

M.Sc. Chemistry

Syllabus

(With effect from the year 2018-2019)



Department of Chemistry
Sri Chandrasekharendra Saraswathi Viswa Mahavidyalaya
(University established under sec 3 of UGC Act 1956)
(Accredited with "A" by NAAC)
Enathur, Kanchipuram – 631 561.Tamilnadu,

M. Sc [Chemistry] – Curriculum & Syllabus
(With effect from 2018-2019)

SEMESTER-I							
Subject Code	Core/ Elective	Title of the Paper	Credits/ Hrs. per week	Duration of Semester Exam	Marks		Total Marks
					IA	EA	
MCHF181T10	Core	Crystalline State and Inorganic Clusters	4	3	40	60	100
MCHF181T20	Core	Principles of Organic Chemistry	4	3	40	60	100
MCHF181T30	Core	Chemical Kinetics and Group Theory	4	3	40	60	100
MCHF181T40	Core	Analytical Chemistry	4	3	40	60	100
MCHF181P50	Core lab	Inorganic Chemistry Laboratory	(6*)	To be continued in semester II			
MCHF181P60	Core lab	Organic Chemistry Laboratory	(6*)	To be continued in semester II			
MCHF181P70	Core lab	Physical Chemistry Laboratory	(6*)	To be continued in semester II			
Distribution of working hours / Week			Theory 16 Hours/credits		Seminar 2 Hours		
SEMESTER –II							
MCHF182T10	Core	Coordination Chemistry	4	3	40	60	100
MCHF182T20	Core	Organic Transformations	4	3	40	60	100
MCHF182T30	Core	Thermodynamics and Quantum Chemistry	4	3	40	60	100
MCHF182T40	Core	Advanced Analytical Methods	4	3	40	60	100
MCHF182P50	Core lab	Inorganic Chemistry Laboratory	6	6	40	60	100
MCHF182P60	Core lab	Organic Chemistry Laboratory	6	6	40	60	100
MCHF182P70	Core lab	Physical Chemistry Laboratory	6	6	40	60	100
Distribution of working hours / Week			Theory 16 Hours/credits	Practical 18 Hours/credits			
SEMESTER-III (Any one elective paper has to be chosen)							
MCHF183T10	Core	Physical Methods in Inorganic Chemistry	4	3	40	60	100
MCHF183T20	Core	Organic Spectroscopy	4	3	40	60	100
MCHF183T30	Core	Electrochemistry and Spectroscopy	4	3	40	60	100
MCHF183T40	Core	Organic Reagents & Reactions	4	3	40	60	100
MCHF183E50	Core Elective- 1 (Any 1 out of 3)	Green Chemistry	4	3	40	60	100
MCHF183E60		Polymer chemistry					
MCHF183E70		Nanomaterials					
MCHF183P80	Core lab	Analytical Chemistry Laboratory	6	6	40	60	100
			Theory 20 Hours/credits	Practical 6 Hours/credits			
SEMESTER-IV (Any Two elective papers have to be chosen)							
MCHF184T20	Core	Soft Skills and Scientific Writing	4	3	40	60	100
MCHF184T10	Core	Surface Chemistry and Photo Chemistry	4	3	40	60	100
MCHF184E40	Elective-2 and 3 (Any 2 out of 4)	Synthetic Organic Chemistry	4	3	40	60	100
MCHF184E30		Nuclear and Bioinorganic Chemistry					
MCHF184E50		Supramolecular Chemistry					
MCHF184E60		Crystal Growth					
MCHF184V60	Core viva	Comprehensive Viva	2	-	-	100	100
MCHF184Z70	Core project	Project Work and Viva-Voce	8	-	-	100	100
Distribution of working hours / Week			Theory 16 Hours/credits	Viva and project & viva-voce 8 credits			
				TOTAL CREDITS		100	
(*) total credits for one year				TOTAL MARKS		2300	

Semester	Sub. Code	Title of the Paper	L	P	T	Credits
I	MCHF181T10	Crystalline State and Inorganic Clusters	4	0	0	4

Aim: To make the student to appreciate the effect of symmetry on properties of crystals, utility of XRD in structure determination.

Objective:

- Understanding on properties of solids on the basis of the internal structure of the crystals.
- Understanding on various types of inorganic clusters.

Outcome:

- Successful completion of the course the students should have knowledge about the X-ray crystallography.

Unit-I Crystal structure

(15 hrs)

Types of solids – crystalline state – order – unit cell- lattice – types – lattice planes- Miller indices. Crystal geometry – symmetry – symmetry elements –space groups – types of crystals- Reciprocal lattice – construction – properties – reciprocal lattices of SC, BCC and FCC lattices - Ewald's sphere -X-ray Diffraction – Bragg's law – methods of diffraction – single crystal – powder crystal and rotating crystal methods -Crystal structure determination – scattering factor – structure factor –phase problem –space group determination.

Unit-II Structure of Ionic Solids

(15 hrs)

Properties of ionic solids – lattice energy – Born-Haber cycle -Packing of atoms – AB and ABC structures – radius ratio rules - Structure of simple ionic solids - AX type NaCl, CsCl, ZnS – AX₂ type CaF₂, TiO₂ – layered structures NiAs, CdI₂ and MoS₂ .Structures of spinels and Perovskite.

Unit-III Defects and electronic structure of solids

(15 hrs)

Crystal defects – types - point, line and plane defects – Schottky and Frenkel defects – colour centers thermodynamics of defect formation – non stoichiometric crystals – consequences of defects. Band theory – refinement of simple band theory – k-space – conductors, insulators and semiconductors on the basis of band theory. Superconductivity – photoconductivity – dielectric properties – pyroelectricity and piezoelectricity (Basic concepts only)

Unit-IV Properties and applications of solids

(15 hrs)

Magnetic materials - metals and alloys – metal oxides –garnets – ilmenites – magneto plumbites – applications – transformer cores – information storage – memory devices – permanent magnets. Solid state electrolytes – types - examples – applications – electrochemical cells – batteries- sensors and fuel cells. Crystallization – growth of single crystals – Czochralski – Bridgman and Stockbarger – zone melting - melt :flux methods

Unit-V Inorganic Rings chains and Clusters**(15 hrs)**

Silicates – chain silicates - 2D and 3D silicates – Beryls – Muscovite – aluminosilicates – zeolites (structures only)-Carboranes – types- nomenclature – metalloboranes (Structures only)- classification-Metal clusters – Re_2C_{18} type clusters – structure – qualitative MO diagram – quadruple bond

Text Books

- I. Chakraborty.D.K, *Solid state chemistry*, New Age India limited, 2005.
- II. Velmurugan.D, *Elementary crystallography*, MJP Publishers, 2010.
- III. West Anthony R. *Solid State Chemistry and Its Applications*. Wiley, 2014
- IV. Shriver and Atkins , *Inorganic Chemistry*, Oxford University Press,2014

Reference Books

1. James Huheey, Ellen A.Keiter and Richard L.Keiter , *Inorganic Chemistry Principles of Structure and Reactivity*, Pearson Education Asia, 2001.
2. J.D. Lee, *Concise Inorganic Chemistry*Wiley India Ltd., Sixth edition, 2008
3. Gurdeep Raj, *Advanced Inorganic Chemistry*, Eleventh edition, Vol. II, Goel Publishing House, 2008.

Semester	Sub. Code	Title of the Paper	L	P	T	Credits
I	MCHF181T20	Principles of Organic Chemistry	4	0	0	4

Aim: To learn about Reaction intermediates and stereochemistry of compounds.

Objectives:

- To learn the Nucleophilic Substitution and Electrophilic Substitution Reactions
- To understand the different types of organic reactions.

Outcome:

- Understanding on organic reaction kinetics and stereochemistry of reactions.
- Understanding on various types of organic reaction and reaction intermediates.

Unit-I Reaction intermediates

(15 hrs)

Nomenclature of aromatic and heteroaromatic compounds: Heterocyclics with not more than two heteroatoms (oxygen/sulfur/nitrogen)

Stability, generation and applications of carbocations, carbanions, free radicals, carbenes, nitrenes, benzyne, ylides, enamines.

Unit-II Reactions: mechanisms and their determinations

(15 hrs)

Principle of Equilibria and free energy, free energy change in relation to bond strengths, activation energy, measurement of activation energy, reaction profile diagrams, rate determining step, thermodynamic and kinetic control, applications of kinetic principles (Hammond postulate, effect of solvent on reaction rate), Curtin-Hammett principle, Hammett equation, Swain-Scott equation, Grunwald-Winstein equation, microscopic reversibility, methods of determining mechanisms.

Unit-III Stereochemistry I

(15 hrs)

Stereoisomerism: Introduction, molecular representation, classification of isomers based on: symmetry criterion, energy criterion, stereoisomerism, conformation and chirality. Nomenclature: Fischer's D and L and R and S. E and Z nomenclature, Stereochemistry of allenes, Biphenyl derivatives and atropisomerism, Stereoselective and stereospecific reactions, Homotopic, enantiotopic and diastereotopic ligands (definitions only)

Unit-IV Stereochemistry II

(15 hrs)

Stereochemistry of cyclic and acyclic systems, conformations of ethane, 1,2-disubstituted ethanes, effect of conformation on reactivity (E_2 elimination, Curtin-Hammett principle, Wagner-Meerwein rearrangement. Conformations of cyclopentane, cyclohexane, methyl cyclohexane, 1,2-1,3- and 1,4-dimethyl cyclohexanes. Molecular dissymmetry and chirotopic properties, circular birefringence, and circular dichroism, Cotton effect, applications of ORD and CD, Axial halo ketone rule, Octant rule conformational effects on reactivity (Ester hydrolysis with a base, Cyclohexanol oxidation with chromium trioxide and water, Intramolecular closure of halohydrin to form epoxide), NGP, Determination of 2-amino cyclohexanol

Unit-V Nucleophilic Substitution Reactions**(15 hrs)**

Aliphatic nucleophilic substitution reactions- Introduction, S_N^2 mechanism, S_N^1 mechanism, (effects of substrate, attacking nucleophile, leaving group and solvent), S_N^1 vs S_N^2 reactions, neighboring group participation and non-classical carbocations. Aromatic nucleophilic substitution reactions – S_NAr general mechanism, Aryl cation mechanism, benzyne mechanism.

Text books:

- I. D. Nasipuri, *Stereochemistry Organic Compounds, Principles and applications, Second edition, New Age International (P) Ltd., 1994, Reprint 2008.*
- II. P.S. Kalsi, *Stereochemistry Conformation and Mechanism, Seventh edition, , New Age International Publishers, 2008.*
- III. P.S. Kalsi, *Organic Reactions and their mechanisms, Third edition, New Age International Publishers, 2010.*

Reference Books:

1. Jerry March, *Advanced Organic Chemistry, Reactions, Mechanisms and structures, Wiley Students edition, 2006.*
2. F.A. Carey and R.I. Sundberg, *Advanced Organic Chemistry, Part A & B, 5th Ed., Springer, 2009.*
3. V.K. Ahluwalia, R.K. Parashar, *Organic Reaction Mechanisms, Third edition, Narosa Publishing House, 2009.*
4. Peter Sykes, *A guide book of mechanism in organic chemistry, Pearson, 6th Ed., 2006.*
5. Ernest.L.Eliel, Samuel H.Wilen, L.N.Mander, *Stereo chemistry of Organic compounds, John Wiley & Sons., New York, 2003.*

Semester	Sub. Code	Title of the Paper	L	P	T	Credits
I	MCHF181T30	Chemical Kinetics and Group Theory	4	0	0	4

Aim: To study about Chemical Kinetics and Group Theory

Objectives:

- To understand the concepts and applications of reaction kinetics.
- To understand the symmetry of molecules and its applications.

Outcome:

- Students will get an idea about the applications of Group Theory to various Molecules.

Unit-I Theories of reaction rates

(15 hrs)

Effect of temperature on reaction rates, Arrhenius equation for simple reactions, Energy of activation, Potential energy surfaces, an introduction, Collision theory, factors affecting effective collision, Weakness of collision theory, reaction cross section, comparison with Arrhenius equation, Transition state theory, thermodynamic treatment, Unimolecular reactions, Lindemann's mechanism, Rice Ramsperger Kassel (RRK) model.

Unit-II Complex reactions

(15 hrs)

Kinetics of reversible reactions, consecutive and parallel reactions, Kinetics of chain reactions, H_2 & Br_2 , H_2 & O_2 , decomposition of CH_3CHO & N_2O_5 , Study of fast reactions, flow technique, stopped flow technique, temperature and pressure jump methods, shock tubes.

Unit III Reactions in solutions

(15 hrs)

Solvent effects, factors affecting reactions rates, ARRT as applied to solution phase, effect of internal pressure, reactions between ions, single sphere and double sphere mechanisms, influence of ionic strength, pressure and dielectric constant, volume of activation, diffusion controlled reactions: an introduction, Linear free energy relations, Hammett equation.

Unit-IV Group theory – fundamentals

(15 hrs)

Theory of groups, classes, sub groups, similarity transformations, point group classification, isomorphism, Matrix representation of symmetry operations, reducible and irreducible representations, decomposition of irreducible representation in to reducible representation, properties of irreducible representation, notations and theorems related to irreducible representations, Projection operator, theorems of representation, construction of character tables for C_{2v} and C_{3v} point groups, direct product representation.

Unit-V Group theory – applications

(15 hrs)

Applications of group theory to molecular vibrations (H_2O & ethylene), group theoretical treatment of hybridization (methane & boron trifluoride), SALC procedure for butadiene. Electronic spectrum of formaldehyde, Selection rules for IR and Raman spectrum, Woodward and Hoffmann rules.

Text Books

- I. *J. Rajaram, J. C. Kuriacose, Kinetics and Mechanisms of Chemical Transformations, First edition, Macmillan, 1993, reprint 2011.*
- II. *Peter Atkins, Julio de Paula, Physical Chemistry, Eighth edition, Oxford press, 2006.*
- III. *P.C. Jain and Monika Jain, Engineering Chemistry, 15th edition Dhanpat Rai Publishing Co., 2008.*
- IV. *F.A. Cotton, Chemical Applications of Group Theory, Third edition, John Wiley & Sons, 1990, reprint 2006.*
- V. *M.S.Gopinathan and V. Ramakrishnan, Group theory in Chemistry, Second edition, Vishal Publications, 1991, reprint 2001.*

Reference Books

1. *Donald A. Mcquarrie, John D. Simon, Physical Chemistry, First edition, Viva Books, 1998.*
2. *K. Veera Reddy, Symmetry and Spectroscopy of Molecules, Second edition, New Age International, 2009.*
3. *Keith.J. Laidler, Chemical Kinetics, Third Edition, Pearson Education, 2004.*

Semester	Sub. Code	Title of the Paper	L	P	T	Credits
I	MCHF181T40	Analytical Chemistry	4	0	0	4

Aim: To Understand the basic concepts of analytical techniques

Objective:

- To impart the knowledge of various analytical chemistry methods.

Outcome:

- The students will acquire knowledge of,
- Data handling and statistical treatment of data
- Principles of wet analytical methods, thermal analytical methods, optical methods, chromatographic techniques and electro analytical techniques and its applications

Unit-I Errors & Laboratory Procedures

(15 hrs)

Significant figures, rules for determination, definition and classification of errors, accuracy and precision, methods of expressing accuracy (absolute error, relative error), comparison between accuracy and precision, methods of expressing precision (mean, median, range, standard deviation, variance), test of significance (F-test, chi square test, Q-test). Classification of chemicals, rules for handling reagents and solutions, measurement of mass (Electronic analytical balance only)

Unit-II Wet Analysis

(15 hrs)

Volumetric analysis – acid base, redox & complexometric titrations- theory and experiment. Gravimetric analysis - precipitation methods- homogeneous precipitation-filtration, washing, drying, weighing-Colorimetric analysis – photoelectric colorimeter – single beam and double beam schematic diagrams, applications.

Unit-III Thermal and Spectral Methods

(15 hrs)

Thermal Analysis: TGA, DTA, DSC - principles, instrumentation and applications. Spectral Methods: UV-Visible spectroscopy- Beer Lamberts Law, Description of UV-Vis spectrophotometer Applications of UV- Visible spectroscopy -Infrared spectroscopy – instrumentation, single beam and double beam spectrometers, sample handling, FTIR spectrometer

Unit-IV Chromatographic Techniques

(15 hrs)

Paper Chromatography – theory, techniques and applications. Column Chromatography – principles, experimental requirements, identification of compounds and applications. Thin layer Chromatography – theory, techniques and applications. Gas Chromatography – principle, theory, instrumentation, identification of chromatogram. High Performance Liquid Chromatography – instrumentation and applications.

Unit-V Electroanalytical Methods**(15 hrs)**

Conductometric titrations – principle, practice and applications-Amperometric titrations – principle, instrumentation and applications-Potentiometry – instrumentation, electrodes, potentiometric titrations-pHmetry -Glass electrode and Ion selective electrodes-Electrogravimetry – theory, electrolysis at constant current and constant voltage-principle, experimental set up and applications-Coulometry – coulomb calculation, silver coulometer, constant current Coulometry.

Text Books

- I. *Dhruba Charan Dash, Analytical Chemistry, PHI Learning Private Ltd., 2011.*
- II. *H. Kaur, Instrumental Methods of Chemical Analysis, Sixth edition, Pragati Prakashan, 2010.*
- III. *Douglas A. Skoog, Donald M. West, F. James Holler, Analytical Chemistry An Introduction, Sixth Edition, Saunders College Publishing, 1994.*

Reference Books

1. *Douglas A. Skoog, F. James Holler, Stanley R. Crouch, Instrumental Analysis, Brooks/Cole Cengage Learning (I) Pvt. Ltd., First Indian Reprint 2008.*
2. *Gurdeep R. Chatwal, Sham K. Anand, Instrumental Methods of Chemical Analysis, Fifth edition, Himalaya Publishing Company, 2007.*
3. *H.H. Willard, L.L. Merritt Jr., J.A. Dean, F.A. Settle, Instrumental Methods of Analysis, Seventh edition, CBS Publishers & Distributors, 1986.*

Semester	Sub. Code	Title of the Paper	L	P	T	Credits
II	MCHF182T10	Coordination Chemistry	4	0	0	4

Aim: *To understand the basic principles of coordination chemistry*

Objectives:

- *Learning about the various theories of complex formation.*
- *Studying and interpreting the magnetic properties of complexes.*

Outcome:

- *Students will get an idea about basics of metal complex formation and explain the properties of complexes on the basis of CFT and MOT.*

Unit-I Theories of metal complexes

(15 hrs)

Co-ordination compounds – detection of formation – isomerism in complexes-Historical background of theories of metal complexes – Werner’s –Sidgwick and valence bond theories Crystal field theory(CFT) – assumptions – splitting of d orbitals in different fields – CFSE calculations – evidences for splitting factors affecting splitting –spectrochemical series – Jahn-teller distortion – limitations of CFT Ligand Filed Theory (LFT) – sigma and pi bonding in complexes – evidences for pi bonding – MO diagrams for Oh and Td complexes – effects of pi donors and pi acceptors on splitting – nephelauxetic effect and series.

Unit-II Stability and reactions of complexes

(15 hrs)

Stability of complexes kinetic and thermodynamic stabilities- formation constants – stepwise and overall formation constants- factors affecting stability of the complexes -Kinetics and mechanisms of ligand substitution reactions in Oh complexes- acid hydrolysis – base hydrolysis - factors affecting the rate of reactions- anation reactions Substitution in SP complexes – trans effect- theories of trans effect –applications Redox reactions of complexes – inner sphere and outer sphere mechanisms- Marcus theory.

Unit-III Magnetic properties of metal complexes

(15 hrs)

Basic definitions in magneto chemistry – thermal energy and magnetic properties- magnetism on the basis of crystal field model .Zeeman effect – second order Zeeman effect on Sm(III) Spin pairing – applications Anomalous magnetic moments – reasons -Co-operative magnetism – antiferro magnetism – direct M- M interaction – super exchange – examples – Ferro magnetism (Concept only)

Unit-IV Organometallics

(15 hrs)

Types of organometallics – 18 e- rule –alkene complexes – Zeise’s salt – Hapticity Metal allyl complexes – metal acetylene complexes -Metal sandwich complexes – Ferrocene – preparation structure and reactivity-Reactions of organometallics – oxidative addition reductive elimination – industrial applications of organometallics – Wilkinson’s catalysts- Reppe’s process- Oxo process-Wacker’s process and Ziegler-Natta catalysts.

Unit-V Metal Carbonyls and Nitrosyls**(15 hrs)**

Metal carbonyls – classification – description of M-CO bond- terminal and bridging CO groups – carbonyls of V, Mn, Fe and Co. Metal carbonyl hydrides and metal carbonyl halides-Metal nitrosyls - liner and bent nitrosyls- preparation and properties - nitrosyls of iron.

Text Books

- I. James Huheey, Ellen A. Keiter and Richard L. Keiter, *Inorganic Chemistry Principles of Structure and Reactivity*, Fourth edition, Pearson Education Asia, 2001.
- II. Shriver and Atkins, *Inorganic Chemistry*, Third edition, Plenum Press, .
- III. Wahid U. Malik, G.D. Tuli and R.D. Madan, *Selected Topics in Inorganic Chemistry*, First Edition, S. Chand and Company Ltd., 1976 (Reprint 1998).
- IV. R. Gopalan and V. Ramalingam, *Concise Coordination Chemistry*, First edition, Vikas Publishing House Private Ltd., 2001 (Third reprint 2007).

Reference Books

1. F. Albert Cotton, *Advanced Inorganic Chemistry*, Sixth edition, Geoffrey Wilkinson, Carlos A. Murilo and Manfred Bochmann, Wiley India, 2004 (Reprint 2008).
2. Gurdeep Raj, *Advanced Inorganic Chemistry*, Eleventh edition, Vol. II, Goel Publishing House, 2008,
3. Agarwal and Keemti Lal, *Advanced Inorganic Chemistry*, Eleventh edition, Pragati Prakashan, 2012.
4. J.D. Lee, *Concise Inorganic Chemistry*, Sixth edition, Wiley India Ltd., 2008.

Semester	Sub. Code	Title of the Paper	L	P	T	Credits
II	MCHF182T20	Organic Transformations	4	0	0	4

Aim: To understand the mechanism of organic reactions

Objectives:

- To understand the mechanism of molecular rearrangements
- To acquire knowledge in natural products

Outcome:

- Students will acquire knowledge in mechanism of various organic reactions
- Learn about the preparation and uses of natural products

Unit-I Electrophilic Substitution Reactions (15 hrs)

Arenium ion mechanism -S_E² reaction (nitration, sulphonation, halogenation, Friedel-Crafts alkylation, acylation), Vilsmeier-Hack formylation, substitution on monosubstituted benzenes – orientation and reactivity – activation and deactivation (inductive effect, mesomeric effect), examples of ortho & para directing groups, meta directing groups, activating and deactivating substituent's and their synthetic applications.

Unit-II Addition and elimination reactions (15 hrs)

Addition to double bonds: Addition of Halogens & Hydrogen Halides, Electrophilic addition to alkynes, Nucleophilic addition to alkenes and alkynes, Nucleophilic addition to carbonyl compounds-Hydride reduction-hemiacetals and acetals. E₂ mechanism, direction of elimination in E₂, rate of E₂ reactions, stereochemistry of E₂ elimination, E₂ elimination from acyclic systems & cyclohexane systems, E₁ mechanism, direction of elimination, E₁ elimination from cyclic compounds, Curtin-Hammett principle.

Unit-III Molecular rearrangements (15 hrs)

Pinacol-pinacolone, Wagner-meerwein, wolff, benzyl-benzilic acid, Beckmann, Hofmann, Curtius, Lossen, Schmidt, Baeyer-Villiger, Hydroperoxide, Dakin, Favorskii, Stevens, Sommelet-Hauser, Wittig, Neber, Fries, Claisen, dienone-phenol rearrangements and their mechanisms.

Unit-IV Organometallic compounds (15 hrs)

Grignard reagents, organolithium, organocopper- Gilman's reagent, Gignard –copper- I reagent-reactions of organo cuprates, epoxide cleavage, conjugate addition, Tandem-1,4-addition, organozinc-alkyl zinc iodides-di alkyl zinc-reformatsky reaction-cyclopropanation-Dibal-H reduction, Julia olefinations, Petersons olefination.

Unit-V Alkaloids (15 hrs)

Occurrence-functions-nomenclature-classification-isolation-general structure determination-synthesis and structural elucidation of quinine, papaverine, morphine.

Text Books

- I. P.S. Kalsi, *Organic Reactions and Their Mechanisms, Third edition, New Age International Publishers, 2010.*
- II. V.K. Ahluwalia, R.K. Parashar, *Organic Reaction Mechanisms, Third edition, Narosa Publishing House, 2009.*
- III. W.Caruthers, Iain Coldhan, *Modern Methods of Organic Synthesis, Cambrodge university press,2015.*
- IV. I.L.Finar, *Organic Chemistry Vol-II, Pearson Education, 2002.*

Reference Book

1. Jerry March, *Advanced Organic Chemistry: Reactions, Mechanisms and Structure, Wiley Student Edition, 2006.*
2. ROC.Norman and J.M coxon, *Principles of organic synthesis Modern synthesis,CRC press,1993*
3. Francis. A Carey and Richard. J Sundberg, *Advanced Organic Chemistry:Part-B:Reaction and synthesis,Springer,2008*

Semester	Sub. Code	Title of the Paper	L	P	T	Credits
II	MCHF182T30	Thermodynamics and Quantum Chemistry	4	0	0	4

Aim: To understand the basics of Thermodynamics and quantum mechanics

Objectives:

- To understand the fundamentals and applications of statistical thermodynamics.
- To study the basics and applications of chemical thermodynamics.
- To study the fundamentals and applications of quantum chemistry.

Out Come:

- Students will get Knowledge about Various types of Quantum Statistics.

Unit-I Thermodynamics of open systems (15 hrs)

Partial molar properties, chemical potential, partial molar volume, partial molar heat content, variation of chemical potential with temp. and pressure, fugacity, determination of fugacity, variation with temp., and pressure. Thermodynamics of ideal and non-ideal solutions. Excess functions for non-ideal solutions. Concepts of activity and activity coefficients, detn. of activity and standard free energy, choice of standard states.

Unit-II Third law of thermodynamics & classical statistics (15 hrs)

Nernst heat theorem, need for third law, third law of TD's, experimental verification of third law, entropies of real gases, entropy changes in chemical reactions, Boltzmann entropy equation, residual entropy, statistical meaning of third law. Introduction to statistical thermodynamics, terminologies, Liouville's theorem, statistical equilibrium, thermodynamic probability, Boltzmann statistics, partition function, translational, rotational, vibrational and electronic partition function, partition functions and thermodynamic functions (internal energy, heat capacity, entropy, work function), partition function for monatomic and diatomic molecules, limitations of Boltzmann's statistics.

Unit-III Quantum statistics (15 hrs)

Bose-Einstein statistics, Bose-Einstein condensation, Fermi-Dirac statistics, Fermi energy, Fermi energy of electron gas in a metal, thermionic emission, comparison between MB, FD & BE statistics.

Unit-IV Basics of quantum mechanics (15 hrs)

Inadequacy of classical mechanics, black body radiation, photoelectric effect, Bohr's quantum theory, Davisson & Germer experiment, wave particle duality, Compton effect, De-broglie's equation, Uncertainty principle, theory of wave motion, Schrodinger's equation for particle waves, wave function and its physical meaning, Postulates of quantum mechanics, operator algebra, Eigen values, Eigen functions, particle in a box (1-D and 3-D), quantum numbers, zero point energy. Self Study (not for exams): Harmonic oscillators and rigid rotors.

Unit-V Applications of quantum mechanics**(15 hrs)**

Approximation methods, perturbation and variation methods, application to hydrogen and helium atom, R-S coupling and term symbols for atoms in the ground state, HFSCF theory, Slater determinant, Born-Oppenheimer approximation, hydrogen molecule ion, hydrogen molecule, Concept of hybridization, Huckel's theory (ethylene, 1,3-butadiene and benzene).

Text Books

- I. *B.R. Puri, L.R. Sharma & Madan S. Pathania, Principles of Physical Chemistry, 42nd edition, Vishal Publishing Company, 2008.*
- II. *R.P. Rasthogi & R.R. Misra, An Introduction to Chemical Thermodynamics, Sixth edition, Vikas Publishing House, 2008.*
- III. *S.K. Sinha, Introduction to Statistical Mechanics, First edition, Narosa Publishing House, 2005.*
- IV. *R. K. Prasad, Quantum Chemistry, Third edition, , New Age International, 2007.*
- V. *Gurdeep Raj, Advanced Physical Chemistry, 22nd edition, Goel Publications, 1998.*

Reference Books

1. *Donald A. Mcquarrie, John D. Simon, Physical Chemistry, First edition, Viva Books, 1998.*
2. *Peter Atkins, Julio de Paula, Physical Chemistry, Eighth edition, Oxford press, 2006.*
3. *Moudgil, The text book of Physical Chemistry, Printice hall publication, 2010.*
4. *Donaua.Mcquarrie, Qunatum Chemistry, Second Edition, University Science books Publication, 2007.*

Semester	Sub. Code	Title of the Paper	L	P	T	Credits
II	MCHF182T40	Advanced Analytical Methods	4	0	0	4

Aim: To know about spectroscopy

Objective:

- To impart the knowledge of various advanced analytical techniques for chemical characterization.

Outcome:

- The students will acquire knowledge of principles, instrumentation and applications of separation techniques, AAS, inductively coupled plasma atomic emission spectroscopy, NMR, XRD, fluorescence spectroscopy, and mass spectrometry.

Unit-I Separation techniques

(15 hrs)

Capillary electrophoresis: Theory, instrumentation and applications. Ion Chromatography: Theory, instrumentation, and applications.

Unit-II AAS & ICP

(15 hrs)

Atomic Absorption Spectrometry: Introduction, basic principles, instrumentation, quantification of elements, applications. Inductively coupled Plasma Atomic Emission Spectroscopy: Introduction, physical and chemical principles, instrumentation, applications.

Unit-III NMR & XRD

(15 hrs)

NMR: Theory, instrumentation, and applications. X-ray diffraction: Introduction, theory, instrumentation and applications.

Unit-IV Fluorescence Spectroscopy & Microscopic Methods

(15 hrs)

Theory, instrumentation and applications of Fluorescence spectroscopy. Principle, instrumentation and applications of SEM and TEM techniques.

Unit-V Techniques of Mass Spectrometry

(15 hrs)

Different ionization techniques, and detectors in mass spectrometers, basic instrumentation of MS, and applications, GC-MS, LC-MS.

Text Books

- I. *Skoog, Holler, and Crouch, Instrumental Analysis, Brooks/Cole, 2007.*
- II. *Willard, Merrit, Dean, Settle, Instrumental Methods of Analysis, Seventh edition, CBS publishers and distributors, 1986.*
- III. *Skoog, West, Holler, Analytical Chemistry: An Introduction, Sixth edition, Saunders College Publishing, 1994.*
- IV. *Khopkar, S.M., Basic Concepts of Analytical Chemistry, New Age International (P) Limited, Publishers, (2008).*

Reference Book

1. *Frank Settle, Handbook of Instrumental Techniques for Analytical Chemistry, Pearson education, 1997.*
2. *Silverstein, Bassler, Morrill, Spectrometric identification of organic compounds, John Wiley & Sons, 1991.*

Semester	Sub. Code	Title of the Paper	L	P	T	Credits
II	MCHF182P50	Inorganic Chemistry Laboratory	0	6	0	6

- Separation and Analysis** of an “Inorganic mixture containing two common and two less common metal ions” including the following:
Common Ions: Pb, Cu, Bi, Cd, Al, Ni, Co, Mn, Zn, Ba, Ca, Sr and Mg; **Less common Ions:** W, Se, Te, Mo, Ce, Th, Zr, Ti, V, U, and Li
- Estimation of metals in a mixture (Volumetry and Gravimetry)**
 - Copper (V) - Nickel (G)
 - Copper (G) – Zinc (V)
 - Iron (V) – Nickel (G)
 - Iron (V) – Magnesium (G)
- Colorimetric Estimation** of Cu, Cr, Fe, Ni and Mn
- Preparation** of any five of the following complexes:
 - Tetraamminecopper(II) sulphate,
 - Potassium trioxalatochromate(III),
 - Hexaureachromium(III) chloride,
 - Sodium trioxalatoferate(III),
 - Tris(acetylacetonato)copper (II),
 - Tris(ethylenediamine)nickel (II) chloride

Reference Books

- V.V. Ramanujam, *Inorganic Semi-micro-Analysis*, 3rd edition, The National publishing company, 1997.
- Gurdeep Raj, *Pragathi Prakasan, Advanced Inorganic Practical*, Meerut.
- Vogel's *Text book of Quantitative Analysis*, Longman Group publishers, 5th edition, 1994.
- G.B. Kauffmann, *Inorganic Coordination Compounds*, Heyden and Son Ltd.
- Burger, *Synthesis of Inorganic Complexes*, 1973.

Scheme of Evaluation

S.No.	Particulars	Max. marks
1	Analysis of the mixture (Group separation-10, Analysis of each cation-10)	50
2	Preparation	30
3	Viva-voce	10
4	Record	10
Total		100

Semester	Sub. Code	Title of the Paper	L	P	T	Credits
II	MCHF182P50	Organic Chemistry Laboratory	0	6	0	6

1. Separation and Analysis of an organic binary mixture and derivatisation of the components.

2. Preparation of organic compounds (Any 8 from the following list): 1. Benzoic acid from benzaldehyde, 2. Salicylic acid from methyl salicylate, 3. o-chlorobenzoic acid from anthranilic acid, 4. Resacetophenone from resorcinol, 5. Para bromoacetanilide from acetanilide, 6. para-nitroacetanilide from acetanilide, 7. Dibenzalacetone from acetone, 8. Benzhydrol from benzophenone, 9. Phenylazo-2-naphthol from aniline, 10. Glucose penta acetate from glucose, 11. Piperidone from ethyl acetoacetate, 12. Naphthylmethyl ether from β -naphthol

Reference Books

1. Jag Mohan, *Organic, Analytical chemistry, theory and practice*. Narose publishing House, 2006.
2. Gnanaprakasam, Ramamurthy. *Organic chemistry lab manual*.

Scheme of Evaluation

S. No.	Particulars	Max. marks
1	Analysis of the mixture (each component -25)	50
2	Preparation	20
3	Pilot separation	10
4	Viva-voce	10
5	Record	10
Total		100

Semester	Sub. Code	Title of the Paper	L	P	T	Credits
II	MCHF182P70	Physical Chemistry Laboratory	0	6	0	6

Electrochemistry Experiments

Conductometry Experiments

1. Titration of : 1. Strong acid Vs strong base, 2. Weak acid Vs Strong base, 3. Weak acid Vs weak base
2. Titration of a strong base Vs mixture of acids.
3. Precipitation titration: 1. BaCl₂ Vs MgSO₄, 2. AgNO₃ Vs mixture of halides
4. Verification of Debye - Huckel – Onsager relation for a strong electrolyte
5. Dissociation constant of a weak electrolyte.
6. Solubility and solubility product of a sparingly soluble salt.

Potentiometry Experiments

1. Dissociation constant of a weak acid: titration method
2. Dissociation constant of a weak acid: Henderson method
3. Redox titration: KMnO₄ Vs Fe²⁺ / KMnO₄ Vs KI
4. Precipitation titration: AgNO₃ Vs mixture of halides
5. Standard reduction potential of Cu / Zn / Ag electrode
6. Formal redox potential of Fe²⁺ / Fe³⁺ or Ce³⁺ / Ce⁴⁺ system
7. Solubility product of a sparingly soluble salt by (i) Single electrode method (ii) Concentration cell method.

Non- Electrochemistry Experiments

1. Determination of partition coefficient of I₂ between water and CCl₄. Equilibrium constant for the formation of I³⁻ ion.
2. Construction of phase diagram for a pair of partially miscible liquids and the effect of added impurity.
3. Construction of phase diagram for a three partially miscible liquids.
4. Construction of phase diagram for a simple eutectic system.
5. Construction of phase diagram for a system with compound formation
6. Determination mol.wt of a non-volatile solute by Rast's method
7. Determination mol.wt of a non-volatile solute by transition temperature method
8. Study of adsorption of oxalic acid on charcoal. (Verification of Freundlich's isotherm)
9. Determination of integral heat of solution by solubility method.
10. Determination of heat hydration of anhydrous CuSO₄.
11. Determination of rate, order of the reaction between K₂S₂O₈ and KI (clock reaction method)
12. Verification of Bronsted – Bjerrum equation with reaction between K₂S₂O₈ and KI.
13. Determination of order of the reaction for base hydrolysis of an ester- Conductometric method
14. Kinetics of acid catalyzed iodination of acetone – spectrophotometric method.
15. Determination of Arrhenius parameters for acid catalyzed hydrolysis of ester.

Reference Books

1. A.Finlay and J.A.Kitchener, *Practical Physical Chemistry*, Longman, 1973.
2. F.Daniels and J.H.Mathews *Experimental Physical Chemistry*, , Longman, 1985.
3. A.M.James, J.A.Churchil,*Practical Physical Chemistry*, 1961.
4. H.H.Willard, L.L.Merritt and J.A.Dean,*Instrumental Methods of Analysis*, Affiliated East-West Press, 1965.
5. D.P.Shoemaker and C.W.Garland, *Experimental Physical Chemistry*, McGraw-Hill, 1974.

Scheme of Evaluation

S.No.	Particulars	Max.marks
1	Aim & Principle	5
2	Procedure, Formula, Model graph & Table	25
3	Reading & Calculation	30
4	Graph	10
5	Result	10
6	Record	10
7	Viva-voce	10
Total		100

Semester	Sub. Code	Title of the Paper	L	P	T	Credits
III	MCHF183T10	Physical Methods in Inorganic Chemistry	4	0	0	4

Aim: To study about utility of spectroscopic techniques in study of inorganic compounds.

Objectives:

- To understand the role of spectroscopic methods in inorganic chemistry.
- To acquire basic knowledge about the application of spectral methods in structural elucidation of inorganic compounds.

Outcome:

- Students will Understand the importance of various spectral methods in structural elucidation of inorganic compounds

Unit-I Infra red & Raman spectroscopy (15 hrs)

Infrared spectroscopy: Principle – molecular vibrations – types- vibrational energy of a molecule – Selection rules – dipole moments in the vibrating molecule –IR activity conditions - anharmonicity of vibrations –consequences – expressions for fundamentals –overtones and hot bands – coupling of rotations and vibrations. Normal mode analysis of C₂V group (H₂O , SO₂ and ClO₂) – ZXY₂ type molecule – square planar XY₄ complexes(AuCl₄). Raman spectroscopy: Raman effect – Raman, Rayleigh and fluorescent scatterings –polarized Raman lines- conditions for Raman activity. Structure of molecules from IR and Raman spectra – mutual exclusion principle – violation of the principles – dynamic modes of molecules – structure determination - identification of coordination – site symmetry lowering (SCN-, NO₃- SO₄²⁻ and Urea as ligands).

Unit-II Electronic spectra (15 hrs)

Free ion configurations –terms and states –spin orbit coupling –L-S coupling scheme –j-j coupling scheme – terms for p² and d² configurations – hole formalism – energy of terms – Hund’s rule – inter electronic repulsion parameters – spin –orbit coupling parameters.Effect of crystal fields on terms – S, P, D and F terms – Ligand field term diagrams – Orgel diagrams – expected electronic transitions – term interactions – Tanabe– Sugano diagrams – uses. Electronicspectra of metal complexes – selection rules – group theoretical treatment of selection rules – relaxation of selection rules – electronic spectra bands – band intensities and widths - Jahn-Tellereffect – spectrochemical series – nephelauxetic series – calculation of **Dq**, **B'** and **β** – graphical method – Konig’s numerical method – charge transfer spectra – spectra of lanthanides and actinides.

Unit-III NMR spectroscopy (15 hrs)

Nuclear magnetic resonance – chemical shift-reference compounds –interpreting chemical shift – spin –spin coupling. Aids in analyzing spectra-FTNMR-advantages- variable temperature NMR. Dynamic NMR spectra –. symmetrical two -site exchange – (slow/fast)-barrier to internal rotation-unsymmetrical site exchange – ring inversion – fluxional molecules –

fluorophosphoranes – organometallic compounds. NMR Spectra of other nuclei ^{13}C , ^{19}F and ^{31}P applications to simple molecules.

Unit-IV ESR spectroscopy**(15 hrs)**

Electron spin resonance- principle-ESR transition -selection rules-g-factor-presentation of spectra-relaxation processes-hyperfine splitting-dipolar interaction-isotropic hyperfine interaction-spin polarization-hyperfine splitting constants-anisotropy in A and g- factor – dynamic processes-electron transfer-proton exchange-fluxional molecules. ESR of systems with more than one unpaired electron Triplet state-spin transition in triplet state-effect of dipolar field – zero field splitting- Kramer’s degeneracy-ESR of transition metal complexes-factors affecting g-value-effect of John-Teller distortion-spectra of 3d series metal ions.

Unit-V Mossbauer, NQR & PES**(15 hrs)**

Mossbauer spectroscopy- Principle – Recoilless transition – Effect of Magnetic field – Quadrupole nuclei – simple application to Iron and Tin complexes. Nuclear Quadrupole Resonance Spectroscopy: Introduction-quadrupole moment – electrical field gradient-asymmetryparameter-effect of external magnetic field-applications. Photo Electron Spectroscopy: UVPES and XPES Koopmann’s theorem –ESCA - Auger effect- AES.

Text Books

- I. K.Veera Reddy, *Symmetry and spectroscopy of molecules*, Second revised edition, New Age International Publishers, 2009.
- II. Russell.S.Drago, *Physical Methods in Inorganic Chemistry*, First edition, Affiliated East-West Press Private Ltd., 1965.
- III. D.N.Sathyanarayana, *Introduction to Magnetic Resonance Spectroscopy ESR, NMR, NQR*, First edition, I. K. International Publishing House Pvt. Ltd., 2009.
- IV. C.N.Banwell & Elaine McCash, *Tata, Fundamentals of Molecular Spectroscopy*, Fourth edition, McGraw- Hill Publishing Co.Ltd., 1994.

Reference Book

1. D.N.Sathyanarayana, *Electronic Absorption Spectroscopy and Related Techniques*, First edition, Universities Press (India) Ltd., 2001.
2. E.A.V.Ebsworth, David, W.H.Rankin, *Structural Methods in Inorganic Chemistry*, ELBS edition, Stephen Cradock, Blackwell Scientific Publications, 1988.
3. D.N.Sathyanarayana, , *Vibrational Spectroscopy Theory and Applications*, Second edition, New Age International Publishers 2004 (Reprint 2007).

Semester	Sub. Code	Title of the Paper	L	P	T	Credits
III	MCHF183T20	Organic Spectroscopy	4	0	0	4

Aim:

- *To study the principles and applications of spectroscopic methods in structural elucidation of simple organic molecules*

Objective:

- *To impart the knowledge of structure elucidation of organic compounds using spectroscopic data.*

Outcome:

- *The students will acquire knowledge of using UV-Visible, IR, NMR and Mass spectral data for elucidating the structure of organic compounds.*

Unit-I UV-Vis spectroscopy**(15 hrs)**

Electronic transitions, red shift, blue shift – effects of solvents, calculation of λ_{max} for isolated double bonds, conjugated double bonds, polyenes, carbonyl compounds (Woodward-Fieser rules), aromatic systems. Spectral problems.

Unit-II Infra-Red spectroscopy**(15 hrs)**

Absorption of IR radiation, Molecular vibrations (Vibrational motion is quantized, dipole moment and IR spectra, fundamental vibrations, symmetry and IR spectra, Overtones and combination bands, coupled vibrations, Fermi resonance), calculation of vibrational frequencies, Interpretation of IR spectra of alkanes, alkenes, alkynes, aromatic rings, alcohols, phenols, ethers, carbonyl compounds, aldehydes, ketones, carboxylic acids, esters, amides, acid chlorides, amines, nitro compounds. Spectral problems.

Unit-III ^1H NMR & ^{13}C NMR spectroscopy**(15 hrs)**

Introduction-chemical shift-TMS scale-spectrum-shielding effect and spin-spin splitting-theory of PMR-internal standard-factors affecting chemical shift-equivalent and non-equivalent protons-theory of spin-spin splitting-magnitude of coupling constant- 2D NMR – ROESY- COSY - NOE-NOESY-DOSY. Spectral problems. Introduction-spectrum-operating frequency-off resonance decoupling-chemical shift equivalence-chemical shifts. Spectral problems.

Unit-IV Mass spectrometry**(15 hrs)**

Introduction-EI ionization method-base peak-molecular ion peak-instrumentation-fragmentation pattern of general and simple organic molecules and derivatives.

Unit-V Combined spectral problems**(15 hrs)**

Combined spectral problems.

Text Books

- I. *P.S. Kalsi, Spectroscopy of Organic Compounds, Fifth edition, New Age International Publishers, 2004.*
- II. *Pavia, Lampman, Kriz, Vyvyan, Spectroscopy, Brooks/Cole, 2007.*

Reference Book

1. *Silverstein, Bassler, Morrill, Spectrometric identification of organic compounds, John Wiley & Sons, 1991.*
2. *William Kemp, Organic Spectroscopy, Palgrave, 1991.*

Semester	Sub. Code	Title of the Paper	L	P	T	Credits
III	MCHF183T30	Electrochemistry and Spectroscopy	4	0	0	4

Aim: To understand the physical principles behind various spectral methods

Objectives:

- To study about the various theories of Electrolytic Conductance & Irreversible Electrode process.
- To study in detail Raman and electronic spectroscopies.
- To study in detail NMR and ESR spectroscopies.

Outcome:

- Students acquire Knowledge about Principles of Spectroscopy & about Irreversible electrode process

Unit-I Theory of Electrolytic Conductance

(15 hrs)

Degree of dissociation, ionic atmosphere, Debye-Huckel theory, mechanism of electrolytic conductance, DHO equation, validity of DHO eqn., deviations from DHO eqn., significance of degree of dissociation, determination of degree of dissociation, conductance ratio and DHO, Debye-Falkenhagen and Wien effects. Debye-Huckel limiting law, Debye-Huckel Bronsted equation, test for DH limiting eqn, extension of DH theory, triple ions (concept only).

Unit-II Electrified Interface

(15 hrs)

Thermodynamics of electrified interface, Lippmann equation, electro-capillary curves, surface excess, determination of surface excess, structure of electrical double layer, Helmholtz-Perrin model, Gouy-Chapman model, Stern model. Electro-kinetic Phenomena, Zeta potential, electro-osmosis, streaming potential, electrophoresis, determination of zeta potential, effect of ions on electro-kinetic phenomena.

Unit-III Irreversible electrode processes & Electrode processes

(15 hrs)

Theories of overvoltage and its determination, factors affecting overvoltage, exchange current density, polarization. Irreversible electrode processes, polarography, theory and experimental set up, Ilkovic equation derivation, Halfwave potential, applications of polarography, amperometric titrations, kinetics of electrode reactions, Butler-Volmer equation derivation, Tafel equation, transfer coefficient (concept only).

Unit-IV Physical principles of spectroscopy, IR & Raman spectra

(15 hrs)

EM radiation, quantization of energy, regions of spectrum, interaction of radiation with matter, representation of spectra, spectrometers, signal to noise ratio, resolving power, parameters for a spectral line (position, intensity, width), factors affecting them, FT spectroscopy, computer averaging. Infra red spectroscopy, the vibrating diatomic molecule, simple harmonic oscillator model, the anharmonic oscillator, diatomic vibrating rotator, break down of Born-Oppenheimer

approximation, vibrations of polyatomic molecules, overtones and combination frequencies, influence of rotation on the spectra of polyatomics, parallel and perpendicular vibrations, skeletal vibrations and group frequencies. Raman effect, classical and quantum theories, rotational raman spectra, symmetric tops and asymmetric tops, vibrational raman spectra, role of mutual exclusion, polarization of light and raman effect, combined use of raman and IR.

Unit-V Electronic and Spin Resonance Spectroscopies (15 hrs)

Electronic spectroscopy of molecules, Born-Oppenheimer approximation, vibrational coarse structure, progressions and sequences, Frank-Condon principle, dissociation energy, rotational fine structure, Fortrat diagram, pre-dissociation. NMR Spectroscopy: Interaction of spin and applied field, population of energy levels, Larmor precession, relaxation, FTNMR, multiple pulse FTNMR, NMR spectrum of hydrogen nuclei, chemical shift, coupling constant, Quadrupole effect. ESR Spectroscopy: Position of ESR absorption, hyperfine structure, fine structure of ESR spectrum, zero field splitting, calculation of electron density.

Text Books

- I. Samuel Glasstone, *An Introduction to Electrochemistry*, First edition, Affiliated East West Press Private Ltd., 1942, reprint 1999.
- II. J. N. Gurtu & A. Gurtu, *Pragati Prakashan, Advanced Physical Chemistry*, Eighth revised edition, 2006.
- III. B.R. Puri, L.R. Sharma & Madan S. Pathania, *Principles of Physical Chemistry*, 37th edition, Shoban Lal Nagin Chand and Co., 1998.
- IV. C. N. Banwell & Elaine McCash, *Fundamentals of Molecular Spectroscopy*, Fourth edition, Tata McGraw-Hill Publishing Co. Ltd., 1994, reprint 2001.

Reference Books

1. Skoog, Holler, and Crouch, *Instrumental Analysis*, Brooks/Cole, 2007.
2. H. Kaur, *Pragati Prakashan, Instrumental Methods of Chemical Analysis*, Sixth edition, 2010.
3. John.O.M Bockris and Amulya K.N Reddy, *Modern Electrochemistry, Vol 1&2*, Springer publications, 2008.
4. O.D. Tyagi & M. Yadav, *A Text book of Spectroscopy*, Anmol publications, 2002.

Semester	Sub. Code	Title of the Paper	L	P	T	Credits
III	MCHF183T40	Organic Reagents & Reactions	4	0	0	4

Aim: To enable the students to learn the principles of Photo chemical reactions and reagents used for various reactions

Objective:

- To impart the knowledge of Oxidation-reduction reactions are widely used to produce chemicals that are used in manufacturing

Outcome:

- Students get knowledge about organic compounds through the name reactions, oxidation and reduction reactions.
- To get an idea about terpenoids.

Unit-I Oxidation reactions

(15 hrs)

Mn(VII) oxidants: for the oxidation of alcohols, alkenes, alkynes, aromatic side chains and rings, aldehydes, ketones, amines, nitro, and carbonyl compounds. Oxidation by MnO_2 . Cr (VI) oxidants: for the oxidation of alcohols, phenols- Jones reagent, Chromium trioxide-pyridine complex, pyridinium chlorochromate complex, pyridinium dichromate, Oxidation of alkanes, alkenes, and aromatic side chains and nucleus-catalytic asymmetric epoxidation, Swern oxidation,

Unit-II Reduction reactions

(15 hrs)

Reduction using: Copper Chromite, LiAlH_4 , Sodium borohydride, Sodium cyanoborohydride, Diborane, asymmetric reductions using Borane complexes Sodium/alcohol, Sodium/liq. NH_3 , Magnesium, Zinc Chloride acid, Hydrazine, Di-amide, Formic acid, silanes, stannous chloride, Sn/HCl , $\text{Zn/CH}_3\text{COOH}$, Zn/NaOH , Sodium metabisulphite, Sodium dithionite, Mg/alcohol .

Unit-III Organic name reactions

(15 hrs)

Aldol condensation, Diels Alder reaction, Enamine reaction, Elbs persulfate oxidation, HVZ reaction, Perkin reaction, Riemer-Tiemann reaction, Rosenmund reaction, Wurtz reaction, Shapiro reaction, Robinson annulations, Chichibabin amination, MPV reduction.

Unit-IV Photochemical reactions

(15 hrs)

Laws of photochemistry, electronic excitation, excited states, chemistry of excited molecules, difference between photochemical and thermal reactions, photochemical reactions of carbonyl compounds and olefins, photoisomerization of cis-trans stilbenes, photochemical cycloaddition reactions.

Unit-V Terpenoids

(15 hrs)

Nomenclature-properties-isolation-isoprene rule-special isoprene rule-gem dialkyl rule-classification-general methods for structure determination-synthesis and structural determination of α pinene-camphor.

Text Books

- I. V.K. Ahluwalia, R.K. Parashar, *Organic Reaction Mechanisms, Third edition, Narosa Publishing House, 2009.*
- II. P.S. Kalsi, *Organic reactions and their mechanisms, Third edition, New Age International Publishers, 2010.*
- III. Gurdeep R. Chatwal, *Organic Chemistry of Natural Products, Vol-I, Fifth edition, Himalaya Publishing Company, 2011.*
- IV. Gurdeep R. Chatwal, *Organic Chemistry of Natural Products, Vol-II, Fifth edition, Himalaya Publishing Company, 2011.*

Reference Book

1. I.L. Finar, *Organic Chemistry, Vol I and II, Longman, 1963.*
2. F.A. Cary and R.I. Sundberg *Advanced Organic Chemistry, Part A & B, 5th Ed., Springer, 2009.*
3. Laszlo Kurti, Barbara Czako, *Strategic Applications of Named reactions in Organic Synthesis, Elsevier Academic press, 2005.*

Semester	Sub. Code	Title of the Paper	L	P	T	Credits
III	MCHF183E50	Green Chemistry	4	0	0	4

Aim: To make the students to understand, appreciate the practices and outcomes of green chemistry.

Objectives:

- To define “green chemistry” and place its birth and expansion in an historical context.
- To introduce the principles of green chemistry, outline examples, and establish the arguments for our need to recognize green criteria in the practice of chemistry.
- To present examples of successful green technologies.

Outcome:

- A functional understanding of the field of green chemistry.
- A working understanding of the twelve principles of green chemistry.
- An understanding of several real world examples where organizations used green chemistry to improve the sustainability performance of their products.
- An appreciation of how the practice of green chemistry enhances competitiveness, innovation and faster time to market.

Unit-I Principles & Concept of green chemistry (15 Hours)

Introduction –Concept and Principles-development of Green Chemistry- Atom economy reactions –rearrangement reactions , addition reactions- atom uneconomic-sublimation elimination-Wittig reactions-toxicity measures- Need of Green Chemistry in our day to day life.

Unit-II Green Metrics - Measuring environmental performance (15 Hours)

Importance of measurement – lactic acid production-safer Gasoline – introduction to life cycle assessment-four stages of Life Cycle Assessment (LCA) –Carbon foot printing-green process Matrics-eco labels -Integrated Pollution and Prevention and Control (IPPC)- REACH(Registration, Evaluation, Authorization of Chemicals)

Unit-III Emerging green technology and alternative energy sources (15 Hours)

Design for Energy Efficiency-Photochemical reactions- Advantages-Challenge faced by photochemical process. Microwave technology on Chemistry- Microwave heating –Microwave assisted reactions-Sono chemistry and Green Chemistry –Electrochemical Synthesis-Examples of Electrochemical synthesis- Organic solvents – effects of solvents – Solvent less synthesis.

Unit-IV Renewable resources (15 Hours)

Biomass –Renewable energy – Fossil Fuels-Energy from Biomass-Solar Power- Other forms of renewable energy-Fuel Cells-Alternative Economics-Syngas economy- hydrogen economy-Bio refinery chemicals from fatty acids-Polymer from Renewable Resources –Some other natural chemical resources.

Unit-V Industrial case studies**(15 Hours)**

Methyl Methacrylate (MMA)-Greening of Acetic acid manufacture-Vitamin C-Leather manufacture –Types of Leather –Difference between Hide and Skin-Tanning –Reverse tanning –Vegetable tanning –Chrome Tanning-Fat liquoring –Dyeing –Application-Polyethylene- Ziegler Natta Catalysis-Metallocene Catalysis-Eco friendly Pesticides-Insecticides.

Text Books

- I. Lancaster, M. *Green Chemistry: An Introductory Text*; The Royal Society of Chemistry: 2002.
- II. Anastas, P. T.; Warner, J. C. *Green Chemistry: Theory and Practice*; Oxford University Press, 1998.
- III. Manahan, S. E. *Green Chemistry and the Ten Commandments of Sustainability*; ChemChar Research Inc, 2005.
- IV. J. Clark, D. Macquarrie, “*Handbook of Green Chemistry & Technology*”, Blackwell Science, 2002.
- V. Ahluwalia, V. K.; Kidwai, M. *New Trends in Green Chemistry*; Kluwer Academic: Dordrecht, The Netherlands, 2004.

Reference Books

1. Sheldon, R. A.; Arends, I.; Hanefeld, U. *Green Chemistry and Catalysis*; Wiley-VCH: Weinheim, 2007.
2. *Renewable Resources: Scope and Modification for Non-Food Applications*; Stevens, C. Verhé, R. G., Eds.; John Wiley & Sons Ltd.: West Sussex, 2004.
3. Tundo, P.; Perosa, A.; Zecchini *Methods and Reagents for Green Chemistry: An Introduction*; F., Eds.; John Wiley & Sons, Inc.: Hoboken, NJ, 2007.

Semester	Sub. Code	Title of the Paper	L	P	T	Credits
III	MCHF183E60	Polymer Chemistry	4	0	0	4

Aim: To understand the basic concepts of polymers

Objectives:

- To gain the knowledge in the preparation, properties, characterization and Uses of polymers.
- To Understand the industrial polymer processing techniques

Outcome:

- Students get knowledge about the various polymerization techniques.
- Learn about the applications of industrial oriented polymers.

Unit-I Basic concepts of polymers

(15 hrs)

Importance of polymers - Monomers - Degree of polymerization – Linear - Branched and Network polymers - Classification of polymers –Polymerization Methods: Condensation, Addition - Radical chain - Ionic and Co-ordination and Co-polymerization-Polymerization conditions and reactions- Polymerization in homogeneous and heterogeneous systems.

Unit-II Kinetics and Mechanisms

(15 hrs)

Kinetics and mechanisms of Condensation, Addition - Radical chain - Ionic and Co-ordination-(Ziegler-Natta) polymerization and Co-polymerization.

Unit-III Polymer characterization

(15 hrs)

Chemical analysis of polymers - Spectroscopic methods - X-ray diffraction studies - Thermal analysis - Physical testing: Tensile strength – Fatigue – Impact - Tear resistance - Hardness and Abrasion resistance. Polydispersion - Molecular weight: Number, Weight and Viscosity average molecular weights - Polydispersity and molecular weight distribution - Practical significance of molecular weight - Measurement of molecular-weights: End-group, Viscosity, Light scattering, Osmotic and Ultracentrifugation methods.

Unit-IV Polymer Structure and properties

(15 hrs)

Molecular forces in polymers - dipole forces, induction forces, dispersion forces, Dependence of physical properties on intermolecular forces. Configuration of polymer chains – Crystal structure of polymers – morphology of crystalline polymers – structural requirements for crystallinity, degree of crystallinity, crystallizability-mechanism of crystallization– Crystalline melting point – glass transition temperature.

Unit-V Synthesis, Applications and polymer processing

(15 hrs)

PE, PS, PMMA, PVA and PTFE -Polymer Processing: Molding – Compression – Injection – Blow – Thermoset – Extrusion – Brief Notes on Recent Advances in Polymers: Conducting Polymers - Polyaniline – Bio-degradable polymers –Polymer composites.

Text Books

- I. *F.W. Billmeyer Jr., Wiley-India Textbook of Polymers Science, Second Edition, Wiley-India, 2007.*
- II. *V.R. Gowarikar, N.V. Viswanathan, Jayadev Sreedhar, Polymer Science, First edition, New Age International (P) Ltd., Publishers, Reprint 2005.*
- III. *Introduction to Polymer Chemistry, Charles E. Carraher. Jr., CRC Press, Taylor and Francis, 2006*

Reference Books

1. *M.S. Bhatnagar, A Text book of Polymer chemistry, S.Chand Publications, 2004.*
2. *B.K. Sharma, polymer Chemistry, Goel Publishing House, 2014*
3. *The Elements of Polymer Science and Engineering, Alfred Rudin, Elsevier Academic Press, 1999.*
4. *Polymer Science and Technology, Premamoy Ghosh, Tata MC Graw Hill, 2011.*

Semester	Sub. Code	Title of the Paper	L	P	T	Credits
III	MCHF183E70	Nanomaterials	4	0	0	4

Aim: To study about nanoscience and nanotechnology

Objectives:

- To understand the basic concepts and chemistry of nanomaterials
- To familiarize with importance and applications of nanotechnology

Outcome:

- Students acquire basic knowledge on nanoscience
- They get an idea about the scope and importance of nanotechnology.

Unit-I Introduction to Nanoscience

(15 hrs)

The Science of Nano - Atomic structures - Molecular and atomic size - Bohr radius – Emergence of Nanotechnology – Differences between bulk and nanomaterials – Reasons - Challenges in Nanotechnology.

Unit-II Growth of Nanomaterials

(15 hrs)

Influence of nucleation - rate on the size of the crystals - macroscopic to microscopic crystals and nanocrystals - large surface to volume ratio, top-down and bottom-up approaches - self-assembly process – template assisted and template free approach – micelles assisted methods - grain boundary volume in nanocrystals - defects in nanocrystals - surface effects on the properties.

Unit-III Types of Nanostructures

(15 hrs)

Different types of nanomaterials - Types of Nanocrystals - One Dimensional (1D) - Two Dimensional (2D) -Three Dimensional (3D) nanostructured materials - Quantum dots - Quantum wire - Core/Shell nanostructures - Synthesis and properties of Carbon Nanotubes (CNT) and Graphene – Metal nanostructures of Au and Ag - Metal oxides (TiO₂, CeO₂, ZnO) - Semiconductors (Si, Ge, CdS, ZnSe) - Ceramics and Composites – Polymer nanocomposites.

Unit-IV Instrumentation Analysis for Nanomaterials

(15 hrs)

Principle, Theory, Working and Applications of X-Ray Diffraction, Scanning Electron Microscopy, Transmission Electron Microscopy, High Resolution Transmission Electron Microscopy, Field Emission Scanning Electron Microscopy, Atomic Force Microscopy.

Unit-V Applications of Nanoscience and Nanotechnology

(15 hrs)

Biological applications - Biochemical sensor - Nanoscience in Drug Delivery - Nanomedical applications of green nanotechnology - Membrane based water purification. Energy applications – Electrocatalysis – Nano Electronics and Nano Optics – Industrial Applications.

Text books:

- I. *A.K.Bandyopadhyay, Nano Materials, New Age International, India, 2008.*
- II. *K.K.Chattopadhyay, A.N.Banerjee Introduction to nanoscience & nanotechnology, PHI India, 2009.*
- III. *T.Pradeep, Nano: the essentials understanding nanoscience & nanotechnology, Mcgraw-Hill Education India Pvt. Ltd, 2007.*
- IV. *C.Carl, Koch, Nanostructured materials: Processing, properties & applications, William Andrew, NY, 2007.*

Reference books:

1. *M. Wilson, K. Kannangara, G Smith, M. Simmons, B. Raguse, Nanotechnology: Basic science and Emerging technologies, Overseas Press India Pvt Ltd, New Delhi, First Edition, 2005.*
2. *C.N.R. Rao, A. Muller, A. K. Cheetham (Eds), The chemistry of nanomaterials: Synthesis, properties and applications, Wiley VCH Verlag GmbH&Co, Weinheim, 2004.*
3. *Kenneth J. Klabunde (Eds), Nanoscale Materials Science, John Wiley & Sons, InC, 2001.*

Semester	Sub. Code	Title of the Paper	L	P	T	Credits
III	MCHF183P80	Analytical Chemistry Laboratory	0	6	0	6

1. Estimation of KMnO_4 by Visible Spectrophotometry.
2. Estimation of Dye by Visible Spectrophotometry.
3. Estimation of Surfactant by UV-Visible Spectrophotometry.
4. Determination of Kinetics by UV-Visible Spectrophotometry.
5. Qualitative analysis of organics by FT-IR Spectrometer – KBr – technique.
6. Qualitative analysis of organics by FT-IR Spectrometer – ATR-technique.
7. Pot. Ferri cyanide and Ferro cyanide by Cyclic Voltammetry.
8. Electrochemical Oxidation of Organics by Cyclic Voltammetry.
9. Estimation of Fluorescence Dye by Spectrofluorometer.
10. Estimation of Quantum Yield by Spectrofluorometer.
11. Estimation of Alkali metals by Flame Photometry.
12. Determination of Reaction Kinetics by FT-IR spectrometer.
13. Analysis of water quality parameters.
14. Estimation of COD of waste water by spectrophotometer.

Reference Book

1. Course material developed by the department of chemistry, SCSVMV.

Scheme of Evaluation

S. No	Particulars	Max. Marks
1	Aim, Principle, Procedure, Model graph and Table	20
2	Graph	10
3	Calculation	10
4	Interpretation of result	10
5	Spectra Interpretation	30
6	Record	10
7	Viva-voce	10
Total		100

Semester	Sub. Code	Title of the Paper	L	P	T	Credits
IV	MCHF184T20	Soft Skills and Scientific Writing	4	0	0	4

Aim: To develop soft skills of students and to introduce about scientific literature to the students.

Objective:

- To impart the knowledge of soft skills, scientific literature survey and report writing.

Outcome:

- The students will acquire knowledge of time management, positive thinking and report writing

Unit-I Memory and study skills

(15 hrs)

Definition and importance of memory-Causes of forgetting-How to forget (thought stopping), how to remember (techniques for improving memory)-The technique of passing exams- management of examination fear.

Unit-II Power of positive thinking

(15 hrs)

Nurturing creativity, decision-making and problem solving-Thinking power- seven steps for dealing with doubt-Traits of positive thinkers and high achievers-Goals and techniques for positive thinking-Enhancement of concentration through positive thinking-Practicing a positive life style-Advantages of time management.

Unit-III Literature survey

(15 hrs)

Chemical nomenclature and literature primary sources - secondary sources including reviews. Treatise and monographs, literature searching, Review of work relevant to the chosen problems. Abstraction of a research paper.

Unit- IV Writing a thesis or paper

(15 hrs)

General format - page and chapter formation. The use of quotation - footnotes - tables and figures - referencing - appendixes - revising the paper or thesis - editing and evaluating the final product - proof reading the final typed copy - Publication of Research paper

Unit-V Oral presentation skills

(15 hrs)

Structure, voice, appearance, body language – delivery Presentation a scientific seminar – appearing in interviews.

Text Books

- I. G.A. Dudley, *Double your learning power*, Thomas Publishing Group Ltd., Delhi, 2004.
- II. J. Anderson, B.H. Dursten and M. Poole, *Thesis and Assignment Writing*, Wiley Eastern, 1977.

Reference Books

1. D.J. Mile, *Power of positive thinking*, Rohan Book Company, Delhi, 2004.
2. H. Lorayne, *How to develop a super power memory*, Thomas Publishing Group Ltd., 2004.
3. J. Anderson, B.H. Dursten and M. Poole, *Thesis and Assignment Writing*, Wiley Eastern, 1977.

Semester	Sub. Code	Title of the Paper	L	P	T	Credits
IV	MCHF184T10	Surface Chemistry and Photo Chemistry	4	0	0	4

Aim:

- To make the students to understand about the basics of surface chemistry and Photochemistry.

Objectives:

- To understand the concepts and applications of surface chemistry.
- To study about Photophysical Processes & Principles of Photochemistry

OutCome:

- Students acquire the knowledge about Catalytic reactions Which are used in day-to-daylife.

Unit-I Adsorption**(15 hrs)**

Gas-Solid interface, types of adsorptions, factors affecting adsorption, physical adsorption, adsorption isotherms, Freundlich's adsorption isotherm, Langmuir adsorption isotherm, BET equation, modification of BET equation, determination of surface area, Harkins and Jura method, Benton and White method, point B method, importance of surface area, heat of adsorption. Adsorption from solutions, types, Gibb's adsorption equation, verification of Gibbs equation, Domain & Barker method, tracer method, surface tension and surface free energy, capillary condensation, wetting phenomena, applications of adsorption.

Unit-II Reaction on Surfaces**(15 hrs)**

Mechanisms of surface reactions, effect of surface heterogeneity, unimolecular surface reactions, bi-molecular surface reactions, combination and formation of atoms at surfaces, exchange reactions, transition state theory of surface reactions, comparison of homogeneous and heterogeneous reaction rates. Classification of catalytic reactions, types of catalysts, metals, semi-conductors, insulators, energetic of adsorption processes.

Unit-III Colloids**(15 hrs)**

Emulsions, types, characteristics of emulsions, emulsifiers, theories of emulsification, importance of emulsion, micellar emulsion, applications, micelles, structure of micelles, ionic micelles, CMC, determination of CMC, solubilization, Donnan membrane equilibrium and its application. Applications of colloids.

Unit-IV Excitation of Molecules**(15 hrs)**

Mechanism of radiation absorption, electric dipole transitions, Einstein's treatment, intensity of electronic transitions, selection rules, directional nature of light absorption, life times of excited states, types of transitions, two photon absorption spectroscopy. Physical properties of excited molecules, changes on electronic excitation, potential energy diagram, shape of absorption band and Frank-Condon principle, emission spectra, environmental effect, dipole moment, acidity

constant, redox potential in excited states, geometry of electronically excited molecule, flash photolysis.

Unit-V Photophysical Processes

(15 hrs)

Types of Photophysical pathways, Jablonski diagram, radiation less transition, internal conversion, intersystem crossing, fluorescence, phosphorescence, emission property and electronic configuration, kinetics of unimolecular processes, state diagram, delayed fluorescence, effect of temperature on emission processes. Kinetic collisions and optical collisions, mechanism of fluorescence quenching in gases, collisions in solution, Stern-Volmer equation, concentration dependence of quenching, excimer formation. Quenching by foreign substances, photosensitization, charge transfer mechanisms, energy transfer mechanism, donor acceptor interaction in energy transfer (qualitative treatment), sensitized delayed emission.

Text Books

- I. Gurdeep Raj, *Advanced Physical Chemistry*, 22nd edition, Goel Publications, 1998.
- II. Keith J. Laidler, *Chemical Kinetics*, Third Edition, Pearson Education, 2004.
- III. J. Rajaram, J.C. Kuriacose, *Kinetics and Mechanisms of Chemical Transformations*, First edition, Macmillan, 1993, reprint 2011.
- IV. K.K. Rohatgi-Mukherjee, *Fundamentals of Photochemistry*, New Age International Publishers, 1978, revised edition 2002.

Reference Book

1. Peter Atkins, Julio de Paula, *Physical Chemistry*, Eighth edition, Oxford press, 2006.
2. Arthur W. Adamson & Aulice P. Gast, *Physical Chemistry of Surface*, Wiley India Pvt Ltd., 2012.
3. Gurudeep Raj, *photochemistry*, Krishna Prakashan publications, 2012.

Semester	Sub. Code	Title of the Paper	L	P	T	Credits
IV	MCHF184E40	Synthetic Organic Chemistry	4	0	0	4

Aim: To teach the synthetic organic methodologies and reagents in organic synthesis

Objective:

- To impart the knowledge of multistep organic synthesis.

Outcome:

- Students get knowledge about the chemical modification of a functional group to obtain chemoselectivity in a subsequent chemical reaction.
- To get an idea about modern synthesis.

Unit-I Heterocyclic compounds

(15 hrs)

Chemistry of heterocyclic compounds, synthesis and reactivity of the following systems-quinoline, isoquinoline, benzofuran, benzothiophene, pyrazole, imidazole, oxazole, isoxazole, thiazole, isothiazole, pyridazine, pyrimidine, and pyrazine.

Unit-II Protecting groups and retero synthetic analysis

(15 hrs)

Requirements for protecting groups-Protection and deprotection of hydroxyl, carboxyl, carbonyl, carboxy amino groups and carbon-carbon multiple bond; chemo- and regioselective protection and deprotection; illustration of protection and deprotection in synthesis.

Disconnection approach to synthesis – disconnection- definition – preferred positions – FGI – Synthons – synthetic equivalents – reterosynthetic analysis of Benzocaine, BHT and saccharine. Types of disconnections – order of disconnections - one group disconnections – RCO-X and ROH disconnections – two group C-X disconnections – types and examples only.

Unit-III Reagents in organic synthesis

(15 hrs)

Preparation and reactions of: Aluminium isopropoxide, NBS, Diazomethane, DDQ, DCC, LTA, LAH, OsO₄, Sodium borohydride, Wittig reagent-hydroboration-oxidation-regio and stereo selectivity.

Unit-IV Modern synthetic methods

(15 hrs)

Baylis-Hillman reaction, Henry reaction, Nef reaction, Kulinkovich reaction, Ritter reaction, Sakurai reaction, Tishchenko reaction and Ugi reaction. Brook rearrangement; Tebbe olefination. Metal mediated C-C and C-X coupling reactions: Heck, Stille, Suzuki, Negishi and Sonogashira.

Unit-V Pericyclic reactions

(15 hrs)

Types of Pericyclic reactions, stereochemistry of Pericyclic reactions, M.O. theory, symmetry properties of reactant and product orbitals, 2+2 cycloadditions, 4+2 cycloadditions, cyclization of 4n systems, 4n+2 systems, correlation diagram, sigmatropic rearrangements.

Text Books

- I. V.K. Ahluwalia, R.K. Parashar, *Organic Reaction Mechanisms, Third edition, Narosa Publishing House, 2009.*
- II. P.S. Kalsi, *Organic reactions and their mechanisms, Third edition, New Age International Publishers, 2010.*
- III. F.A. Carey and R.I. Sundberg., *Advanced Organic Chemistry, Part A & B, 5th Ed., Springer, 2009.*

Reference Book

1. Jerry March., *Advanced Organic Chemistry: Reactions, Mechanisms and Structure, Wiley Student Edition, 2006.*
2. R.O.C. Norman and James.M. Coxon, *Principles of Organic Synthesis, Modern synthesis, CRC press, 1993*
3. S.Warren, *The Disconnection Approach, John Wiley & Sons, 2004.*

Semester	Sub. Code	Title of the Paper	L	P	T	Credits
IV	MCHF184E30	Nuclear and Bioinorganic Chemistry	4	0	0	4

Aim: To study about basic concepts of nuclear chemistry and bioinorganic Chemistry

Objectives:

- To understand the basic concepts of nuclear reactions and nuclear reactor.
- To understand the biological importance of inorganic chemistry.

Outcome:

- Students will get an idea nuclear reactions and applications of inorganic compounds in biological systems.

Unit-I Structure of nucleus

(15 hrs)

size and shape of nucleus – nuclear stability - nuclear angular momentum – magnetic properties of nuclei – quadrupole moment – nuclear parity-forces and interactions. Nuclear models: Shell, liquid drop and Fermi gas models – collective model –optical model. Detection and measurement of radioactivity: Radio activity – units of radio activity - characteristics of decay – decay kinetics – theories of alpha and beta decay (primitive treatment only) – gamma emission – artificial radio activity – detectors –ionization chamber scintillation and – semiconductor detectors.

Unit-II Nuclear reactions and applications

(15 hrs)

Nuclear reactions: Bethe's notation – types of reactions –cross section- compounds nuclear theory – photo and thermo nuclear reactions – fusion reactors – origin and evolution of elements. Applications of radioactivity: Nuclear reactors – breeder reactor –India's nuclear energy – recovery of U and Pu from spent fuel – applications of radio isotopes – probing – Szilard-Chalmers' reaction – cow and milk systems –tracers. Elementary particles of nucleus: classification – particles and antiparticles – Parton structure –Quarks and Gluons – classification of Quarks – Higgs Boson.

Unit-III Bioinorganic Chemistry

(15 hrs)

Metal ions in biological systems: Electron transfer systems –cytochrome and Fe –S proteins - Structure and functions -Transport and storage of oxygen – Haemoglobin –structure and functions –cyanide poisoning –Myoglobin-Chlorophyll – Cyanocobalamine- structure and functions- Calcium in biological systems –sodium-potassium ion pumps-Metals in medicine – Ptbinding to DNA.

Unit-IV Acids, Bases and Non-Aqueous Solvents

(15 hrs)

Acids and Bases: Arrhenius theory –Bronsted –Lowry theory –Lux-Flood definition – Solvent system definition – Lewis concept – Usanovich definition – generalized acid base concept - HSAB concept – basis of classifications – applications – pi bonding contributions –electro negativity and hard soft species – limitations of the principle. Non aqueous solvents:

classification of solvents – leveling and differentiating solvents ionizing solvents – Liq.NH₃ – Liq.SO₂ - Liq.N₂O₄ - Liq. BrF₃ – acetic acid.

Unit-V Inorganic nomenclature and redox stability (15 hrs)

Affixes used in naming- general naming – names of ions- radicals – acids – salts and salt like compounds- boron hydrides-isopolyanions and heteropolyanions- organometallics
Redox stability in water – hydrogen over voltage – oxygen over voltage – Latimer, Frost and Pourbaix diagrams – Electrometallurgy - Ellingham diagram.

Text Books

- I. H.J.Arnika., *Essentials of nuclear chemistry, Revised Fourth edition, 1995, New Age International Publishers, Reprint 2009.*
- II. P.S.Kalsi and J.P.Kalsi., *Bioorganic, Bioinorganic and Supramolecular chemistry, Fourth edition, New Age International Publishers, 2007.*
- III. R.Gopalan and V.Ramalingam. *Concise coordination chemistry, First edition, 2001, Vikas Publishing House Private Ltd., Third reprint, 2007.*
- IV. Wahid U.Malik, G.D.Tuli and R.D.Mada.n, *Selected Topics in Inorganic Chemistry, First edition, S.Chand and Company Ltd., 1976 (Reprint 1998).*
- V. F.Albert Cotton, Geoffrey Wilkinson, Carlos. A.Murilo and Manfred Bochmann., *Advanced inorganic chemistry, Sixth edition, Wiley India, 2004 (Reprint 2008).*
- VI. G.S.Manku., *Theoretical principles of Inorganic chemistry, First edition, Tata McGraw-Hill Publishing Company Ltd., 1980 (Twentieth reprint).*

Reference Books

1. Bodie Douglas, Darl McDaniel and John Alexander., *Concepts and Models of Inorganic Chemistry, Third edition, Wiley India Ltd., 2006.*
2. Asim.K.Das., *Bioinorganic Chemistry, First edition, Books and Allied (P) Ltd., 2007 (Reprint 2009).*
3. M.Satake and Y.Mid., *Bioinorganic Chemistry, First edition, Discovery Publishing House, 2001(Reprint 2003).*
4. Stephen J. Lippard, Jeremy M. *Principles of bioinorganic chemistry Berg.Mill Valley, Calif. University Science Books, 1994.*

Semester	Sub. Code	Title of the Paper	L	P	T	Credits
IV	MCHF184E50	Supramolecular Chemistry	4	0	0	4

Aim: To introduce and demonstrate the importance of supramolecular (non-covalent interactions) complex materials and applications.

Objective: To impart knowledge of types of supramolecules, structures their applications as organic materials, sensors, and devices.

Outcome: The students will acquire knowledge of,

- Molecular recognition and nature of bindings involved in biological systems
- Structure of supramolecules of various types in solution and solid state
- Applications of supramolecules in miniaturization of molecular devices

Unit-I Supramolecular chemistry: Basic concepts, principles and history (15 hrs)

Introduction to Supramolecular chemistry- Basic concepts, principle and history. Nature of binding interactions in supramolecular structures: ion-ion, ion-dipole, dipole-dipole, H-bonding, cation- π , anion- π , π - π and vander waal interactions.

Unit-II Receptors: synthesis, structure and binding (15 hrs)

Synthesis and structures of crown ethers, Lariat ethers, Podands, Cryptands, Spherands, Calixarene, Cyclodextrins, Cyclophanes, Cryptophanes, Carcerands and hemicarcerands, Host-guest interactions, Preorganisation and complimentarity, Lock and key analogy. Binding of cationic, Anionic, Ion pair and neutral guest molecules.

Unit-III Self-assembly molecules (15 hrs)

Design, Synthesis and Properties of the molecules, Self-assembly by H-bonding, Catenanes, Rotaxanes, Dendrimers and Supramolecular gels. Relevance of supramolecular chemistry to mimic biological system.

Unit-IV Supramolecular Reactivity and Catalysis (15 hrs)

Catalysis by reactive macrocyclic cation receptor molecules. catalysis by reactive anion receptor molecules. catalysis with cyclophane type receptors. supramolecular metalocatalysis. cocatalysis: catalysis of synthetic reactions. biomolecular and abiotic catalysis. Supramolecular chemistry in solution: cyclodextrin, micelles, dendrimers, gelators. classification and typical reactions- applications.

Unit-V Supramolecular devices and sensors (15 hrs)

Various types of supramolecular devices, supramolecular light conversion and energy transfer devices. supramolecular electronic conducting devices - molecular wires, modified and switchable molecular wires. ion and molecule sensors.

Text Books

- I. Atwood, J., Steed, J., *Supramolecular Chemistry - 2nd ed.* Chichester: John Wiley & Sons, Ltd., 2009.
- II. Hans-Joerg Schneider and Anatoly Yatsimirsky, *Principles and Methods in Supramolecular Chemistry*, J. Wiley and Sons; 1st Ed. 2000.
- III. Kalsi, P.S., and Kalsi, J.P., *Bioorganic, Bioinorganic and Supramolecular Chemistry*, New Age International (P) Limited, Publishers, 2010.

Reference Books

1. Lehn, J. M., *Supramolecular Chemistry-Concepts and Perspectives*, Wiley –VCH, 1995.
2. Beer, P.D., Gale, P. A., and Smith, D. K., *Supramolecular Chemistry*, Oxford University Press.1999.
3. Steed, J. W., and Atwood, J. L., *Supramolecular Chemistry*, Wile, 2000.
4. Kunitake, T., Ariga, K., *Supramolecular Chemistry – Fundamentals and Applications. Advanced Textbook*. Berlin: Springer-Verlag Heidelberg, 2006.

Semester	Sub. Code	Title of the Paper	L	P	T	Credits
IV	MCHF184E60	Crystal growth	4	0	0	4

Aim: To create interest in the field of crystal growth techniques

Objectives:

- To study the Crystal Growth Theories.
- To understand the Characterization of Crystals.

OutCome:

- NLO organic single crystals have been identified as potential candidates in optical and electro-optical devices.

Unit-I Nucleation

(15 hrs)

Nucleation concept – Kinds of nucleation – Classical theory of nucleation - Spherical nucleus – Induction period – Measurement - Heterogeneous nucleation – Equilibrium concentration of embryos – Energy of formation of a critical nucleus - Free energy of formation of a critical heterogeneous cap shaped and disc shaped nuclei –Nucleation rate.

Unit-II Crystal Growth Theories

(15 hrs)

Surface energy theory – Diffusion theory – Adsorption layer theory – Volmer theory –Bravais theory – Kossel theory – Two-dimensional nucleation theory – Free energy of formation of a two-dimensional nucleus – Possible shapes – Rate of nucleation.

Unit-III Crystal Growth Methods

(15 hrs)

Growth from Melt, Vapor, Solution (High & Low Temperature Solution Growth). Low Temperature Solution Growth – Slow Cooling, slow Evaporation & Temperature Gradient Method.

Unit-IV Characterization of Crystals

(15 hrs)

Different techniques for analysis - FTIR, UV as applied to solid crystals - Single Crystal XRD, SEM, NLO, Micro hardness. Principles of NLO -SHG. Steps in Crystal structure analysis

Unit-V Effects of impurities on crystals

(15 hrs)

Doping, Types of Dopants-Imperfections due to doping – Thresholds concentration of doping in Crystals. Effect of doping on crystals. Methods of detecting imperfections.

Text books:

- i. *Crystal growth for beginners*, Ivan.V. Markov, World scientific Private Ltd.,2016.
- ii. *Introduction to crystal growth: Principles and practice*, H. L. Bhat, CRC Press, 2014.
- iii. *Solid state chemistry*, D.K.Chakrabarthy, New Age International Ltd, 2010.
- iv. *Solid state chemistry and its applications*, Anthony.R. West, John Wiley& sons, 2014.
- v. *Introduction to Solid state physics*, Neil W Ashcroft, N. David Mermin, Cengage Ltd, 2003.

Reference books:

1. *Introduction to crystal growth*, Klaus-Werner Benz, Wolfgang Neumann, Wiley-VCH, 2014.
2. *Crystal Growth*, Brain R. Pamplin., Pergamon Press. Oxford, 1980.
3. *The growth of crystals from melt*, Brice, J.C.. North Holland, Amsterdam, 1973.
1. *Crystal Growth in Gels*, Heinz K. Henish.. Cambridge University Press, 1973.
2. *Cryst allization Mullin*, J.W. Academic Press. London.1972.