Central University of Punjab, Bathinda



Course Structure and Syllabus

M.Sc. Chemistry

Session: 2019-21

Department of Chemical Sciences

School of Basic and Applied Sciences

Program Outcomes

Department of Chemical Sciences was established in Jul, 2015. The department offers M.Sc. Chemistry, M.Sc. Chemistry (Specialization: Applied Chemistry) and Ph.D. in Chemistry.

Upon successful completion of the graduate program, student should be able

- Demonstrate an understanding and applications of major concepts in all disciplines of chemistry.
- Instrumentation in chemical proof of scientific/research concepts at an advanced level.
- Design and execute experiments with proper use of good laboratory practices and proper handling of waste generated in the laboratory.
- Critical think and design, carry out, record and analyze the results of chemical experiments as per the research standards.
- Identify, formulate research out literature and analyze complex problems reaching substantial conclusions using principles of chemical sciences.

S. No.	Paper Code	Course Title	Course Type	L	Т	P	Cr
1	CHM.506	Fundamental Biology (Non-medical CF group)				_	2
	CHM.507	Fundamental Mathematics (Medical group)		2	-		4
2	CHM.508	Analytical Chemistry and Instrumental Methods	CF	3	-	-	3
3	CHM.509	Inorganic Chemistry-1	CC	3	-	-	3
4	CHM.510	Organic Chemistry-I	CC	3	-	-	3
5	CHM.511	Physical Chemistry-I	CC	3	-	-	3
6	CHM.512	Quantum Chemistry	CC	3	_	_	3
7	CHM.513	Practical Inorganic Chemistry-I (P)	CC	-	-	4	2
8	CHM.514	Practical Organic Chemistry-I (P)	CC	-	-	4	2
9	XXX	Inter-Disciplinary Course (ID) (Opt any one from other Departments)	EC	2	-	-	2
10.	CHM.541	Seminar	EC	1			1
		Total		20	0	8	24

CC: Core Course, **EC**: Elective Course, **CF**: Compulsory Foundation, **EF**: Elective Foundation

L: Lectures T: Tutorial P: Practical Cr: Credits

S.	Paper	Course Title	Course	L	T	P	Cr
No.	Code		Type				
1	CHM.521	Inorganic Chemistry-II	CC	3	_	-	3
2	CHM.522	Organic Chemistry-II	CC	3	_		3
3	CHM.523	Physical Chemistry-II	CC	3	_		3
4	CHM.524	Spectroscopic Analysis	CF	3	_	-	3
5	CHM.525	Molecular Spectroscopy	CC	3	_	-	3
6	CHM.526	Practical Inorganic Chemistry-II (P)	CC	-	-	4	2
7	CHM.527	Practical Physical Chemistry- II (P)	CC	_	-	4	2
8	CHM.542	Seminar	EC	_	1	-	1
9	XXX	Inter-Disciplinary Course (ID)	EC	2	-	-	2
		(Opt any one from other Departments)					
1.0							
10.	XXX	Value Based Course	EF	1			1
		Total		18	1	8	23

CC: Core Course, **EC**: Elective Course, **CF**: Compulsory Foundation, **EF**: Elective Foundation

Mode of Transactions: Lecture, Demonstration, Lecture cum demonstration, Experimentation, Problem solving, Brain storming, Tutorial, Case study, Dialogue Mode, Seminar.

S. No.	Paper Code	Course Title	Course Type	L	Т	P	Cr
1.	CHM.556	Research Methodology	CF	2	_	-	2
2.	CHM.551	Inorganic Chemistry-III	CC	3	_	-	3
3.	CHM.552	Organic Chemistry-III C		3	-	_	3
4.	CHM.553	Bioinorganic and Biophysical Chemistry	СС	3	-	-	3
5.	CHM.554	Practical Organic Chemistry-III (P)	CC	-	-	4	2
6.	CHM.555	Practical Physical Chemistry- III (P)	CC	-	-	4	2
7.	XXX*	Value Based Course	CF	1			1
8.	CHM.599	Project	EC	-	_	12	6
	Total			14	-	20	24

CC: Core Course, **EC**: Elective Course, **CF**: Compulsory Foundation, **EF**: Elective Foundation

Mode of Transactions: Lecture, Demonstration, Lecture cum demonstration, Experimentation, Problem solving, Brain storming, Tutorial, Case study, Dialogue Mode, Project.

S. No.	Paper Code	Course Title	Course Type	L	Т	P	Cr
1	CHM.571	Polymer and Solid State Chemistry	CC	4	_	_	4
2.	CHM.572	Concepts in Chemistry –I	CC	2	_	_	2
3.	CHM.573	Concepts in Chemistry –II	CC	2	_	_	2
4.	CHM.599	Project	EC	-	_	12	6
Opt	Opt any one of the following courses:						
	CHM.574	Advanced Organic Synthesis					
_	CHM.575	Chemistry of Natural Products	EC				
5.	CHM.576	Organotransition Metal Chemistry		4	-	-	4
	CHM.577	Environmental Chemistry					
Opt	any one of	the following courses:			l		
_	CHM.578	Inorganic Photochemistry					
6.	CHM.579	Current Trends in Organic Synthesis	EC 4				
5.	CHM.580	Supramolecular Chemistry			-	_	4
	CHM.581	Material Chemistry					
		Total		16	-	-	22

CC: Core Course, **EC**: Elective Course, **CF**: Compulsory Foundation, **EF**: Elective Foundation

Mode of Transactions: Lecture, Demonstration, Lecture cum demonstration, Experimentation, Problem solving, Brain storming, Tutorial, Case study, Dialogue Mode, Project.

Course Title: Fundamental Biology (Non-medical group)

Paper Code: CHM.506 Total Contact Hours: 30

L	T	P	Cr
2	0	0	2

Course Outcome: After this course completion, the students will be able to analyze and apply the knowledge of

- 1. Molecular structure and interactions present in various biomolecules like proteins, nucleic acids, lipids etc.
- 2. Organization and working principles of various components present in living cell.
- 3. Physical principles of structure, function, and folding of biomolecules.

Unit 1 7 Hours

Introduction: Cell structure and functions, thermodynamics and kinetics of biological processes, ATP. Interactions in aqueous solutions, Role of water in life, pH, Acidic and basic buffers, Biological buffers, solution equilibria, Henderson-Hasselbalch equation, Hofmeister series, Chaotropic and kosmotropic ions/co-solvents.

Unit 2 7 Hours

Amino Acids and Peptides: Classification and properties of amino acids, peptide and polypeptides, primary structures, structure of peptide bond, synthesis of peptides, different protecting groups in peptide chemistry, N-terminal, C-terminal and sequence determination.

Carbohydrates: Biologically important monosaccharides, disaccharides and polysaccharides, glycoproteins, role of sugars in biological recognition.

Unit 3 8 Hours

Proteins: Secondary structure of proteins with emphasize on supramoelcular characteristics of \Box -helix, \Box -sheets, supersecondary structure and triple helix structure of collagen, tertiary structure of protein-folding, quaternary structure of protein, in-vivo and in-vitro protein folding, protein misfolding and conformational diseases.

Unit 4 8 Hours

Nucleic Acids: Purine and pyrimidine bases, nucleotides, nucleosides, base pairing via H-bonding, structure of ribonucleic acids (RNA) and deoxyribonucleic acids (DNA), double helix model of DNA, different types of RNA and their functions, the chemical basis for heredity, overview of replication of DNA, transcription, translation and genetic code.

Lipids: Lipid classification, lipid bilayers, liproproteins-composition.high density (HDL) and low-density (LDL) lipoproteins and function, membrane proteins - integral membrane proteins.

Suggested Readings

- 1. Voet, D., Voet, J. G., and Pratt, C. W. (2008). *Principle of Biochemistry*. John Wiley and Sons .
- 2. Berg, J. M., Stryer, L., and Tymoczko, J. L. (2015). StryerBiochemie. Springer-Verlag.
- 3. Garrett, R. H., and Grisham, C. M. (2013). *Biochemistry*, Brooks/Cole, Cengage Learning.
- 4. Conn, E., and Stumpf, P. (2009). *Outlines of Biochemistry*. John Wiley and Sons.

Course Title: Fundamental Mathematics (Medical group)

Paper Code: CHM.507 Total Contact Hours: 30

	L	T	P	Cr
ſ	2	0	0	2

Course Outcome: The students should be able to demonstrate and apply the various mathematical operations including matrix operations, differentiation, integration, complex, quadratic and differential equations.

Unit 1 7 Hours

Trigonometry and Algebra

Trigonometric functions of sum and differences of angles, addition and subtraction formulas. Polynomial equations and their solutions: binomial theorem and expansion. Common series and expansions used in chemistry.

Complex Algebra: Complex numbers, the graphical interpretation of complex numbers, characterizations of the exponential function, the trigonometric functions of complex argument ($e^{i\theta}$, $e^{-i\theta}$).

Unit 2 8 Hours Differential Calculus

Functions, limits, differentiation, basic rules of differentiation, maxima and minima, exact and inexact differentials, partial differentiation.

Matrix Algebra: Addition and multiplication; inverse, adjoint and transpose of matrices, matrix equation, Introduction to vector spaces, matrix Eigen values and Eigen vectors, diagonalization, determinants (examples from Huckel theory).

Unit 3 8 Hours Integral Calculus

Basic rules for integration, integration by parts, partial fraction and substitution, definite integrals, evaluation of definite and some standard integrals related to chemistry

Unit 4 7 Hours

Elementary Differential Equations: Variables-separable and exact, first-order differential equations, homogenous, exact and linear equations. Applications to chemical kinetics, quantum chemistry, etc. solutions of differential equations by the power series method, spherical harmonics, second order differential equations and their solutions.

Suggested Readings

- 1. Steiner, E. (2008). The Chemistry Maths Book. Oxford University Press.
- 2. Doggett, G., and Sutcliffe, B. T. (1995). *Mathematics for Chemistry*. Longman Pub Group.
- 3. Daniels, F. (2003). *Mathematical Preparation for Physical Chemistry*. McGraw Hill Publishers.
- 4. Tebbutt, P. (1998). Basic Mathematics for Chemists. Chichester: Wiley.

Course Title: Analytical Chemistry and Instrumental

Methods

Paper Code: CHM.508 Total Contact Hours: 45

L	T	P	Cr
3	0	0	3

Course Outcome: The students should be able to choose the method of analysis based on the sample amount/volume, accuracy and precision required for analysis and interference. The student should be able to able to demonstrate the understanding and application of the principles of instrumental analysis.

Unit 1 11 Hours

Errors in Quantitative Analysis: Accuracy, precision, sensitivity, specificity, mean and standard deviation, classification of errors and their minimization, significant figures, linear regression, covariance and correlation coefficient. Standard reference materials, criteria for selection of analytical method.

Quantitative Analysis: Concepts important to quantitative analysis, classification of methods for quantitative analysis, choice of method for analysis, theory of volumetric and gravimetric methods of analysis.

Unit 2 11 Hours

Analytical Spectroscopy: Principle, applications and limitations of spectrophotometery, Beer-Lambert law, analysis of mixtures, sources and treatment of interferences and detection limits to be considered in each of the techniques, fluorescence spectrometry, atomic absorption spectrometry (AAS); flame AAS, electrothermal AAS (ETAAS).

Unit 3 12 Hours

Potentiometry: General principles, reference electrodes, ion selective electrodes, ion selective electrode construction, membrane electrode, glass electrodes, liquid membrane electrodes, biosensors ISFET and MOSFETS.

Coulometry: Basic principles of electrogravimetry, ohmic potential, kinetic and concentration polarization, overpotential, constant current and constant potential coulometry. coulometric titrations and application.

Voltammetry: Principles, dropping mercury electrode (DME), polarography, half-wave potential, diffusion current and Illkovic equation, different wave forms-linear scan, square scan and triangular scan, cyclic voltammetry, voltammograms. Anion/cation striping voltametry and its applications.

Unit 4 11 Hours

Chromatography: Partition and distribution, principles of chromatography, plate and rate theory. retention time and retention factor, resolution and separation factor; general idea about adsorption, partition and column chromatography, paper and thin layer chromatography, gas chromatography (GC) and high performance liquid chromatography (HPLC) - instrumentation, methodology and applications. SFC LC, hyphenated techniques. Ion exchange resins and extraction, Ion Chromatography, anion supressors and ion speciation analysis.

Suggested Readings

- 1. Skoog, D. A., Holler, F. J., and Crouch, S. R. (2017). *Principles of Instrumental Analysis*. Cengage learning.
- 2. Willard, H. H., Merritt Jr, L. L., Dean, J. A., and Settle Jr, F. A. (1988). *Instrumental Methods of Analysis*.CBS Publishers.
- 3. Mendham, J., Denney, R. C., Barnes, J. D., and Thomas, M. J. K. (2008). *Vogel's Textbook of Quantitative Chemical Analysis*, Dorling Kindersley.
- 4. Skoog, D. A., West, D. M., Holler, F. J., and Crouch, S. (2013). *Fundamentals of Analytical Chemistry*. Nelson Education.
- 5. Christian, G. D. (1994). *Analytical Chemistry*. John Wiley and Sons, USA, 331.
- 6. Bard, A. J., and Faulkner, L. R. (2001). *Electrochemical Methods*, 2nd. John Wiley New York, 669.
- 7. Rouessac, F., and Rouessac, A. (2013). *Chemical Analysis: Modern Instrumentation Methods and Techniques*. John Wiley and Sons.
- 8. Danzer, K. (2007). Analytical Chemistry: Theoretical and Metrological Fundamentals. Springer Science and Business Media.

Course Title: Inorganic Chemistry - I

Paper Code: CHM.509 Total Contact Hours: 45

L	T	P	Cr
3	0	0	3

Course Outcome: The completion of this course will endow

- 1. To predict the reaction mechanism, formation constant and stability of the coordination complexes.
- 2. Interpretation of the electronic and magnetic properties.

Unit 1 11 Hours

Metal-Ligand Equilibria in Solution: Stepwise and overall formation constant 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 and its thermodynamic origin, determination of binary formation constants by spectrophotometry and potentiometric (pH) methods.

Unit 2 11 Hours

Reaction Mechanisms of Transition Metal Complexes: Introduction, potential energy diagram and reactivity of metal complexes, ligand substitution reactions, labile and inert metal complexes, acid hydrolysis, factors affecting acid hydrolysis, base hydrolysis, conjugate base mechanism, anation reaction, substitution reactions in square planar complexes, trans effect, mechanism of the substitution reaction reactions without metal ligand bond cleavage, electron transfer processes outer and inner sphere.

Unit 3 12 Hours

Ligand field theory and molecular orbital theory; nephelauxetic series, structural distortion and lowering of symmetry, electronic, steric and Jahn-Teller effects on energy levels, conformation of chelate ring, structural equilibrium, magnetic properties of transition metal ions and free ions presentive, effects of L-S coupling on magnetic properties, quenching of orbital angular momentum by crystal fields in complexes in terms of splitting. effect of spin-orbit coupling and A, E and T states mixing.

Unit 4 11 Hours

Crystal Fields Splitting: Spin-spin, orbital-orbital and spin orbital coupling, LS and J-J coupling schemes, determination of all the spectroscopic terms of pⁿ, dⁿ ions, determination of the ground state terms for pⁿ, dⁿ, fⁿ ions using L.S. scheme, determination of total degeneracy of terms, order of interelectronic repulsions and crystal field strength in various fields, spin orbit coupling parameters (λ) energy separation between different j states, the effect of octahedral and tetrahedral fields on S, P, D and F terms. Splitting patterns of and G, H and I terms. selection rules of electronic transitions in transition metal complexes, relaxation of the selection rule in centrosymmetric and non-centrosymmetric molecules, Orgel diagrams, Tanabe Sugano diagrams, spectrochemical series, band intensities, factors influencing band widths.

Suggested Readings

1. Cotton, F. A., and Wilkinson, G. (1988). *Advanced Inorganic Chemistry* (Vol. 545). New York: Wiley.

- 2. Huheey, J. E., Keiter, E. A., Keiter, R. L., and Medhi, O. K. (2006). *Inorganic Chemistry: Principles of Structure and Reactivity*. Pearson Education India.
- 3. Greenwood, N. N., and Earnshaw, A. (2012). *Chemistry of the Elements*. Elsevier.
- 4. Miessler, G. L. and Tarr, D. A. (2011) *Inorganic Chemistry*, Pearson Education.
- 5. Atkins, P. (2010). Shriver and Atkins' Inorganic Chemistry. Oxford University Press, USA.
- 6. Dutta, R. L., and Syamal, A. (1993). *Elements of Magnetochemistry*. Affiliated East-West Press.
- 7. Drago, R. S. (1992) *Physical Methods for Chemists*. Saunders College Publishing.

Course Title: Organic Chemistry-I

Paper Code: CHM.510 Total Contact Hours: 45

L	T	P	Cr
3	0	0	3

Course Outcome: Students will apply the knowledge of

- 1. Structure activity relationship and predict the mechanism of various organic reactions.
- 2. Mechanistic and synthetic aspects of nucleophilic and electrophilic substitution for various organic reactions.
- 3. Mechanistic and synthetic aspects of addition and elimination for various organic reactions.

Unit 1 11 Hours

Reaction mechanism, structure and reactivity: Classification and determination of reaction mechanisms, kinetic and thermodynamic control, Hammond's postulate, Curtin-Hammett principle, methods of determining mechanisms, isotope effects, effect of structure on reactivity: Hammett equation, Taft equation.

Reactive intermediates: Generation, structure and reactions of carbocations, carbanions, free radicals, carbenes, nitrenes and benzynes. Neighbouring group participation, classical and non-classical carbocations, phenonium ions and norbornyl system.

Aromaticity: Aromaticity in benzenoid and non-benzenoid compounds, antiaromaticity, homoaromatic compounds.

Unit 2 11 Hours

Aliphatic nucleophilic substitution reaction: The S_N^2 , S_N^1 , mixed S_N^2 and S_N^1 , the S_N^i mechanism. Energy profile diagram, nucleophilic substitution at an allylic, aliphatic and vinylic carbon. reactivity effects of substrate structure, attacking nucleophile, leaving group and reaction medium, ambident

nucleophile, regioselectivity, effect of solvent in substitution reaction, competition between $S_N{}^2$ and $S_N{}^1$ mechanisms.

Aromatic nucleophilic substitution: The S_N^{Ar} , bimolecular displacement mechanism and benzyne mechanism, reactivity effect of substrate structure, leaving group and attacking nucleophile.

Aromatic electrophilic substitution: The arenium ion mechanism, orientation and reactivity, energy profile diagrams, *ortho/para* ratio, *ipso* attack, orientation in other ring systems, quantitative treatment of reactivity in substrates and electrophiles.

Unit 3 12 Hours

Elimination reactions: E2, E1 and E1cB mechanisms and their spectrum, orientation of the double bond, effects of substrate structures, attacking base, the leaving group and the medium, mechanism and orientation in pyrolytic elimination.

Addition to carbon-carbon multiple bonds: Mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals, addition of halogen polar reagents to alkenes, Regio- and chemoselectivity, orientation and reactivity, hydroboration, epoxidation and hydroxylation.

Unit 4 11 Hours

Addition to carbon-hetero multiple bonds: Structure and reactivity of carbonyl group towards nucleophilic addition: addition of CN, ROH, RSH, H₂O, hydride ion, ammonia derivatives, LiAlH₄, NaBH₄, organozinc and organolithium reagents to carbonyl and conjugated carbonyl compounds, Arndt-Eistertsynthesis. Mechanism of condensation reactions involving enolates: Aldol, Knoevenagel, Claisen, Dieckmann, Mannich, Benzoin, Perkin and Stobbereactions. Carboxylic acids and derivatives, hydrolysis of esters and amides, ammonolysis of esters.

Suggested Readings

- 1. Clayden, J., Greeves, N., Warren, S. and Wothers, P. (2012) *Organic Chemistry*,Oxford University Press.
- 2. Finar, I. L. (1996). *Textbook OfOrganic Chemistry*. ELBS, Pearson Education UK.
- 3. McMurry, J. (1996). Organic Chemistry, Brooks. Cole, New York, 657.
- 4. Smith, M. B., and March, J. (2013). *March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure*. John Wiley and Sons.
- 5. Ahluwalia, V. K., and Parashar, R. K. (2011). *Organic Reaction Mechanisms*. Narosa Publishing House (P) Ltd.
- 6. Bansal, R. K. (2012). *A Textbook of Organic Chemistry*. New Age International.
- 7. Bansal R.K. (2010) *Organic Reaction Mechanism.* New Age International (P) Ltd.
- 8. Kalsi, P.S. (2010) Organic Reactions and Their Mechanisms. New Age International, New Delhi.

- 9. Lowry, T. H. and Richardson K. S. (1998) *Mechanism and Theory in Organic Chemistry*, Addison-Wesley Longman Inc., New York.
- 10. Morrison, R.T. and Boyd, R.N. (2011) *Organic Chemistry*, Prentice- Hall of India.
- 11. Mukherjee, S.M. and Singh, S.P. (2009) *Reaction Mechanism in Organic Chemistry*. Macmillan India Ltd., New Delhi.
- 12. Robert, J. D. And Casereo, M.C. (1977) Basic Principle of Organic Chemistry. Addison-Wesley.
- 13. Solomon, T.W.G, Fryhle, C.B. and Snyder, S. A. (2013) *Organic Chemistry*. John Wiley and Sons, Inc.
- 14. Sykes, P. A. (1997) Guide Book to Mechanism in Organic Chemistry, Prentice Hall.

Course Title: Physical Chemistry-I

Paper Code: CHM.511 Total Contact Hours: 45

L	T	P	Cr
3	0	0	3

Course Outcome: The students will acquire knowledge of

- 1. Classical thermodynamics and understanding thermodynamic phenomenon in a chemical system
- 2. Statistical thermodynamics and understanding thermodynamic properties in terms of partition functions,
- 3. Maxwell-Boltzmann, Bose-Einstein and Fermi-Dirac statistics, theories of specific heat for solids.

Unit 1 11 Hours

Partial Molar Properties and Fugacity: Partial molar properties. Chemical potential of a perfect gas, dependence of chemical potential on temperature and pressure, Gibbs- Duhem equation, fugacity, its importance and determination, standard state for gases.

Thermodynamics of Simple Mixtures: Thermodynamic functions for mixing of perfect gases. Chemical potential of liquids. Raoult's law, thermodynamic functions for mixing of liquids (ideal solutions only). Real solutions and activities. Activity coefficient; determination of activity and activity coefficients.

Unit 2 11 Hours

Solid-Liquid Solutions: Solutions of nonelectrolytes and electrolytes. Colligative properties of solutions, such as osmotic pressure, depression of the freezing point and elevation of the boiling point.

Phase transition: Phase rule, water, CO₂ phase transition, binary and ternary component phase transitions. Clausius-Clapeyron equation and its application to solid-liquid, liquid-vapour and solid-vapour equilibria.

Unit 3 12 Hours

Statistical Thermodynamics: Statistical concepts and examples, Thermodynamic probability and entropy, Partition function, molar partition function, thermodynamic properties in term of molecular partition function for diatomic molecules, monoatomic gases, rotational, translational, vibrational and electronic partition functions for diatomic molecules, calculation of equilibrium constants in term of partition function.

Unit 4 11 Hours

Theories of Statistical Thermodynamics: Concept of Maxwell-Boltzmann, Bose-Einstein and Dermi-Dirac statistics, Difference between Maxwell-Boltzmann, Bose-Einstein and Fermi-Dirac statistics, Applications of Maxwell-Boltzmann, Bose-Einstein and Fermi-Dirac statistics., Monoatomic solids, theories of specific heat for solids.

Suggested Readings

- 1. Barrow, G. M. (2007) Physical Chemistry. Tata McGraw-Hill Publishers.
- 2. Kapoor, K. L. (2011) *Text Book of Physical Chemistry*.3/5, Macmillan Publishers.
- 3. Atkins, P. and De Paula, J. (2009) *Atkins' Physical Chemistry*. Oxford University Press.
- 4. McQuarrie, D. A. and Simon, J. D. (1998) *Physical Chemistry: A Molecular Approach*. Viva Books.
- 5. Moore, J. W. and Pearson, R. G.(1981) *Kinetics and Mechanism.* John Wiley and Sons.
- 6. Silbey, R. J. Alberty, R. A. and Bawendi, M. G. (2004) *Physical Chemistry*. Wiley-Interscience Publication.
- 7. Engel, T., Reid, P. and Hehre, W. (2012) *Physical Chemistry*. Pearson Education.
- 8. Puri, B.R., Sharma L.R. and Pathania, M.S. (2013) *Principles of Physical Chemistry*. Vishal Publishing Company.
- 9. Rastogi, R. P. and Mishra, R. R. (2013) An Introduction to Chemical Thermodynamics. Vikas Publishing
- 10. Rajaram, J. and Kuriacose, J. C.(2013) Chemical Thermodynamics, Classical, Statistical and Irreversible Thermodynamics. Pearson Education.
- 11. Laurendeau N. M.(2005) Statistical Thermodynamics: Fundamentals and Applications. Cambridge University Press.
- 12. Nash, L. K. (2012) *Elements of Statistical Thermodynamics*. Dover Publication Inc.
- 13. Hill, T. L. (1986) An Introduction to Statistical Thermodynamics. Dover Publications Inc

Course Title: Quantum Chemistry

Paper Code: CHM.512 Total Contact Hours: 45

L	T	P	Cr
3	0	0	3

Course Outcome: The students will be able to

- 1. Interpret and solve the Schrodinger equation various particle in a boundary model, Electronic and Hamiltonian operators for molecules.
- 2. Interpret and demonstrate the Quantum chemical description of angular momentum and term symbols for a one and many-electron systems.
- 3. Relate the Born-Oppenheimer approximation, the Pauli principle, Hund's rules, Hückel theory and the variation principle with the atomic and molecular phenomena.

Unit 1 11 Hours

Fundamental Background: Review of essential mathematical concepts required for quantum chemistry, Postulates of quantum mechanics, Eigen values and Eigen functions, operators, Schrodinger equation.

Unit 2 11 Hours

Translational, Rotational and Vibrational Motions: - Free particle and particle in a box and its application (*i.e.*, quantum tunnelling effect), one-dimensional harmonic oscillator and rigid rotor, particle in a ring, particle on a sphere, hydrogen like atoms

Variation Methods: The variation theorem and its application, linear variation principle, perturbation theory up to second order in energy and its applications.

Unit 3 12 Hours

Angular Momentum: Ordinary angular momentum, generalized angular momentum, Eigen functions and Eigen values for angular momentum, Ladder operator, addition of angular momenta, spin, antisymmetry and Pauli exclusion principle, Slatter determinantal wave functions.

Electronic Structure of Atoms: Electronic configuration, term symbols and spectroscopic states, Russell-Saunders terms and J-J coupling schemes, Term separation energies of pn and dn configurations, Magnetic effects: spin-orbit coupling and Zeeman splitting.

Unit 4 11 Hours

Born-Oppenheimer Approximation: LCAO-MO and VB treatments of the H_2^+ and H_2 , hybridization and valence MOs of H_2O and NH_3 . Huckel Theory of acyclic and cyclic conjugated systems, bond order and charge density calculations.

Suggested Readings

1. Levine, I.N. (2000) Quantum Chemistry. Pearson Education Inc.

- 2. Chandra, A.K. (1994) *Introductory Quantum Chemistry*. Tata Mcgraw-Hill.
- 3. Prasad, R.K., (2009) Quantum Chemistry. New Age Science.
- 4. McQuarrie, D. A. and Simon, J. D. (1998) *Physical Chemistry: A Molecular Approach*. Viva Books.
- 5. Murrell, J.N., Kettle S.F.A. and Tedder, J. M. (1965) *Valence Theory*. John Wiley Publishers.
- 6. Lowe, J. P. and Peterson, K., (2006). *Quantum Chemistry*. Academic Press.

Course Title: Practical Inorganic Chemistry-I (P)

Paper Code: CHM.513 Contact Hours: 60
 L
 T
 P
 Cr

 0
 0
 4
 2

Course outcome: The students will be updated to analyse of

- 1. Volumetric and gravimetric analysis of cations and anions within reaction mixtures.
- 2. Standardization and titrations of various inorganic compounds.

Experiments:

Introduction to good laboratory practices in chemistry. Gravimetric Estimation

- 1. Determination of Ba²⁺ as its sulphate/chromate.
- 2. Estimation of lead as its lead sulfate.
- 3. Estimation of Nickel (II) as its nickel dimethyl glyoximate.
- 4. Estimation of Cu²⁺as cuprousthiocyanate.

Precipitation Titrations

- 1. AgNO₃ standardization by Mohr's method.
- 2. Volhard's method for Cl- determination.

Oxidation-Reduction Titrations

- 1. Standardization of KMnO₄with sodium oxalate and determination of Ca²⁺ ion.
- 2. Standardization of ceric sulphate with Mohr's salt and determination of Cu^{2+} , NO_2 and $C_2O_4^{-2}$ ions.
- 3. Standardization of $K_2Cr_2O_7$ with Fe^{2+} and determination of Fe^{3+} (Ferric alum)
- 4. Standardization of hypo solution with potassium iodate / K₂Cr₂O₇ and determination of available Cl₂ in bleaching powder, Sb³⁺ and Cu²⁺.
- 5. Determination of hydrazine with KIO₃ titration.

Suggested Readings

1. Pass, G. and Sutcliffe H. (1979) *Practical Inorganic Chemistry*. Chapman and Hall Ltd.

- 2. Jolly, W.L. (1961) Synthetic Inorganic Chemistry. Prentice Hall, Inc.
- 3. Nakamoto, K.(1997) *Infrared and Raman Spectra of Inorganic and Coordination Compounds: Part A and B.* John Wiley and Sons,.
- 4. Mendham, J., Denney, R.C., Barnes, J.D.and Thomas, M. J. K.(2000) *Vogel's Textbook of Quantitative Chemical Analysis*, Pearson Education Ltd.
- 5. Svehla, G. and Sivasankar, B. (1996) *Vogel's Qualitative Inorganic Analysis*. Pearson Education Ltd.
- 6. Skoog, D.A., Holler, F.J. and Crouch, S.R.(2007) *Principles of Instrumental Analysis*. Thomson Learning.

Course Title: Practical Organic Chemistry-I (P)

Paper Code: CHM.514 Total Contact Hours: 60

L	T	P	Cr
0	0	4	2

Course Outcome: At the end of this course student will

- (i) Demonstrate and practice good laboratory practices including safe handling of hazardous chemicals, laboratory glassware and equipment(s).
- (ii) Apply various experimental skills for purification, isolation and recrystallization of organic molecules.
- (iii) Analyse the progress of a given reaction on thin layer chromatography.

Experiments:

Safety and Handling of hazardous chemicals:

- (i) Good laboratory practices, handling and disposal of hazardous chemicals.
- (ii) Awareness about different types of glassware, heating devices, equipment(s), how to conduct organic reaction etc.

A. Techniques:

Chromatography: Thin layer chromatography (TLC): Monitoring the progress of chemical reactions, R_f values: identification of unknown organic compounds by comparing the R_f values with known standards. Column chromatography.

Purification Techniques: crystallization, distillation, sublimation.

Determination of melting point and mixed melting point.

- **B. Single Stage Synthesis**: Synthesis of compounds and their purification, aspects such as conversion, theoretical yield and percentage yield should be paid attention. (Attempt any six)
 - 1. Synthesis of chalcones *via* Claisen-Schmidt condensation.
 - 2. Reduction of benzophenone to benzhydral using NaBH₄.
 - 3. Conversion of benzaldehyde to cinnamic acid (Knoevenagel condensation)
 - 4. Conversion of benzaldehyde to dibenzylidene acetone (Aldol condensation)

- 5. To prepare phenylpropene *via* dehydration of corresponding phenyl propanol.
- 6. To prepare ethyl cinnamate *via* acid catalyzed esterification of cinnamic acid.
- 7. Conversion of phthalic anhydride to phthalimide
- 8. To synthesize acylinide analogue of Meldrum acid.
- 9. Synthesis of alcohol *via* addition of Grignard reagent to an aldehyde.
- **C. ChemDraw-Sketch:** Draw the structure of simple aliphatic, aromatic, heterocyclic organic compounds with substituents. Get the correct IUPAC name.

Suggested Readings

- 1. Harwood, L.M. and Moody, C.J. (1989) *Experimental Organic Chemistry*. Blackwell Scientific Publishers.
- 2. Vogel, A.I. (1978) *Textbook of Practical Organic Chemistry*. ELBS, Longman Group Ltd.
- 3. Mann, F.G. and Saunders, B.C. (1975) *Practical Organic Chemistry*. Orient Longman Pvt. Ltd.
- 4. Leonard, J. andLygo, B. (1995) *Advanced Practical Organic Chemistry*. Chapman and Hall,.
- 5. Armarego, W.L. and Chai, C. (2012) *Purification of Laboratory Chemicals*. Butterworth-Heinemann.
- 6. Young, J.A. (1991) *Improving Safety in the Chemical Laboratory: A Practical Guide*. Wiley Publishing.

Course Title: Seminar Paper Code: CHM.541 Total Contact Hours: 15

L	T	P	Cr
1	0	0	1

Course Outcome: The student should elucidate and demonstrate the technical writing and present the problem in hand highlighting the various ways the problem is addressed in the literature.

The seminar must include discussion on topics such as awareness about weapons of mass destruction (chemical, biological, radiological, and nuclear weapons), disarmament, peaceful uses of chemistry, International Regulation of Biological and Chemical or Weapons of Mass Destruction.

Course Title: Inorganic Chemistry-II

Paper Code: CHM.521 Total Contact Hours: 45

I	,	T	P	Cr
3		0	0	3

Course Outcome: The students will be able to

- 1. Elaborate the point group within any chemical structure, character tables and projection operator techniques.
- 2. Relate and apply symmetry and group theory in spectroscopy.
- 3. Demonstrate and explain the structural properties of organometallic complexes and their uses.

Unit 1 11 Hours

Symmetry: Symmetry elements, symmetry operations and their matrix representation, group postulates and types, multiplication tables, point group determination.

Unit 2 11 Hours

Group theory: Determination of reducible and irreducible representations, character tables, construction of character tables for C_2v , C_3v , use of symmetry in obtaining symmetry of orbitals in molecules.

Unit 3 12 Hours

Metal Complexes: Organic-transition metal chemistry, complexes with π -acceptor and σ -donor ligands, 18-electron and 16-electron rules, isolobal analogy, Synthesis and important reaction of metal carbonyls. Structure and bonding of metal carbonyls, metal nitrosyl, dinitrogen and dioxygen complexes, tertiary phosphine as ligand and vibrational spectra of metal carbonyls for bonding and structure elucidation.

Unit 4 11 Hours

Inorganic cages: Metallocenes, metal cluster compounds, metal-metal bond, metal carbenes, carbonyl and non-carbonyl clusters, fluxional molecules, application of organometallic compounds as catalysts in organic synthesis. Cage compounds of boron: boron cage compounds, boranes, carboranes and metallocene carboranes.

Suggested Readings

- 1. Cotton, F. A., and Wilkinson, G. (1988). *Advanced inorganic chemistry* (Vol. 545). New York: Wiley.
- 2. Huheey, J. E., Keiter, E. A., Keiter, R. L., and Medhi, O. K. (2006). Inorganic chemistry: principles of structure and reactivity. Pearson Education India.
- 3. Greenwood, N. N., and Earnshaw, A. (2012). Chemistry of the Elements. Elsevier.

- 4. Lever, A.B.P. (1984) *Inorganic Electronic Spectroscopy*. Elsevier Science Publishers B.V.
- 5. Atkins, P. (2010). Shriver and Atkins' inorganic chemistry. Oxford University Press, USA.
- 6. Dutta, R. L., and Syamal, A. (1993). *Elements of magnetochemistry*. Affiliated East-West Press.

Course Title: Organic Chemistry-II

Paper Code: CHM.522 Total Contact Hours: 45

L	T	P	Cr
3	0	0	3

Course Outcome: The students to be able to

- 1. Interpret and predict the energetically favoured Conformation of cyclic and acyclic compounds, chirality and reactivity.
- 2. Demonstrate, explain and apply basic photochemical reactions, photochemistry of carbonyl and aromatic compounds, various thermally or photochemically driven pericyclic reactions and explain their stereochemical aspects.
- 3. Explain and apply various molecular rearrangements in organic synthesis for the conversion of different functional group.

Unit 1 11 Hours

Stereochemistry: Chirality, projection formulae, configurational conformational isomerism in acyclic and cyclic compounds; stereogenicity, diastereoselectivity, R/S, stereoselectivity. D/L, E/Zand configurational notations, threo and erythro isomers, optical purity, enantiotopic and diastereotopic atoms, groups and faces, stereospecific and stereoselective synthesis, optical activity in the absence of chiral carbon (biphenyls, allenes and spiranes), chirality due to helical shape, conformational analysis of acyclic compounds and cyclic compounds such as cyclopentane, cyclohexane, cyclohexanone derivatives, decalins, 1,2, 1,3-, 1,4-disubstituted cyclohexane derivatives and D-Glucose, effect of conformation on reactivity,

Unit 2 11 Hours

Photochemistry: Jablonski diagram, singlet and triplet states, photosensitization, quantum efficiency, photochemistry of carbonyl compounds, Norrish type-I and type-II cleavages, Paterno-Buchi reaction, Photoreduction, Di π – methane rearrangement.

Photochemistry of aromatic compounds, Photo-Fries reactions of anilides, Photo-Fries rearrangement, Barton reaction, Singlet molecular oxygen reactions.

Unit 3 12 Hours

Pericyclic chemistry: Introduction, Phases, nodes and symmetry properties of molecular orbitals in ethylene, 1,3-butadiene, 1,3,5- hexatriene, allyl cation, allyl radical, pentadienyl cation and pentadienyl radical.

Electrocyclic reactions: Conrotation and disrotation, 4n and 4n+2 systems. Woodward-Hoffmann rules.(i) Symmetry properties of HOMO of open chain partner (ii) Conservation of orbital symmetry and correlation diagrams.

Cycloaddition reactions: Suprafacial and antarafacial interactions. $\pi^2 + \pi^2$ and $\pi^4 + \pi^2$ cycloadditions and stereochemical aspects. Diels-Alder reaction. Woodward-Hoffmann Selection rules. Explanation for the mechanism by (i) Conservation of orbital symmetry and correlation diagrams (ii) FMO theory

Sigmatropic reactions: [1,j] and [i,j] shifts; suprafacial and antarafacial, selection rules for [l, j] shifts; Cope and Claisen rearrangements; explanation for the mechanism by (i) symmetry properties of HOMO (ii) Introduction to cheletropic reactions and the explanation of mechanism by FMO theory.

Unit 4 11 Hours

Rearrangements: General mechanistic considerations-nature of migration, migratory aptitude, mechanistic study of the following rearrangements: Pinacol-pinacolone, Wagner-Meerwein, Benzil-Benzillic acid, Favorskii, Neber, Beckmann, Hofmann, Curtius, Lossen, Schmidt, Carroll, Claisen, Cope, Gabriel-Colman, Smiles and Sommelet-Hauser rearrangements.

Selective Name Reactions: Ene/Alder-ene reaction, Dakin reaction, Reformatsky, Robinson annulation, Michael addition, Hofmann-Loffler Fretag, Chichibabin reaction.

Suggested Readings

- 1. Clayden, J., Greeves, N., Warren, S. and Wothers, P. (2012). *Organic Chemistry*. Oxford University Press.
- 2. Bansal, R. K. (2012). *A Textbook of Organic Chemistry*. New Age International.
- 3. Carey, F. A., and Sundberg, R. J. (2007). *Advanced Organic Chemistry: Part A: Structure and Mechanisms*. Springer Science and Business Media.
- 4. Kalsi, P. S. (2010). *Stereochemistry Conformation and Mechanism*. New Age International.
- 5. Eliel, E. L., and Wilen, S. H. (2008). *Stereochemistry of Organic Compounds*. John Wiley and Sons.
- 6. Carey, F. A., and Sundberg, R. J. (2007). *Advanced Organic Chemistry: Part B.* Springer Science and Business Media.
- 7. Finar, I. L. (1996). Textbook of Organic Chemistry. ELBS, Pearson Education UK.
- 8. Katritzky, A. R., Ramsden, C. A., Joule, J. A., andZhdankin, V. V. (2010). *Handbook of Heterocyclic Chemistry*. Elsevier.
- 9. Norman, R.O.C. and Coxon, J.M. (1998). *Principles of Organic Synthesis*. Blackie Academic and Professional.

- 10. Fleming, I. (2015). Pericyclic Reactions. Oxford University Press.
- 11. Singh, J. (2005). *Photochemistry and Pericyclic Reactions*. New Age International.
- 12. McMurry, J. (1996). Organic Chemistry, Brooks. Cole, New York, 657.

Course Title: Physical Chemistry-II

Paper Code: CHM.523 Total Contact Hours: 45

L	T	P	Cr
3	0	0	3

Course Outcome: The students should be able to

- 1. Evaluate and predict the spontaneity of a redox processes in electrochemical systems
- 2. Evaluate and apply activity coefficient calculated from Debye-Huckel theory in real chemical solutions.
- 3. Establish and evaluate the kinetics and Mechanism for chemical reactions including fast reactions, homogenous and heterogeneous catalysis reactions.
- 4. Understanding of techniques for fast reaction monitoring.

Unit 1 12 Hours

Electrochemistry: Ionic equilibria, electrolytic conductance –Kohlrausch's Law, activity-coefficients, mean activity coefficients; Debye-Huckel treatment of dilute electrolyte solutions, derivation of Debye-Huckel limiting law, extended Debye-Huckel law and conductometric titrations.

Electrochemical Cells: Nernst equation, redox systems, electrochemical cells, application of electrochemical cell, concentration cells with and without liquid junction, thermodynamics of reversible electrodes and reversible cells, potentiometric titration.

Unit 2 11 Hours

Reaction Kinetics: Introduction, rates of chemical reactions, complex reactions, steady state approximation, determination of mechanisms of chemical reactions, temperature dependence of rate constant, Arrhenius and Eyring equations and their applications, collision and transition state theories of rate constant, treatment of unimolecular reactions, steric factor, ionic reactions: salt effect,.

Unit 3 11 Hours

Photochemical Reactions and Processes: Laws of photochemistry and kinetics of photochemical reactions, measurement of fluorescence and phosphorescence lifetimes and photoinduced electron transfer rates, photosensitization, quenching and photodimerization.

Fast Reaction Kinetics: Introduction to time-resolved techniques for absorption and emission measurements, relaxation method, study of kinetics

of fast reactions by millisecond stopped-flow, nanosecond flash photolysis techniques, detection and kinetics of reactive intermediates,

Unit 4 11 Hours

Adsorption and Catalysis: Adsorption of solids, Gibbs adsorption isotherm, BET adsorption isotherm, Langmuir and Fredulich Isotherms. Homogeneous catalysis and heterogeneous catalysis, enzyme catalysis. Michealis-Menten mechanism, Lineweaver-Burk Plot, competitive, non-competitive and uncompetitive bindings, kinetics of catalytic reactions.

Suggested Readings

- 1. Laidler, K. J. (1987). Chemical Kinetics. Pearson Education Ltd.
- 2. Atkins, P. and De Paula, J. (2009) *Atkins' Physical Chemistry*. Oxford University Press.
- 3. Silbey, R. J. Alberty, R. A. and Bawendi, M. G. (2004) *Physical Chemistry*. Wiley-Interscience Publication.
- 4. Engel, T.andReid, P. (2012). *Thermodynamics, Statistical Thermodynamics, and Kinetics*. Pearson Education.
- 5. Lakowicz, J. R. (2006). Principles of Fluorescence Spectroscopy. Springer.
- 6. Barrow, G. M. (2007) Physical Chemistry. Tata McGraw-Hill Publishers.
- 7. Kapoor, K. L. (2011) *Text Book of Physical Chemistry*.3/5, Macmillan Publishers.
- 8. McQuarrie, D. A. and Simon, J. D. (1998) *Physical Chemistry: A Molecular Approach*. Viva Books.
- 9. Moore, J. W., and Pearson, R. G. (1981). *Kinetics and Mechanism*. John Wiley and Sons.
- 10. Raj, G. (2002). Surface Chemistry (Adsorption). Goel Publishing House.
- 11. Moore, J. W. and Pearson, R. G. (1981) *Kinetics and Mechanism.* John Wiley and Sons.
- 12. Puri, B.R., Sharma L.R. and Pathania, M.S. (2013) *Principles of Physical Chemistry*. Vishal Publishing Company.

Course Title: Spectroscopic Analysis

Paper Code: CHM.524 Total Contact Hours: 45

L	T	P	Cr
3	0	0	3

Course Outcome: At the end of this course student will be able to

- Elucidate and demonstrate the application of various spectroscopic techniques (UV, IR, NMR and MS) in organic synthesis.
- Predict NMR spectra and various fragment-ions/peaks in MS of a given molecular structure.
- Analyse and interpret the combined spectroscopic data (UV-Vis, IR, ¹H & ¹³C NMR) for structural elucidation of unknown organic molecules.

Unit 1 11 Hours

UV-Visible spectroscopy: Introduction, role of solvents, chromophores and their interaction with UV-visible radiation. Woodward-Fieser rule for conjugated dienes and carbonyl compounds

Infrared Spectroscopy: Infrared radiation and its interaction with organic molecules, vibrational mode of bonds, effect of hydrogen bonding and conjugation on absorption bands, interpretation of IR spectra. FTIR.

Unit 2 12 Hours

Nuclear magnetic resonance spectroscopy: Introduction, chemical shift and factors influencing chemical shift, reference standards and solvents. spin-spin coupling, effect of deuteration, coupling constants, integration of signals, interpretation of spectra, spin decoupling, double resonance and shift reagent methods, long range coupling, resonance of other nuclei e.g. ¹⁹F, ¹⁵N, ³¹P.

Unit 3 11 Hours

13C NMR: Introduction, Proton coupled and proton decoupled ¹³C NMR, nuclear overhauser enhancement (NOE), DEPT techniques, 2D NMR Correlation spectroscopy (COSY), Homo COSY (¹H-¹H COSY), Hetro COSY (¹H-¹³C COSY, HMQC), long range ¹H-¹³C COSY (HMBC), NOESY.

Unit 4 11 Hours

Mass spectrometry: Basic principles and brief outline of instrumentation. Ion formation: EI, CI, FAB, MALDI, ESI, metastable ion, □-cleavage, McLafferty rearrangement, Retro-Diels-Alder Cleveage, nitrogen rule, fragmentation process of organic molecules in relation to molecular structure determination. Relative abundance of isotopes, High resolution mass spectrometry (HRMS) and recent advances in mass spectrometry.

Problems for structure elucidation using the above spectroscopic techniques.

Suggested Readings

- 1. Banwell, C. N., and McCash, E. M. (1994). Fundamentals of Molecular Spectroscopy(Vol. 851). New York: McGraw-Hill.
- 2. Dyer, J. R. (1965). Applications of Absorption Spectroscopy of Organic Compounds. Phi Learning.
- 3. Kalsi, P. S. (2007). Spectroscopy of Organic Compounds. New Age International.
- 4. Kemp, W. (1998). Organic Spectroscopy, ELBS.
- 5. Khopkar, S. M. (1998). *Basic Concepts of Analytical Chemistry*. New Age International.
- 6. Melinda, J.D. (2010). *Introduction to Solid NMR Spectroscopy*. Wiley India Pvt Ltd.
- 7. Mendham, J., Denney, R. C., Barnes, J. D., and Thomas, M. J. K. (2008). *Vogel's Textbook of Quantitative Chemical Analysis*, Dorling Kindersley.

- 8. Pavia, D. L., Lampman, G. M., Kriz, G. S., and Vyvyan, J. A. (2008). *Introduction to Spectroscopy*. Cengage Learning.
- 9. Silverstein, R. M., Webster, F. X., Kiemle, D. J., and Bryce, D. L. (2014). *Spectrometric Identification of Organic Compounds*. John wileyand sons.
- 10. Gross, J. H. (2006). Mass Spectrometry: A Textbook. Springer Science and Business Media.

Course Title: Molecular Spectroscopy

Paper Code: CHM.525 Total Contact Hours: 45

	L	T	P	Cr
(3	0	0	3

Course Outcome: The students will be able to

- 1. Apply microwave, infrared-vibration-rotation Raman and infra-red Spectroscopy for chemical analysis and prediction of molecular structure
- 2. Demonstrate and apply electronic spectroscopy of different elements and simple molecules.
- 3. Demonstrate and elucidate the physical principles of nuclear magnetic and electron spin resonance spectroscopy.

Unit 1 11 Hours

Electronic Spectroscopy: Electronic transition, energy of electronic transition, selection rules, the Franck-Condon principle.

Microwave Spectroscopy: Classification of molecules, rigid rotor model, effect of isotopic substitution on the transition frequencies, intensities of spectral lines, non-rigid rotor, Stark effect, applications.

Unit 2 12 Hours

Vibrational Spectroscopy: Review of harmonic oscillator, Selection rules, vibrational energies of diatomic molecules, zero point energy, force constant and bond strength, anharmonicity, vibration-rotation spectroscopy, Morse potential energy diagram, P, Q, R branches, vibrations of polyatomic molecules, overtones, hot bands and applications.

Raman Spectroscopy: Classical and quantum theories of Raman Effect, vibrational-rotational Raman spectra, selection rules, mutual exclusion principle, resonance Raman Spectroscopy, surface enhanced Raman spectroscopy, coherent anti stokes Raman spectroscopy.

Unit 3 11 Hours

Magnetic Resonance Spectroscopy: Basic principles of NMR and ESR, instrumentation of NMR and ESR, magnetization vector and relaxation, NMR transitions, Bloch equation, relaxation effects and mechanism, effect of

quadrapole nuclei, nuclear overhauser effect (NOE), multiple pulse methods, Hyperfine splitting in ESR.

Unit 4 11 Hours

Lasers and Laser Spectroscopy: Principles of laser action, pulsed lasers, examples of lasers: He-Ne, Nd-YAG, dye lasers.

Photoelectron spectroscopy: The photoelectric effect, UV photoelectron spectroscopy UPES, X-ray photoelectron spectroscopy XPES.

Suggested Readings

- 1. Hollas, J. M. (2004). Modern Spectroscopy. John Wiley and Sons.
- 2. Lakowicz, J. R. (2006). *Principles of Fluorescence Spectroscopy*. Springer.
- 3. Barrow, G. M. (2007) *Physical Chemistry*. Tata McGraw-Hill Publishers.
- 4. Banwell, C. N., and McCash, E. M. (1994). Fundamentals of Molecular Spectroscopy (Vol. 851). New York: McGraw-Hill.
- 5. Carrington, A., and McLachlan, A. D. (1967). *Introduction to Magnetic Resonance: With Applications to Chemistry and Chemical Physics*. Chapman and Hall, London.
- 6. Lynden-Bell, R. M., and Harris, R. K. (1969). *Nuclear Magnetic Resonance Spectroscopy*. Appleton-Century-Crofts.
- 7. Reilley, C. N., Everhart, D. S., and Ho, F. F. L. (1982). *Applied Electron Spectroscopy for Chemical Analysis. Chemical Analysis*, 63, 105. John Wiley.
- 8. Chang, R. (1971). Basic Principles of Spectroscopy. McGraw-Hill.
- 9. Ghosh, P. K. (1983). *Introduction to Photoelectron Spectroscopy*. John Wileyand Sons, New York.
- 10. Günther, H. (2013). NMR Spectroscopy: Basic Principles, Concepts and Applications in Chemistry. John Wiley and Sons.

Course Title: Practical Inorganic Chemistry -II (P)

Paper Code: CHM.526 Total Contact Hours: 60

L	T	P	Cr
0	0	4	2

Course Outcome: The students will be able to do

- 1. Preparation and purification of different inorganic complexes.
- 2. Analysis via application of UV-Vis, FT-IR, Magnetic moment measurement, Conductivity measurements, NMR and Thermogravimetric analysis for characterization of coordination complexes.
- 3. Preparation of Chloropentaammine cobalt (III) CHMoride and its IR measurements.

- 4. Preparation of [Co(en)₂Cl₂] Cl, Na₂ [Fe(CN)₅ NH₃]. H₂O, [UO₂ (NO₃)₂ Py₂], Cu₂ (CH3COO)₄ (H₂O)₂.
- 5. Preparation of Hg[Co(CNS)₄] and used as standard for the magnetic moment measurement
- 6. Preparation of cis-and trans-K [Cr $(C_2O_4)_2$ $(H_2O)_2$ and its IR study.
- 7. Preparation of bis(2,4-pentanedione)vanadium(IV) acetate and its piperidine or pyridinecomplex. Study of both the complexes with the help of infrared, UV-vis spectroscopy and magnetic susceptibility.
- 8. Preparation of lead tetraacetate.
- 9. Preparation and separation of isomers of $K_3[Fe(C_2O_4)_3]$, Cu(II) and Ni(II) complexes of Schiff base.
- 10. Determination of Chlorophyll content
- 11. Determination of gross calorific value (GCV) for fuels.
- 12. Determination of pour point, flash point and cloud point of liquid fuel.

Suggested Readings

- 1. Pass, G. and Sutcliffe H. (1979). *PracticalInorganicChemistry*. Chapman and Hall Ltd.
- 2. Nakamoto, K. (1997). *Infrared and Raman Spectra of Inorganic and Coordination Compounds: Part A and B.* John Wiley and Sons,.
- 3. Mendham, J., Denney, R.C., Barnes, J.D. and Thomas, M. J. K. (2000). *Vogel's Textbook of Quantitative Chemical Analysis*, Pearson Education Ltd.
- 4. Kolthoff, I. M., and Sandell, E. B. (1944). *Text Book of Quantitative Inorganic Analysis*. The Macmillan; New york.
- 5. Marr, G., andRockett, B. W. (1960). *Practical Inorganic Chemistry*. John Wiley and Sons.
- 6. Jolly, W.L. (1961). Synthetic Inorganic Chemistry. Prentice Hall, Inc.

Course Title: Practical Physical Chemistry-II (P)

Paper Code: CHM.527 Total Contact Hours: 60

L	T	P	Cr
0	0	4	2

Course Outcome: The students will acquire knowledge of development of experimental skills on conductivity meter, potentiometer, pH meter, viscometer, refractometer, spectrophotometer, CD and FTIR for different applications.

- 1. Determination of strength of a given base by titrating with an acid conductometrically.
- 2. Determination of solubility and solubility product of sparingly soluble salts (e.g., PbSO₄, BaSO₄) conductometrically.
- 3. Determination standard electrode potential of Fe²⁺/Fe³⁺ system by potentiometer using potassium permanganate solution.
- 4. Determination of pK_a of acetic acid and glycine by potentiometric titration using NaOH.

- 5. Determination of relative and absolute viscosity of a given liquid.
- 6. Determination of surface tension of alcohols.
- 7. Determination of refractive indices (RI) of given liquids and determination of the concentration from RI.
- 8. Determination of concentrations of proteins and DNAusing spectrophotometer
- 9. Preparation of buffers and measurement of their pH.
- 10. Verification of the Lambert Beer's law.
- 11. Structural analysis of amino acids and proteins using CDand Fluorescencespectrometer.
- 12. Study of chemical and thermal denaturation(T_m and $\Box H_m$) of proteins and DNA using UV-Visible and CD spectrometer.
- 13. Molecular weight of a non-electrolyte by cryoscopy method.
- 14. Determination of stability constant of Fe(III)-salicyclic acid complex by spectrophotometer.
- 15. Determination of mean, median, standard errors, standard deviation, coefficient of variance using software.

Suggested Readings

- 1. Nad, A. K., Mahapatra, B. andGhoshal, A. (2014). *An Advanced Course in Practical Chemistry*. New Central Book Agency (P) Ltd.
- 2. Maity S.,and Ghosh, N.(2012). *Physical Chemistry Practical*. New Central Book Agency (P) Ltd.
- 3. Elias, A. J. (2002). A Collection of Interesting General Chemistry Experiments. Universities Press.
- 4. Khosla, B.D., Garg, V.C., and Gulati A.R. (2007). Senior Practical Physical Chemistry. S. Chandand Sons.
- 5. Yadav, J. B. (2006). *Advanced Practical Physical Chemistry*. Krishna Prakashan Media.
- 6. Das, R. C., and Behera, B. (1983). Experimental Physical Chemistry. Tata McGraw-Hill.
- 7. Das, R.C., and Behra, B.(1983). Experimental Physical Chemistry. 1983, Tata McGraw-Hill.
- 8. James, A. M., and Prichard, F. E. (1974). *Practical Physical Chemistry*. New York: Longman.
- 9. Ghosh, J.C. (1990). Experiments in Physical Chemistry, BharatiBhavan.

Course Title: Seminar Paper Code: CHM.542 Total Contact Hours: 15

L	T	P	Cr
0	1	0	1

Course Outcome: The student would be able to

- 1. Investigate various aspects related to the chemistry problem.
- 2. Appreciate the literature and its relevance to his/her topic of interest

- 3. Technical write and presentation the chemical problem in hand.
- 4. Should generate interest in current topics of research and commercial worth of chemistry.

Seminar would emphasize on problem solving approach and use of various techniques to prove a chemical process /techniques. The seminar would emphasize upon the writeup of introduction, review of literature and cited references. The presentation would promote the use of graphical features of MS-Office and Chemdraw,® apart from spreadsheets and imaging software

Course Title: Research Methodology

Paper Code: CHM.556 Total Lecture: 60

L	T	P	Cr
2	-	-	2

Unit 1 15 Hours

General principles of research: Meaning and importance of research, Critical thinking, Formulating hypothesis and development of research plan, Review of literature, Interpretation of results and discussion.

Bibliographic index and research quality parameters: citation index, impact factor, h index, i10 index, etc. Research engines such as google scholar, Scopus, web of science, etc

Unit-2 15 Hours

Technical and scientific writing: Technical and Scientific writing - theses, technical papers, reviews, electronic communication, research papers, etc., Poster preparation and Presentation and Dissertation. Reference Management using various softwares such as Endnote, reference manager, Refworks, etc. Communication skills-defining communication; type of communication; technicques of communication, etc.

Unit-3 15 Hours

Library: Classification systems, e-Library, Reference management, Web-based literature search engines.

Plagiarism: Plagiarism, definition, Search engines, regulations, policies and documents/thesis/manuscripts checking through softwares, Knowing and Avoiding Plagiarism during documents/thesis/manuscripts/ scientific writing.

Unit-4 15 Hours

Intellectual Property Rights: Intellectual Property, intellectual property protection (IPP) and intellectual property rights (IPR), WTO (World Trade Organization), WIPO (World Intellectual Property Organization), GATT (General Agreement on Tariff and Trade), TRIPs (Trade Related Intellectual Property Rights), TRIMS (Trade Related Investment Measures) and GATS (General Agreement on Trades in Services), Nuts and Bolts of Patenting, Technology

Development/Transfer Commercialization Related Aspects, Ethics and Values in IP.

Suggested Readings:

- 1. Gupta, S. (2005). Research Methodology and Statistical Techniques. Deep and Deep Publications (p) Ltd.
- 2. Kothari, C. R. (2008.) Research Methodology(s). New Age International (p) Limited.
- 3. Web resources: www.sciencedirect.com for journal references, www.aip.org and www.aps.org for reference styles.
- 4. Web resources: www.nature.com, www.sciencemag.org, www.springer.com, www.pnas.org, www.tandf.co.uk, www.opticsinfobase.org for research updates.

Course Title: Inorganic Chemistry-III

Paper Code: CHM.551
Total Contact Hours: 45

L	T	P	Cr
3	0	0	3

Course Outcome: The students will be able to do

- 1. Workout of chemistry of f-block elements
- 2. Structural analysis of inorganic compounds through spectroscopic techniques

Unit 1 11 Hours

Lanthanides, actinides and super-heavy elements: Coordination chemistry, magnetic and spectral properties, comparison of general properties of lanthanides and actinides, comparison with d-block elements, organo lanthanides and actinides, analytical application of lanthanides and actinideslanthanides as shift reagents and high temperature super conductors.

Unit 2 Nuclear Magnetic Resonance (NMR) and Electron Spin Resonance (ESR) Spectroscopy:

NMR: Basic concepts of NMR with emphasis on ³¹P, ¹⁹F, ²⁹Si, ¹¹B, ¹⁰B, ⁵⁷Se, ¹²⁵Te, ⁹⁵Mo, ¹⁰⁹Ag, ¹⁹⁵Pt, ¹¹⁹Sn and an explanations with appropriate examples. NMR study in Fluxional organometallic compounds.

ESR: Hyperfine coupling, spin polarization for atoms and transition metal ions, spin orbit coupling and significance of *g*-tensors, application of transition metal complexes (having one unpaired electron) including biological systems.

Unit 3 11 Hours

Mossbauer Spectroscopy: Basic principles, spectral parameters and spectrum display, application of the technique to the studies of (1) bonding and structures of Fe^{2+} and Fe^{3+} compounds including those of intermediate spin ,

(2) Sn²⁺ and Sn⁴⁺ compounds- nature of M-L bond, coordination number, structure and (3) detection of oxidation state and non-equivalent MB atoms.

Unit 4 11 Hours

Nuclear Chemistry: Classification of nuclides, nuclear stability, atomic energy, types of nuclear reactions-fission and fusion, nuclear decay laws, radioanalytical techniques.

Suggested Readings

- 1. Cotton, F.A. and Lippard, S.J., (1998). *Progress in Inorganic Chemistry*.Vol. 8, Wiley Internationals.
- 2. Lever, A.B.P.,(1984). *Inorganic Electronic Spectroscopy*. Elsevier Science Publishers B.V.
- 3. Parish, R.V.,(1990). NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry. Ellis Harwood.
- 4. Silverstein, R.M., Bassler, G.C., and Morrill, T.C. (2002). Spectrometric Identification of Organic Compounds. John Wileyand Sons.
- 5. Abraham, R. J., Fisher, J., and Loftus, P. (1988). *Introductionto NMR spectroscopy*. Wiley.
- 6. Martin, M. L., Delpuech, J. J., and Martin, G. J. J. (1980). *Practical NMR spectroscopy*. Heyden.
- 7. Williams, D. H., and Fleming, I. (1980). Spectroscopic Methods in Organic Chemistry. McGraw-Hill.
- 8. Greenwood, N. N., and Earnshaw, A. (2012). Chemistry of the Elements. Elsevier.

Course Title: Organic Chemistry-III

Paper Code: CHM.552 Total Contact Hours: 45

L	T	P	Cr
3	0	0	3

Course Outcome: The students will acquire knowledge of:

- 1. Designing a retrosynthetic approach for the synthesis of a target molecule.
- 2. Oxidation and reduction reagents and their application for functional group conversion in organic synthesis.
- 3. Nomenclature, synthesis and reactivity of smaller, five and six membered heterocyclic compounds.

Unit 1 11 Hours

Retrosynthesis: Synthon, synthetic equivalent, functional group interconversion (FGI), functional group addition, functional group elimination, criteria for selection of target, linear and convergent synthesis, retrosynthetic analysis involving chemoselectivity, reversal of polarity (umpolung), importance of the order of events in organic synthesis. One group and two group C-X disconnections, two group C-C disconnections; Diels-Alder reaction, control in carbonyl condensation.

Unit 2 12 Hours

Metal and non-metal mediated oxidation: Mechanism, selectivity, stereochemistry and applications of oxidation reactions, Baeyer-Villiger, Oppenauer oxidation, oxidation reactions using DDQ, NBS, Pb(OAc)₄, Selenium dioxide, PCC, PDC, Cr and Mnreagents, phase transfer catalysis, Periodic acid, Ceric ammonium nitrate,OsO₄, Swern oxidation, hydroboration, Sharpless asymmetric epoxidation, epoxidations using peracids. Recent approaches for oxidation using green oxidants.

Unit 3 11 Hours

Metal and non-metal mediated reduction: Mechanism, selectivity, stereochemistry and applications of catalytic hydrogenations using Pd, Pt and Ni catalysts (Lindlar, Rosenmund, Adam's catalysts)Clemmensen reduction, Wolff-Kishner reduction, Meerwein-Pondorff-Verley reduction, dissolving metal reductions, metal hydride reductions using NaBH₄, NaBH₃CN, NaBH(OAc)₃, LiAlH₄, DIBAL. Wilkinson's catalysis, Birch reduction.

Unit 4 11 Hours

Heterocyclic Chemistry: Systematic nomenclature (Hantzsch-Widman system) for monocyclic, fused and bridged heterocycles, aromatic heterocycle, non-aromatic heterocycle: bond angle and torsional strains and their consequences in small ring heterocycles, conformation of six-membered heterocycles and their synthesis.

Three-membered and four-membered heterocycles: aziridines, oxiranes, thiranes, azetidines, oxetanes. Five membered heterocycles containing two heteroatoms (S,N,O): Diazoles (imidazole, pyrazole), triazoles, oxazoles and thiazoles.

Benzo-fused five-membered and six membered heterocycles:Indoles, benzofurans and benzimidazoles.

Six-membered heterocycles: Synthesis and reactions of coumarins, chromones, pyridine.

Suggested Readings

- 1. Ahluwalia, V. K., and Parasar R. K., (2011). Organic Reaction Mechanism. Narosa Publishing House (P) Ltd., New Delhi.
- 2. Bansal, R. K. (2012). *A Textbook of Organic Chemistry*. New Age International.
- 3. Bansal, R.K. Hetrocyclic Chemistry, 5thEdition, 2010, New Age International (P) Ltd., New Delhi.
- 4. Carey, F. A., and Sundberg, R. J. (2007). *Advanced organic chemistry:* part B. Springer Science and Business Media.
- 5. Finar, I. L. (1996). Textbook of Organic Chemistry. ELBS, Pearson Education UK.
- 6. Gilchrist, T.L.,(1997). *Heterocyclic Chemistry*. Addison Wesley Longman Publishers, US.

- 7. Gupta R.R., Kumar M., and Gupta V., (2010). *Heterocyclic Chemistry-II Five Membered Heterocycles*. Vol. 1-3, Springer Verlag, India.
- 8. Joule, J.A., and Mills, K., (2010). *Heterocyc1ic Chemistry*. Blackwell Publishers, New York.
- 9. Smith, M. B.,(2013). March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure. John Wiley and Sons.
- 10. Warren, S., (2010). Organic synthesis: The Synthon Approach. John Wileyand Sons.
- 11. Warren, S.,andWyatt, P., (2010). Designing Organic synthesis: A Disconnection Approach. John Wiley and Sons.
- 12. Corey, E.J., and Cheng X.-M., (1989). *The Logic of Chemical Synthesis*. John Wiley and Sons.

Course Title: Bio-inorganic and Biophysical Chemistry

Paper Code: CHM.553
Total Contact Hours: 45

L	T	P	Cr
3	0	0	3

Course Outcome: The students will acquire knowledge of

- 1. Structure and biological functions of proteins and enzymes.
- 2. The role of metals in biology
- 3. Factors that govern the thermodynamic stability, folding, and dynamics of proteins.
- 4. Kinetics, thermodynamics, and mechanism of protein folding.

Unit 1 11 Hours

Inorganic Chemistry of Enzymes – I: Metalloporphyrins: Hemoglobin and myoglobin, nature of heme-dioxygen binding, model systems, cooperativity in hemoglobin, structure and function of hemoglobin and myoglobin. Other iron-prophyrin biomolecules, peroxidases and catalases, cytochromes, cytochrome P450 enzymes, other natural oxygen carriers, hemerythrins, electron transfer. Biochemistry of iron, iron storage and transport, ferritin, transferrin.

Unit 2 12 Hours

Inorganic Chemistry of Enzymes – II: Metallothioneins: Ferridoxins, carboxypeptidase, carbonicanhydrase, blue copper proteins, superoxide dismutase, hemocyanines.

Enzymes: Structure and function, inhibition and poisoning vitamin B_{12} and B_{12} coenzymes metallothioneins, bio-inorganic chemistry of Mo and W.

Unit 3 11 Hours

Metal Ions in Biological Systems: Role of metal ions in replication and transcription process of nucleic acids. Biochemistry of calcium as hormonal messenger, muscle contraction blood clotting, neurotransmitter, metals in the regulation of biochemical events.

Unit 4 11 Hours

Biophysical Chemistry: Principles of biophysical chemistry (pH, buffer, reaction kinetics, thermodynamics), physical principle of structure, function, and folding of proteins, conformations of proteins (Ramachandran plot, secondary, tertiary and quaternary structure; domains; motif and folds), determination of protein structures by spectroscopic methods (CD, FTIR, NMR), thermodynamics of protein folding by spectroscopic and calorimetric methods, protein conformational study by NMR and fluorescence spectroscopy,

Suggested Readings

- 1. Huheey, J. E., Keiter, E. A., Keiter, R. L., and Medhi, O. K. (2006). Inorganic chemistry: principles of structure and reactivity. Pearson Education India.
- 2. Douglas, B. E., and McDaniel, D. H. (1965). Concepts and models of inorganic chemistry. John Wiley and Sons.
- 3. Cotton, F. A., and Wilkinson, G. (1988). *Advanced inorganic chemistry* (Vol. 545). New York: Wiley.
- 4. Elschenbroich, C. (2016). Organometallics. John Wiley and Sons.
- 5. Atkins, P., Overtone, T., Rourke, J., Weller, J., and Armstrong, F.,(2010). *Shriver and Atkins' inorganic chemistry*. Oxford University Press.
- 6. Cowan, J.A.(1997). *Inorganic Biochemistry: An Introduction*. Wiley VCH.
- 7. Lippard, S. J. (1991). Progress in Inorganic Chemistry. Vol. 18, Wiley-Interscience.
- 8. Lippard, S. J. (1991). *Progress in Inorganic Chemistry*. Vols. 38, Wiley-Interscience.
- 9. Lesk, A.M., (2010). *Introduction to Protein Science: Architecture, Function, and Genomics*. Oxford University Press.
- 10. Cantor, C.R. and Schimmel, P.R., (980). *Biophysical Chemistry*. Freeman.
- 11. Van Holde, K.E., Johnson, W.C., and Ho, P.S., (2006). *Principles of Physical Biochemistry*. Pearson Education.
- 12. Harding, S.E. and Chowdhry, B. Z. (2001). *Protein-Ligand Interactions*. Oxford University Press.

Course Title: Practical Organic Chemistry-III (P)

Paper Code: CHM.554
Total Contact Hours: 60

L	T	P	Cr
0	0	4	2

Course Outcome: The students will acquire knowledge of

- 1. Various reactions conditions including modern coupling strategies and their implications.
- 2. Various techniques for purification, isolation, recrystallization and charcetrization of synthesized organic molecules.

Experiments:

- **1. Synthesis**: Separation and purification of organic compounds by column chromatography, percentage yield calculation
 - 1. Preparation of allylic alcohols *via*Baylis-Hillman reaction using DABCO as a catalyst and their characterization through various spectroscopic techniques.
 - 2. To study Buchwald-Hartwig reaction of aryl halide with an amine using Cu-based catalyst.
 - 3. Synthesis of triazole *via* reaction of phenylacetylene with azide in water (Huisgen cycloaddition).
 - 4. Synthesis of stilbenes *via* Heck coupling Strategy.
 - 5. To study decarboxylation of Ferulic acid under microwave irradiation.
 - 6. Regionselective reduction of a,β -unsaturated carbonyl compound under microwave irradiation.
 - 7. Synthesis of imidazolium and pyridinium based ionic liquids.
 - 8. To study dehydration of benzylic alcohols using imidazolium based ionic liquid.
 - 9. To synthesize 2-phenyl-1,3,4-oxadiazole from benzhydrazide.
 - 10. To synthesize substituted benzodiazepine from chalcone *via* reflux conditions.
 - 11. Synthesise of benzothiazole starting from 2-aminothiophenol.
 - 12. To study amination of benzothiazole with various amines.
 - 13. To synthesize acylidineanalogue of Meldrum acid.

Suggested Readings

- 1. Harwood, L.M.andMoody, C.J. (1989) Experimental Organic Chemistry. Blackwell Scientific Publishers.
- 2. Vogel, A.I. (1978) *Textbook of Practical Organic Chemistry*. ELBS, Longman Group Ltd.
- 3. Mann, F.G. and Saunders, B.C. (1975) *Practical Organic Chemistry*. Orient Longman Pvt. Ltd.
- 4. Leonard, J. andLygo, B.(1995) *Advanced Practical Organic Chemistry*. Chapman and Hall,.
- 5. Armarego, W.L.and Chai, C. (2012) *Purification of Laboratory Chemicals*. Butterworth-Heinemann.
- 6. Young, J.A. (1991) *Improving Safety in the Chemical Laboratory: A Practical Guide*. Wiley Publishing.

Course Title: Practical Physical Chemistry-III (P)

Paper Code: CHM.555
Total Contact Hours: 60

Ι	,	T	P	Cr
C)	0	4	2

Course Outcome: The students will acquire knowledge of

- 1. Experimental techniques for controlling the chemical reactions.
- 2. Measurement of various physical and chemical properties.

3. Applying related experiments for their research work.

Experiments:

- 1. To verify Freundlich and Langmuir adsorption isotherms for adsorption of acetic acid on activated charcoal.
- 2. Determination of partition coefficient of benzoic acid between organic solvent and water.
- 3. Determination of partition coefficient of iodine between water and octanol and determination of equilibrium constant of tri-iodide.
- 4. Determination of rate constant of hydrolysis of an ester and to study the effect of ionic strength on reaction rate.
- 5. To study kinetics of inversion of cane sugar by optical rotation measurement.
- 6. Determination of activation energy of a reaction by spectrophotometer.
- 7. Energy of activation of acid catalyzed hydrolysis of methyl acetate.
- 8. Kinetics of acid-catalysed reaction between acetone-iodine
- 9. Determination of order of $S_2O_8^{2-} + I^- \rightarrow SO_4^{2-} + I_2$ reaction
- 10. Determination of energy of activation of $S_2O_8^{2-}+I^- \rightarrow SO_4^{2-}+I_2$ reaction
- 11. Studies on the effect of variation of ionic strength on the rate of $S_2O_8^{2-}$ +I $^ \rightarrow$ SO_4^{2-} + I₂reaction
- 12. Determination of the rate constant for the oxidation of iodide ions by hydrogen peroxide studying the kinetics as an iodine clock reaction.
- 13. Curve fitting using linear and non-linear (Activation thermodynamic parameter, equilibrium thermodynamic parameter) regression analysis using software.
- 14. Determination of Michaelis-Menten (K_m) constant in enzyme kinetics.

- 1. Nad, A. K., Mahapatra, B. andGhoshal, A. (2014). *An Advanced Course in Practical Chemistry*. New Central Book Agency (P) Ltd.
- 2. Maity S., and Ghosh, N.(2012). *Physical Chemistry Practical*. New Central Book Agency (P) Ltd.
- 3. Elias, A. J. (2002). A Collection of Interesting General Chemistry Experiments. Universities Press.
- 4. Khosla, B.D., Garg, V.C., and Gulati A.R. (2007). Senior Practical Physical Chemistry. S. Chand and Sons.
- 5. Yadav, J. B. (2006). *Advanced Practical Physical Chemistry*. Krishna Prakashan Media.
- 6. Das, R. C., and Behera, B. (1983). Experimental Physical Chemistry. Tata McGraw-Hill.
- 7. Yadav, J.B., (2008). *Advanced Practical Physical Chemistry*. Krishna Prakashan Media.
- 8. James, A. M., and Prichard, F. E. (1974). *Practical Physical Chemistry*. New York: Longman.
- 9. Ghosh, J.C. (1990). Experiments in Physical Chemistry, Bharati Bhavan.

Course Title: Project
Paper Code: CHM.599
Total Contact Hours: 12

L	T	P	Cr
0	0	12	6

Course Outcome: The student would be able to

- 1. Investigate various aspects related to the chemistry problem.
- 2. Appreciate the literature and its relevance to his topic of interest
- 3. Write synopsis independently
- 4. Would generate interest in current topics of research.

Project supervisor would be allocated at the start of the semester and research project would be undertaken in discussion with the project supervisor. At the end of the semester the student has to prepare a project report as per the university guidelines. Upon submission of the project report, the projects would be evaluated based on a project presentation.

SEMESTER 4

Course Title: Polymer and Solid State Chemistry

Paper Code: CHM.571
Total Contact Hours: 60

L	T	P	Cr
4	0	0	4

Course Outcome: After completion of this course, the students will acquire knowledge of

- 1. Different mechanisms of polymerization, number, weight and viscosity average molecular weights with various techniques
- 2. Processing of thermoplastic and thermosetting polymers, concept of conducting polymers and their applications.
- 3. Physicochemical properties, defects in solid, diffraction techniques, electrical and magnetic properties of materials.

Unit 1 15 Hours

Polymers: Importance of polymers, basic concepts: monomers, repeat Units, degree of polymerization. linear, branched and network polymers, classification of polymers. polymerization: condensation, addition, radical chain-ionic, coordination and copolymerization, polymerization conditions and polymer reactions, polymerization in homogeneous and heterogeneous systems.

Application of Polymers: Phenol-formaldehyde, urea-formaldehyde, melamine-formaldehyde, epoxy resins and curing agents, polyamides: nylon-6, nylon-6, 6,

Unit 2 15 Hours

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, light scattering, osmotic and ultracentrifugation methods, analysis and testing of polymers, chemical analysis of polymers, thermal analysis and physical testing-tensile strength.

Unit 3 15 Hours

Solid State Structure: Primitive lattice vectors, reciprocal lattice, crystal systems and symmetry, bravais lattices, lattice energy, crystal structure of diamond, NaCl, KCl, CsCl, TiO₂, etc,

Defects: Intrinsic and extrinsic defects, point, line and plane defects, vacancies, Schottky defects, Frenkel defects, Thermodynamic and structural aspects.

Diffraction Methods: Basic concepts of X-ray, electron and neutron diffraction methods, structure of simple lattices and X-ray intensities, structure factor and its relation to intensity and electron density, phase identification, X-ray structure analysis, XRD and its applications, polymorphism and cocrystallization.

Unit 4 15 Hours

Semiconductor and Superconductors: Band theory, band gap, metals and semiconductors, intrinsic and extrinsic semiconductors, p-n junctions and other applications

Magnetic Optical Properties: Classification of magnetic materials, Langevin diamagnetism, magnetic domains and hysteresis, optical reflectance, Raman scattering in crystals, photoconduction, lasers, photovoltaic and photocatalytic effects.

Nanomaterials: Nanoparticles: zero dimensional nanostructure, homogeneous and heterogeneous nucleation, metallic nanoparticles- synthesis and applications; nanowires and nanorods: one dimensional nanostructures, spontaneous growth, VLS, electro spinning, lithography; thin film: two dimensional nanostructure- preparation techniques; Langmuir-Blodgett (LB) filmgrowth techniques, photolithography properties and applications.

- 1. Gowariker, V. R., Viswanathan, N. V., and Sreedhar, J. (1986). *Polymer Science*. New Age International.
- 2. Odian, G. (2004). Principles of Polymerization. John Wiley and Sons.
- 3. Peacock, A. J., and Calhoun, A. (2012). *Polymer Chemistry: Properties and Application*. Carl HanserVerlag GmbH Co KG.
- 4. Chandra, R., and Adab, A. (1994). Rubber and Plastic Waste: Recycling, Reuse and Future Demand. CDB Publishers.
- 5. Bahadur, P., and Sastry, N. V. (2005). *Principles of Polymer Science*. Narosa Publishing House, New Delhi .
- 6. Ashcroft, N. W., and Mermin, N. D. (1976). *Introduction to Solid State Physics*. Saunders.

- 7. Callister Jr, W. D., and Rethwisch, D. G. (2012). Fundamentals of Materials Science and Engineering: An Integrated Approach. John Wiley and Sons.
- 8. Anderson, J. C., Leaver, K. D., Rawlings, R. D., and Leavers, P. S. (2004). *Materials Science for Engineers*. CRC Press.
- 9. Keer, H. V. (1993). Principles of the Solid State. New Age International.

Course Title: Concepts in Chemistry-I

Paper Code: CHM.572 Total Contact Hours: 30

L	T	P	Cr
2	0	0	2

Course Outcome: The student will able to exercise and understand various applications of

- 1. Spectroscopic techniques for structural elucidation of unknown compounds.
- 2. Various reagent and organic transformations, their mechanism and stereochemical aspects.
- 3. Reactivity of heterocyclic compounds and utility of natural products

Unit 1 7 Hours

Combined Structure problems: Exercises of structure elucidation of unknown compounds *via* combined spectral interpretation of IR, UV-vis, Hand Hand MR and mass spectra, along with two-dimensional NMR spectroscopy. IUPAC nomenclature of organic molecules including regio- and stereoisomers.

Unit 2 7 Hours

Organic reaction mechanisms: involving addition, elimination and substitution reactions with electrophilic, nucleophilic or radical species. Determination of reaction pathways.

Various strategies for asymmetric synthesis and its applications in natural products and drug molecules.

Unit 3 8 Hours

Organic transformations and reagents: Functional group interconversion including oxidations and reductions; common catalysts and reagents: organic, inorganic, organometallic and enzymatic. Chemo, regio and their applications in organic synthesis. stereoselective transformations. Green catalysts in organic synthesis. Exercises on stereochemical aspects of various pericyclic reactions.

Unit 4 8 Hours

Reactivity of common heterocyclic compounds containing one or two heteroatoms (O, N, S) and their utility in organic synthesis. Chemistry of natural products: Carbohydrates, proteins and peptides, fatty acids, nucleic acids, terpenes, steroids and alkaloids.

Suggested Readings

- 1. Pavia, D.L., Lampman, G. M., Kriz, G. S., and Vyavan, J. R., (2010). *Introduction to Spectroscopy*. Harcourt College, NY.
- 2. Dewick, P.M., (2009). *Medicinal Natural Products: A Biosynthetic Approach*. Wiley and Sons, UK.
- 3. Finar, I.L. (2006). *Organic Chemistry: Stereochemistry and the Chemistry of Natural Products*. Dorling Kindersley Pvt. Ltd., India.
- 4. Claydon, J., Gleeves, N., Warren, S. AndWother, P., (2001). *Organic Chemistry*. Oxford University Press, UK.
- 5. Fleming, I., (2015). Pericyclic Reactions. Oxford University Press.
- 6. Carey B. F. A., and Sundberg R.J., (2007). *Advanced Organic Chemistry Part B.* Springer Science and Business Media Ltd.

Course Title: Concepts in Chemistry-II

Paper Code: CHM.573 Total Contact Hours: 30

L	T	P	Cr
2	0	0	2

Course Outcomes: The student will acquired understanding of physical concept involving in quantities errors, Kinetics, thermodynamics, photochemistry and electrochemistry.

Unit 1 7 Hours

Structure and bonding: Electronic configuration of atoms (L-S coupling) and the periodic properties of elements; Ionic radii, Ionisation potential, electron affinity, electronegativity; concept of hybridisation. Molecular orbitals and electronic configuration of homo- and hetero-nuclear diatomic molecules. Shape of polyatomic molecules; VSEPR theory, Symmetry elements and point groups for simple molecules. Acid and bases concepts, pH and pKa, HSAB concept, Buffer solution. Properties of solid state and solution phase.

Unit 2 8 Hours

Aspects of s, p, d and f-block elements: General characteristics of each block. Chemistry of representative (s and p-block) elements, Coordination chemistry of transition elements. Chemistry of lanthanide and Actinides.

Unit 3 7 Hours

Thermodynamics: Concepts involved in first, second and third law of thermodynamic, Maxwell relations, Helmholtz and Gibbs Energies, equilibrium constant, temperature-dependence of equilibrium constant and Van't Hoff equation, Colligative properties of solutions.

Unit 4 8 Hours

Electrochemistry: Ionic equilibria, ion conduction mechanism, solutions of nonelectrolytes and electrolytes, electrolytic conductance –Kohlrausch's Law,

transport number and its determination, Nernst equation, redox systems, electrochemical cells.

Basics of Photochemistry: Absorption, excitation, laws of photochemistry, quantum yield, lifetime of excited states, photochemical stages-primary and secondary process.

Kinetics: Introduction, rates of chemical reactions, Kinetics of photochemical reactions.

Suggested Readings

- 1. Cotton, F. A., and Wilkinson, G. (1988). *Advanced Inorganic Chemistry* (Vol. 545). New York: Wiley.
- 2. Huheey, J. E., Keiter, E. A., Keiter, R. L., and Medhi, O. K. (2006). *Inorganic Chemistry: Principles of Structure and Reactivity*. Pearson Education India.
- 3. Greenwood, N. N., and Earnshaw, A. (2012). Chemistry of the Elements. Elsevier.
- 4. Miessler, G. L. and Tarr, D. A. (2011) *Inorganic Chemistry*, Pearson Education.
- 5. Atkins, P. (2010). Shriver and Atkins' Inorganic Chemistry. Oxford University Press, USA.
- 6. Barrow, G. M. (2007) *Physical Chemistry*. Tata McGraw-Hill Publishers.
- 7. Kapoor, K. L. (2011) *Text Book of Physical Chemistry*. 3/5, Macmillan Publishers.
- 8. Atkins, P. and De Paula, J. (2009) *Atkins' Physical Chemistry*. Oxford University Press.
- 9. Moore, J. W. and Pearson, R. G.(1981) *Kinetics and Mechanism.* John Wiley and Sons.
- 10. Puri, B.R., Sharma L.R. and Pathania, M.S. (2013) *Principles of Physical Chemistry*. Vishal Publishing Company.
- 11. Laidler, K. J. (1987). Chemical Kinetics. Pearson Education Ltd.
- 12. Rohatgi-Mukherjee, K. K., (1986). Fundamentals of Photochemistry. New Age International.

Course Title: Advanced Organic Synthesis

Paper Code: CHM.574
Total Contact Hours: 60

L	T	P	Cr
4	0	0	4

Course Outcomes: The students will apply the knowledge of

- 1. Asymmetric synthesis and chiral resolution.
- 2. Various reagents including organometallic compounds, experimental conditions and their applications in organic synthesis.
- 3. Some important reactions utilizing phosphorus and sulphur ylides.

Unit 1 15 Hours

Asymmetric synthesis: Chiral pools, chiral catalysis: chiral auxiliaries, methods of asymmetric induction – substrate, reagent and catalystcontrolled reactions; determination of enantiomeric and diastereomeric excess; enantio-discrimination. resolution – optical and kinetic, chemo- regio- and stereoselective transformations, organocatalysis and biocatalysis

Unit 2 15 Hours

Reaction of ylides: Phosphorus ylide; structure and reactivity, stabilized ylides, effects of ligands on reactivity, Witting, Wittig-Horner and Wadsworth, Emmons reactions-mechanistic realization; E/Z selectivity for olefin formation, Schlosser modification: Sulphur ylides; stabilized and non-stabilized ylides: thermodynamically and kinetically controlled reactions with carbonyl compounds, regio- and stereo-selective reactions. Nitrogen Ylides, Stevens rearrangement.

Unit 3 15 Hours

Organometallic compounds: Organoboranes: Preparation of organobornaesviz dicylohexyl hvdroboration with BH₃-THF, borane. disiamvlborane. thexylborane, 9-BBN, diisopinocampheyl borane. functional transformations oxidation. protonolysis of organo boranes: and rearrangements. formation of carbon-carbon-bonds υiz organoboranescarbonylation.

Organolithium, organozinc, organosilicon, organopalladium and organostannous compounds: applications in C-C coupling reactions.

Unit 4 15 Hours

Reagents in organic synthesis: Gilman'sreagent, Lithium diisopropylamide(LDA), 1,3-Dithiane (Umpolung reagent), Trimethylsilyl iodide, Bakersyeast,Prevost Hydroxylation, Crown ether, Merrifield resin, Fenton's reagents, Ziegler-Natta catalyst, Lawsson reagents, K-selecteride and L-selecteride, IBX,Fetizon reagent, Dioxiranes, Tebbe reagent, Corey-Nicolaou reagent and macrolactonisation, Mosher's reagent.

- 1. Claydon, J., Gleeves, N., Warren, S., and Wother, P., (2001). *Organic Chemistry*. Oxford University Press, UK.
- 2. Finar, I.L., (2012). Organic Chemistry. Pearson Education, UK.
- 3. Li, J. J., (2014). Name Reactions: A Collection of Detailed Reaction Mechanism. Springer-Verlag.
- 4. Smith, M. B., (2013). March's Advanced Organic Chemistry: Reactions, Mechanisms, And Structure. John Wiley and Sons.
- 5. Corey, E.J. and Cheng, X.-M.(1989). *The Logic of Chemical Synthesis*. John Wiley and Sons.
- 6. Fuhrhop, J. H., Penzlin, G., and Li, G., (2003). *Organic Synthesis: Concepts And Methods*. John Wiley and Sons.

- 7. Davies, S. G., (2013). Organotransition Metal Chemistry: Applications to Organic Synthesis: Applications to Organic Synthesis (Vol. 2). Elsevier.
- 8. Aitken, A., and Kilényi, S. N., (Eds.). (1992). Asymmetric Synthesis. CRC Press.
- 9. Proctor G. (1996). Asymmetric Synthesis. Academic Press.
- 10. Mundy, B. P., Ellerd, M. G., and Favaloro Jr, F. G., (2005). *Name Reactions And Reagents In Organic Synthesis*. John Wiley and Sons.

Course Title: Chemistry of Natural Products

Paper Code: CHM.575
Total Contact Hours: 60

L	T	P	Cr
4	0	0	4

Course Outcome: At the end of this course student will be

- 1. familiar with various types of natural products and their importance.
- 2. Identify various types of natural products including their properties, occurrence, structure and biosynthesis.

Unit 1 15 Hours

Terpenoids and Carotenoids: Classification, nomenclature, occurrence, isolation, general methods of structure determination, isoprene rule. Structure determination, stereochemistry, biosynthesis and synthesis of the following representative molecules: Geraniol, Menthol and β -Carotene

Unit 2 15 Hours

Alkaloids: Nomenclature and physiological action, isolation, general methods of structure elucidation, degradation, classification based on nitrogen heterocyclic ring, structure, stereochemistry, synthesis of the following: Ephedrine, Nicotine and Morphine.

Unit 3 15 Hours

Steroids: Occurrence, nomenclature, basic skeleton and stereochemistry, structure determination and synthesis of cholesterol, partial synthesis of testosterone and progesterone, chemical tests for steroids

Unit 4 15 Hours

Plant pigments: Occurrence, nomenclature and general methods of structure determination. isolation and synthesis of anthocyanins

Carbohydrates: Introduction of sugars, structures of triose, tetrose, pentose, hexose, stereochemistry and reactions of glucose, conformation and anomeric effects in hexoses

- 1. Bhat, S.V., Nagasampagi, B.A., and Meenakshi, S. (2009). *Natural Product Chemistry and Applications*. Narosa Publishing House, New Delhi.
- 2. Bhat, S.V., Nagasampagi, B.A., and Sivakumar, M. (2005). *Chemistry of Natural Products*. Narosa Publishing House, New Delhi.

- 3. Cseke, L.J., (2009). Natural Products from Plants. CRC Press.
- 4. Dewick, P.M. (2009). *Medicinal Natural Products: A Biosynthetic Approach*. Wiley and Sons, UK.
- 5. Finar, I.L.,(2006). Organic Chemistry: Stereochemistry and the Chemistry of Natural Products. Dorling Kindersley Pvt. Ltd., India.
- 6. Peterson, F. and Amstutz, R., (2008). *Natural Compounds as Drugs*. Birkhauser-Verlay.

Course Title: Organotransition Metal Chemistry

Paper Code: CHM.576 Total Contact Hours: 60

L	T	P	Cr
4	0	0	4

Course Outcome: At the end of this course student will be able to

- 1. The chemistry of transition metal complexes and compounds of transition metal-carbon multiple bonds
- 2. Chemistry on alkyls and aryls of transition metals and fluxional organometallic compounds
- 3. Workout on homogeneous catalysis with appropriate planning.

Unit 1 15 Hours

Compounds of Transition Metal-Carbon Multiple Bonds: Alkylidenes, alkylidynes, low valent carbenes and carbynes-synthesis, nature of bond, structural characteristics, nucleophilic and electrophilic reaction on the ligands, role in organic synthesis

Unit 2 15 Hours

Transition Metal Complexes: Transition metal complexes with alkyl and unsaturated organic molecules, alkenes, alkynes, allyl, diene, dienyl, arene and trienyl complexes, preparations, properties, nature of bonding and structural features important reactions relating to nucleophilic and electrophilic attack on ligands and to organic synthesis.

Unit 3 15 Hours

Aryls of Transition Metals: Types, routes of synthesis, stability and decomposition pathways, applications in organic synthesis.

Unit 4 15 Hours

Homogeneous Catalysis: Stoichiometric reaction for catalysis, homogeneous catalytic hydrogenation, Zeigler-Natta polymerization of olefins, catalytic reactions involving carbon monoxide such as hydrocarbonylation of olefins (oxo reaction) oxo-palladation reactions, activation of C-H bond.

Suggested Readings

- 1. Collman, J.P., Norton, J.R., Hegsdus, L.S. and Finke, R.G., (1987) *Principles and Application of Organotransition Metal Chemistry*. University Science Books.
- 2. Crabtree, R.G. (2011). The Organometallic Chemistry of the Transition *Metals*. John Wiley.
- 3. Mehrotra, R. C., and Singh, A., (2005). Organometallic Chemistry. New Age International.
- 4. Cotton, F.A., and Wilkinson, G., (1999). *Advanced Inorganic Chemistry*. John Wiley.
- 5. Pearson, A.J., (1985). Metallo-Organic Chemistry. Wiley.

Course Title: Environmental Chemistry

Paper Code: CHM.577
Total Lectures: 60

L	T	P	Cr
4	0	0	4

Course Outcome: The student will acquire knowledge of

- 1. Various chemical processes in the air water and soil environment
- 2. Various policy implication for applied chemists
- 3. Treatment technologies adopted for various wastewaters

Unit 1 15 Hours

Aquatic chemistry: Surface, ground water, marine and brackish water resources - assessment and utilization; Rivers and Lakes in India; hydrological cycle; Structure and properties of water, Water quality parameters, Physicochemical concepts of color, odour, turbidity, pH, conductivity, DO, COD, BOD and its kinetics, Carbonates and alkalinity, redox potential, Pourbiax diagram, pH-pE diagrams for Iron, oxoanions and anions, Environmental Issues: Ground water depletion; Water logging and salinity; Water Conservation and management techniques; Rain water harvesting; Watershed management; Eutrophication; Restoration of Lakes, transboundary river water sharing and interlinking of rivers.

Interfacial Interactions: Environmental chemistry of arsenic, chromium, Chemical potential, fugacity and its application to fugacity model.

Unit 2 15 Hours

Water treatment Technologies: Chemical and Physical Methods of wastewater treatment with emphasis on sedimentation, coagulation, adsorption, water softening, defluoridation and ion exchange process.

Membrane Processes: Reverse Osmosis, Types of membrane, characterization of membranes, nano-membranes and their formation, efficiency of different membranes in removal of different elements.

Biological wastewater treatment including Activated sludge process, trickling filter and Membrane bioreactor, biological treatment processes - process description, design and application.

Unit 3 15 Hours

Atmospheric chemistry: Composition of air, Chemical speciation, particles, ion and radicals, Formation of particulate matter, Photochemical reactions in the atmosphere, Chemistry of air pollutants, Photochemical smog, Acid rain, Ozone Chemistry and Montreal Protocol, Greenhouse gases and Global warming, Clean Development Mechanism and Kyoto Protocol, Persistant Organic Pollutants (POP) and Stockholm Convention.

Sources of Natural and Artificial Radiations: Dosimetry, types of dosimeters, radioactive substances, applications and handling of isotopes and other radionuclides in environment. Biochemical and Toxicological aspects of arsenic, cadmium, lead, mercury, carbon monoxide, O₃, PAN, MIC and other carcinogens.

Unit 4 15 Hours

Chemistry of Soil: Physio-chemical composition of soil, humus, inorganic and organic components of soil, nutrients (NPK) in soil, significance of C:N ratio, cation exchange capacity (CEC), reactions in soil solution, ion exchange (physiosorption), ligand exchange (chemisorption), complexations, chelation; precipitation / dissolution.

Environmental Geochemistry: Concept of major, trace and REE. classification of trace elements, mobility of trace elements, geochemical cycles.

Waste Management: Biomass waste management, biomedical waste management and chemical waste management, design and construction of waste management site. Regulations for waste management.

- 1. Baird, C., and Cann, M., (2008). Environmental Chemistry. W.H. Freeman, USA
- 2. Manahan, S. E., (2008). Fundamentals of Environmental Chemistry. CRC Press, USA
- 3. Connell D. W. (2005). Basic concepts of Environmental Chemistry, CRC Press, USA
- 4. Girard, J., (2010). *Principles of Environmental Chemistry*. Barlett Publishers, USA.
- 5. Harrison, R. M., (2007). *Principles of Environmental Chemistry*. RSC Publishing, UK
- 6. Hillel, D., (2007). Soil in the Environment: Crucible of Terrestrial Life. Academic Press, USA.
- 7. Manahan, S. E., (2010). Water Chemistry: Green Science and Technology of Natures Most Renewable Resource. CRC Press, USA.

- 8. Tchobanoglous, G., Burton, F. L., and Stensel, H. D., (2003). Wastewater Engineering: Treatment and Reuse. McGraw-Hill Science, USA.
- 9. American Public Health Association, American Water Works Association and Water Environment Federation, (2005). *Standard Methods for the Examination of Water and Wastewater*. American Public Health Association.
- 10. Eckenfelder, Jr., W.W., Ford, D.L., and Englande, A.J., Jr. (2009). *Industrial water quality.* McGraw-Hill.
- 11. Crittenden, J. C., Trussell, R. R., and Hand, D. W., (2005). *Water treatment: principles and design*. Wiley Publishers, USA.
- 12. Grady Jr, C. L., Daigger, G. T., Love, N. G., and Filipe, C. D. (2011). *Biological Wastewater Treatment*. CRC Press.

Course Title: Inorganic Photochemistry

Paper Code: CHM.578
Total Contact Hours: 60

L	T	P	Cr
4	0	0	4

Course Outcomes: The student will be able to handle

- 1. Inorganic photochemistry and photophysical chemistry.
- 2. The characterization of transient intermediates by ultrafast modern techniques.
- 3. The theory of photoreaction.
- 4. The photochemistry and photophysical chemistry of macromolecules.

Unit 1 15 Hours

Basics of Photochemistry: Electronic transitions, Jablonski diagram and photophysical processes, radiative transitions, absorption and emission, phosphorescence, intersystem crossing, mechanisms of singlet-triplet conversion (spin-orbit coupling), examples of ISC between states of different configurations, radiative rates, radiationless transitions, internal conversion, energy gap.

Unit 2 15 Hours

Photochemical Mechanism: Properties of excited states- structure, dipole moment, photochemical kinetics- calculation of rates of radiative process; bimolecular deactivation- quenching; excited states of metal complexes comparison with organic compounds, electronically excited states of metal complexes, charge transfer excitation.

Unit 3 15 Hours

Ligand Field Photochemistry: Photosubstitution, photooxidation and photoreduction, ground state and excited state, energy content of the excited state, development of redox potentials of the excited states; redox reactions by excited metal complexes- energy transfer(FRET and SET), exciplex formation,

Unit 4 15 Hours

Applications of Photochemistry: Measurement of fluorescence and phosphorescence and lifetimes, introduction to time-resolved techniques for absorption and emission measurements, detection and kinetics of reactive intermediates, photochromic reactions and memory devices, sensors, switches and molecular machines, TiO₂photocatalysis, flash photolysis.

Suggested Readings

- 1. Lakowicz, J. R., (2006). Principles of Fluorescence Spectroscopy, Springer.
- 2. Rohatgi-Mukherjee, K. K., (1986). Fundamentals of Photochemistry. New Age International.
- 3. Kryukov, A. I., and Yakuchmii, S., (1990). Fundamentals of Photochemistry of Coordination Compounds.
- 4. Kavarnos, G. J. (1993). Fundamentals of Photoinduced Electron Transfer. Vch Pub.
- 5. Valeur, B., and Berberan-Santos, M. N. (2012). *Molecular Fluorescence: Principles and Applications*. John Wiley and Sons.
- 6. Turro, N. J., Ramamurthy, V., and Scaiano, J. C. (2012). *Modern Molecular Photochemistry of Organic Molecules*. Wiley Publishers.
- 7. Ninomiya, I., and Naito, T. (2012). *Photochemical Synthesis*. Academic Press.

Course Title: Current Trends in Organic Synthesis

Paper Code: CHM.579
Total Contact Hours: 60

L	T	P	Cr
4	0	0	4

Course Outcome: At the end of this course student will be able to

- 1. Understand and apply the concept of free radical chemistry for various coupling reactions including metal free C-H bond activation/fictionalization
- 2. Apply the concept of enolate chemistry for controlling the selectivity of various organic transformations.
- 3. Design various processes taking into consideration the protection and deprotection.

Unit 1 15 Hours

Free radical reactions: Types of free radical reactions, free radical substitution mechanism at an aromatic substrate, free radical rearrangement, 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), auto-oxidation. Coupling of alkynes and arylation of aromatic compounds by diazonium salts. Recent trends in oxidative functionalization of C-H bond *via* free radical chemistry.

Unit 2 15 Hours

Enolate Chemistry: Regio- and stereo-selectivity in enolate generation. "O" versus "C" alkylation, effect of solvent, counter-cation and electrophiles; symbiotic effect; thermodynamically and kinetically controlled enolate formations; various transition state models to explain stereoselectiveenolate formation; enamines and metallo-enamines; regioselectivity in generation, application in controlling the selectivity of alkylation.

Unit 3 15 Hours

Protection and deprotection of various functional groups:Protection of alcohols by ether, silyl ethers and ester formations and their deprotection, protection of carbonyls by acetal and ketal formation and their deprotection, protection of 1, 2 diols- by acetal, ketal and carbonate formation and their deprotection, protection of amines by acetylation, benzylation, benzyloxy carbonyl, *t*-butoxycarbonyl (Boc), fmoc, triphenyl methyl groups and their deprotection, protection of carboxylic acids by ester formation and their deprotection: Recent advances in protection-deprotection free organic synthesis.

Unit 4 15 Hours

New synthetic reactions: Baylis-Hillman reaction, Biginelli reaction, Mukaiyama aldol reaction, Mitsunobu reaction, McMurrey reaction, Julia-Lythgoe olefination, and Peterson's stereoselective olefination, Buchwald-Hartwig coupling, Eishenmosher-Tanabe fragmentation and Shapiro reaction, Stork-enamine reaction, Aza-Cope, Aza-Wittig reaction, Ugi reaction, Robinson-Gabriel synthesis, Vilsmeier-Haack reaction.

- 1. Finar, I.L., (2012). Organic Chemistry Vol. 1. Pearson Education, UK.
- 2. Finar, I.L., (2012). Organic Chemsitry Vol. 2: Stereochemistry and the Chemistry of Natural Products. Pearson Education, UK.
- 3. Fleming I., (2011). *Molecular Orbitals and Organic Chemical Reactions*. John Wiley and Sons.
- 4. Li, J. J., (2014). Name Reactions: A Collection of Detailed Reaction Mechanisim. Springer-Verlag.
- 5. Kalsi, P.S. (2010). Organic Reactions and Their Mechanisms. New Age International Pub.
- 6. McMurry, J. (1996). Organic Chemistry, Brooks Cole,.
- 7. Mukherjee, S.M., and Singh, S.P., (2009). *Reaction Mechanism in Organic Chemistry*. Macmillan India Ltd.
- 8. Smith, M. B., (2013). *March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure.* John Wiley and Sons.
- 9. Solomon, T.W.G., Fryhle, C.B. and Snyder, S. A., (2013). *Organic Chemistry*. John Wiley and Sons, Inc.
- 10. Sykes, P. A.(1997). Guide Book to Mechanism in Organic Chemistry. Prentice Hall.

11. Carruthers, W. (2004). Some Modern Methods of Organic Synthesis. Cambridge Uni. Press, UK.

Course Title: Supramolecular Chemistry

Paper Code: CHM.580 Total Contact Hours: 60

L	T	P	Cr
4	0	0	4

Course Outcome: The students will acquire knowledge of

- 1. Various supramolecular aspects of interaction between two chemical systems.
- 2. Devising supramolecular systems based on complementarily and preorganizational requirements of host.

Unit 1 15 Hours

Introduction: Definition and development of supramolecular chemistry, nature of binding interactions in supramolecular structures: ion-ion, ion-dipole, dipole-dipole, h-bonding, cation , anion , anion , and van der waals interactions, supramolecular chemistry in life, ionophores, porphyrin and other tetrapyrrollic macrocycles, coenzymes, neurotransmitters, DNA and biochemical self-assembly. Classification of supramolecular host-guest compounds, pre- organization and complementarily, receptors, nature of supramolecular interactions.

Host-guest chemistry: synthesis and structure of crown ethers, lariat ether and podands, cryptands, spherands, calixarenes, cylcodextrins, cyclophanes, carcerands and hemicarcerands. Concepts of selectivity, macrocyclic, macrobicyclic synthesis and template effects,

Unit 2 15 Hours

Cation Binding: Binding Constant and its determination, concept of coordination chemistry, cation complexation using various preorganized host, soft ligands including N, S and P based macrocycles, Schiff's base, proton and ammonium ion complexation, carbon donor and π - acid ligands, siderophores. **Anion Receptor:** Anion recognition and its biological relevance, concepts on anion host design, from cation to anion hosts- a simple change in pH,

anion host design, from cation to anion hosts- a simple change in pH, guanidinium- based receptors, neutral receptors, organometallic receptors, coordination interactions. Chromogenic and cluorogenic receptors, dosimeters, ion pair recognition and zwitterion recognition.

Inclusion Complexes: Molecular guests and their inclusion complexation with Cyclodextrin, molecular clefts, tweezers, cryptophanes, cyclophanes, carcerands and hemicarcerands, solid state inclusion including clathrate formation, solid-liquid, solid-gas inclusions.

Unit 3 15 Hours

Molecular Self-assembly: Supramolecular polymers: definition, kineic and thermodynamic consideration of self-assembly. self-assembly molecules: design, synthesis and properties of the molecules, self-assembly by H-bonding,

proteins and foldamers, DNA, catenanes, rotaxanes, molecular knot: topology and examples including trefoil and borromean rings, surfactants self assembly, liquid crystals.

Dendrimers structure and nomenclature, synthesis and characterization, supramolcular chemistry of dendrimers and its assembly, dendritic nanodevices

Supramolecular polymers including amphiphilic block polymers and molecular imprinter polymers, biological self assembly in amyloids, actins and fibrin, COF and supramolecular gels.

Unit 4 15 Hours

Supramolecular and Molecular Devices: Supramolecular photochemistry and catalysis, molecular electronic devices: molecular electronic devices, molecular wires, molecular rectifiers, molecular switches and molecular logic gates, non linear optical devices, organics for photonics and electronics.

Molecular Machines: Molecular machine terminology and bio-inspiration, ratchet mechanism including pulsating and tilt mechanism, covalent and supramolecular motors and their controlling mechanisms, machines based on catenanes and rotaxanes. Applications as molecular walkers, switchable catalysts, surface analysis at molecular dimensions.

Suggested Readings

- 1. Steed, J. W., and Atwood, J. L. (2013). Supramolecular chemistry. John Wiley and Sons.
- 2. Lehn, J. M., (1995). Supramolecular Chemistry-Concepts and Perspectives. Wiley –VCH.
- 3. Beer, P.D., Gale, P. A., and Smith, D. K., (1999). Supramolecular Chemistry. Oxford University Press.
- 4. Martin, N. and Nierengarten J.-F. (2012). Supramolecular Chemistry of Fullerenes and Carbon Nanotubes. Wiley-VCH.
- 5. Vicens, J. and Harrowfield J. (2007). *Calixarenes in the Nanoworld*. Springer.
- 6. Schalley, C. A. (2012). *Analytical Methods in Supramolecular Chemistry*. Vol. 1 and 2, Wiley-VCH.
- 7. Erbas-Cakmak, S., Leigh, D. A., McTernan, C. T., andNussbaumer, A. L. (2015). Artificial molecular machines. *Chemical Review*, 115(18), 10081-10206.

Course Title: Material Chemistry

Paper Code: CHM.581 Total Contact Hours: 60

L	T	P	Cr
4	0	0	4

Course Outcome: The students will acquire knowledge of

- 1. Inorganic, organic and mixed materials
- 2. Characterization of these materials

3. The relationship between material structure and physical attributes associated with them.

Unit 1 15 Hours

Magnetic Materials (Ferrites) Introduction, structure and classification, hard and soft ferrites, synthesis of ferrites by various methods (precursor and combustion method), characterization of ferrites by Mossbauer spectroscopy, significance of hysteresis loop and saturation magnetization in ferrites, magnetic properties of ferrites, applications of ferrites.

Glasses, Ceramics, Composites and Nanomaterials: Glassy state, glass formers and glass modifiers, applications. ceramic structures, mechanical properties, clay products. microscopic composites; dispersion-strengthened and particle-reinforced, fibre-reinforced composites, macroscopic composites, nanocrystalline phase, preparation procedures, special properties, applications.

Unit 2 15 Hours

Mesmorphic behaviour, thermotropic liquid crystals, positional order, bond orientational order, nematic and smecticmesophases; smectic - nematic transition and clearing temperature -homeotropic, planar and sCHMieren textures, twisted nematics, chiral nematics, molecular arrangement in smectic A and smectic C phases, optical properties of liquid crystals. dielectric susceptibility and dielectric constants. lyotropic phases and their description of ordering in liquid crystals.

Thin Films and Langmuir- Blodgett Films

Prepartion techniques; evaporation/sputtering, chemical process, sol gel etc. Langmuir – Blodgett (LB) films, growth technique, photolithography, properties and applications of thin and LB films

Materials for Solid State Devices

Rectifiers, transistors, capacitors –IV-V compounds, low–dimensional quantum structure; optical properties.

Unit 3 15 Hours

Types of ionic conductors, mechanism of ionic conduction, interstitial jumps (Frenkel); vacancy mechanism, diffusion superionic conductors; phase transitions and mechanism of conduction in superionic conductors, examples and applications of ionic conductors.

Molecular Conductor: Oligo (phenylenevinylene)s, oligo(phenyleneethynylene)s, oligo (eneyne)s, oligo(thiophenevinylene), oligo (thipheneethynylene) etc. and their applications.

Preparation and characterization of silica and zirconia based stationary phases by (a) dynamic chemical modification, in which chiral selector is adsorbed on the surface of the zirconia by physical forces, (b) permanent chemical modification, in which a CS is chemically bonded onto the zirconia surface, and (c) physical screening, in which zirconia surface is coated with a polymer or carbon layer, and their application in chiral separations by LC

Unit 4 15 Hours

Fullerenes, Carbon Nanotubes and Graphene: Types and Properties, methods of preparation and separation of carbon nanotubes, applications of fullerenes, CNTs and graphene.

Nonlinear optical materials:Non-linear optical effects, second and third order – molecular hyperpolarisability and second order electric suspceptibility – materials for second and third harmonic generation.

Suggested Readings

- 1. Ashcroft, N. W., and Mermin, N. D. (1976). *Introduction to Solid State Physics*. Saunders.
- 2. Callister Jr, W. D., and Rethwisch, D. G. (2012). Fundamentals of Materials Science and Engineering: An Integrated Approach. John Wiley and Sons.
- 3. Anderson, J. C., Leaver, K. D., Rawlings, R. D., and Leevers, P. S. (2004). *Materials Science for Engineers*. CRC Press.
- 4. Keer, H. V. (1993). Principles of the Solid State. New Age International.

Course Title: Project
Paper Code: CHM.599
Total Contact Hours: 432

L	T	P	Cr		
0	0	12	6		

Course Outcome: The student would be able to

- 1. Investigate various aspects related to the chemistry problem.
- 2. Appreciate the literature and its relevance to his topic of interest
- 3. Write research proposal independently
- 4. Would generate interest in current topics of research.

Project supervisor would be allocated at the start of the semester and research project would be undertaken in discussion with the project supervisor. At the end of the semester the student has to prepare a project report as per the university guidelines. Upon submission of the project report, the projects would be evaluated based on a project presentation.

Interdisciplinary Courses Offered by Centre for Chemical Sciences

ID	ID Courses offered by the faculty of Centre for Chemical Sciences (For										
stu	students of other Centres)										
1	CHM.515	1 - 1		-	-	2	10	15	15	10	50
		Inorganic Chemistry									
2	CHM.516	Introduction to Green		-	-	2	10	15	15	10	50
		Chemistry and Sustainability									
3	CHM.517	Chemistry of Nanomaterials		-	-	2	10	15	15	10	50
		and Fabrication									
4.	CHM.528	General Laboratory Practices		-	_	2	10	15	15	10	50

Course Title: Basic Perspectives in Inorganic Chemistry

Paper Code: CHM.515

L	T	P	Cr
2	0	0	2

Total Contact Hours: 30

Course Outcome: The completion of this course will enable the students for

- 1. Handling the coordination chemistry of d-group elements with understanding of structures.
- 2. Workout on the environmental chemistry and metal hydrides.

Unit 1 7 Hours

Chemistry of d-block elements. coordination chemistry, models and stereochemistry, theories, spectra and bonding.

Unit 2 8 Hours

Ions role in bioscience: ionophores, pophyrin and other tetrapyrrollic macromolecules, coenzymes, neurotransmitters, metal binding to dna.

Unit 3 8 Hours

Metals in aqueous environment: Introduction, environmental chemistry, environmental composition, chemical processes, complexes, metal speciation of calcium, copper and mercury, their behaviour in hydrosphere.

Unit 4 7 Hours

Hydrogen Energy: introduction, synthesis and structures of metal hydrides, coordination modes of hydrogen atom, hydrogen storage, H_2 evolution under solar energy, thermal energy and acidifications.

- 1. Lippard, S.J. and Berg, J.M., (1994) *Principles of Bioinorganic Chemistry*. University Science Books.
- 2. Cotton, F. A., and Wilkinson, G. (1988). *Advanced Inorganic Chemistry* (Vol. 545). New York: Wiley.
- 3. Huheey, J. E., Keiter, E. A., Keiter, R. L., and Medhi, O. K. (2006). *Inorganic Chemistry: Principles of Structure and Reactivity*. Pearson Education India.
- 4. Greenwood, N. N., and Earnshaw, A. (2012). *Chemistry of the Elements*. Elsevier.
- 5. Van-Loon G.W. and Duffy S.J. (2011) *Environmental Chemistry: A Global Perspective*. Oxford University Press.
- 6. Rao C.S. (2006) *Environmental Pollution Control Engineering*. New Age International Publishers, New Delhi,
- 7. Peruzzini, M. and Poli, R. (2005) Recent Advances in Hydride Chemistry, Elsevier Science B.V., Amsterdam.

L	T	P	Cr
2	0	0	2

Course Title: Introduction to Green Chemistry and

Sustainability

Paper Code: CHM.516 Total Contact Hours: 30

Learning objective: To introduce basic concepts of green chemistry and their importance for sustainable development.

Unit 1 7 Hours

Introduction: Adverse effect of some of the current chemical practices on health and environment, concept and need of green chemistry, basic principles of green chemistry with examples— atom economy, wastage minimization, selection of starting materials etc. limitations/obstacle in the persuit of the goals of green chemistry, types of solvent.

Unit 2 7 Hours

Emerging non-conventional techniques: Microwave heating as energy efficient source, mechanism of microwave heating, Examples of microwave assisted organic synthesis, sono-chemistry and green chemistry,

Unit 3 8 Hours

Green solvents: Ionic liquids: properties and advantages, use ofionic liquids as solvent as well as catalyst, recyclability of ionic liquids. Solvent-free synthesis.

Unit 4 8 Hours

Value addition of abundantly available precursors: Need for the use of renewable precursors over petroleumbased feedstocks, biomass conversion (carbohydrates, lignocellulose biomass) into value added molecules.

Course Outcome: The students will be acquainted with

- 1. Modern concepts and tools of green chemistry and their importance in sustainable development.
- 2. Utilization of abundantly available precursors for the production of value added chemicals.

- 1. Anastas, P.T. and Warner J. C. (2000) *Green chemistry: Theory and Practical.* Oxford University Press, US.
- 2. Ahluwalia, V.K and Kidwai, M. (2004) New Trends in Green Chemistry. Springer.
- 3. Malhotra, S. V. (2007) *Ionic Liquids in Organic Synthesis*. Oxford University Press, US.

- 4. Ahluwalia, V.K. (2011) *Green Chemistry: Greener Alternatives to Synthetic Organic Transformations*. Alpha Science International Limited.
- 5. Klass, D. (1998) Biomass for Renewable Energy, Fuels, and Chemicals. Elsevier.

Course Title: Chemistry of Nanomaterials and Fabrication

Paper Code: CHM.517 Total Contact Hours: 30

L	T	P	Cr
2	0	0	2

Course Outcome: The students will acquire knowledge of Nanotechnology, fabrication and characterization of nanomaterials, properties and applications of nanomaterials.

Unit 1 7 Hours Background to Nanotechnology:

Scientific revolution- Atomic structures-molecular and atomic size-Bohr radius -emergence of nanotechnology-challenges in nanotechnology. definition of a nano system - types of nanocrystals-one dimensional (1D)-two dimensional (2D)-three dimensional(3D) nanostructured materials - quantum dots - quantum wire- multifunctional nanostructures.

Unit 2 7 Hours

Fabrication and Characterization of Nanomaterials: Top-down and bottom-up approaches: chemical routes for synthesis of nanomaterials: chemical precipitation and coprecipitation; metal nanocrystals by reduction, sol-gel synthesis; microemulsions or reverse micelles, myle formation; solvothermal synthesis; thermolysis routes, microwave heating synthesis; sonochemical synthesis; electrochemical synthesis. physical methods: -inert gas condensation, arc discharge, plasma arc technique, MW plasma, laser pyrolysis, molecular beam epitaxy, chemical vapour deposition method and electro deposition. diffraction analyses, imaging techniques, spectroscopic techniques.

Unit 3 8 Hours

Nanomaterials and properties: Influence of nucleation rate on the size of the crystals- macroscopic to microscopic crystals and nanocrystals - large surface to volume ratio. Metals (Au, Ag) - metal oxides (TiO2, CeO2, ZnOetc) - semiconductors (Si, Ge, CdS, ZnSe) - carbon nanotubes (CNT) - ceramics and composites - dilute magnetic semiconductor- biological system - DNA and RNA - lipids - size dependent properties - mechanical, physical and chemical properties.

Unit 4 8 Hours

Applications of Nanomaterials: Photocatalysis- solar cell-water splitting-energy harvesting- LSPR- molecular electronics and nanoelectronics- quantum

electronic devices - CNT based transistor and field emission display -biological applications - biochemical sensor-MRI agent - nanomedicine: molecular manufacturing - MEMS - NEMS - Bio-MEMS - protein nanoarrays - nano fluidics and micro fluidics -self-assembly of nanoparticles for biomedical applications-bacterial structures- cubosomes-dendrimers-DNA nanoparticle conjugates- bioactive nanomaterials-Au nanoparticles and CdSe quantum dots - molecular motors -nanoparticle and protein interactions.

Suggested Readings

- 1. Rao, C. N. R., Müller, A. and Cheetham, A. K. (Eds.) (2004). The Chemistry of Nanomaterials: Synthesis, Properties and Applications. Willy-VCH.
- 2. Poole, Jr., C. P. and Owens F. J. (2006). Introduction to Nanotechnology, Willy-VCH
- 3. Mukhopadhyay, S. M., (2012) Nanoscale Multifunctional Materials: Science and Applications. Willy-VCH
- 4. Kelsall, R. W., Hamley, I. W. and Geoghegan, M. (2005). *Nanoscale Science and Technology*. 2005, John Wiley and Sons.

Course Title: General Laboratory Practice

Paper Code: CHM.528 Total Contact Hours: 30

L	T	P	Cr
2	0	0	2

Course Outcome: The students will acquire knowledge of

- 1. Good laboratory practices
- 2. Quality control and Quality assurance
- 3. Chemical, biological and radiational hazards in laboratory and safety.
- 4. General know how of analytical sample preparation.

Unit 1 7 Hours

Good Laboratory Practices: Introduction and WHO guidelines on GLP and GMP. History of GLP. Quality assurance in GLP. Quality control laboratory, responsibilities, routine controls, instruments reagents, sampling plans.

Unit 2 8 Hours

Quality Standards and Quality Assurances: Advantages and disadvantages of quality standards, concepts of quality control, quality assurance its functions and advantages. Standard test procedures, protocols, non-clinical testing, controls on animal house, data generation and storage, quality control documentation, retention samples, records. Complaints and recalls, evaluation of complaints, recall procedures, related records and documents.

Unit 3 8 Hours

Safety and Hazard Analysis: Chemical classification of hazards, Radiation hazard, AERB regulation for Fire and its prevention, biosafety and biohazard. Weapons of Mass destruction

Unit 4 7 Hours

Basic Analytical practices: Titrimetry, Gravimetric analysis, Potentiometry and Spectrophotometric analysis. Pesticides and pesticide residue extraction, Solid phase extraction etc. Trace metal sample preparations and analysis. Proteomic and metabolomic sample preparations

- 1. Miller, J. C. Miller, J. N. (1998) Statistics for Analytical Chemistry. Wiley.
- 2. http://www.who.int/water_sanitation_health/resourcesquality/wqmchap9.pdf
- 3. https://www.unece.org/fileadmin/DAM/env/water/publications/documents/guidancela boratories.pdf.