MASTER OF SCIENCE IN CHEMISTRY

(SEMESTER PATTERN)

CHOICE BASED CREDIT SYSTEM SYLLABUS TWO YEAR FULL TIME PROGRAMME

COURSE OF STUDIES

(AS PER U.G.C. MODEL SYLLABUS)

(2023 -2024)

P. G. DEPARTMENT OF CHEMISTRY
M.P.C. AUTONOMOUS COLLEGE, TAKHATPUR, BARIPADA,
MAYURBHANJ, ODISHA, PIN-757003

M.P.C. AUTONOMOUS COLLEGE
COURSE OF STUDIES
FOR THE
M. Sc. EXAMINATION IN CHEMISTRY
(2023-2024)

PREFACE

*Master of Science (M.Sc.) in Chemistry is a full time two years post-graduation programme of M.P.C.Autonomous College. The choice based credit system (CBCS) syllabus in M. Sc. Chemistry is comprised of four semesters, having total of **100** credits (**2000** marks). There are **16** theory papers carrying four credits each with 100 full marks. Out of which mid and end semester examinations carry 20 marks and 80 marks, respectively. The duration of end semester examination is three hours. Besides there are **4** practical papers (**5** credit each and full mark **100**) with end semester examination of six hours duration. The fourth semester has a compulsory project work of 5 credits (100 marks). Students are required to undertake a project work after completion of 2nd semester and submit project report in the 4th semester for evaluation. Questions will be set unit wise with long and short answer type questions.*

PROGRAM OBJECTIVES:

- To impart knowledge in fundamental aspects of all branches of chemistry (Organic, Inorganic, Physical, Polymer and Analytical Chemistry) along with the current scientific status and new developments in Chemistry.
- To acquire deep knowledge in the specific areas like spectroscopy, materials chemistry, research methodology etc.
- To teach the students about good laboratory practices, safety of oneself and others in the laboratory.
- To acquire the different practical skills, hand on training on basic equipment, and data analysis for research and better job prospective.
- To train the students in accepting the challenges in Chemistry and to become a responsible citizen in the society.

PROGRAM OUTCOMES:

On completion of the M.Sc. Chemistry programme, the students will:

- Acquire the in-depth functional knowledge of the fundamental principles and contemporary practices of chemistry and ability to use them to investigate, explain and predict the new phenomena.
- Acquire skills to design, execute and document of laboratory experiments at a level suitable to succeed at an entry level position in research, academia, or chemical industry.
- Develop an awareness of social, economic, environmental and technological implication of chemistry.
- Find job opportunities in Chemical, pharmaceutical, and other chemistry based industries; Research & Development in various scientific/academic institutions.
- Have the ability to disseminate research results orally, and in writing.

Structure Of Syllabus For Semester Pattern Choice Based Credit System
M.Sc.(Chemistry) Programme Effective From The Session- 2023 – 2024

FIRST SEMESTER

Course code	Title of the Paper	Credits	Max. Marks		Total
			Mid Sem	End Sem	
CC-101	Inorganic Chemsitry-I	05	20	80	100
CC-102	Organic Chemistry-I	05	20	80	100
CC-103	Physical Chemistry-I	05	20	80	100
CC-105	Polymer Chemistry	05	20	80	100
CC-105	Inorganic Chemistry Practical	05	-	100	100
	Total	**25**	**80**	**420**	**500**

SECOND SEMESTER

Course code	Title of the Paper	Credits	Max. Marks		Total
			Mid Sem	End Sem	
CC-201	Organic Chemistry-II	05	20	80	100
CC-202	Inorganic Chemsitry-II	05	20	80	100
CC-203	Physical Chemistry-II	05	20	80	100
CC-205	Organic Spectroscopy	05	20	80	100
CC-205	Physical Chemistry Practical	05	-	100	100
	Total	**25**	**80**	**420**	**500**

THIRD SEMESTER

Course code	Title of the Paper	Credits	Max. Marks		Total
			Mid Sem	End Sem	
CC-301	Inorganic Chemistry-III	05	20	80	100
CC-302	Organic Chemsitry-III	05	20	80	100
CC-303	Research Methodology	05	20	80	100
OEC-305	OEC-Industrial Chemistry	05	_	100	100
CC-305	Organic Chemistry Practical	05	-	100	100
	Total	**25**	**60**	**420**	**500**

FOURTH SEMESTER

Course code	Title of the Paper	Credits	Max. Marks		Total
			Mid Sem	End Sem	
DEC-401	Bio-Inorganic Chemistry and Supra-Molecular Chemistry	05	20	80	100
DEC-402	Organometallic Chemistry	05	20	80	100
DEC-403	Molecular Spectroscopy	05	20	80	100
DEC-405	Applied Chemistry Practical	05	-	100	100
DC-405	Dissertation	05		100	100
	Total	**25**	**60**	**420**	**500**

SEMESTER -I

INORGANIC CHEMISTRY-I

Course Code: CC-101	**End Sem-80 marks**	**Time-3 hour**
Credits: 05	**Mid Sem-20 marks**	**Time- 1hour**

Objective: (*i) To understand the concepts of bonding and stereochemistry of main group elements,*

(ii) To introduce the concept of symmetry and group theory and their application in chemistry

***Outcome**: At the end of the course the student will*

(i).Acquire the knowledge and have the ability to describe the bonding and stereochemistry of different inorganic compounds and ions. (ii) To understand importance of group symmetry and group theory in chemistry, classifying different compounds in to point groups and derive the character tables for various applications.

UNIT-I *Stereochemistry and Bonding in main group compounds*:-VSEPR, Walsh diagram (triatomic molecules), dπ-Pπ bonds, Bent rule and energetics of hybridization, some simple reactions of covalently bonded molecules.

UNIT-II *Symmetry and Group Theory Symmetry elements and Symmetry operation*:- Symmetry elements & Symmetry Operations, Groups and Subgroups, Relation between orders of a finite Groups and its sub-groups, Symmetry point group. Schonflies symbols, Conjugacy relation and classes, Matrix representations of groups,Representation of Group Operaters, Character of a representation. The Great Orthogonality theorem (without proof) and its explanation, Irrreducible & Reducible Representation, Basis of Representation,Character tables and their uses. Reduction formula. Derivation of character table for C2v , C3v.

UNIT-III *Chemistry of Main Group elements* A:General characteristics, Allotropes, Structure and Reactions of simple and industrially important compounds: Boranes, Carboranes, Silicones, Silicates, Boron nitride, Borazines and Phosphazenes, Wade's rule , Styx Number, Isolabal analogy.Lipscom Topology,Application of Boron Compounds,Synthesis and structures of S-N Cyclic compounds

UNIT-IV *Chemistry of Main Group elements* B : General characteristics, Structure and Reactions of simple and industrially important compounds: Hydrides, Oxides and Oxoacids of pnictogens (N, P), chalcogens (S, Se & Te) and halogens, Xenon compounds, Pseudo halogens and Interhalogen compounds.

Books and References:

1. Symmetry & Group Theory by K.Veera Reddy, New age Publishers.
2. Chemical Application of Group Theory: F. A. Cotton, John Wiley.
3. Symmetry in Chemistry: Orchin and Jaffe.
4. Group theory: K. V. Raman, Tata McGraw Hill.
5. Advanced Inorganic Chemistry: F. A. Cotton and G. Wilkinson, John Wiley.
6. Inorganic Chemistry: J.E. Huheey, E. A. Keiter, R. L. Keiter, Pearson Education.
7. Chemistry of the Elements: N. N. B. Greenwood and A. Earnshow, Pergamon.
8. Comprehensive Coordination Chemistry eds.,- G. Wilkinson, R. D. Gillars and J. A. McCleverty, Pergamon.
9. Inorganic Chemistry by Catherine E.Housecroft & Alan G.Sharpe.
10. Fundamentals Concepts of Inorganic Chemistry,Volume-2,Asim K. Das and Mahua Das,CBS Publishers and Distributors Pvt. Ltd.

ORGANIC CHEMISTRY-I

Course Code: CC-102	**End Sem-80 marks**	**Time-3 hour**
Credits: 05	**Mid Sem-20 marks**	**Time- 1hour**

Objective: *To understand the molecular details in greater depth on following topics: aromaticity, stereochemistry, and substitution reactions in aliphatic compounds.*

Outcome: *Upon completion of this course students will be able to: (i) Understand the fundamental aspects of aromaticity, nonaromaticity and antiaromaticity, (ii) Feel the structural details of organic compounds and the origin of optical activity of the chiral molecules, (iii) Understand the origin of stereoselectivity as far as asymmetric catalysis is concern, and the basic mechanism of substitution reactions in aliphatic compounds.*

UNIT-I *Nature of Bonding &Reaction Mechanism*:

(a) Delocalised Chemical bonding-Conjugation Cross conjugation, Resonance,Hyper Conjugation, Bonding in fullerenes,tautomerism. Aromaticity in Benzenoid & Non-Benzenoids compounds, Alternant & Non-Alternant Hydrocarbons, Huckle's Rule: Energy level of Pie Molecular Orbitals, annulenes,anti-aromaticity,Pseudo-aromaticity,Homo-aromaticity,

(b) Types of mechanism, types of reactions, thermodynamic and kinetic requirements, kinetic and thermodynamic control, Hammond's postulate, Curtin - Hammett principle. Potential energy diagrams, transition states and intermediates, methods of determining mechanisms, isotope effects. Hard and soft acids and bases. Effect of structure on reactivity: resonance and field effect, steric effect, quantitative treatment. The Hammett equation and linear free energy relationships, substitutent and reaction constants. Taft equation.

UNIT-II (a) *Aliphatic Nucleophilic substitution*:

The SN2, SN1, mixed SN1 and SN2 and SET mechanisms. The neighbouring group mechanism, neighbouring group participation by σ and π bonds, anchimeric assistance. Classical and nonclassical carbocations, phenonium ions, norbornyl system, common carbocation rearrangements. Application of NMR spectroscopy in the detection of carbocations. The SN1 mechanism: Nucleophilic substitution at an allylic, aliphatic trigonal and a vinylic carbon. Reactivity effects of substrate structure, attacking nucleophile, leaving group and reaction medium, phase transfer catalysis and ultrasound, ambident nucleophile, regioselectivity.

(b)*Aromatic Nucleophilic Substitution*:

The SNAr, SNi benzyne and SRN^1 mechanisms. Reactivity-effect of substrate structure, leaving group and attacking nucleophile. The von Richter, Sommelet-Hauser, and Smiles rearrangements.

UNIT-III (a) *Aliphatic Electrophilic Substitution*

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

(b) ***Aromatic Electrophilic Substitution***: The areniun ion mechanism, orientation and reactivity, energy profile diagrams. The ortho/para ratio, Ipso attack, orientation in other ring systems. Quantitative treatment of reactivity in substrates and electrophiles. Diazonium coupling, Vilsmeier reaction, Gattermann- Koch reaction.

UNIT–IV (a) *Free Radical Reactions*:

Types of free radical reactions: Free radical substitution, mechanism, mechanism at an aromatic substrate, neighbouring group assistance. Reactivity for aliphatic and aromatic substrates at a bridgehead. Reactivity in the attacking radicals. The effect of solvents on reactivity. Allylic halogenation (NBS), oxidation of aldehydes to carboxylic acids, auto-oxidation, coupling of alkynes and arylation of aromatic compounds by diazonium salts. Sandmeyer reaction, free radical rearrangement, Hunsdiecker reaction.

(b) *Elimination Reactions*: The E2, EI and E1cB mechanisms. Orientationof the double bond. Reactivity: Effects of substrate structures, attacking base, the leaving group and the medium. Mechanism and orientation in pyrolytic elimination.

Books and References:

1. Organic chemistry: J. Clayden, N. Greeves, S. Warren and P. Wothers, Oxford University Press.
2. Advanced Organic Chemistry Reactions, Mechanism and Structure: Jerry March. John Wiley and Sons.
3. Advanced Organic Chemistry: F. A. Carey and R. J. Sundberg. Plenum.
4. A Guide Book to Mechanism in Organic Chemistry: Peter Sykes, Longman/Pearson Education.
5. Structure and Mechanism in Organic Chemistry: C. K. Ingold. Cornell University Press.
6. Organic Chemistry: R. T. Morrison and R. N. Boyd. Prentice Hall/Pearson Education.
7. Modern Synthetic Reactions: Second Edition, H. O. House, Benjamin, Menlo Park, 1972.
8. Principles of Organic Synthesis: R. O. C. Norman and J. M. Coxon. Blackie Academic and Professional / CBS Publishers.
9. A logical Approach to Modern Organic Chemistry: Dr. Jagdamba Singh and Dr. S. Anandvardhan. Pragati Prakasan.
10. Reaction Mechanism in Organic Chemistry: S. Mukherji and S. P. Singh, Macmillan.
11. Advanced Organic Chemistry: Reactions and Mechanism: B. Miller and R. Prasad. Pearson-Education.

PHYSICAL CHEMISTRY-I

Course Code: CC-103 **End Sem-80 marks** **Time-3 hour**
Credits: 05 **Mid Sem-20 marks** **Time- 1hour**

Objective: *The topics covered under the course are inherently very fundamental and intended to provide the basic understanding at atomic, subatomic, interfacial and ion- solvent interaction*

Outcome: *Students will able to understand the underlying concepts and realization of quantum mechanics. They will able to solve problems at realistic atomic and molecular level, in particularly in the field of spectroscopy and analytical chemistry. They will also able to analyze the surface phenomenon and distribution of solvent molecules around the ion.*

UNIT-I (a) *Quantum Chemistry*:

The Schrodinger equation and the postulates of quantum mechanics. Discussion of solutions of the Schrodinger equation to some model systems viz. particle in a box, the harmonic oscillator, the rigid rotor, the hydrogen atom.

(b) *Approximation Methods*:

The Helium atom. 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 *Molecular Orbital Theory*:

H2 + and H2 molecules: Valance bond theory (VBT) and molecular orbital theory (MOT) approaches. Homonuclear and Heteronuclear diatoms. Huckel theory of conjugated systems, bond order and charge density calculation. Applications to ethylene, butadiene, cyclopropenyl radical, and cyclobutadiene.

UNIT-III *Surface Chemistry*: ***(a) Adsorption***: Surface tension, capillary action, pressure difference across curved surface (Laplace equation), vapour pressure of droplets (Kelvin equation). Gibbs adsorption isotherm, estimation of surface area (BET equation), surface films on liquids (Electrokinetic phenomenon), catalytic activity at surfaces.

(b) Micelles: Surface active agents, classification of surface active agents, micellization, hydrophobic interaction, critical micellar concentraion (CMC), factors affecting the CMC of surfactants counter ion binding to micelles, thermodynamics of micellization, phase separation and mass action models, solubilization, micro emulsion, reverse micelles.

UNIT-IV *Electrochemistry*:

Electrochemistry of solutions. Debye-Huckel–Onsager treatment and its extension, ion solvent interactions. Deby-Huckel-Bjerrum model. Solution of Strong electrolytes. Debye Huckel theory for activity coefficient of electrolytic solutions; determination of activity and activity coefficients; ionic strength. Thermodynamics of electrified interface equations. Derivation of electro-capillarity, Lippmann equations (surface excess), methods of determination. Structure of electrified interfaces, Helmltoz-Perrin, Guoy–Champman,

Stern models. Over potentials, exchange current density, derivation of Butler– Volmer equation, Tafel plot

Books and References:

1. Atkin's Physical Chemistry: P. W. Atkins, J. D. Paula, Oxford University Press
2. Introductory to Quantum Chemistry: 4th Ed., A. K. Chandra, TataMc Graw Hill.
3. Quantum Chemistry: Ira N. Levine, Prentice Hall.
4. A text Book Of Quantum Chemistry, R.K.Prasad
5. D. Chandler, Introduction to Modern Statistical Mechanics, Oxford University Press 1987.
6. Physical Chemistry Vol-II: .K. L. Kapoor, Mcmillan Publication.
7. Micelles, Theoretical and Applied Aspects, V. Moroi, Plenum.
8. Modem Electrochemistry: Vol.-I and Vol. II, J. O. M. Bockris and A. K. N. Reddy, Plenum.
9. An Introduction to electrochemistry: S. Glasstone, Affiliated East-West Press Pvt. Ltd.
10. Quantum Chemistry,Donald A. McQuarrie,Viva Books Private Limited.

POLYMER CHEMISTRY

Course Code: CC-105	**End Sem-80 marks**	**Time-3 hour**
Credits: 05	**Mid Sem-20 marks**	**Time- 1hour**

Objective: *To study the fundamental concepts of polymer chemistry, structure of monomers, functionality, and classification of polymers on the basis of source, composition, conditions, molecular weight, geometry, industrial polymer fabrication process, and nomenclature of polymers.*

Outcome: *After the completion of course students will able to understand about the basics of polymer and the differences between crystalline melting temperature and glass transition temperature, as well as the effect of kinetics on both, develop specific skills, competencies, and thought processes sufficient to support further study or work in this field of polymer chemistry, evaluate the effect of factors such as polymer structure, molecular weight, branching and diluents on crystallinity, and apply knowledge to build up small scale industry for developing endogenous plastic product*.

UNIT I ***Basics Importance of Polymers Basic concepts***: Monomers, repeat units, degree of polymerization, Linear, branched and network polymers. Classification of Polymers. Polymerization Process, 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 weights-End-group, viscosity, light scattering, osmotic and ultracentrifugation methods.

UNIT III ***Structure, morphology and properties of polymer***: Morphology and order in crystalline polymers-configurations of polymer chains. Crystal structures of polymers- Crystalline, Amorphous structure. Factors affecting crystallinity, degree of crystallinity, techniques to determine the degree of crystallinity, morphology of crystalline polymer, strain induced morphology, properties affected by crystallinity, Glass transition temperature: effects of molecular weight, diluents, chemical structure, chain topology, branching and cross linking on glass transition temperature. Tm-melting points of homogeneous services: effect of chain flexibility, steric factor, entropy, and heat of fusion on Tm. Relation between Tg and Tm, Property requirements and polymer utilization.

UNIT IV ***Polymer Processing***: Plastics, elastomers, and fibers. Resin, Compounding, Additives (crosslinking agent, UV stabilizer, fire retardant, coloring agent, plasticizer, and others). Processing techniques: Calendaring, die casting, rotational casting, film casting, injection molding, blow molding, extrusion molding, reinforcing, pultrusion and fiber spinning. Properties of Commercial Polymers Polythylene, polyvinyl chloride, polyamides, polyesters, phenolic resins, epoxy resins and silicone polymers. Functional polymers – Fire retarding polymers and electrically conducting polymers

(PANI, Polyacetylene). Polymer in Biomedical applications: contact lens, dental polymers, artificial heart, kidney, skin, and blood cells.

Books and References

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.

INORGANIC CHEMISTRY PRACTICAL

Course Code: CC-105 **End Sem-100 marks** **Time-6 hour**
Credits: 05

Objective: (i) Qualitative analysis of inorganic salts mixture containing acid and basic radicals with insoluble compound (ii) To separate the mixture of metal ions by volumetric and gravimetric analysis (iii) To learn the best laboratory practice for the synthesis of some inorganic materials.

Outcome: (i) Ability to separate and identify different cations and anion from a mixture of inorganic salts. (ii) Understanding the principles of separation and analysis of different metal ions and their applications in real fields. (iii) Learn the synthesis and applications of Wilkinson's catalyst.

1. Qualitative analysis of mixtures containing not more than eight radicals [less common metal ions Mo, W, Ti, V, Zr, U (two metal ions in cationic / anionic forms), insoluble-oxides, sulphates and halides may be included].
2. Separation and determination of two metal ions Cu-Ni, Ni-Zn, Cu-Fe etc. involving volumetric and gravimetric methods.
3. Synthesis of bulky Schiff base (Ketimine/ diketimine/ phenolate) transition metal complexes.
4. Preparation of some selected inorganic compounds and their study. Handling of air and moisture sensitive compounds. (**a**) $Mn(acac)_3$, (**b**) $K_3[Fe(C_2O_4)_3$, (**c**) $[Ni(NH_3)_6]Cl_2$,(**d**) [$Ni(dimg)_2$, (**e**) $[Cu(NH_3)_4]. SO_4.H_2O$, (**f)** Cis - and Trans $[Co(en)_2]Cl_2$.
5. **A**. Synthesis of Wilkinson's catalyst
   B. Reaction of Wilkinson's catalyst with Cyclohexene
   C. Reaction of Wilkinson's catalyst with Hydrogen.

Books and References:

1. Inorganic Experiments: J. Derck Woollins, VCH.
2. Microscale Inorganic-chemistry; Z.Szafran, RM. Pike and M.M.Singh. Wiley.
3. Practical Inorganic Chemistry: G.Marr and B.W. Rockett, van,Nostrand.
4. Vogel'-s Qualitative Inorganic Analysis (revised) : G. Svehla, Longman.

SEMESTER -II

ORGANIC CHEMISTRY-II

Course Code: CC-201 **End Sem-80 marks** **Time-3 hour**
Credits: 05 **Mid Sem-20 marks** **Time- 1hour**

Objective:

To understand the molecular details in greater depth on following topics: aromaticity, stereochemistry, and substitution reactions in aliphatic compounds.

Outcome: *Upon completion of this course students will be able to: (i) Understand the fundamental aspects of aromaticity, nonaromaticity and antiaromaticity, (ii) Feel the structural details of organic compounds and the origin of optical activity of the chiral molecules, (iii) Understand the origin of stereoselectivity as far as asymmetric catalysis is concern, and the basic mechanism of substitution reactions in aliphatic compounds.*

Unit-I (a) ***Stereochemistry***: Conformational analysis of cycloalkanes, decalins, effect of conformation on reactivity, conformation of sugars, steric strain due to unavoidable crowding. Elements of symmetry, chirality, molecules with more than one chiral center, R-S and E-Z conventions, threo and erythro isomers, methods of resolution, optical purity, enantiotropic and diastereotropic atoms, groups and faces, stereospecifjc and, steroselective synthesis. Asymmetric synthesis, Optical activity in the absence of chiral carbon (biphenyls, allenes, spiranes, transcycloalkene and metallocenes), chirality due to helical shape. Stereochemistry of the compounds containing nitrogen, sulphur and phosphorus.

UNIT–II (a) ***Addition to Carbon-Carbon Multiple Bonds***: Mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals, selectivity, orientation and reactivity, Electrophilic cyclization, Baldwin's rule. Hydrogenation of double and triple bonds, hydrogenation of aromatic rings. Hydroboration, Michael reaction. Sharpless asymmetric epoxidation.

(b) ***Addition to Carbon-Hetero Multiple Bonds***: Mechanism of metal hydride reduction of saturated and unsaturated carbonyl compounds, acids, esters and nitriles. Addition of Grignard reagents, organozinc and organolithium reagents to carbonyl and unsaturated carbonyl compounds. Wittig reaction. Mechanism of condensation reactions involving enolates, Aldol, Knoevenagel, Claisen, Mannich, Benzoin, Perkin and Stobbe reactions.

UNIT-III ***Pericyclic Reactions***: Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3- butadiene, 1, 3, 5 – hexatriene and allyl system. Classification of pericyclic reactions. WoodWard –Hoffmann correlation diagrams. FMO and PMO approach. Electrocyclic reactions, conrotator and disrotatory motions; 4n, 4n+2 and allyl systems. Cycloadditions, antarafacial and suprafacial additions; 4n and 4n+2 systems, 2+2 addition of ketenes. 1, 3 - dipolar cycloadditon and cheletropic reactions. Sigmatropic rearrangements - suprafacial and antarafacial shifts of H, sigmatropic shifts involving carbon moieties, 3, 3 - and 5, 5 – 10 sigmatropic rearrangements: Claisen, Cope and aza-Cope rearrangements. Fluxional tautomerism. Ene reaction.

UNIT IV *Photochemistry:*

(a) Principles, Thermal and photochemical reactions, Laws of photochemistry, Interaction of electromagnetic radiation with matter, types of excitations, fate of excited molecule (singlet, triplet state), Jablonski diagram (fluorescence, phosphorescence, delayed fluorescence), Excimer, Exciplex, quantum yield/quantum efficiency, transfer of excitation energy (Sensitization & quenching), Actinometry. Types of photochemical reactions – photo-dissociation, gas-phase photolysis.

(b) Intramolecular reactions of the olefinic bond – geometrical isomerism, cyclisation reactions, rearrangement of 1,4 – and 1,5 – dienes, Di-π methane rearrangement. Intramolecular reactions of carbonyl compounds – saturated, cyclic and acylic, β,γ-unsaturated and α,β- unsaturated compounds, Norrish type I and II reaction, Paterno-Buechi Reaction, Cyclohexadienones, Photodimerisation of carbonyl compounds.

Books and References:

1. Organic chemistry: J. Clayden, N. Greeves, S. Warren and P. Wothers, Oxford University Press.
2. Advanced Organic Chemistry Reactions, Mechanism and Structure: Jerry March. John Wiley and Sons.
3. Modern Methods of Organic Synthesis, W. Carruthers and I. Coldham, Oxford University Press.
4. Modern Organic Synthesis An Introduction, George S. Zweifel and Michael H. Nantz, W.H. Freeman and Company, New York
5. Advanced Organic Chemistry: FA Carey and RJ. Sundberg. Plenum.
6. Photo Chemistry and Pericyclic Reactians: Jagdamba Singh and Jaya Singh, New Age Internatianal.
7. Sereochemistry : Conformation and mechanism, P.S. Kalsi, New Age International Publication
8. Stereochemistry of Organic Compounds: Principles and Applications, D. Nasipuri, New Age International Publication
9. Stereochemistry of Organic Compounds: E. L. Eliel and S. H. Wilen. John Wiley
10. Stereochemistry of Organic Compounds: P. S. Kalsi, New Age International.
11. Pericyclic Reactions, S. M. Mukherji, Macmillan, India.
12. Conversion of Orbital Symmetry, R.B. Woodward and R. Hoffman
13. Organic Reactions and Orbital Symmetry,R. C. Storr, T. L Gilchrist
14. Fundamentals of Photochemistry, K.K.Rohtagi-Mukherji, Wilcy-Eastern.
15. Molecular Photochemistry, N.J.Turro, W.a.Benjamin.
16. Introductory Photochemistry, A.Cox and T.Camp. McGraw-Hill.
17. Photochemistry, R.P.Kundall and A.Gibert, Thomson Nelson.
18. Organic Photochemistry, J.Coxon and B.Halton, Cambridge University Press.

INORGANIC CHEMISTRY-II

Course Code: CC-202	**End Sem-80 marks**	**Time-3 hour**
Credits: 05	**Mid Sem-20 marks**	**Time- 1hour**

Objective: *1. To understand the theoretical basis of boding of structurally different coordination compounds. 2. To understand the basis of electronic spectra of metal complexes as well as to understand the basis of anomalous magnetic behaviour of metal complexes. 3. To impart knowledge on preparative methods, structure and bonding of metal-π complexes and cultures.*

Outcome: *On completion of this course student will be able to: 1. Understand and explain the bonding in coordination and organometallic compounds. Describe the fundamental requirement to interpret the electronic spectra of metal complexes for prediction of their properties. 2. Describe the synthesis, structure and bonding of metal carbonyls, metal nitrosyls, dioxygen, dinitrogen complexes as well as metal clusters.*

UNIT-I: ***Electronic Spectra of Transition Metal Complexes***: Spectroscopic ground states, Orgel diagrams for d1 -d9 states in Oh and Td symmetry, Tanabe-Sugano diagrams for d2 configuration in Oh and Td symmetry. Calculations of Dq, B and β parameters.

UNIT-II ***Metal-Ligand Bonding***:

Crystal-Field Theories: Limitation of Crystal Field Theory, Molecular orbital theory for Octahedral, Tetrahedral and Square Planar Complexes, σ and π bonding in Molecular Orbital Theory. Application of MOT to Correlation diagrams.

UNIT-III: ***Chemistry of Transition Elements***: Coordination chemistry of Transition Metal ions, Stabilization of Unusual oxidation states, Stereochemistry of coordination compounds, Splitting of d-orbitals in Low symmetry environment, Jahn-Teller effect, Interpretation of Electronic Spectra including Charge Transfer Spectra, Spectrochemical series, Nephelauxetic series, Fluxional molecules, Iso and Hetero Poly acids. Structures of Mixed Metal Oxides: Spinel & Inverse Spinel, lleminite and Perovskite structure, Coloured Minerals and Gem quality crystals.

UNIT-IV: ***Chemistry of Inner Transition Elements***:

Chemistry of Lanthanides and Actinides: Lanthanide Contraction, Separation of Lanthanide elements, Oxidation state, Spectral and Magnetic Properties, Stereochemistry, Use of Lanthanide Compounds as Shift reagents, Actinide contraction, Oxidation states, Comparisons between Lanthanides and Actinides.

Books and References:

1. Advanced Inorganic Chemistry: A Comprehensive Text: F. A. Cotton and G. Wilkinson, John Wiley.

2. Inorganic Chemistry: Principles of Structure and Reactivity: J. E. Huheey, E. A. Keiter and R. L. Keiter, Addition Wisley Publishing Company.

3. Comprehensive Coordination Chemistry eds.: G. Wilkinson, R. D. Gillars and J. A. McCleverty, Pergamon.

4. Inorganic chemistry: Gary L. Miessler, Donald A. Tarr, Pearson

PHYSICAL CHEMISTRY-II

Course Code: CC-203 **End Sem-80 marks** **Time-3 hour**
Credits: 05 **Mid Sem-20 marks** **Time- 1hour**

Objective: *The topics covered under the course are inherently very fundamental and intended to provide the basic understanding at atomic and subatomic level. The objective of the course to study and understand the concept of energy, the transfer of energy into work, capacity of energy to function, entropy, enthalpy, chemical potentials, thermodynamic laws, criterion for determination of the feasibility or spontaneity of a given transformation, partial molar properties, their determinations. The course is designed in a manner in which a bridge between classical thermodynamics and quantum mechanics can be established.*

Outcome: *Understanding the underlying concepts and realization of quantum mechanics will be useful in solving problems at realistic atomic and molecular level, in particularly in the field of spectroscopy and analytical chemistry. Understanding thermodynamics requires knowledge of how the microscopic world operates and importance of reversible and irreversible processes*.

UNIT-I *Classical Thermodynamics*: Brief resume of concepts of laws of thermodynamics, entropy and free energy. The concept of chemical potential and partial molar properties; partial molar free energy, partial molar volume and partial molar heat content and their significance. Determination of these quantities. Concept of fugacity and determination of fugacity. Activity, activity coefficient, Debye-Huckel theory for activity coefficient of electrolytic solutions; determination of activity and activity coefficients, ionic strength.

UNIT-II *Phase Diagram*: Phase behavior of one and two component systems (solid-solid, solid-liquid, solid-vapor, liquid-liquid, liquid-vapor equilibrium). Ehrenfest classification of phase transitions.

UNIT–III *Statistical Thermodynamics*:

Concept of distribution, thermodynamic probability and most probable distribution. Ensemble averaging, postulates of ensemble averaging, Canonical, grand canonical and microcanonical ensembles, corresponding distribution laws (using Lagrange's method of undetermined multipliers) Partition functions-translational, rotational, vibrational and electronic partition functions, calculation of thermodynamic properties in terms of partition function. Fermi-Dirac statistics, distribution law and application to metal. Bose-Einstein statistics - distribution law and application to helium.

UNIT–IV *Chemical Dynamics* : Potential energy surfaces. Collision theory of reaction rates, Conventional transition state theory (CTST); CTST as applied to ionic reactions, kinetic salt effects. steady state kinetics. Kinetic and thermadynamic control of reactions. Treatment of unimolecular reactians. dynamics of unimolecular reactions (Lindemann- Hinshelwood and Rice Rampsberger - Kassel Marcus (RRKM) theories of unimolecular reactions). Dynamics chain (hydrogen-bromine reaction, pyrolysis of acetaldehyde, decomposition of ethane), photochemical (hydrogen -bromine and hydrogen - chlorine reactions) and oscillatory reactions (Belousov- Zhabotinski reaction), homogeneous catalysis, kinetics of enzyme reactions. General features of

fast reactions, study of fast reactions by flow methods, relaxation methods, Flash photolysis. Dynamics of barrier less chemical reactions in solution.

Books and References

1. A textbook of Physical chemistry – H.K. Moudgil
2. Physical Chemistry, T. Engel and P. Reid, Pearson, 2006, 1st edition, New Delhi.
3. Thermodynamics, G. N. Lewis and M. Randall, McGraw Hill, 2nd edition, 1961, New York.
4. Molecular Thermodynamics, D. A. McQuarrie and Simon. Viva, 2009, 1st edition, New Delhi.
5. Non Equilibrium Thermodynamics, S.R. deGroot and Mazur, Dover, New York.
6. Introductory Statistical Thermodynamics, T. Hill, Dover, 1986, New York.
7. Statistical Thermodynamics, Oxford, Oxford Chemistry Primer vol. 58, 1997.
8. Introduction to Statistical Mechanics, R. Bowley and M. Sanchez, Clarendon press,
9. Statistical Mechanics and Thermodynamics, C. Garrod, Oxford Univ. Press, 1995, New York.
10. Introduction to thermodynamics of irreversible processes, 2nd edition, Interscience, 1961, New York
11. Chemical Kinetics, K.J.Laidler, Mcgraw-Hill.
12. Kinetics and Mechanism of Chemical Transformations, J.Rajaraman and J.Kuriacose, McMillan.
13. Fast Reaction – D.N.Hague
14. Chemical Kinetics and Dynamics–2 nd Edn. , JISteinfild, J.S.Fransis Co, W.L.Hase , Beutic Hall (1999).
15. Physical Chemistry- G. K Vemulapalli
16. Physical Chemistry- George Woodbury, Brooks cole
10. Statistical Thermodynamics: M. C. Gupta, New Age Pvt Publication..

ORGANIC SPECTROSCOPY

Course Code: CC-205 **End Sem-80 marks** **Time-3 hour**
Credits: 05 **Mid Sem-20 marks** **Time- 1hour**

Objective: *To impart knowledge of different spectroscopic technique for structural elucidation of organic compounds*.

Outcome: *Upon completion of this course students will be able to understand how Ultraviolet and Visible Spectroscopy, Infrared Spectroscopy, Nuclear Magnetic Resonance Spectroscopy and Mass Spectrometry are powerful technique to analyze the structural details of organic compounds, and predict different unknown compound based on UV-Vis, IR, 1HNMR, 13CNMR and mass spectroscopic data.*

UNIT-I ***Ultraviolet and Visible Spectroscopy***:
Various electronic transitions, Beer Lambert law, effect of solvent on electronic transitions, ultraviolet bands for carbonyl compounds, unsaturated carbonyl compounds, dienes, conjugated polyenes, Woodward- Fieser rules for conjugated dienes and carbonyl compounds, ultraviolet spectra of aromatic and heterocyclic compounds, steric effect in biphenyls.

UNIT-II ***Infrared spectroscopy*****:** Instrumentation and sample handling, characteristics vibrational frequencies of alkanes, alkenes, alkynes, aromatic compounds, alcohols, ethers, phenols and amines, Detail study of vibrational frequencies of carbonyl compounds (ketones, aldehydes, esters, amides, acids, 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, FTIR, IR of gaseous, solid and polymeric materials.

UNIT III: (a)*Nuclear Magnetic Resonance Spectroscopy (NMR*):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, aldehydic, and aromatic compounds) and other nuclei (alcohols, phenols, enols, carboxylic acids, amines, amides, and mercapto), chemical exchange, effect of deuterium, complex spin-spin interaction between two, three, four and five nuclei (first order spectra), virtual coupling, stereochemistry, hindered rotation, karplus curve-variation of coupling constant with dihedral angle, simplification of complex spectra, nuclear magnetic double 13 resonance, NMR shift reagents, solvent effects, Fourier transform technique, nuclear overhauser (NOE). Resonance of other materials.

(b) ***Carbon-13 NMR spectroscopy***: General considerations, chemical shift (aliphatic, olefinic, alkyne, aromatic, heteroaromatic and carbonyl carbon), coupling constants. Two dimension NMR spectroscopy – COSY, NOESY, DEPT, APT and INADEQUATE techniques.

UNIT IV ***Mass spectrometry***: Introduction, ion production – EI, CI and FAB factors affecting fragmentation, ion analysis, ion analysis, ion abundance, mass spectral fragmentation of organic compounds, common functional groups, molecular ion peak, metastable peak, McLafferty rearrangement, nitrogen rule, high resolution

mass spectrometry, examples of mass spectral fragmentation of organic compounds with respect to their structure determination.

Books and References

1. Introduction to Spectroscopy , Donald L. Pavia, Garry M. Lampman and George S. Kriz, Cengage India Pvt. Ltd
2. Spectroscopy of Organic compounds, P.S. Kalsi, New Age Publishher
3. Silverstein, R. M.; Webster, F. X. Spectrometric identification of organic compounds; 6th ed.; Wiley: New York, 1998.
4. Lambert, J. B; Shurvell, H. F, Organic structural spectroscopy, Prentice Hall, 1998.
5. Kemp, W. Organic spectroscopy; 3rd ed.; Macmillan Education: Houndmills, Basingstoke, Hampshire, 1991.
6. Levitt, Malcolm H.; Spin Dynamics-Basics of Nuclear Magnetic Resonance, Second edition; John Willey & Sons Ltd.

PHYSICAL CHEMISTRY PRACTICAL

Course Code: CC-205 **End Sem-100 marks** **Time-6 hour**

Credits: 05

Objective: The laboratory course is framed on the basis of instruments such as conductivity meter, pH meter and potentiometer, where a number of experiments based on conductivity measurement, pH measurement and potential measurement can be performed.

Outcome: It is believed that students performing the experiments will be capable of handling the conductivity meter, pH meter and potentiometer. Also it gives a real feel of the electrochemistry, such a verification of Debye-Huckel-Onsager equation, neutralisation of weak acids, determination of Ksp of sparingly soluble salt and conductometric titrations, which are taught in theory.

Chemical Kinetics:

1. Saponification of ethylacetate with sodium hydroxide by chemical method.
2. Comparison of strength of acids by ester hydrolysis
3. Determination of energy of activation of acid catalyzed hydrolysis of methyl acetate.
4. Determination of velocity constant of hydrolysis of an ester/ionic reaction in micellar media.

Adsorption:

1. Adsorption of acetic acid and oxalic acid on animal charcoal and verification of Freundlich isotherm.
2. Study of the surface tension – concentration relationship for solutions (Gibb's equation)

Phase equilibria:

1. Determination of critical solution temperature of phenol-water system.

2.Construction of phase diagram for a three component system (chloroform-acetic acid – water).

Electrochemistry:

Conductometry:

1. Determination of strength of strong acid and weak acid in given mixture conductometrically.
2. Determination of solubility and solubility product of a sparingly soluble salt (i.e., $PbSO_4$, $BaSO_4$) conductometrically.
3. Determination of hydrolysis constant of aniline hydrochloride conductometrically

***Potentiometry*:**

4. Determination of strength of halides in a mixture potentiometrically.
5. Determination of the formation constant of silver amine complex and stochiometry of the complex potentiometrically.
6. Estimation of ferrous iron in ferrous ammonium sulphate potentiometrically.
7. Potentiometric titration of a strong acid with strong base using quinhydrone electrode.

***pH metry*:**

8. Determination of first and second ionization constants of phosphoric acid by pH meter.
9. Determination of hydrolysis constant of aniline hydrochloride by pH meter.
10. Verification of Debye-Huckel-Onsagar equation of conductance.

Books and References:

1. Experimental physical chemistry: R. C. Das and B. Behera, Tata McGraw Hill.
2. Findlay's practical chemistry (revised): B. P. Levitt, Longman.
3. Advanced practical physical chemistry: J. B. Yadav, Goel publishing house, Meerut. 21

SEMESTER – III

INORGANIC CHEMISTRY III

Course Code: CC-301 **End Sem-80 marks** **Time-3 hour**
Credits: 05 **Mid Sem-20 marks** **Time- 1hour**

Objective: (i) *To learn about the formation and stability of metal complexes and their determination and (ii) Mechanistic aspects of different types of reaction of metal complexes in solution.*

Outcome: *At the end of the course the student will (i) Be able understand the concept stability constant, its determination and application in different fields (ii) Understand the reactions and mechanism of different types of reactions in coordination compounds and their applications in practical fields*

UNIT –I (a) ***Metal π –Complex*****:** Metal Carbonyls, Structure and Bonding, Important reactions of metal carbonyls; Preparation, Bonding, Structure and Important Reactions of Transition Metal Nitrosyl, Dinitrogen and Dioxygen Complexes ligands. ***(b) Metal clusters:*** Metalloboranes, Metallocarboranes, Metal carbonyls and Metal halide clusters.

UNIT –II ***Metal -Ligand Equilibria in Solution***: Stepwise and Overall formation constants and their interaction, trends in stepwise constants. Factors affecting the Stability of metal complexes with reference to the nature of metal ion and ligand. Chelate effect, Macrocyclic effect and its thermodynamic origin. Determination of Binary Formation Constants by pHmetry and Spectrophotometry.

UNIT-III ***Reaction Mechanism of Transition Metal Complexes (Part-A):*** Energy profile of a reaction, Reactivity of metal complexes, Inert and Labile complexes, Kinetic application of Valence Bond and Crystal field theories, Kinetics of Octahedral substitution, Acid hydrolysis, Factors affecting acid hydrolysis and base hydrolysis, Conjugate base mechanism, direct and indirect evidences in favour of conjugate base mechanism.

UNIT-IV ***Reaction Mechanism of Transition Metal Complexes (Part-B):*** Anation reactions, k-exchange, reaction without metal ligand bond cleavage. Substitution reactions in square planar complexes. The trans effect, mechanism of one electron transfer reactions, Outer sphere reactions, Marcus-Hush Theory, Inner sphere type reactions.

Books and References:

1. Advanced Inorganic Chemistry: A Comprehensive Text: F. A. Cotton and G. Wilkinson, John Wiley.
2. Inorganic Chemistry: Principles of Structure and Reactivity: J. E. Huheey, E. A. Keiter and R. L. Keiter, Addition Wisley Publishing Company.
3. Comprehensive Coordination Chemistry eds.: G. Wilkinson, R. D. Gillars and J A McCleverty, Pergamon.
4. Advanced Inorganic Chemistry: F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann, John Wiley and Sons.
5. Fundamentals Concepts of Inorganic Chemistry,Volume -5,Asim K. Das and Mahua Das,CBS Publishers and Distributors Pvt. Ltd.

ORGANIC CHEMISTRY-IV

Course Code: CC-302 **End Sem-80 marks** **Time-3 hour**
Credits: 05 **Mid Sem-20 marks** **Time- 1hour**

Objective: *To impart knowledge of oxidation, reduction , some selective name reactions, disconnection approach and heterocyclic chemistry*

Outcome: *Upon completion of this course students will be able to understand the reactivity pattern and underlying reaction mechanism of different oxidizing and reducing reagents, and understand the art of selective protection and deprotection of alcohol, amine, carbonyl and carboxyl groups in organic compounds and the chemistry of heterocyclic compounds*

UNIT- I (a) ***Oxidation****:* Introduction, different oxidative processes, hydroborations alkanes, alkenes, aromatic rings, saturated C-H groups (active and unactivated), alcohols, diols, aldehydes, ketones, ketals, and carboxylic. Amines, hydrazines and sulphides, Oxidation with ruthenium tetraoxide, iodobenzene diacetate and thallium III) nitrate, oxidation with IBX, Dess-martin periodinane, PDC (Pyridinium Dichromate), PCC (Pyridinium Chlorochromate). Swern oxidation.

(b*) Reduction*: Introduction: Different reductive processes, hydrocarbonsalkanes, alkenes, alkynes and aromatic ring, Carbonyl compounds: aldehydes, ketones, acids and their derivatives. Epoxides, Nitro, nitroso, azo, oxime groups, hyrogenolysis, Clemmenson's reduction,Wolff kishner reduction & Luche reduction.

UNIT- II ***Selective organic name reactions*:** Favorski reaction, stock enamine reaction, Mannich reaction, Sharpless asymmetric epoxidation, ene reaction, barton reaction, Baeyer-Villiger reaction, Chichibabin reaction, Claisen condensation, Claisen reduction, Curtius Rearrangement, Demjanov rearrangement, Dieckmann condensation, Favorskii rearrangement, Horner-Wadsworth-Emmons olefination, Wittig olefination, Wolff-kishner reduction, Mitsunobu reaction, Fries rearrangement, Peterson olefination, Mcmurry Coupling.

UNIT-III ***Disconnection approach***: An introduction to synthons and synthetic equivalents, disconnection approach, functional group interconversions, the importance of the order of events in organic synthesis, one group C-X and two groups C-X disconnections, chemoselectivity, reversal of polarity (umpolung reaction), cyclisation reactions, amine synthesis. (b) Protecting groups: Principle of protection of alcohol, amine, carbonyl, carboxyl groups and Umpolung Reaction (c) One group C-C disconnection: Alcohols and carbonyl compounds, regioselectivity. Alkene synthesis, use of acetylenes and aliphatic nitro compounds in organic synthesis. (d) Two group C – C disconnection: Diels-Alder reaction, 1,3 – difunctionalized compounds, alpha, beta- unsaturated carbonyl compounds, control in carbonyl condensations, 1,5 – difunctionalized compounds, Michael addition and Robinson annelation. (e) Chemistry of Natural Products: Application of Disconnection approach in the construction of biomolecules like Synthesis of Camphor, Longifoline & Juvabione.

UNIT-IV ***Heterocyclic Chemistry*** : Principles of heterocylic synthesis involving cyclisation reactions and cycloadditions. Three-membered and four-membered

heterocycles: Synthesis and reactions of Aziridines, Oxiranes, thiranes, azetidines, Oxetanes and thietanes. (ii) Benzo fused Five-Membered Heterocycles: Synthesis and

reactions including medicinal applications of benzopyrroles, benzofurans and benzothiophenes. (iii) Nitrogen Containing heterocyclic: Synthesis and reactivity of pyridine, quinoline, Isoqunoline and Indole. Skraup Synthesis, Fisher Indole Synthesis.

Books and References:

1. Advanced Organic Chemistry; Reactians Mechanism and Structure: Jerry March, John.Wiley.
2. Advanced Organic Chemistry: F. A. Carey and R. J. Sundberg, Part-B. 3. Principles of Organic Synthesis: R. O. C. Norman and J. M. Coxon, Blackie Academic & Professianal
4. Reactian Mechanism in Organic Chemistry: S. M. Mukherjee and S. P. Singh, Macmillian. India. Ltd.
5. Organic Chemistry: J. Clayden, N. Greeves, S. Warren and P. Wothers, Oxfard University Press.
6. Organic Reactians and Orbital Symmetry: T. L. Gilchrist and R. C. Storr, Cambridge at the University Press.
7. Photo Chemistry and Pericyclic Reactians : Jagdamba Singh and Jaya Singh, New Age Internatianal.
8. Mechanism and Theory in Organic Chemistry: Thomas H. Lowry, Additian Wesley.
9. Named reaction by Jie Jack Lie.

RESEARCH METHODOLOGY

Course Code: CC-303 **End Sem-80 marks** **Time-3 hour**
Credits: 05 **Mid Sem-20 marks** **Time- 1hour**

Objective: *To impart knowledge of Scientific research,documentation and scientific writing, data analysis and computer applications.*

Outcome: *Upon completion of this course students will be able to understand the research methodology, formulation of objective, literature survey, scientific writing and computer applications in chemistry.*

UNIT-I(a)*Scientific Research*-

Defination,characterstics,types, need of research,Identification of the problem,assessing the status of the problem, formulating the objectives, preparing design,Actual investigation**.**

(b) *Literature Survey*:- primary sources (Journals and Patents),Secondary resources (abstract,CA,collective indexes,reviews, awareness service, general treatise, monographs on specific areas, reference books),basic ideas of literatures,search on web(sci-finder,scopus,Scirus,sciencedirect),Citiation index,impact factor of research papers**.**

UNIT-II *Documentation and scientific writing*:-organization and writings of manuscripts papers,monographs,authored books,thesis writings,srtructure and components of research reports,Type of report:Research papers,thesis,Research project reports,picture and graphics,citiation styles,writing a review paper,bibliography**.**

UNIT-III *Statstical methods of data analysis*

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 precission,significant figures,Test of significance(F-test,student T-test,paired test,T-test),mean value and deviation,average and standard deviation,median value ,confidence intervals,least square methods of fitting lionear equations,correlation co-efficients and co-efficient of determination.

UNIT-IV- *Computer applications in chemistry*:-introduction to computer and IT,data and information,General features of a computer,softwares and its types,application of softwares packages in chemistry,computatio0nal chemistry.Application of some computer packages(MS-Excel,Origin,Chem-Draw) to chemistry,computer techniques used in chemistry with special reference to UV-Visible spectroscopy,FTIR,XRD.

***Books and References*:-**

1. Research Methodology: Methods & Technique, C.R. Kothari, Wiley EastenLtd, New Delhi 1985.
2. Research Methodology, G. C. Ramamurthy, Dreamtech Press.
3. Research Methodology: A step by step Guide for Beginners 2nd edn. Kumar Ranjit, Pearson Education, Singapore, 2005.
4. Introduction to Research & Research Methodology, M. S. Sridhar.
5. Analytical Chemistry, G. D. Christian, 6th Edn, Wiley Student Edition.

OPEN ELECTIVE

INDUSTRIAL CHEMISTRY

Course Code: OEC-305 **End Sem-100 marks** **Time- 3 hour**

Credits: 05

Objective: *To impart knowledge on Silicate, fertilizers, cements, sugars, oils, fats, sugars, soaps & detergent and fuel industries.*

Outcome: *Upon completion of this course students will be able to understand the synthetic methods and applications of glass, ceramics, fertilizers, cements, and can able to analyze chemical products for industrial applications.*

Unit-I, *Silicate Industries:-*

(A) Glass: Glassy state and its properties, classification (silicate and non-silicate glasses). Manufacture and processing of glass. Composition and properties of the following types of glasses: Soda lime glass, lead glass, armoured glass, safety glass, borosilicate glass, fluorosilicate, coloured glass, photosensitive glass.

(B) Ceramics: Important clays and feldspar, ceramic, their types and manufacture. High technology ceramics and their applications, superconducting and semiconducting oxides, fullerenes carbon nanotubes and carbon fibre.

Unit-II

(A) Fertilizers:-

Different types of fertilizers. Manufacture of the following fertilizers: Urea, ammonium nitrate, calcium ammonium nitrate, ammonium phosphates; polyphosphate, superphosphate, compound and mixed fertilizers, potassium chloride, potassium sulphate.

(B) Cements:-

Classification of cement, ingredients and their role, Manufacture of cement and the setting process, quick setting cements.

(C) ***Sugar:-*** **E**xtraction of juice, Purification of juice:-defection, classification by sulphitation and carbonation process; Concentration and crystallization, Recovery of sugar from molasses and bagasse, Testing of purity of sugar.

Unit-III, Oil, Fats & Wax; Soaps and Detergents:-

(A) Chemical nature of oil, fats, and wax, distinction between oil & fat. Manufacture of vegetable oil by solvent extraction, Hydrogenation of oil.

(B) Analysis of oils, fats, and waxes:- Sapofication of value, Acid value, Ester value, Iodine value, RM value, Elaiden test, Aniline temperature.

(C) Soaps:- ingredients, Manufacture of soaps, Toilet soap, Transparent soap, Shaving soap. ***Detergents:-*** Cationic, Anionic and zwitterionic detergents. Advantages and disadvantages over soap. Shampoos.

Unit-IV, Liquid Fuels:- Liquid fuels, Petroleum, Occurrence, Origin, Composition, Grading of petroleum, Flash point and its determination, Knocking and anti knocking agents, Octane number, Cetane number. Upgradation by chemical treatment i.e. Reforming,

Polymerization, Catalytic polymerization, Alkylation, Isomerisation, Aromatization. Rocket fuel, Propellants of rocket and guided missiles fuels for jet engine. Fuel oil or boiler oils.

Books and References

1. E. Stocchi: *Industrial Chemistry*, Vol-I, Ellis Horwood Ltd. UK.
2. R. M. Felder, R. W. Rousseau: *Elementary Principles of Chemical Processes*, Wiley Publishers, New Delhi.
3. W. D. Kingery, H. K. Bowen, D. R. Uhlmann: *Introduction to Ceramics,* Wiley Publishers, New Delhi.
4. J. A. Kent: Riegel's *Handbook of Industrial Chemistry*, CBS Publishers, New Delhi.
5. P. C. Jain, M. Jain: *Engineering Chemistry,* Dhanpat Rai & Sons, Delhi.
6. R. Gopalan, D. Venkappayya, S. Nagarajan: *Engineering Chemistry,* Vikas Publications, New Delhi.
7. B. K. Sharma, & H. Kaur, *Industrial Chemistry,* Goel Publishing House, (Meerut) (1996)

ORGANIC CHEMISTRY PRACTICAL

Course Code: CC-305 **End Sem-100 marks** **Time-6 hour**
Credits: 05

Objective: To impart knowledge of basic separation techniques and purification of organic samples using TLC and column chromatography

Outcome: Upon completion of this course students will be able to 1) purify and separate mixture of organic samples 2) Can able to perform synthesis of derivatives of simple functional groups and purify them 3) Can able to identify the functional groups present in organic molecules, 4) can able to isolate organic compounds from a mixture of organic samples

1. Separation, purification and identification of compounds of binary mixtures (solid-solid, solid-liquid, liquid-liquid) using TLC and column chromatography, Chemical tests.
2. **Quantitative Analysis**: (a) Determination of amino group by acetylation method. (b) Detennination of hydroxyl group by acetylation method. (c) Estimation of Keto group. (d) Determination of iodine value and saponification value of an oil sample.

3. **Organic Synthesis**: Preparation of adipic acid, p-chlorotoluene, p-nitroaniline, pbromoaniline, triphenylmethanol. Preparation of PDC (Pyridinium dichromate) & PCC(Pyridinium chloro chromate) reagents and it's application on benzyl alcohol Grignard reagent preparation and reactions on aldehyde.

Books and References:

1. The Systematic Identification of Organic Compounds: R.L. Shriner, C. K. F. Harmann, T.C. Morrill, D.Y. Curtin, R.C. Fusion, John Wiley and Sons.
2. Organic Analytical Chemistry (Theory and Practice): Jagmohan, Narosa Publishing House.
3. A Text Book of Practical Organic Chemistry: Arthur I.Vogel, .E.L.B.S. and Longman.
4. Experiments and Techniques in Organic Chemistry: D. Pasto, C. Johnson. 5. Laboratory Mannual of Organic Chemistry: B.B. Dey and M.V.Siaram (Revised)-:T.R.Govindachari, Allied Publishers.
6. Systematic Qualitative Organic Analysis: H. Middleton, Orient Longman. 7. A Hand Book of Organic Analysis (Qualitative and Quantitative): H.T. Clarke, Revised, B. Haynes, Arnold Publishers.

SEMESTER – IV

BIOINORGANIC AND SUPRAMOLECULAR CHEMISTRY

Course Code: DEC-401 **End Sem-80 marks** **Time-3 hour**
Credits: 05 **Mid Sem-20 marks** **Time- 1hour**

Objective:

1. To study the role on the role of metals in biological systems and medicine.
2. To introduce the student on structure, stereochemistry and biological functions of different metalloenzymes.
3. To study the structure and function of biomolecules in nitrogen fixation and photosynthesis.
4. To introduce concept molecular recognition, interactions in supramolecular systems and their applications

Outcome:

On completion of the course the student will
1. Understand and acquire knowledge of effect of deficiency and toxicity of metals in both human and plant systems.
2.Describe the structural and functional relationships, mechanisms and importance of metaloenzymes.
3. Understand the fundamentals of supramolecules, supramolecular reactions and catalysis, devises

UNIT -I Biological roles of metal ions, Calcium Biochemistry, Oxygen Transport and storage: Hemoglobin, Myoglobin, Cobalt containing models of oxygen binding, Iron containing models of oxygen carrier, Hemocyanin; Iron storage and transport: Ferritin, Transferrin, Siderophores.

UNIT-II *Enzymes exploiting acid catalysis*:

Carbonic anhydrase, Carboxypeptidases, Superoxide dismutase, Xanthine oxidase. Redox catalysis: Iron-sulfur proteins: Ferredoxins and Rubbredoxins, Non-heme iron, Cytochromes, Cytochrome P-450 enzymes, Blue Copper Proteins, Coenzyme B12 Nitrogen Fixation, Photosynthesis.

UNIT-III *Metals in medicine*: Ionophores, Importance of Na and K, Metal deficiency and diseases, Toxic effects of metals, Metals used for diagnosis and chemotherapy, Anticancer drugs

UNIT-IV *Supramolecular Chemistry*:

Host guest chemistry, chiral recognition and catalysis, molecular recognition, biomimetic chemistry, crown ethers, cryptates. Cyclodextrine, cyclodextrinbased enzyme models, calixarenes, Ionophores

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Books and References:

1. Priciple of Biochemistry (Lehninger): D. L Nelson and M. M Cox, W. H. Freeman and company, New York.
2. Fundamentals of Biochemistry: D. Voet, J. G. Voet and C. W. Pratt; John wiley and sons.
3. Inorganic Chemistry of Biological process- M. Huges.
4. Bio Inorganic Chemistry – E. Ochiai 24

ORGANOMETALIC CHEMISTRY

Course Code: DEC-402 **End Sem-80 marks** **Time-3 hour**
Credits: 05 **Mid Sem-20 marks** **Time- 1hour**

Objective: *1. To introduce the students on preparations, structure and bonding aspects of simple organometallic compounds*

2. To study the methods of synthesis, properties and reactivity of organometallic compounds with metal-carbon multiple bonds.

3. To introduce on types of common organometallic reactions, reagents and mechanistic study of some homogeneous catalytic reaction systems involving organometallic compounds

Outcome:

On completion of this course, the student will be able to

1. Describe the structure and bonding aspects of different organotransition metal compounds and their correlations with the stability and reactivity of such compounds.

2. Identify the different types of organotranstion metal complexes catalyzed reactions and explain mechanistic pathways of different catalytic reactions.

3. Describe the important applications of organometallic homogeneous catalysis in the production of organic chemicals

UNIT-I *Organometallic Chemistry*:

18-Electron Rule, Ligands in Organomettallics, Synthesis, bonding and reactions of Alkyl, Aryl, Alkylidenes, Alkylidynes, Allyl, Dienyl, Arene & Trienyl complexes, Cyclic π systems (3 to 8 membered rings) and Fullerene complexes. Spectral analysis of Organometallic Complexes.

UNIT –II *Homogenous and Heterogenous catalysis*:

Stiochiometric reactions for Organometallic catalysts: Dissociation & Substitution, Oxidative addition & carbonylation, Oxygen transfer from Peroxo and Oxo Species, Reductive & Hydride elimination, Insertion, Displacement and Isomerization reaction. Hydrogenation, Hydrosilation and Hydrocynation of unsaturated compounds, Hydroformylation, Wacker (Smidt) Process, Olefin Metathesis, Fischer-Tropsch synthesis, Zeigler-Natta polymerization, Water gas reaction.

UNIT –III (a) Organometalic reagents: Principle, Preparations, properties and application of the following in organic Synthesis with mechanistic details. (i) Group I and II Metals: Li, Mg, Hg, Cd, Zn, (ii) Transition metals: Cu, Pd, Ni, Co (iii) Group I and II metal Organic Compounds: Li, Mg, Hg, Cd, Zn (b) Organo main group chemistry-Boron, Silicon and Tin.

UNIT –IV *Magneto Chemistry & EPR*:

(a) Induction and susceptibility. Lande interval rule, calculation of g-values, Van Vleck's equation and its use. Effect of spin orbit coupling. Magnetic properties of A.E.T terms with reference to Co(I) and Ni(II) complexes.

(b) Electron Paramagnetic Resonance Spectroscopy: Hyperfine splitting, Spin orbit coupling, Significance of g-tensor, Zero field splitting, Kramer's degeneracy, Application to inorganic systems

Books and References:

1. Advanced Inorganic Chemistry: F. A. Cotton and G. Wilkinson, John Wiley.
2. Inorganic Chemistry: J. E. Huheey, E. A. Keiter, R. L. Keiter, Pearson Education.
3. Inorganic Electronic Spectroscopy: A. B. P. Lever, Elsevier.
4. Magnetochemistry, R. L. Carlin, Springer Verlag.
5. Comprehensive Coordination Chemistry eds.,-G. Wilkinson, R. D. Gillars and J. A. McCleverty, Pergamon.

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Molecular Spectroscopy

Course Code: CC-403	**End Sem-80 marks**	**Time-3 hour**
Credits: 05	**Mid Sem-20 marks**	**Time- 1hour**

Objective: *To impart knowledge of fundamentals of molecular spectroscopy from theoretical point of view and different instrumental analysis.*

Outcome:

Upon completion of this course students will be able to understand rotational, vibrational and electronic spectroscopy and their applications to different molecules.

UNIT-I Spectroscopy: (*a) Rotational Spectroscopy*: The rigid diatomic rotor, selection rules, intensity of rotational transitions, the role of rotational level degeneracy, the role of nuclear spin in determining allowed rotational energy levels. Classification of polyatomic rotors and the non-rigid rotor.

(***b) Vibrational Spectroscopy***: Review of linear harmonic oscillator, vibrational energies of diatomic molecules, zero point energy, force constant and bond strength; anharmonicity, Morse potential energy diagram, vibration-rotation spectroscopy. Breakdown of Oppenheimer approximation, vibrations of polyatomic molecules, Selection rules, normal modes of vibration, group frequencies, overtones, hot bands, factors affecting the band positions and intensities; metal-ligand vibrations.

UNIT-II ***(a) Electronic Spectroscopy***: Electronic transitions, Franck-Condon principle. Vertical transitions. Selection rules, parity, symmetry and spin selection rules. Polarization of transitions. Fluorescence and phosphorescence.(b) Raman Spectroscopy: Classical and quantum theories of Raman effect Pure rotational, vibrational and vibrational-rotational Raman spectra, selection rules, Mutual exclusion principle.

UNIT-III ***Electron Spin Resonance (ESR) spectroscopy***: g-factor, electron-nuclear coupling, double resonance in ESR electron-electron coupling. Techniques of ESR spectroscopy **Mössbauer Spectroscopy**: Basic principles, instrumentation, spectral parameter and displays, applications. Mossbauer parameters- isomer shift, quodropole splitting, Magnetic hyperfine interaction, Doppler effect. Applications of Mossbauer spectroscopy.

UNIT-IV ***Instrumental Method of Analysis***: ***X-ray diffraction***: Crystals and the diffractions of X-ray, Bragg's law concept of symmetry in crystals, lattice planes and Miller indices, systematic absence of reflections, multiplicities, the x-ray diffraction experiment, powder method, single crystal method, x-ray intensities, structure factor, particle size measurement by x-ray diffraction. ***Polarography***: Current-voltage relationship, theory of polarographic waves, instrumentation, qualitative and quantitative applications. ***Thermal analysis:*** Theory, methodology, instruments and applications of theromo-gravimetric analysis (TGA), and differential scanning calorimetry (DSC).

Books and References: 1. Fundamentals of Molecular Spectroscopy: C. N. Banwell, McGraw-Hill.

2. Basic Principles of Spectroscopy: R. Chang, Mc Graw Hill 3. Application of spectroscopy of organic compounds, J. R. Dyer, Prentice hall

4. Spectroscopic methods in organic chemistry, D. H. Williams, I. Fleming, Tata McGraw Hill.

5. Organic spectroscopy, W. Kemp, ELBS

6. Spectroscopy of organic compounds, P. S. Kalsi, New Age International.

7. Mössbauer Spectroscopy and Transition Metal Chemistry, P. Gütlich, R. Link, A. Trautwien, Springer-Verlag (1978).

8. Mössbauer Spectroscopy, N. N. Greenwood, T. C. Gibb, Chapman and Hall Ltd. (1971).

APPLIED CHEMISTRY PRACTICAL

Course Code: CC-405 **End Sem-100 marks** **Time-6 hour**

Credits: 05

***Objective*:**

1.To acquire a minimum practical skill to determine the molecular weight of polymers and thier characterization by other methods

2. To learn the conventional techniques of analysis of different water parameters and specific components in different samples by classical/instrumental methods.

3. The laboratory course is designed based on UV Visible spectrophotometer. Experiments such as determination of indicator constant, stoichiometry of a metal complex by Job's method are included

Outcome:

After the completion of course students will be able

1. To perform experiment on polymers and their basic characterizations.

2. To perform the analysis of different water parameters using classical and instrumental methods.

3. To understand the principles behind the experiment performed in the laboratory

4. To understand BeerLambert's law in a better manner.

i. Determination of viscosity average molecular weight of polystyrene (PS), polyninyl alcohol (PVA), polyethyleneglycol (PEG), Polyacrylamide (PA).

ii. Determination of (i) Dissolved Oxygen (DO), (ii) Chemical Oxygen Demand (COD) and (iii) Biochemical Oxygen Demand (BOD) in water samples.

iii. Analysis of a ground water sample for sulphate by titrimetry (EDTA) and turbidimetry.

iv. Determination of fluoride in drinking water/ground water by spectrophotometry (alizarin red lake method).

v. phosphate by molybdenum blue method Miscellaneous

vi. Spectrophotometric estimation of phosphate in cola drinks

vii. Analysis of fat in a butter sample

viii. Spectrophotometric estimation of hexavalent chromium in water samples.

ix. Determination of ascorbic acid in vitamin C tablets.

x. Verification of Beer's Lambert's law

xi. Determination of partial molar volume of solute (e.g.,KCL) and solvent in a binary mixture.

xii. Determination of the temperature dependence of the solubility of a compound in two solvents having similar intermolecular interactions (benzoic acid in water and in DMSO-water mixture) and calculate the partial molar heat of solution.

xiii. Determination of pKa of an indicator (e.g., methyl red) in (a) aqueous and (b) micellar media.

xiv. Determination of stoichiometry and stability constant of inorganic (e.g. ferric – salicyclic acid) and organic (e.g. amine-iodine) complexes.

xv. Estimation of Pb2+ and Cd2+ / Zn+ and Ni2+ ions in a mixture of Pb2+ and Cd2+ / Zn+ and Ni2+ by polarography.

xvi. Determination of dissolved oxygen in aqueous solution of organic solvents.

xvii. Determination of rate constant for hydrolysis / inversion of sugar using a polarimeter

xviii. Determination of stoichiometry and stability constant of inorganic (e.g. ferric-salicylic acid) and organic (amine-iodine) complex. .

Books and References:

1. Vogel's Text Book of Quantitative Chemical Analysis By J.Mendham, R.C.Denney, J.D.Barnes, M.J.K. Thomas, Pearson Education Publishers, 6thy Edition.

2. Hand book of Environmental analysis by Pradyot Patnaik, Lewis Publishers, USA (1997).

3. Standard Methods for the Examination of Water and Wastewater, APHA, AWWA, WPCF, Washington, DC, USA, 17th Edition.

DISSERTATION

Course Code: DC-405 **End Sem-100 marks** **Time-3 hour**
Credits: 05

The dissertation shall comprise of conducting a small project under faculty members of the department. The title and execution of the project work shall be decided in consultation with the faculty members of the dept by a committee constituting HOD and other senior faculty members. The committee may also extend the provision of co-opting the external guide as per the provision provided by the M.P.C. Autonomous College, Baripada. In general, the student is expected to do literature survey in the assigned topic, and to do some kind of experimental investigation, and result analysis. However, final decision regarding the execution of project work rests with the supervisor/co-supervisor and the committee on mutual discussion to the best benefit of the student for academic career. The guideline provided by UGC shall be also taken into account in this regard.