course the student will be able to

- Familiarize themselves about the basic elements of practical spectroscopy such as components of a spectrometer, resolving power and signal to noise ratio.
- Learn about microwave activity of different types of molecules. Gain in-depth knowledge on rotational spectra of diatomic molecules using both rigid rotor and non-rigid rotor models. Apply these concepts to calculate different molecular properties.
- Get detailed insight into the infrared spectra of diatomic molecules by treating them using both harmonic and anharmonic oscillator model. Apply these concepts to calculate different molecular properties.
- Learn about Raman activity of molecules using the polarizability ellipsoids, analyze the rotational and vibrational bands in Raman spectra.
- Learn about the coarse spectra of hydrogen-like species, learn about their spectral fine

structure. Learn about the term symbols in multi-electron atoms, and about the spectra of helium and alkaline earth metals.

- Understand the molecular spectra at dissociation and predissociation limits. Apply these concepts to understand the spectrum of the simplest molecule, H_2.
- Learn about the basic principles of photoelectron spectroscopy and apply to study spectra of simple molecules.
- Learn about the basic principles of spin resonance spectroscopy of NMR and ESR. Learn to explain NMR spectra through chemical shift and coupling of nuclear spins. Learn about the g-factor, electron-nucleus coupling and hyperfine structure.
- Do research in Pharmaceutical Sector

Books Recommended:

1. Fundamentals of molecular spectroscopy, C.N Banwell and E. M. McCash
2. Modern Spectroscopy, J.M. Hollas, John Wiley.
3. Applied Electron Spectroscopy for Chemical Analysis Ed. H. Windawi and F.L. Ho, Wiley Interscience.
4. Introduction to molecular spectroscopy, G .M Barrow
5. Introduction to photoelectron spectroscopy, P.K Ghosh
6. Atomic structure and chemical Bonding including molecular spectroscopy, Manas Chandra.

CH - 410 **Marks-100 (6 Credits)**

PHYSICAL GENERAL PRACTICAL

OBJECTIVES:

The objective of this paper, obviously, is to give students practical and hands-on experience to many of the concepts they learn in physical chemistry. Here, the students handle equipment and chemicals to do experiments in order to verify and determine themselves several concepts they learn in theory.

CHEMICAL KINETICS

1. To determine the rate constant of acid catalysed hydrolysis of ethyl acetate by volumetric titration method.
2. To determine the rate constant of base-catalysed hydrolysis of ethyl acetate - by volumetric titration method.
3. To determine the bimolecular rate constant of the oxidation of iodide ions by hydrogen peroxide in aqueous medium.

HETEROGENEOUS EQUILIBRIA

1. To determine the partition coefficient of iodide between carbon tetrachloride and water.
2. To determine the equilibrium constant of the tri-iodide formation $I_2 + I^- \rightleftharpoons I_3^-$ in aqueous solution.

CONDUCTOMETRY:

1. Conductometric titration of a mixture of HCL + CH_3COOH against NaOH.
2. To determine the rate constant of saponification of ethyl acetate - conductometrically
3. To determine the ionization constant of weak acid.

POTENTIOMETRY

1. Potentiometric titration of a strong acid vs strong base.
2. Solubility product of a sparingly soluble salt.

POLARIMETER

1. To determine the rate constant of Inversion of cane sugar in acid medium.
2. To determine the concentration of unknown sugar.

SPECTROPHOTOMETER

1. Verification of Beer-Lambert's law.

COURSE OUTCOMES:

On completion of the course the student will be able to

- Determine the rate constant of acid catalysed hydrolysis of ethyl acetate by volumetric titration method.
- Determine the rate constant of base-catalysed hydrolysis of ethyl acetate - by volumetric titration method.
- Conductometric titration of a mixture of HCL + CH_3COOH against NaOH.
- Potentiometric titration of a strong acid vs strong base.
- Determine the rate constant of Inversion of cane sugar by polarimetry method and concentration of unknown sugar.
- Verification of Beer-Lambert's law and determination of extinction coefficient

Book Recommended:

1. Experimental Physical Chemistry by R.C. Das and B. Behera, Tata, Mc Graw Hill.

OE-CH - 412 **Marks- 80 (5 Credits)**

GENERAL ENVIRONMENTAL CHEMISTRY

OBJECTIVES:

The objectives of environmental education is to increase public awareness about environmental issues, explore possible solutions, and to lay the foundations for a fully informed and active participation of individual in the protection of environment and the prudent and rational use of natural resources.

CONTENTS:

UNIT - I

Introduction to Environmental Chemistry

Concept and scope of environmental chemistry, Environmental terminology and nomenclatures, Environmental segments

Atmosphere

Regions of atmosphere, Earth's radiation balance, chemistry of ozone layer, role of chemicals in ozone destruction, ozone hole, green-house gases and its effect, Global warming, measures to check global warming, El-Nino phenomenon.

UNIT - II

Air Pollution

Air Pollutants: sources, classification, sampling and monitoring. Aerosols, Acid Rain, Photochemical smog, Auto exhausts, Air-quality standards.

Water Pollution

Water pollutants (sources, sampling and monitoring), Water-quality parameters and standards: physical and chemical parameters (colour, odour, taste and turbidity). Effects of fluoride in drinking water. Fresh water conservation in India.

UNIT - III

Chemical Toxicology

Toxic chemicals in the environment, impacts of toxic chemicals on enzymes, biochemical effects of arsenic, cadmium, lead, mercury, carbon monoxide, pesticides, insecticides and carcinogens. Bioaccumulation and biomagnifications.

UNIT - IV

Green Chemistry: Basic concept, History, rules of green chemistry, Environmental impact, pollution control, industrial applications of green chemistry. Application of Green Chemistry in Sustainable development.

COURSE OUTCOMES:

On completion of the course the student will be able to

- Understand the scope of environmental chemistry and its basic terminology.
- Understand ozone destruction, green-house effect, global warming and El-Nino effects.
- Understand sources, classification and monitoring of air pollution.
- Able to identify water pollutants and understand water quality parameters.
- Understand phenomenon like acid rain, photochemical smog.
- Understand air quality standards.
- Identify effect of metals and other toxic pollutants and their biochemical effects.
- Understand the phenomenon of Bioaccumulation and biomagnifications.
- Outline the principles of green chemistry and its industrial applications.
- Understand application of green chemistry in sustainable development.

Books Recommended:

1. Environmental Chemistry, S.E. Manahan, Lewis Publishers
2. Environmental Chemistry, Shariha & Krishna Publishers
3. Environmental Chemistry, A.K. De, Wiley Eastern.
4. Environmental Pollution Analysis, S.M. Khopkar, Wiley Eastern
5. Standard Method of Chemical Anal., F.J. Welcher Vil. - III, Van Nostrand Reinhold Co.
6. Environmental Toxicology, Ed. J. Rose, Gordon and Breach Science Publication.
7. Elemental Analysis of Airborne Particles, Ed. S. Landsberger and M. Creatchman, Gordon and Breach Science Publication.
8. Environmental Chemistry, C. Baird, W.H. Freeman
9. Hand Book of Environmental Analysis, Pradyot Patnaik, Lewis Publishers (1997)
10. Standard Methods for the Examination of Water and Wastewater, APHA, AWWA, WPCF, Washington D.C. 20005, USA, 17th Edition (1998)

SEMESTER - III

CH - 501 **Marks- 80 (5 Credits)**

ADVANCED ENVIRONMENTAL CHEMISTRY

OBJECTIVES:

The objectives in environmental science are to understand the relationships and processes in the natural world, how humans and the natural world interact with each other, and how humans and human activities affect the natural world. Through the understanding generated

by pursuing these objectives, environmental science is also applied to solving environmental problems caused by human activities and develop new ways to serve human interests while minimizing the negative environmental impacts of such activities.

CONTENTS:

UNIT - I

Environment

Introduction, Earth, Environment, Types of Environment, Environmental Segments, Vertical Temperature of Atmosphere, Heat Budget of Earth's Atmospheric System, Human Interference with Environment, biogeochemical cycles in environment: water, carbon, oxygen and nitrogen.

UNIT - II

Atmosphere

Chemical Composition of Atmosphere: Introduction, Particulates, Ions, Radicals, Smog

Chemical and Photochemical Reactions in the Atmosphere: Introduction, Oxygen, Ozone, Nitrogen, Oxides of Nitrogen, Oxides of Sulphur, Oxides of carbon.

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UNIT - III

Soil Pollution

Introduction, Formation of Soil and its Characteristics, Soil Profile, Types of Soil, Alkaline, Acidic, and Neutral Soil, Plant Nutrients, Environmental Concerns of Soil Pollution, Harmful Effects of Soil Pollution.

Water Pollution

Types of Water Pollutants, Water, Pollution in Various Water bodies, Harmful Effects of Water Pollution, Sewage and Domestic Wastes, Industrial Effluents, Agricultural Discharge, Detergents, Toxic Metals.

UNIT - IV

Radioactive Pollution

Introduction, Radioactive Pollution, Sources of Radioactive Pollution, Effects of Radioactive Pollution, Disposal of Radioactive Waste.

Environmental Toxicology

Chemicals in the Environment, Biodegradation, Microbial Transformations, Effect of Toxic Chemicals on Enzymes, Biochemical Effects of Some Toxic Substances.

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COURSE OUTCOMES:

On completion of the course the student will be able to

- Understand types of environment and human interference with the environment
- Understand various photochemical reactions in the atmosphere.
- Describe soil profile and harmful effects of soil pollution.

- Describe source and effects of radioactive pollution, and disposal of radioactive waste.
- Identify effect of metals and other toxic pollutants in the environment and their effect on human health.
- Get employability in Pharmaceutical & NGO Sector

Books Recommended:

1. Advanced Environmental Chemistry, V K Ahluwalia, Teri (The Energy and Resource Institute), 2017
2. Environmental Chemistry, S.E. Manahan, Lewis Publishers
2. Environmental Chemistry, Shariha & Krishna Publishers
3. Environmental Chemistry, A.K. De, Wiley Eastern.
4. Environmental Pollution Analysis, S.M. Khopkar, Wiley Eastern
6. Environmental Toxicology, Ed. J. Rose, Gordon and Breach Science Publication.
7. Environmental Chemistry, C. Baird, W.H. Freeman

CH-503 **Marks-80 (5 Credits)**

COMPUTER FOR CHEMISTS

OBJECTIVES:

To impart basic idea about the applications of computer in Chemistry.

CONTENTS:

UNIT-I

Introduction to computer

History of development of computer, basic structure of a computer: the CPU, the input-output devices, the internal memory, commonly storage secondary media, data representation, overview of binary, octal and hexadecimal number systems.

UNIT-II

The softwares

Concept of low level low level and high level languages, computer interpreter, editor, operating system concept (salient features).

General awareness of commonly used software packages like MS-Excel and Power Point.

UNIT-III

C Language programming – I

C Language fundamentals

Character set, identification, keywords, Data types, constant and variables, Statements, operators, Precedence of operators, Input- output assignments, control structure, decision making and branching, decision making and looping.

Arrays and string

One dimensional, multidimensional and their applications, declarations, manipulation and string handling functions.

C Functions

Users defined vs standard functions, formal vs actual arguments, functions category, function prototypes, parameter passing, recursion, storage classes: auto, extern, global, static.

UNIT-IV

Computer applications in Chemistry

Development of small computer codes involving simple formulae in chemistry such as van der Waals equation, pH-titration, kinetics and radiation decay.

Evaluation of lattice energy and ionic radii from experimental data. Execution of X-Y plots.

COURSE OUTCOMES:

On completion of the course the student will be able to

- Get brief account on history of development of computer, know about basic structure of a computer: the CPU, the input-output devices, the internal memory, hard disk drive, etc. Get idea on data representation on a computer: binary, octal and hexadecimal number systems.
- Know about the concept of low level and high level languages, computer interpreter, assembler and compilers, text editors, basic idea on work of operating systems (examples: Windows, Linux, Unix, Android, etc). Have general awareness of commonly used software packages like MS-Word, MS-Excel and Power Point.
- Learn about the fundamentals of C Language programming. One-dimensional, multidimensional arrays and their applications, declarations, manipulation and string handling functions. Know about C Functions: Users defined vs standard functions, formal vs actual arguments, etc.
- Write simple codes in C Programming language to express equations and to solve problems in Chemistry, such as van der Waals equation, pH-titration equation, kinetics and radiation decay. Apply to evaluation of lattice energy and ionic radii from experimental data and make 2-dimensional X-Y plots.

Books recommended:

1. Fundamentals of computer, V. Rajaraman
2. Computational chemistry, A. C. Narris
3. Computer Aids to Chemistry, Ed. G. Vernini and M. Chanon

4. Programming in C, E. Balaguruswamy, Tata Mcgraw Hill.
5. C the complete reference, H. Schildt, Tata Mcgraw Hill.
6. Let us C, Y. Kanetkar, BPB publications.

CH - 505 **Marks- 80 (5 Credits)**

PHYSICAL CHEMISTRY-II

OBJECTIVES:

The principal objective of this paper is to introduce students a modern branch in thermodynamics, that is, the statistical thermodynamics. Here they learn how classical thermodynamical quantities like, enthalpy, entropy, pressure, internal energy, free energy etc can be expressed in terms of atomic and molecular energy states that comes from quantum mechanics. In addition, students also learn about rates of irreversible or spontaneous processes.

CONTENTS

UNIT – I

Classical thermodynamics

Brief resume of law of thermodynamics, free energy in closed system, thermodynamics of open systems: partial molar properties, chemical potential, Gibbs-Duhem equation, chemical potential and its relations to other partial molar properties and phase equlibrium, chemical potential of a system of ideal gas, determination of partial molar volume: slope and intercept method, concept of fugacity and determination of fugacity of a gas. Activity, activity coefficient, ionic strength

UNIT-II

Equilibrium statistical thermodynamics

Concepts: distribution of molecular states, microstates and macrostates of a system, equilibrium state and entropy, most probable distribution, canonical ensemble, grand canonical and microcanonical ensemble, time average and ensemble average of thermodynamic property

Statistical distribution formula: Bose-Einstein statistics, Fermi-Dirac statistics, Maxwell-Boltzman statistics

UNIT - III

Partition functions

Boltzman factor and partition function, canonical partition function for a system of noninteracting particles, Atomic and molecular partition functions: electronic, translational,

rotational and vibrational partition functions, thermodynamic properties in terms of ensemble partition function

UNIT-IV

Application of partition function

Application to a system of monoatomic and diatomic ideal gas, heat capacity behavior of monoatomic crystals: Einsten and Debye theory, equilibrium constant of ideal gas reactions in terms of partition functions.

Non-equilibrium thermodynamics

Phenomenological laws and Onsager's reciprocal relations, entropy production in spontaneous processes - due to flow of heat and matter, Prigogines principle of minimum entropy production

COURSE OUTCOMES:

On completion of the course the student will be able to

- Differentiate between thermodynamics of closed and open systems. Learn about free energy in closed system as opposed to partial molar properties and chemical potential in open systems. Learn about the concept of fugacity and its determination for a real gas by graphical method.
- Learn about the concepts in statistical thermodynamic such as, distribution of molecular states, microstates and macrostates of a system, equilibrium state and entropy, most probable distribution. Derive the statistical distribution formula for Maxwell-Boltzman statistics, Fermi-Dirac statistics and Bose-Einstein statistics.
- Derive expressions for atomic and (diatomic) molecular partition functions for different degrees of motion: electronic, translational, rotational and vibrational partition functions. Derive and express thermodynamic properties in terms of ensemble partition function.
- Apply of the concept of partition function to evaluate thermodynamic properties of some realistic systems. Study of heat capacity behavior of monoatomic crystals using Einstein and Debye theory. Learn about the thermodynamics of systems that are not in equilibrium and about spontaneous processes. Derive expression for entropy production in spontaneous processes both due to flow of heat and matter.

Books Recommended:

1. Physical Chemistry by Ira N Levine
2. Molecular Thermodynamic by D. A. McQuarrie and J. D. Simon
3. Physical Chemistry by P. Atkins and J. de Paula
4. Statistical Thermodynamics by M.C. Gupta
5. Fundamentals of Statistical Mechanics by B. B. Laud
6. Introduction to Modern Statistical Mechanics, by D. Chandler, Oxford University Press (NY)
7. An introduction to Statistical Thermodynamics by T. L. Hill Dover (NY).

CH – 507 (Elective-I, Group-A) **Marks- 80 (5 Credits)**

ORGANIC SYNTHESIS - I

OBJECIVES:

The objective of the course is io impart knowledge on organometallic reagents and their applications in organic chemistry and to learn about oxidation and reduction reactions of different catagories of carbon-carbon and carbon-heteroatom bonds.

CONTENTS:

UNIT - I

Organometallic reagent

Application of organometalic reagent in organic synthesis: Group - I and Group - II metal : Li, Mg, and Zn. Transition metals : Cu, Pd, Ni, Rh and Other elements Si and B.

UNIT - II

Oxidation

Use of modern Methods, reactivity, selectivity and representative examples in oxidation of hydrocarbons, alcohols, activated and unactivated C-H bond, carbon-carbon double bond, ketones, palladium-catalyzed oxidation of alkenes, oxidation with ruthenium and thallium (III) nitrate.

UNIT - III

Reduction

Use of modern methods, reactivity, selectivty and representative examples in reductions : catalytic hydrogenation, reductions with metals in solutions, hydride transfer reagents, borane, dialkyl-boranes and trialkyltin hydrides and trialkyl-silanes.

UNIT - IV

Heterocyclic synthesis

Principles of heterocyclic synthesis involving cyclization reactions and cycloaddition reactions involving small ring heterocycles Three-membered and four-membered heterocycles-synthesis and reaction of aziridines, oxiranes, thiiranes, azetidines, oxetanes and thietanes.

COURSE OUTCOMES:

On completion of the course the student will be able to

- Assess the mechanism and synthetic uses of selected organometallic reagent in organic synthesis.

- Predict the structure, mechanism and stereochemistry of reactions involving selected oxidizing and reducing agents on organic molecules.
- Understand the principles of constructing small ring (three and four membered) heterocycles involving cyclization and cycloaddition reactions.
- Get employability in Pharmaceutical Sector

Books Recommended:

1 Warren, S. Organic Synthesis: The Disconnection Approach John Wiley & Sons (1984).
2. Organic Synthesis - Concept, Methods and Starting Materials, J. Furhrop and G. Penzillin, Verlage VCH.
3. Modern Methods of Organic Synthesis, Cambridge University Press; 4th edition. 2015
4. Principles of Organic Synthesis, R. Norman and J. M. Coxon, Blackie Academic & Professional.
5. Advanced Organic Chemistry Part B, F.A. Carey and R.J. Sundberg, Plenum Press.
6. Organic Chemistry, Jonathan Clayden , Nick Greeves, Stuart Warren, Oxford University Press; 2nd edition 2014.
7. Organic Synthesis, Jagdamba Singh & L D S Yadav, Pragati Prakashan, Meerut, 2015
7. Wiley's Problems in Organic Chemistry, K. Singh, Wiley, 2015.
8. Heterocyclic Chemistry, Raj K Bansal, New Age International Publishers, 6 thEdition, 2019
9. Heterocycle, Joules, Mills & Smith

CH – 507 (Elective-I, Group-B) **Marks- 80 (5 Credits)**

PHOTOINORGANIC AND SUPRAMOLECULAR CHEMISTRY

OBJECTIVES:

This course is aimed to gather knowledge on photo inorganic chemistry and basics & applications of supramolecular chemistry which deals with various non covalent interactions, molecular self assembly and supramolecular devices.

CONTENTS:

UNIT – I

Excited state of Metal complexes

Excited state of Metal complexes, comparison with organic compounds, electronically excited states of metal complexes, CT spectra, CT excitations.

Metal complex sensitizers:

Metal complex sensitizers**,** Electron relay, metal colloid systems, semiconductor supported metal oxide systems, water-photolysis, nitrogen fixation and CO2 reduction.

UNIT – II

Redox Reactions in Metal Complexes

Redox reactions of metal complexes in excited states, excited electron transfer, examples using [Ru(bpy)3]2+ complex and [Fe(bpy)3]3+ complex. Role of spin-orbit coupling, life-times of excited states in these complexes.

Introductory idea of Photo Chemistry of transition metal carbonyls with examples.

UNIT - III

Fundamentals of Supramolecular Chemistry

Concept of Supramolecular Chemistry, Supramolecular Structure through noncovalent interactions

Molecular recognition:Molecular receptors for neutral,cationic and anionic substrates, design and synthesis of co-receptors and multiple recognition,

Introduction to molecular self assembly in Supra Molecular Chemistry with Examples

UNIT - IV

Applications

Supramolecules in transport processes and carrier design, Supramolecular reactivity and catalysis,

Supramolecular devices, Supramolecular photochemistry, Supramolecular electronic, ionic switching devices.

COURSE OUTCOMES:

On completion of the course the student will be able to

- Learn on excited state of metal complexes and their comparison with organic compounds, Charge transfer spectra , Charge transfer excitation and metal complex sensitizers.
- Know about Electron relay, metal colloid systems, semiconductor supported metal oxide systems, water-photolysis, nitrogen fixation and CO_2 reduction.
- Know about Redox reactions of metal complexes in excited states and life-times of excited states in these complexes along with introductory idea of Photo Chemistry of transition metal carbonyls.
- Acquire knowledge on Concept of Supramolecular Chemistry, Supramolecular Structure through non covalent interactions, Molecular receptors for neutral, cationic and anionic substrates, design and synthesis of co-receptors and multiple recognition, molecular self assembly in Supra Molecular Chemistry with Examples
- Acquire knowledge on Supramolecules in transport processes and carrier design, Supramolecular reactivity and catalysis, Supramolecular photochemistry, Supramolecular electronic, ionic switching devices.
- Get employability in Pharmaceutical and drug design Sector

Books recommended:

1. An Introduction to Supramolecular Chemistry, Asim K. Das & Mahua Das

2. Progress in Inorganic Chemistry, Vols. 18 and 38 ed.
3. Supramolecular Chemistry - J.M. Lehn, VCH
4. Inorganic photochemistry, J. Chem Education, Vol. 60, No. 10, 1983.
5. Photochemistry of Coordination compounds, V. Balzari and V. Carassti, Acdemic Press

CH – 507 (Elective-I, Group-C) **Marks- 80 (5 Credits)**

BIOPHYSICAL CHEMISTRY

UNIT - I

Biological cell and its constituents

Biological cell, Structure and functions of proteins, enzymes, DNA and RNA in living systems, Helix coil transition.

Bioenergetics

Standard free energy change in biochemical reactions, exergonic, endergonic, Hydrolysis of ATP from ADP.

UNIT-II

Statistical mechanics in bioplolymers

Chain configuration of macromolecules, Statistical distribution end to end dimensions, calculation of average dimensions for various chain structures, Polypeptides and protein structures, Introduction to protein folding problem.

UNIT - III

Bioploymer interactions

Forces involved in biopolymer interactions, Electrostatic changes and molecular expansion, hydrophobic forces, dispersion force interactions, Multiple equilibria and various types of binding processes in biological systems, Hydrogen ion titration curves.

Thermodynamics of bioploymer solutions

Thermodynamics of biopolymer solutions, Osmotic pressure, Membrane equilibrium, Muscular contraction and energy generation in mechanochemical system.

UNIT - IV

Cell membrane and transport of ions:

Structure and functions of cell membrabe, Ion transport through cell membrane, Irreversible thermodynamic treatment of membrane transport, Nerve conduction.

Bioploymers and their molecular weight

Evaluation of size, shape, molecular weight and extent of hydration of biopolymers by various experimental techniques, Sedimentation equilibrium, hydrodynamic methods diffusion, sedimentation velocity, Viscocity, Electrophoresis and rotational motions.

Books Recommended:

1. Principles of Biochemistry by Lehninger, D.L. Nelson and M. Cox.
2. Bio-chemistry by Voet and Voet
3. Biothermodynamics by T.T. Edsall and H. Gutfreund, Wiley (NY)
4. BioPhysical Chemistry by J. Edsall and J. Wyman, Academic (NY)
5. Bioenergetics, A.L. Lehinger, Benjamin (NY)

COURSE OUTCOMES:

On completion of the course the student will be able to

- Learn on structure and functions of proteins, enzymes, DNA and RNA in living systems, Standard free energy change in biochemical reactions
- Learn on statistical distribution end to end dimensions calculation of average dimensions for various chain structures.
- Acquire knowledge on various bioploymer interactions Thermodynamics of bioploymer solutions.
- Cell membrane and transport of ions Bioploymers and their molecular weight

CH – 507 (Elective-I, Group-D) Marks- 80 (5 Credits)

MACROMOLECULAR SYNTHESIS AND CHARACTERIZATIONS

UNIT - I

Ionic and Coordination Polymerization

Chemistry of Non-radical chain polymerization, Cationic polymerization, Mechanism & Kinetic with examples, Anionic polymerization, mechanism and Kinetics with example. Coordination polymerization (Zingler - Natta Catalyst), Steroregular polymerization, mechanism and kinetics of ring opeing polymerizatiion.

UNIT - II

Synthesis of Polymer

Bulk, Solution, Suspension, Emulsion, Precipitatiion Gas Phase, Solid State and interfacial methods of polymerization.

Polymerization and hydrogen transfer polymerization: Preparation Nylon 6.6 Poly (1.1. - undecanoamide). Poly (Decamethylene oxamide) Poly (Ethylene Terepthalate). Poly sulphone from Bio-Phenol - A & dichlorophenyl sulphone.

Thermal polymerization of styrene in Bulk, Emulsion polymerization of styrene with persulfate, suspension polymerization of styrene solution and emulsion polymerization of vinyl acetate, solution polymerization of Acrylamide.

UNIT - III

Ring - opening Polymerization

Fast polymerization of caporolactam to Nylon-6 with anion catalysts, low temperature polymerization of L-Piperidine to Nylon-5, polymerization of Ethylene oxide and Tetrahydrofuran and Preparation of linear polysilcons.

Non-classical routes to polymers-polymerization of Anhydrous formaldehyde to polyoxymethylene, solid state polymerization of Troioxane. Preparation of n-butylisolyanate, Diazomethan and Norbornlene.

Preparation of Pehnol-formaldehyde resin, Urea-formadehyde resin, Epoxy resin, Allyl resins.

UNIT - IV

Characterisation of Polymers

UV-VIS Spectroscopy of Polymers, characterisation of polymer and copolymer by IR. NMR & EPR of polymers. X-ray difraction and electron diffraction of polymers, composites. Thermal analysis of polymers by TG, DTG, DTA, DSC chromatograCH - Pyrolysis Gas chromatograCH and other chromatographic characterisation.

Course Outcome

On completion of the course the student will be able to

- Learn on Ionic and Coordination Polymerization.
- Learn on different synthetic methods to prepare different types of Polymer.
- Acquire knowledge on Ring - opening Polymerization of different polymers
- Learn on spectral characterization of polymers.

Books recommended:

1. Polymer Science, Gowariker, Viswanathan & Sreedhar
2. Polymer Scince, Premamaya Ghosh
3. Organic Polymer Chemistry, K.J. Saunders
4. Organic Chemistry of Macromolecules, A. Rayve
5. Polymer Chemistry, A.B. Seymour & C.E. Carraher
6. Experiments in Polymer Science, Edw and A. Collin & F.W. Billmeyer
7. Principle of Polymerization, Flory
8. Characterization of POlymer, N.M. Bikales
9. NMR of Polymers, I.Y. Slorium & A.N. Lyubimor
10. FT-IR Characterization of Polymer, H. Ishida

CH - 509 **Marks - 100 (6 Credits)**

ORGANIC GENERAL PRACTICAL

OBJECIVES:

The objective of the course is to synthesize small molecules from commercially available starting materials and to estimate the functional group present in organic compounds

CONTENTS:

1. **Analysis of Organic Compound**

   Separation and identification of components of a mixture of two organic compounds (solid-solid, solid-liquid, liquid-liquid).

2. **Organic Synthesis (Single Step)**

   a) Preparatiion of p-bromoacetanilide.
   b) Preparation of 3, 5 -dibromobenzoic acid.
   c) p-bromo aniline preparation from aromatic electrophilic substitution reaction.
   d) Preparation of p-chlorotolune.
   e) Preparation of Methyl orange.
   f) Preparation of Asprin
   g) Preparation of Anthranilic acid.

3. **Estimation**

   a) Estimation of Keto Group (>c=o)
   b) Estimation of Acetyl group (-C - CH_3)

4. **Separation**

   Acetylation of Cholesterol and separation of cholesteryl acetate by column chromatography.

COURSE OUTCOMES

On completion of the course the student will be able to

- Acquire skills in different laboratory techniques such as melting point, distillation, TLC, column chromatography, crystallization and preparation of dry solvents.
- Separation and qualitative analysis of two component mixtures of organic compounds: characterization of derivatives and identification of the components.
- Design single stage synthesis of simple organic compounds and execute them in the laboratory.
- Single stage preparation of organic compounds using some classical organic reactions.
- Extraction of caffeine from tea leaves, piperine from pepper, lachanoric acid from lichens and casein from milk.

Books Recommended:

1. Vogel's Text Book of Practical Organic Chemistry, Furniss, S. B.; Hannaford, A. J.; Smith, P. W. G.; Tatchell, A. R. 5th Ed.; Longman Scientific & technical, England, 1989.

2. Laboratory Manual of Organic Chemistry, Dey and Sitaraman, Allied Publishers, 1992.
3. Laboratory Manual of Organic Chemistry, Raj K Bansal, New Age International Publishers, 2008

SEMESTER – IV

CH - 502 **Marks - 80 (5 Credits)**

SPECTROSCOPY-II

OBJECIVES:

- ✓ To impart knowledge on in-depth concepts, instrumentations and applications of organic spectroscopy
- ✓ To learn about basic idea, instrumentations and applications of mass spectrometry.
- ✓ To gain the idea about problem solving approach using the concepts of different types of spectroscopic techniques.

CONTENTS:

UNIT - I

(a) Vibrational Rotational Spectroscopy.

Group vibration concept and its limitations, Use of symmetry arguments to determine the number of active infrared and Raman lines. Applications of infrared and Raman spectroscopy for determination of inorganic structures.

(b) **Mossbauer Spectroscopy.**

Basic principles, interpretation of isomeric shift, electronic quadrupole intractions, spectrum display. magnetic interaction, mossbaur emmission spectroscopy, application of Mossbauer Spectroscopy to the studies of (1) bonding and structures of Fe^{+2} and Fe^{+3} compounds including those of intermediate spin, (2) Sn^{+2} and Sn^{+4} compounds - nature of M-L bond, coordination number, structure and (3) detection of oxidation state and inequivalent MB atoms.

UNIT - II

Ultraviolet and Visible Spectroscopy

Various electronic transitions (185- 800 mm.) Beer-Lambert Law, effect of solvent on electronic transitions, ultraviolet bands for carbonyl compounds, unsaturated carbonyl compounds, dienes, conjugated polyenes. Fieser- Woodward rules for conjugated dienes and carbonyl compounds, ultraviolet spectra of aromatic compounds.

Infrared Spectroscopy

Instrument and sample handling. Characteristic vibrational frequencies of alkanes, alkenes, alkynes, aromatic compounds, alcohols, ethers, phenols aryl amines. Detailed study of

vibrational frequencies of carbonyl compounds (Ketones, aldehydes, esters, amides, acids, anhydrides, lactones, lactams and conjugated carbonyl compounds). Effect of hydrogen bonding and solvent effect on vibrational frequencies, overtones, combination bands and Fermi resonance.

UNIT - III

Nuclear Magnetic Resonance Spectroscopy

General introduction and definition, chemical shift, spin-spin interaction, shielding mechanism, mechanism of measurement, chemical shift values and correlation for protons bonded to carbon (Aliphatic, olefinic, enols, carboxylic acids, amines, amides & mercapto), chemical exchange, effect of deuteration, complex spin-spin interaction between two, three, four and five nuclei (first order spectra), virtual coupling. Stereochemistry, hindred rotation, Karplus curve-variation of coupling constant with dihedral angle. Simplification of complex spectra nuclear magnetic double resonance, contact shift reagents, solvent effects. Fourier transform technique, nuclear Overhauser effect (NOE), Resonance of other nuclei-F, P

UNIT – IV

Mass Spectrometry

Introduction ion production - EI, CI, FD and FAB, factors affecting fragmentation, ion analysis,ion abundance. Mass spectral fragmentation of organic compounds,common functional groups, molecular ion peak, metastable peak, Mc Lafferty rearrangement. Nitrogen rule. High resolution mass spectrometry. Examples of mass spectral fragmentation of organic compounds with respect to their structure determination.

COURSE OUTCOMES:

On completion of the course the student will be able to

- Learn the principles of Infrared and Raman spectroscopy, correlate with the molecular modes of vibration and apply the rules to interpret the spectra of organic molecules.
- Understand the basic principles of Mossbauer spectroscopy and apply to elucidate the structure of inorganic molecules.
- Learn the concept and rules of electronic transitions in organic molecules and their correlation with UV absorption spectroscopy.
- Describe the applications of UV-Visible spectroscopy in the identification of conjugation in organic compounds.
- Understand the basic principles of NMR and able to analyze the ^{1}H NMR data of simple organic compounds.
- Analyze and apply the rules of Mass spectroscopy for the fragmentation pattern in different types of organic functional groups.
- Analyze and identify simple organic molecules by using UV, IR, Mass and ^{1}H NMR data.
- Get Employability in Pharmaceutical Sector and Govt. organization

Books Recommended:

1. Structural Methods in Inorganic Chemistry, E.A.V. Wbsworth, D.W.H. Rankin and S. Cradock, ELBS.
2. Infrared and Raman Spectra: Inorganic and Coordination Compounds, K. Nakamoto, Wiley.
3. Symmetry in bonding and spectra: An Introduction by B.E Douglas, Academic Press.
4. Fundamental of Molecular Spectroscopy, C.N.Banwell & Elaine M. McCASH, Fourth edition (2017)
5. Spectrometric Identification of Compounds, R. M. Silverstein, G.C. Bassler and T.C. Morrill, John Wiley.
6. Spectroscopy of Organic Compounds, P. S. Kalsi, New Age International Publishers, 2020, 8 th Ed
7. Spectroscopy, H Kaur, Pragati Prakashan, 2017
8. Introduction to Spectroscopy, Donald J Pavia, Gary M. Lampman & George S. Kriz Cengage Learning India Private Limited; 5th edition (2015)
9. Organic spectroscopy by William Kemp 3rd ed., W.H.Freeman & Co, 1991
10. Spectroscopy Methods in Organic Chemistry, D. H. Williams, I. Fleming, Tata McGraw.

CH – 504 (Elective-II, Group-A) **Marks- 80 (5 Credits)**

ORGANIC SYNTHESIS - II

COURSE OBJECIVES:

- ✓ To understand the basic concepts on retrosynthetic analysis.
- ✓ To deliver the tricks and techniques about the retrosynthesis and synthesis of different types of compounds including biologically important small molecules, agrochemicals, cosmetics and drug molecules
- ✓ To impart knowledge about protection and deprotection of functional groups
- ✓ To apply the tricks of retrosynthetic analysis towards the logical synthesis of complex molecules and natural products.

CONTENTS:

UNIT - I

Disconnection approach

An introduction to synthons and synthetic equivalents, disconnection approach, functional group inter-conversion, the importance of the order of events in organic synthesis, one group

C-X and two group C-X disconnections, chemoselectivity, reversal of polarity, cyclisation reaction andamine synthesis.

Protecting groups

Principle of protection of alcohol, amine, carbonyl and carboxyl groups.

UNIT - II

One group c-c disconnections

Alcohols and carbonyl compounds, regioselectivity. Alkene synthesis, use of acetylenes and aliphatic nitro compounds in organic synthesis.

Two group c-c disconnections

Diels-Alder reaction, 1,3-difunctionalised compounds, unsaturated carbonyl compounds, control in carbonyl condensations, 1,5-difunctionalised compounds, Micheal addition and Robinson annelation.

UNIT – III

Ring synthesis

Saturated heterocycles, synthesis of 3-, 4-, 5- and 6- membered rings, aromatic heterocycles in organic synthesis.

UNIT - IV

Synthesis of some complex molecules

Application of the above in the synthesis of following compounds: Camphor, Cortisone, Reserpine, Vitamin D, Aphidicolin and Fredericamycin A.

COURSE OUTCOMES:

On completion of the course the student will be able to

- Acquire knowledge on disconnection approach as well as role of modern synthetic reagents in organic transformations.
- Compile and demonstrate knowledge on retrosynthesis and various terminologies, retro synthesis of simple molecules-alcohols, alkenes and dicarbonyl compounds, formation of C-C bond using different coupling reactions.
- Analyze and formulate the chemistry of protection and de-protection strategies involved in hydroxyl group by ether and ester, carbonyl group, and amino groups and functional group interconversion by substitution reactions.
- Describe the important concepts of the organic chemistry for the synthesis of new molecule, introduction of different functional group.
- Understand the principles of ring synthesis involving saturated and aromatic heterocycles.
- Retrosynthetic analysis and synthesis of some complex molecules.
- Get employability in Pharmaceutical Sector and public sector undertaking

Books Recommended:

1. Warren, S. Organic Synthesis: The Disconnection Approach John Wiley & Sons (1984).
2. Organic Synthesis - Concept, Methods and Starting Materials, J. Furhrop and G. Penzillin, Verlage VCH,
3. Modern Methods of Organic Synthesis, Cambridge University Press; 4th edition. 2015
4. Principles of Organic Synthesis, R. Norman and J. M. Coxon, Blackie Academic & Professional.
5. Advanced Organic Chemistry Part B, F.A. Carey and R.J. Sundberg, Plenum Press.
6. Organic Chemistry, Jonathan Clayden , Nick Greeves, Stuart Warren, Oxford University Press; 2nd edition 2014.
7. Organic Synthesis, Jagdamba Singh & L D S Yadav, Pragati Prakashan, Meerut, 2015.
Wiley's Problems in Organic Chemistry, K. Singh, Wiley, 2015.
8. Heterocyclic Chemistry, J A Joule & K. Mills, Wiley, 5 th Edition.
9. Organic Chemistry, Volume 2: Stereochemistry and the Chemistry Natural Products, I. L. Finar, Pearson, 5th Edition

CH - 506 PRACTICAL (Elective, Group -A) Marks -100 (6 Credits)

COURSE OBJECIVES:

- ✓ To synthesize small molecules from commercially available starting materials.
- ✓ To analyze qualitatively the organic molecules in a mixture of compounds
- ✓ To characterize the compounds using different analytical techniques such as UV, FTIR, NMR Spectroscopy and Mass spectrometry.
- ✓ Isolation and characterization of organic compounds from natural sources.

CONTENTS:

1. Qualitative analysis

Separation and identification of Organic Compound of binary mixture (one liquid and one solid)

2. Organic synthesis (single step)

a) Preparation of Salicylaldehyde.
b) Preparation of quinoline
c) Cannizzaro reaction : 4 - chlorobenzaldehyde as substrate.
d) Aldol condensation : Dibenzal acetone from benzaldehyde.

3. Organic synthesis (multi step)

Benzene Nitrobenzene Aniline Phenol

4. Quantitative analysis

Determination of the percentage or number of hydroxyl groups in an organic compunds by acetylation method.

5. Spectrophotometric estimation

Amino Acids.

COURSE OUTCOMES:

On completion of the course the student will be able to

- Reduction of camphor to borneol with Sodium Borohydride
- Isolation of Caffeine from tea bags.
- Isolation of lactose from milk.
- Preparation of phenylazo-2-napthol from aniline.
- Separation and qualitative analysis of three component mixtures of organic compounds: characterization of derivatives and identification of the components.

Books Recommended:

1. Vogel's Text Book of Practical Organic Chemistry, Furniss, S. B.; Hannaford, A. J.; Smith, P. W. G.; Tatchell, A. R. 5Th Ed.; Longman Scientific & technical, England, 1989.
2. Laboratory Manual of Organic Chemistry, Dey and Sitaraman, Allied Publishers, 1992.
3. Laboratory Manual of Organic Chemistry, Raj K Bansal, New Age International Publishers, 2008

CH – 504 (Elective-II, Group-B) Marks- 80 (5 Credits)

ORGANO-TRANSITION METAL CHEMISTRY

OBJECTIVES: This course is aimed to gather knowledge on transition metal sigma bonded and π bonded complexes, transition metal-carbon multiple bonded complexes and various organometallic reactions and catalysis.

CONTENTS:

UNIT - I

Alkyls and Aryls of Transition Metals

Types, routes of synthesis,stability and decomposition pathways, organo-copper in organic synthesis.

Transition Metal Compounds with Bonds to Hydrogen

Transition metal compounds with bonds to hydrogen

Compounds of Transition Metal- Carbon Multiple Bonds

Alkylidenes, alkylidynes, low valent carbenes and carbynes- synthesis, nature of bond, structural characteristics, nucleophilic and electrophilic reactions on the ligands, role in organic synthesis.

UNIT - II

Transition Metal pi -**Complexes**

Transition Metal -complexes with usaturated organic molecules, alkenes, alkynes, allyl, diene, dienyl, arene and trienyl complexes, preparation, properties, nature of bonding and structural features. Important reactions relating to nucleophilic and electrophilic attack on ligands and to organic synthesis.

UNIT - III

Fluxional Organometallic Compounds

Fluxionality and dynamic equilibria in compounds such as h^2 - olefin, h^3 - allyl and dienyl complexes.Organometallic Reagents - Synthesis, structure of organometallic reagents of transition metals such as Pd, Rh, Ni, and Fe and their applications in organic synthesis.

UNIT - IV

Organometallic reactions and catalysis

Fundamental reactions: insertion (CO and SO_2) and elimination reactions,oxidative and reductive eliminations,activation of C-H bond.

Stoichiometric reactions for catalysis, homogeneous catalytic isomerisation, hydrogenation of olefines, Zeigler-Natta polymerization of olefins, hydrocarbonylation of olefins (oxo reaction).

COURSE OUTCOMES:

On completion of the course the student will be able to

- Learn about synthesis, stability and decomposition pathways of transition metal alkyl and aryl complexes, role of organo-copper in organic synthesis.
- Learn about Transition metal compounds with bonds to hydrogen, synthesis, nature of bond, structural characteristics, nucleophilic and electrophilic reactions on the ligands of carbene and carbyne complexes.
- Learn about preparation, properties, nature of bonding , structural features and important reactions relating to nucleophilic and electrophilic attack on ligands of alkenes, alkynes, allyl, diene, dienyl, arene and trienyl complexe
- Acquire knowledge on fluxionality and dynamic equilibria in compounds such as h^2 - olefin, h^3 - allyl and dienyl complexes. Synthesis, structure of organometallic reagents of transition metals such as Pd, Rh, Ni, and Fe and their applications in organic synthesis.
- Acquire knowledge on fundamental reactions like insertion (CO and SO_2) , elimination reactions, oxidative and reductive eliminations

Learn about Stoichiometric reactions for catalysis, homogeneous catalytic isomerisation, hydrogenation of olefines, Zeigler-Natta polymerization of olefins, hydrocarbonylation of olefins (oxo reaction).

Books Recommended:

1.Principles and Application of Organo transition Metal Chemistry, J.P. Collman, L.S. Hegsdus, j.R. Norton and R.G. Finke, University Science Books.

2. The Organometallic Chemistry of the Transition Metals, R.H. Crabtree, John Wiley

3. Metallo-organic Chemistry, A.J. Pearson, Wiley

4. Organometallic Chemistry, R.C. Mehrotra and A. Singh, New Age International.

5. Concepts and Models of Inorganic Chemistry by B.E. Douglas, D.H.McDaniel and J.J Alxendar, John Wiley, 1993 3rd Ed.

6. Reaction mechanism in Inorganic Chemistry by R.R.Jordan Oxford Univ. Press, 1998 2nd ED.

7. Advanced Inorganic Chemistry by F.A. cotton and G.W. Wilkison.John-Wiley & Sons, 1988, 5th Ed.

CH-506 PRACTICAL (Elective, Group-B) Marks-100 (6 Credits)

OBJECTIVES: This course is aimed to equip the students with various practical knowledges on preparation of transition metal complexes and determination of free acids and metal contents present in metal salt solutions by ion exchange methods.

CONTENTS:

1. Preparation and Characterization

Preparation of simple complex compounds of Cr(III)/Co(III). Estimation of the metal content and other components of the complexes such as:

Cis - $K[Cr(C_2O_4)_2(H_2O)_2]$

Tranns- $[Co(en)_2Cl_2]Cl$

2. Ion exchange methods of separation and estimation

(i) Separation of mixtures of cations (Co-Ni, Fe-Zn, Zn-Mg, Cd-Zn) by ion exchange method and estimation of the components after separation.

(ii) Determination of metal content and free acid in $FeCl_3/CuCl_2$ solution.

3. Spectrophotometry

(i) Determination of composition of a complex compound in solution by Job's continuous variation method.

(ii) Determination of acid dissociation constant of pentaammine(salicylato)-cobalt(III) complex.

4. Quantitative analysis

Analysis of solder and brass.

5. Potentiometry

Determination of acid dissociation constants of simple coordinated ligands by pH metry.

COURSE OUTCOME:

After completion of this course student will be able to

- Prepare complexes of Cr (III)/Co(III)and estimate the amount of constituents.
- Determine the free acid and metal content in $FeCl_3$ /$CuSO_4$solution by ion exchange methods
- Determine the composition of a complex compound in solution by job's continuous variation method.

Books Recommended:

1. A Text book of Qualitative Analysis, A. I. Vogel
2. A Text book of Quantitative Analysis, A. I. Vogel
3. Inorganic synthesis, Vol. 1 -20

CH - 504 (Elective-II, Group-C) Marks-80 (5 Credits)

SURFACE CHEMISTRY

UNIT - I

Adsorption

Surface tension, capillary action, pressure difference across curved surface, vapour pressure of droplets, Gibbs adsorption isotherm, estimation of surface area (BET) equations, catalytic activity at surfaces.

UNIT - II

Micelles

Surface active agents, classification of surface active agents, micellization, hydrophobic interactions, critical micellar concentration (CMC) factors affection CMC, Solubilization, micromulsion and reverse micelles.

UNIT-III

Macromolecules: Polymer-definition, types of polymer, electrically conducting, fire resistant, liquid crystral polymer. Molecular mass, number and mass average molecular mass, molecular mass determination (osmometry, viscometry, diffusion and light scattering), sedimentation, chain configuration of macromolecules, calculation of average dimension of various chain structures.

UNIT-IV

Surface reactions**:** General aspects, coadsorption, poisoning and promotion effects, model reactions, Examples of surface reactions, detection of adsorbates on surfaces. High pressure catalytic reactions on single crystal surfaces: examples - CO oxidation and methanation, ammonia synthesis, epoxidation reactions.

Books Recommended:

1. Adsorption and Catalysis, by D.K. Chakraborty
2. Solid state chemistry and its application, by A.R. West
3. Physical chemistry, by G.M. Barrow.
4. Solid state chemistry, by H.V. Keer

CH - 506 PRACTICAL (Elective, Group -C) Marks - 100 (6 Credits)

1. Spectrophotometry

Verification of additivity law.
Characterization of complexes by spectroscopic data.
Estimation of metal ions by spectrophotometric titration.
To determine of pH of an indicator

2. Potentiometery

To determine first and second ionization constant of multi basic acid.
To determine the standard electrode potential of Ferrous-Ferric system.

3. Conductometry

To determine hydrolysis constant of aniline hydrochloride.
To determine solubility and solubility product of a sparingly soluble salt.
Verification of Debye-Huckel and Onsager's limiting law.

4. Surface / phase

To study the adsorption of acetic acid on activated charcoal.
To determine the demerization constant of benzoic acid in benzene medium by partition method.

5. Solid state

XRD of simple solids (NaCl, CsCl, Graphite etc. Spectral data analysis only)

6. Viscometery

Determination of molecular weight by Ubbelhood Viscometer.

CH - 504 (Elective - II, Group -D) Marks - 80 (5 Credits)

PHYSICAL CHEMISTRY OF POLYMERS

UNIT - I

Thermodynamic of Polymer Mixture

Partial molar function, ideal and non-ideal solution, enthalpy and entropy of mixing & florykingbaurn theory. Free energy of mixing of a polymer with a solvent - Thermodynamics of swelling of cross-linked polymers.

UNIT - II

Morphology and Crystallinity

Cofiguraion of Polymer chain, Crystal structure of polymers, Morphology of Polymer single crystals structure of polymers crystallised from melt. Crystalizatiion. Orientation and drawing. Amorphous Polymers.

UNIT - III

Rheology and Mechanical Properties of Polymers

Viscous flow, viscoelasticity, the glassy state and the glass transition. Mechanical properties of crystalline polymers. Statistical behavious of polymer moleculars. Random fight - chain model freely rotating chain model, Hindered rotation model. Rotationl Isomeric state model.

UNIT - IV

Technology of Polymers

Additives of Polymers: Filleers and Rainforcement Plasticisers, Antioxidants, Stabilsers, Crosslinking agents, Activators, accelerations, Lubricating agents, antistatic agents colourants.

Fabrication Film casting, casting of casting of articles in models, compression and transfer molding. Thermoforming and welding, calendering, multipolymer systems & composites. Laminates, Foam, Coatings, Adhesives, Pressure sensitive Adhesive.

Books Recommended:

1. Introduction to Polymer Science and Technology, H.S. Kaufman & J.J. Falcetta.
2. Viscoelastic properties of the Polymers, J.D. Ferry
3. Physical Chemistry of Polymer, A. Tagor
4. Statistical Mechanis of Polymers, P.J. Flory
5. Text Book of Polymer Science and Engineering, Anil Kumar Gupta.
6. Plastic Materials, J.A. Brydson.
7. Essential Fiber Chemistry, M.E. Cartel
8. Textile Fibers, J. Peters.

CH - 506 PRACTICAL (Elective, Group -D) Marks-100 (6 Credits)

POLYMER CHEMISTRY

1. Determination of Molecualr weight of given Polymer by Ubblehode Viscometer.
2. Determination of molecular weight of a given polymer by end group analysis.
3. Chemical Testing of polymers.

4. Determination of Tg of a given polymer by Thermogravimetric analysis.
5. Polymerisation of vinyl monomer by free radical method and characterization.
6. Polymerization of PMMA by emulsion polymerisation method.

CH-508 **Marks-100 (5 Credits)**

PROJECT WORK

The project work will consist of experimental / review work under direct supervision of faculty members. Students develops their skill with long term hands - on -training on various organic, inorganic, physical and nanotechnological techniques along with data analysis software training for application of the research theme chosen for the Dissertation and further research and development in Industries, Institutes and Academics

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