COCHIN UNIVERSITY OF SCIENCE AND TECHNOLOGY

DEPARTMENT OF APPLIED CHEMISTRY

OUTCOME BASED SYLLABUS

FOR

M. Sc. CHEMISTRY

(WITH EFFECT FROM 2020-2021)

Programme Objective

This post-graduate course in Chemistry aims to build human resources in the area of Chemical Science and train competent manpower who can take challenges in teaching and research.

Programme Outcomes

On successful completion of M. Sc. Chemistry programme, students will be able to

P.O.1: acquire systematic and coherent understanding of the fundamental concepts.

P.O.2: demonstrate comprehensive knowledge and understanding of both theoretical and experimental/applied chemistry in various fields.

P.O.3: design and perform the chemical synthesis and characterise the products.

P.O.4: design and execute experimental routines for detection and quantification of chemical entities.

P.O.5: analyse the kinetics and energetics of chemical processes and infer the mechanism.

P.O.6: demonstrate the basic principles of instrumental methods of analysis.

P.O.7: operate advanced instruments and related soft-wares to execute in-depth analysis of chemical problems.

P.O.8: acquire core competency in the subject.

DEPARTMENT OF APPLIED CHEMISTRY

M. Sc. CHEMISTRY

(FOUR SEMESTERS / FULL TIME)

COURSE STRUCTURE AND SYLLABUS

(WITH EFFECT FROM 2020-2021)

SEMESTER: 1							*Semester Credit: 18 (Core: 16; Elective: 2) Cumulative Credit: 18*
Course No.	Course Name	Course Type	Credits	L-T-P	CE	ESE	Total Marks
CHE 2101	Chemistry of Main Group Elements (Inorganic Chemistry – I)	Core	3	3-1-0	50	50	100
CHE 2102	Structure and Reactivity (Organic Chemistry – I)	Core	3	3-1-0	50	50	100
CHE 2103	Introduction to Quantum Chemistry (Theoretical Chemistry – I)	Core	3	3-1-0	50	50	100
CHE 2104	Group Theory and Spectroscopy (Theoretical Chemistry – II)	Core	3	3-1-0	50	50	100
CHE 2105	Equilibrium and Nonequilibrium Thermodynamics	Elective	2	2-1-0	50	50	100
CHE 2106	Basic Concepts of Analytical Chemistry (Analytical Chemistry – I)	Core	2	2-1-0	50	50	100
CHE 2107	Inorganic Chemistry Laboratory	Core	2	0-0-6	100	-	100
CHE 2108	Open-ended Laboratory – I	Core	-	-	100	-	100
CHE 2109	Environmental Chemistry	Elective	2	2-1-0	50	50	100
CHE 2110	Solid State Chemistry	Elective	2	2-1-0	50	50	100
SEMESTER: 2							*Semester Credit: 19 (Core: 15; Elective: 4) Cumulative Credit: 37*
Course No.	Course Name	Course Type	Credits	L-T-P	CE	ESE	Total Marks
CHE 2201	Chemistry of d-and f-block Elements (Inorganic Chemistry – II)	Core	3	3-1-0	50	50	100
CHE 2202	Reactions and Mechanisms (Organic Chemistry – II)	Core	2	2-1-0	50	50	100
CHE 2203	Reagents and Synthesis (Organic Chemistry – III)	Core	2	2-1-0	50	50	100
CHE 2204	Spectroscopy of Organic Compounds (Organic Chemistry – IV)	Core	2	2-1-0	50	50	100
CHE 2205	Statistical Thermodynamics (Physical Chemistry – I)	Core	2	2-1-0	50	50	100
CHE 2206	Chemical Bonding and Computational Chemistry	Elective	2	2-0-2	50	50	100

CHE 2207	Bioanalytical Chemistry	Elective	2	2-1-0	50	50	100
CHE 2208	Organic Chemistry Laboratory	Core	2	0-0-6	100	-	100
CHE 2209	Open-ended Laboratory – II	Core	2	-	50	50**	100
CHE 2210	Introduction to Theory of Orbital Interactions in Chemistry	Elective	2	2-0-2	50	50	100
CHE 2211	Nuclear and Radiation Chemistry	Elective	2	2-0-2	50	50	100
CHE 2212	Supramolecular Chemistry	Elective	2	2-0-2	50	50	100
SEMESTER: 3	*Semester Credit: 21 (Core: 13; Elective: 8) Cumulative Credit: 58*						
Course No.	Course Name	Course Type	Credits	L-T-P	CE	ESE	Total Marks
CHE 2301	Instrumental Methods of Analysis (Analytical Chemistry – II)	Core	2	2-1-0	50	50	100
CHE 2302	Organometallic and Bioinorganic Chemistry (Inorganic Chemistry – III)	Core	3	3-1-0	50	50	100
CHE 2303	Natural Products (Organic Chemistry – V)	Core	3	3-1-0	50	50	100
CHE 2304	Kinetics, Adsorption and Catalysis (Physical Chemistry – II)	Core	3	3-1-0	50	50	100
CHE 2305	Electrochemistry and Crystallography	Elective	2	2-1-0	50	50	100
CHE 2306	Physical Chemistry Laboratory	Core	2	0-0-6	100	-	100
CHE 2307	Oleochemicals, Nutraceuticals and Surfactant Technology	Elective	2	2-1-0	50	50	100
CHE 2308	Molecular Modeling in Chemistry	Interdepartmental Elective*	4	4-1-0	50	50	100
CHE 2309	Spectroscopic Techniques	Interdepartmental Elective*	4	4-1-0	50	50	100
CHE 2310	Advanced Photochemistry	Elective	2	2-1-0	50	50	100
CHE 2311	Polymer Chemistry	Elective	2	2-1-0	50	50	100
SEMESTER: 4	*Semester Credit: 16 (Core: 16; Elective: 0) Cumulative Credit: 74*						
Course No.	Course Name	Course Type	Credits	L-T-P	CE	ESE	Total Marks
CHE 2401	Project Dissertation	Core	16	-	200	200**	400

*courses offered to the students of other departments.

**presentation and viva-voce.

L-T-P ≡ Lecture-Tutorial-Practical Hours

CE ≡ Continuous Evaluation; ESE ≡ End Semester Evaluation

Note:

1 Hour Lecture is equivalent to 1 credit

3 Hours Practical is equivalent to 1 credit

SEMESTER: 1

CORE

CHE 2101

Chemistry of Main Group Elements

(Inorganic Chemistry – I)

Credit 3 **48 hours**

Course Outcome After completion of the full course the students should be able to	**Cognitive level**
C.O.1: identify the structure-activity relationship of simple molecules based on their qualitative molecular orbitals.	Analyse
C.O.2: predict the stability and topology of different polyhedral boranes and related compounds.	Analyse
C.O.3: assess the strength of various acids and bases and their reactivity.	Analyse
C.O.4: explain behavior of different non-aqueous solvent systems towards different reactions.	Apply
C.O.5: interpret the structure and properties of compounds of sulfur, nitrogen, phosphorous and group 14 elements.	Apply

MAPPING of CO's and PO's

	Programme Outcomes							
Course Outcomes	P.O.1	P.O.2	P.O.3	P.O.4	P.O.5	P.O.6	P.O.7	P.O.8
C.O.1	x	x			x			x
C.O.2	x	x						x
C.O.3	x	x			x			x
C.O.4	x	x			x			x
C.O.5	x	x			x			x

Unit 1

Qualitative molecular orbital theory, symmetry of molecular orbitals, MOs for homo and heteronuclear diatomic molecules, H_2 to F_2, HF, CO, NO, BeH_2, CO_2, H_2O, BH_3, NH_3, B_2H_6, $B_3N_3H_6$, S_3N_3, $N_3P_3Cl_6$, Si_2H_2. Importance of frontier molecular orbitals, Shape, energy and reactivity of molecules.

Unit 2

Electronic structure and allotropes of boron, boron halides, boron heterocycles, borazine Structure and bonding in polyhedral boranes and carboranes, styx notation; electron count in polyhedral boranes;

Wade's rule; topological approach to boron hydride structure. Importance of icosahedral framework of boron atoms in boron chemistry. Closo, nido and arachno structures. Synthesis of polyhedral boranes; electron counting in polycondensed polyhedral boranes, mno rule. Carboranes, Metallocarboranes.

Unit 3

Relative strength of acids, Pauling rules, Lux-Flood concept, Lewis concept, Measurement of acid base strength, Lewis acid –base interactions, steric and solvation effects, acid –base anomalies, Pearson's HSAB concept, acid-base strength and hardness and softness, Symbiosis, theoretical basis of hardness and softness, electronegativity and hardness.

Unit 4

Chemistry in non-aqueous solvents reactions in NH_3, liquid SO_2, solvent character, reactions in SO_2, acetic acid, solvent character, reactions in CH_3COOH and some other solvents. Molten salts, Green solvent: supercritical CO_2, Ionic liquids and deep eutectic solvents.

Unit 5

Sulphur-Nitrogen compounds: Tetrasulphur tetranitride, disulphur dinitride and polythiazyl. SxNy compounds. S-N cations and anions. Sulphur-phosphorus compounds: Molecular sulphides such as P_4S_3, P_4S_7, P_4S_9 and P_4S_{10}. Phosphorus-nitrogen compounds: Phosphazenes and poly phosphazenes. Transition metal dichalcogenides, MoS_2. Structure, bonding and reactivity of 2D and 3D Carbon, Silicon and Germanium materials. Carbon nitrides, fullerenes, carbon nanotubes (CNT's) and graphenes.

References:

1. G. L. Miessler, P. J. Fischer, D. A. Tarr, Inorganic Chemistry, 5th ed., Pearson, 2014.
2. E. Huheey, E. A. Keiter, R. L. Keiter, Inorganic Chemistry: Principles of Structure and Reactivity, 4th ed., Harper Collin College Publishers, 1993.
3. F. A. Cotton, G. Wilkinson, C. A, Murillo, M. Bochmann, Advanced Inorganic Chemistry, 6th ed., Wiley-Interscience: New York, 1999.
4. D. F. Shriver, P. W. Atkins, C. H. Langford, Inorganic Chemistry, 3rd ed., ELBS, 1999.
5. B. Douglas, D. McDaniel, J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd ed., Wiley, 1994.
6. N. N. Greenwood, A. Earnshaw, Chemistry of the Elements, 2nd ed., Butterworth-Heinemann, 1997.
7. C. E. Housecroft, A. G. Sharpe, Inorganic Chemistry, 5th ed., Pearson, 2018.
8. E. Wiberg, A. F. Holleman, N. Wiberg, Inorganic Chemistry, Academic Press, 2001.
9. A. V. Kolobov, J. Tominaga, Two-Dimensional Transition Metal Dichalcogenides, Springer, 2016.
10. Yu-Chuan Lin, Properties of Synthetic Two-dimensional Materials and Heterostructures, Springer, 2018.
11. C. Wu, X. Wu, et al, Inorganic Two-dimensional Nanomaterials: Fundamental Understanding, Characterization and Energy Applications, RSC, 2017.

12. D. R. MacFarlane, M. Kar, J. M. Pringle, Fundamentals of ionic liquids, Wiley-VCH, 2017.
13. Y.izhak Marcus, Deep Eutectic Solvents, Springer, 2019.
14. J. M. DeSimone, W. Tumas, Green Chemistry Using Liquid and Supercritical Carbon dioxide, D.U.P, 2003.
15. F. M. Kerton, R. Marriott, et al., Alternative Solvents for Green Chemistry, 2nd ed., RSC, 2013.

CORE

CHE 2102

Structure and Reactivity

(Organic Chemistry – I)

Credit 3 **48 hours**

Course Outcome After completion of the full course the students should be able to	**Cognitive level**
C.O.1: review different bonding models with emphasis on understanding three dimensional structures of molecules.	Analyse
C.O.2: study Qualitative Molecular Orbital Theory and group orbital concepts to sketch MO's of common organic structures, functional groups etc.	Evaluate
C.O.3: interpret structure and stability of reactive intermediates.	Evaluate
C.O.4: develop concepts on solvent scales, acidity and basicity of organic compounds and correlate with the structure of the molecules.	Analyse
C.O.5: study the concepts of isomerism and its classification.	Understand
C.O.6: apply the concepts of conformation and configuration in organic chemistry.	Apply
C.O.7: apply methods and techniques to study mechanisms of organic reactions.	Apply
C.O.8: apply the concepts of Frontier orbital theory in the study of ionic, radical and pericyclic reactions.	Analyse

MAPPING of CO's and PO's

	Programme Outcomes							
Course Outcomes	P.O.1	P.O.2	P.O.3	P.O.4	P.O.5	P.O.6	P.O.7	P.O.8
C.O.1	x	x			x			x
C.O.2	x	x			x			x
C.O.3	x	x			x			x
C.O.4	x	x			x			x
C.O.5	x	x						x
C.O.6	x	x			x			x
C.O.7	x	x			x			x
C.O.8	x	x			x			x

Unit 1

Structure and Models of bonding: Study of Lewis Structures, Formal Charge, VSEPR, Hybridization, localised σ and π bonds, polar covalent bonding, Bond dipoles, molecular dipoles and quadrupoles, polarizability, Resonance, Bond Lengths and Bond energy.

Study of Qualitative Molecular Orbital Theory, Group Orbitals, MO's of Methyl, methylene and Formaldehyde, Methane, ethane. Mo's of π systems such as ethylene, propene, butadiene, benzene, benzyl and allyl.

Study of Structure and Stability of Reactive intermediates: Carbocations, Carbanions, Carbenes, Nitrenes, and Radicals.

Study of Bonding Weaker than Covalent Bonds: Ion pairing interactions, ion – dipole interactions, dipole – dipole interactions, Hydrogen bonding, Factors affecting strength and stability of hydrogen bonds, cations – π, polar – π, π-stacking, π-donor – acceptor interactions, induced dipole interactions, the hydrophobic effect.

Study of solvent and solution properties, different solvent scales.

Study of Acid – Base properties, pKa in aqueous and non-aqueous systems, acidity scales, Super Acids

Unit 2

Study of Conformations and Configuration in Organic Chemistry. Study of Strain and stability: Types of strain including *B, F, I*, Pitzer strain, Beyer strain. Conformational analysis, Acyclic sp^3–sp^3, sp^3-sp^2 systems, structure and stability of small, medium, and large rings, cyclohexane, substituted cyclohexanes, *A* values, cyclohexenes, decalins, bicyclic systems.

Geometrical isomerism, origin – structural features including C-C and C-hetero atom double bonds, cyclic systems and other systems exhibiting restricted rotation, different nomenclature including, cis-tarns, E-Z, syn-anti, endo-exo, in-out, relative acidity of maleic and fumaric acids.

Stereogenicity and Stereoisomerism: origin of chirality, chiral centres, axes and planes, helicity, enantiotopic and diastereotopic atoms, groups and faces, prochiral centres and faces, allenes, cumulenes, biphenyls, and spirans. Compounds containing chiral atoms other than carbon.

Unit 3

The study of reactions and the methods of studying reaction mechanisms.

Classification of reactions according to IUPAC conventions. Reaction mechanism: guidelines on Pushing of electrons. Reactive intermediates: Formation, stability and general reactivity. Methods of determining reaction mechanisms (kinetic and non kinetic methods): The Hammond postulate, reactivity vs selectivity principle, the Curtin-Hammett principle, microscopic reversibility, kinetic vs thermodynamic control.

Isotope effects: Primary, secondary and Equilibrium isotope effects, Tunneling effects, solvent isotope effects and heavy atom Isotpe effects.

Linear free energy relationships: Hammett and Taft parameters, Solvent effects (Grunwald-Winstein plots and Schleyer adaptation), nucleophilicity and nucleofugality. Isokinetic and Isoequilibrium temperature, Enthalpy – entropy compensation.

Experimental techniques to determine reaction mechanisms: identification of intermediates by trapping and competition experiments, cross - over experiments, isotope scrambling, radical clocks and traps, matrix isolation.

Conformations and Control of reactivity. Stereoselective and stereospecific reactions. Baldwin ring closure rules. Study of representative examples.

Unit 4

Applications of Molecular Orbital Theory in Understanding reactions and Mechanisms.

Frontier Orbitals, HSAB concept, Nucleophiles and Electrophiles, Perturbation theory of reactivity.

Application of Frontier Orbital theory in studying ionic reactions: aliphatic nucleophilic substitution reactions, Ambident nucleophiles, Ambident electrophiles, α-effect.

Application of Frontier Orbital theory in studying radical reactions.

Unit 5

Pericyclic reactions: study of the principle of conservation of orbital symmetry: Orbital symmetry diagrams for cycloaddition and electrocyclic reactions.

Study of Frontier Molecular Orbital Theory, Aromatic Transition State Theory and The Generalized Woodward – Hoffmann rule applied to cycloaddtions, Electrocyclic reactions, Sigmatropic rearrangements and Chelotropic reactions.

Pericyclic Reactions in Organic Synthesis: Stereochemistry and Regiochemistry of Cycloaddtions. Substituent and medium effects, Secondary Orbital Interactions in [4+2] cycloadditions, Intramolecular Diels–Alder reactions.

Stereochemistry of Electrocyclic Reactions and Sigmatropic rearrangements. Cope rearrangement, Claisen rearrangement and ene-reaction.

1,3-dipolar cycloaddition reactions, Photochromism and thermochromism, Pericyclic reactions in Organic synthesis – case studies.

References:

1. J. March, Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 7th ed., Wiley, 2013.
2. T. H. Lowry, K. S. Richardson, Mechanism and Theory in Organic Chemistry, 3rd ed., Benjamin-Cummings Publishing Company, 1997.
3. F. A. Carey, R. J. Sundberg, Advanced Organic Chemistry (parts A and B), 5th ed., Springer, 2008.
4. E. V. Anslyn, D. A. Dougherty, Modern Physical Organic Chemistry. University Science Books, 2006.
5. F. A. Carroll, Perspectives on structure and mechanism in organic chemistry, Wiley, 2011.
6. N. S. Issacs, Physical Organic Chemistry, 2nd Edition, Prentice Hall, 1995.
7. A. Pross, Theoretical and Physical Principles of Organic Chemistry, 1st ed., Wiley, 1995.
8. J. Clayden, N. Green, S. Warren, P. Wothers, Organic Chemistry, 2nd ed., Oxford University Press, 2012.
9. I. Flemming, Frontier orbitals and organic chemical reactions, Wiley-Blackwell, 1976.
10. I. Flemming: Molecular orbitals and organic chemical reactions, student ed., Wiley, 2009.
11. J. McMurry, Organic Chemistry, 5th ed., Brooks/Cole, 2000.
12. R. Bruckner, Advanced organic chemistry: Reaction Mechanisms. Academic Press, 2001.
13. P. S. Kalsi, Stereochemistry, Conformation and Mechanism, 3rd ed., New Age Publications.
14. E. L. Eliel, S. H. Wilen, Stereochemistry in Organic Compounds, John Wiley, 1994.
15. D. Nasipuri, Stereochemistry of Organic Compounds: Principles and Applications, 2nd ed., Wiley Eastern Limited, New Delhi, 1994.

CORE

CHE 2103

Introduction to Quantum Chemistry

(Theoretical Chemistry – I)

Credit 3 **48 hours**

Course Outcome After completion of the full course the student should be able to	**Cognitive level**
C.O.1: account for the basic principles and concepts of quantum mechanics.	Analyse
C.O.2: apply the postulates of quantum mechanics to simple systems of chemical interest, such as the particle-in-a-box, harmonic oscillator, rigid rotor, and hydrogenic atoms.	Apply
C.O.3: derive the variational principle, use it to calculate properties for simple systems of chemical interest.	Analyse
C.O.4: use perturbation theory to calculate properties for simple systems of chemical interest.	Analyse
C.O.5: define and explain the Hartree-Fock self-consistent field method.	Understand

MAPPING of CO's and PO's

	Programme Outcomes							
Course Outcomes	P.O.1	P.O.2	P.O.3	P.O.4	P.O.5	P.O.6	P.O.7	P.O.8
C.O.1	x	x						x
C.O.2	x	x			x			x
C.O.3	x	x			x			x
C.O.4	x	x			x			x
C.O.5	x	x						x

Unit 1

Wave-particle duality, uncertainty principle, postulates of quantum mechanics, Schrödinger equation, Time dependent and time independent Schrodinger wave equation. Its application on some model systems viz., free particle, particle in one, two and three-dimensional box (rectangular and cubical), separation of variables, concept of degeneracy, introduction to quantum mechanical tunnelling.

Unit 2

Vibrational motion, Harmonic oscillator, Method of power series, Hermite equation and Hermite Polynomials, Recursion formula, wave function and energy.

Rigid rotator, Wave function in spherical polar coordinates, Planar rotator, phi equation, theta equation and solutions Lagendre equation and Lagendre polynomials, Spherical harmonics, Angular momentum operator L^2 and L_z, Space quantization.

Unit 3

H atom, separation into three equations and solutions, Laguerre equation and Laguerre polynomials wave equation and energy of H like systems, quantum numbers and their importance, Radial wave function and radial distribution functions, angular wave function, Shapes of s, p, d and f atomic orbitals. Postulate of electron spin-orbital and spin functions. Zeeman effect.

Unit 4

Many electron atoms. Approximate methods in quantum mechanics: The variation theorem, linear variation principle and perturbation theory (first order and non-degenerate), application of variation method and perturbation theory to the Helium atom, antisymmetry, Pauli exclusion principle, Slatter determinantal wave functions. Electron spin.

Unit 5

Hartree-Fock Self Consistent Field method, The Coulomb and Exchange Operators, The Fock Operator, Koopmans' theorem, Brillouin's theorem, The Roothaan Equations, Slater's treatment of complex atoms, Slater orbitals. Pauli principle, Slater determinant and wave function.

References:

1. D. A. McQuarrie, Quantum Chemistry, 3rd ed., Univ. Sci. Books, Mill Valley, California, 1983.
2. I. N. Levine, Quantum Chemistry, 6th ed., Pearson Education, London, 2008.
3. P. W. Atkins, R.S Friedman, Molecular Quantum Mechanics, 5th ed., OUP, Oxford, 2012.
4. J. P. Lowe, Quantum Chemistry 3rd ed., Academic Press, New York, 2008.
5. A. Szabo, N. S. Ostlund, Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory, Dover Book ed., Mc.Graw-Hill, New York, 1982.
6. P.W. Atkins, Physical Chemistry, 8th ed., Wiley, New York, 2006.
7. R. K. Prasad, Quantum Chemistry, 3rd ed., New Age International, 2006.
8. D. J. Griffiths, Introduction to Quantum Mechanics, 2nd ed., 2004.
9. J. J. Sakurai, Modern Quantum Mechanics, 2nd ed., 2010.

CORE

CHE 2104

Group Theory and Spectroscopy

(Theoretical Chemistry – II)

Credit 3 **48 hours**

Course Outcome After completion of the course, the student will be able to	Cognitive level
C.O.1: analyze the symmetrical aspects of any given molecule.	Analyze
C.O.2: apply symmetry and Group Theory in Quantum mechanics, Spectroscopy, Inorganic or Organic chemistry.	Apply
C.O.3: explain the factors affecting the intensity and broadening of lines in spectra and methods to enhance the sensitivity.	Understand
C.O.4: explain the principles of rotational, vibrational, Raman, electronic, NMR and ESR.	Understand
C.O.5: calculate energy required for a particular type of energy transition and determine the parameters involved.	Apply
C.O.6: apply various theoretical aspects to various spectroscopic techniques for prediction of different spectroscopic observations.	Analyse

MAPPING of CO's and PO's

	Programme Outcomes							
Course Outcomes	P.O.1	P.O.2	P.O.3	P.O.4	P.O.5	P.O.6	P.O.7	P.O.8
C.O.1	x	x						x
C.O.2	x	x						x
C.O.3	x	x						x
C.O.4	x	x				x		x
C.O.5	x	x						x
C.O.6						x		

Unit 1

Molecular symmetry: Symmetry elements and operations, Point groups, Matrix representation of symmetry operations, character, Application of Group theory to symmetry properties of molecules, Definition of a mathematical group, Abelian group, cyclic group, symmetry operations as group elements, similarity transformation and classes, Direct product, Group multiplication table – Symmetry classification of molecules into point groups (Schoenflies symbol)- Application of symmetry to predict polar and chiral compounds.

Unit 2

Reducible and Irreducible representations - Great Orthogonality theorem and its consequences (statement only, proof not needed), Character tables- reduction formula- Construction of character tables for point groups with order ≤6- Interpretation of character tables. Wave functions as bases for irreducible representations, Construction of hybrid orbitals for AB_3(planar), $AB_4(T_d)$, $AB_5(D_{3h})$ and $AB_6(O_h)$ type of molecules - Symmetry adapted linear combinations, Projection operators, Application of projection operators to π-bonding in ethylene, cyclopropenyl systems, benzene and Naphthalene.

Unit 3

Nature of electromagnetic radiation, its interaction with matter, intensity and width of spectral lines, Classical and quantum chemical approach to absorption of radiation by molecules. Energy levels in molecules. Population of energy levels. Induced quantum transitions. Integrated absorption coefficient. Einstein's coefficients of absorption. Basis of selection rules, transition moment integral. Beer's Law. Induced absorption and emission of radiation by molecules, Factors affecting the intensity and width of spectral lines, Methods to reduce line broadening.

Unit 4

Rotational and vibrational energies of diatomic molecules. Linear molecules, Symmetric top and asymmetric top molecules. Rotation spectra: Diatomic and polyatomic molecules, Selection rule.

Vibration spectra of diatomic molecules, Morse potential of real molecules, overtones, combination and hot bands, Fermi resonance, rotational character of vibration spectra. Coupling of rotation and vibration. Parallel and perpendicular bands.

Vibration spectra of polyatomic molecules, Normal modes of vibrations of polyatomic molecules. Raman Spectroscopy. Rotational Raman spectra. Vibrational Raman spectra, Resonance Raman, mutual exclusion principle. Selection rules and applications to IR and Raman spectra, Surface enhanced Raman spectroscopy.

Applications of Group theory for molecular vibration, symmetry of group vibrations. Selection rules and applications to IR and Raman spectra.

Unit 5

Electronic energy states of molecules. Selection rules for electronic transitions, Vibrational structure of electronic bands. Electronic transitions and absorption bands. Electronic spectra of diatomic and polyatomic molecules, its relation to electronic arrangement and symmetry of molecules. Different types of electronic transitions, Electronic spectra of conjugated systems.

Unit 6

Magnetic resonance spectroscopy: Theory of nuclear magnetic resonance, Chemical shifts, Factors affecting chemical shifts, First order and second order spectra, relaxation effects. Fourier Transformation in NMR, Measurement of relaxation time, Spin echo, NOE, 2D NMR, NQR Spectroscopy. MRI, Solid state NMR.

Principle of electron spin resonance.

References:

1. F. A. Cotton, Chemical Applications of Group theory, Wiley Eastern, Singapore, 2nd ed., 1992.
2. V. Ramakrishnan, M. S. Gopinathan, Group theory in Chemistry, Vishal Pub. New Delhi, 1996.
3. P. W. Atkins, Physical Chemistry 8th ed., W. H. Freeman, New York, 2006.
4. R. A. Alberty, Physical Chemistry 8th ed., Wiley, New York, 1994.
5. G. M. Barrow, Introduction to Molecular Spectroscopy, McGraw Hill, New York, 1962.
6. C. N. Banwell, Fundamentals of Molecular Spectroscopy, 4th ed., Tata McGraw Hill, 1996.
7. A. E. Derome, Modern NMR Techniques for Chemical Research, Pergamon Press, 1987.
8. R. S. Drago, Physical Methods for Chemists, 2nd ed., Saunders College Publication, 1992.
9. D. H. Williams, I. Flemming, Spectroscopic Methods in Organic Chemistry, 4th ed., McGraw-Hill, 1985.
10. H. Gunther, NMR Spectroscopy, 2nd ed., John Wiley, 2005.
11. N. B. Colthup, L. H. Daly, S. E. Wiberley, Introduction to Infrared and Raman Spectroscopy, 3rd ed., 1982.

ELECTIVE

CHE 2105

Equilibrium and Nonequilibrium Thermodynamics

Credit 2 **32 hours**

Course Outcome After completion of the full course the student should be able to	**Cognitive level**
C.O.1: apply the concepts of thermodynamics to derive relations between molecular properties and to predict spontaneity of processes.	Analyse
C.O.2: describe the wider significance of chemical potential in physical and chemical processes, with detailed understanding of phase transitions and chemical equilibrium.	Apply
C.O.3: understand thermodynamics of phase transitions and obtain phase diagram of a few phase transitions.	Understand
C.O.4: interpret dependence of chemical equilibrium on pressure, temperature and concentration.	Evaluate
C.O.5: study the basics of transport phenomena's viz., osmosis, biological motors and electro kinetic effects.	Understand

MAPPING of CO's and PO's

	Programme Outcomes							
Course Outcomes	P.O.1	P.O.2	P.O.3	P.O.4	P.O.5	P.O.6	P.O.7	P.O.8
C.O.1	x	x			x			x
C.O.2	x	x			x			x
C.O.3	x	x			x			x
C.O.4	x	x			x			x
C.O.5	x	x			x			x

Unit 1
Language and Mathematics of Thermodynamics. Second law of thermodynamics, Entropy as a state function, The Clausius inequality, Entropy changes accompanying expansion, phase transition and heating. Free energy functions - Variation with

temperature and pressure. Gibbs Helmholtz equation. Relation between thermodynamic functions. Maxwell relations-significance.

Third law of thermodynamics: Nernst Heat Theorem, Calculation of absolute entropy, Unattainability of absolute zero.

Thermodynamic systems of variable composition – Partial molar properties. Chemical Potential, Significance of Chemical potential, Gibbs Duhem Equation and Duhem Margules Equation. Thermodynamics of mixing. Concepts of activity and fugacity, Standard states.

Unit 2

Solutions- Ideal solutions, Raoults law, Henry's Law, Deviations from ideality, Real and Regular solutions, Excess functions, Ideal Dilute Solutions- Colligative Properties- van't Hoff factor.

Physical transformation of Pure substances- Stability of a phase, Phase transitions and phase boundaries- Thermodynamic aspects, Ehrenfest Classification of Phase transitions. Phase rule – Application to one component systems- Water, S, CO_2 and He.

Two component systems- Liquid-vapour equilibria of binary systems – Vapour pressure-composition diagrams and Temperature composition diagrams. Distillation of binary mixtures –Azeotrope formation. Liquid-liquid equilibria- Partially miscible and immiscible liquids- CST, Nernst Distribution Law, Partition co-efficient, Principle of Steam distillation.

Solid-liquid Equilibria-Cooling curve, Eutectic mixture, Application, Compound formation with Congruent and Incongruent melting points.

Solid-Vapour Equilibria- $CuSO_4$-water system. Three component systems.

Unit 3

Chemical Equilibria and free energy, Equilibrium Constants, Applications of free energy function to physical and chemical charges. Effect of temperature and pressure on chemical equilibrium- van't Hoff reaction isotherm and isochore.

Unit 4

General theory, Local entropy production, balances equation for concentration. Energy conservation in open systems. Entropy balance equation. Forces and Fluxes, Steady state and local equilibrium conditions. Linear phenomenological laws. Phenomenological coefficient, Systems with heat, matter and electrical transport, Onsager Reciprocal relation, Application to Diffusion -Thermal diffusion, Thermal Osmosis and Electrokinetic effects, Soret Coefficient, Seebeck effect, biological motors, earths energy balance.Wave-particle duality, uncertainty principle, postulates of quantum mechanics, Schrödinger equation, Time dependent and time independent Schrodinger wave equation. Its application on some model systems viz., free particle, particle in one, two and three-dimensional box (rectangular and cubical), separation of variables, concept of degeneracy, introduction to quantum mechanical tunneling.

References:

1. P. W. Atkins, Physical Chemistry, 8th ed., Wiley, New York, 2006.
2. I. M. Klotz, R. M. Robsenberg, Chemical Thermodynamics, 3rd ed., A. Benjamin, INC.1972.
3. L. K. Nash, Elements of Chemical Thermodynamics, 2nd ed., Addison Wesley, 2005.
4. I. Prigogine, Introduction to Thermodynamic Irreversible Processes, 3rd ed., Wiley Interscience, 1968.
5. S. R. de Groot, P. Mazur, Non-equilibrium Thermodynamics, Dover Publications, 2011.
6. G. Lebon, D. Jou, J. Casas, Understanding Non-equilibrium Thermodynamics, Springer. 2008.
7. S. Kjelstrup, D. Bedeaux, E. Johannessen, J. Gross, Non-Equilibrium Thermodynamics for Engineers: Second Edition, World Scientific Publishing Company, 2017.

CORE

CHE 2106

Basic Concepts of Analytical Chemistry

(Analytical Chemistry – I)

Credit 2 **32 hours**

<u>Course Outcome</u> After the completion of the course, the student will be able to	**<u>Cognitive level</u>**
C.O.1: perform various statistical evaluation of experimental data.	Apply
C.O.2: choose proper chromatographic technique for the separation of mixture of compounds.	Apply
C.O.3: explain the theory and applications of biochemical analysis like RIA, IRMA, ELISA.	Understand
C.O.4: analyse the curves of TG, DTA and DSC.	Analyse
C.O.5: explain the instrumentation of UV-Visible and IR spectrophotometry and perform calculations based on photometric laws.	Apply

MAPPING of CO's and PO's

	Programme Outcomes							
Course Outcomes	P.O.1	P.O.2	P.O.3	P.O.4	P.O.5	P.O.6	P.O.7	P.O.8
C.O.1	x	x						x
C.O.2	x	x		x				x
C.O.3	x	x				x		x
C.O.4	x	x				x		x
C.O.5	x	x				x		x

<u>Unit 1</u>
Evaluation of analytical data - significant figures, Accuracy, Types of errors, Precession, Standard deviation, Pooled standard deviation, Coefficient of variation, Confidence interval and confidence limits, students T test, rejection of suspected value -Q test.

Unit 2

Separation Techniques. Distribution law-Liquid-liquid extractions, synergistic extraction. Counter current extraction, super critical fluids, Electrophoresis- theory and applications.
Chromatography-classification-column-paper, thin layer chromatography, HPLC-Instrumentation, Theory of Ion exchange chromatography, Gel Permeation Chromatography, Important applications of chromatographic techniques

Unit 3

Gas chromatography – basic instrumental set up-carriers, columns, detectors and comparative study of TCD, FID, ECD and NPD. Qualitative and quantitative studies using GC, Preparation of GC columns, selection of stationary phases of GLC, CHN analysis by GC. Super Critical Fluid Chromatography.

Unit 4

Radioimmunoassay (RIA), Immunoradiometric assay (IRMA), Enzyme linked immunosorbent assay (ELISA)-Principles and practical aspects
Thermal methods of Analysis TG, DTA and DSC - Instrumentation and Theory – Factors affecting TGA - effect of atmosphere on DTA. TG of copper sulphate pentahydrate and calcium oxalate monohydrate. Application of thermal methods for identification of substances.

Unit 5

Basic instrumentation for UV-Vis and IR spectrophotometry-single beam and double beam instruments, FT-IR, Fundamental laws of photometry, Beer lambert's law, deviations from Beer's law - photometric accuracy, relative photometric error, Simultaneous determination of two components.

References:

1. D. A. Skoog, D. M. West, F. J. Holler, S. R. Crouch, Fundamentals of Analytical Chemistry, 8th ed., Saunders College Pub., 2007.
2. G. D. Christian, Analytical Chemistry, 6th ed., John Wiley & Sons, 2007.
3. J. M. Mermet, M. Otto, R. Kellne, Analytical Chemistry, Wiley-VCH, 2004.
4. H. Gunzler, A. Williams, Handbook of Analytical Techniques, Volume 2, Wiley-VCH, 2001.
5. S. Higson, Analytical Chemistry, OUP Oxford, 2003.
6. A. Zschunke, Reference Materials in Analytical Chemistry, Springer, 2000.
7. K. Wilson, J. Walker, Practical Biochemistry-Principles and techniques, 4th ed., Cambridge University Press, 1997.

CORE

CHE 2107

Inorganic Chemistry Laboratory

Credit 2 **96 hours**

Course Outcome After completion of the full course the students should be able to	**Cognitive level**
C.O.1: identify the cations in a mixture of unknown salts.	Analyse
C.O.2: estimate the amount of a given metal ion by complexometric and cerimetric reactions.	Analyse
C.O.3: synthesise metal complexes and characterize them by various physicochemical methods.	Apply
C.O.4: record and interpret electronic spectrum of different metal complexes.	Apply

MAPPING of CO's and PO's

	Programme Outcomes							
Course Outcomes	P.O.1	P.O.2	P.O.3	P.O.4	P.O.5	P.O.6	P.O.7	P.O.8
C.O.1	x	x						x
C.O.2	x	x		x				x
C.O.3	x	x	x			x		x
C.O.4	x	x				x	x	x

Reactions of titanium, vanadium, chromium, manganese, iron, cobalt, nickel and copper ions. Reactions of some less common metal ions (Tl, W, Mo, V, Zr, Th, U). The spot test technique for metal ions. Semimicro qualitative analysis of common and rare cations in a mixture.

Estimation of metal ions by complexometric and cerimetric titrations. Estimation of Mg, Ca, Mn, hardness of water.

Synthesis of inorganic complexes and their characterization by various physicochemical methods, such as IR, UV, Visible, NMR, magnetic susceptibility etc. Selection can be made from the following or any other complexes for which references are available in the literature.

Tris(oxalato)manganese(III)

Tetrapyridinesilver(II)peroxidisulphate

Tris(acetylacetonato) iron(III)

Bis(N,N-diethyldithiocarbamato)nitrosyliron(I)

Optical isomers of tris(ethylenediamine)cobalt(III)chloride
Nitropentamminecobalt(III) chloride
Tri(acetylacetonato)manganese(III)
Tris(thiourea) copper(I) sulphate
Phenyl lithium
Tetraphenyl lead
Ferrocene
Phosphonitrilic chloride
Anhydrous copper(II) nitrate
Interpretation of its electronic spectrum and calculation of D_q values. Determination of crystal field splitting energy for certain ligands and construction of a part of the spectrochemical series.

References:

1. G. Pass, H. Sutcliffe. Practical Inorganic Chemistry 2nd ed., Chapman & Hill. 1974.
2. G. Marr, B. W. Rockett, Practical Inorganic Chemistry, Van Nostrand, 1972.

CORE

CHE 2108

Open-ended Laboratory – I

Credit 0

<u>Course Outcome</u> After completion of the full course the student should be able to	**<u>Cognitive level</u>**
C.O.: identify and hypothesise an independent research problem.	Analyse

MAPPING of CO's and PO's

	Programme Outcomes							
Course Outcomes	P.O.1	P.O.2	P.O.3	P.O.4	P.O.5	P.O.6	P.O.7	P.O.8
C.O.	x	x	x	x	x	x		x

The students shall identify a research problem by conducting a literature survey.

The students shall formulate a hypothesis on his/her research problem.

The students shall submit a review report on the literature.

ELECTIVE

CHE 2109

Environmental Chemistry

Credit 2 **32 hours**

Course Outcome After completion of the full course the student should be able to	**Cognitive level**
C.O.1: describe various natural cycles existing in atmosphere.	Understand
C.O.2: identify various air pollutants and explain how they pollute/disturb the atmosphere.	Understand
C.O.3: devise various methods to control air pollution.	Apply
C.O.4: explain the composition and reactions occurring in soil and identify soil pollutants.	Understand
C.O.5: describe water quality criteria and identify various water pollutants.	Understand
C.O.6: determine various water quality parameters.	Apply
C.O.7: explain various instrumental techniques in environmental analysis.	Understand

MAPPING of CO's and PO's

	Programme Outcomes							
Course Outcomes	P.O.1	P.O.2	P.O.3	P.O.4	P.O.5	P.O.6	P.O.7	P.O.8
C.O.1	x	x						x
C.O.2	x	x			x			x
C.O.3	x	x						x
C.O.4	x	x			x	x		x
C.O.5	x	x						x
C.O.6	x	x				x		x
C.O.7	x	x				x		x

Unit 1

Global warming - Ozone hole. Environmental segments – The hydrological cycle – The oxygen cycle – The nitrogen cycle – The sulphur cycle – Composition of atmosphere – Earth's radiation balance – Green house effect.

Unit 2
Air pollution – Primary pollutants, Acid rain – Air quality standards – Sampling – Monitoring – Analysis of CO, nitrogen oxides, sulphur oxides, hydrocarbons and particulate matter – Control of air pollution.
Unit 3
Soil pollution – Inorganic and organic components in soil – Acid – Base and ion exchange reactions in soils – Micro and macro nutrients – Wastes and pollutants in soil.
Unit 4
Water pollution – Water pollutants – Eutrophication – Water quality criteria for domestic and industrial uses – Trace elements in water – Determination of quality parameters – Total hardness, TDS, pH, chloride, heavy metals, etc. Principles of water and waste water treatment – Aerobic and anaerobic treatment – Industrial waste water treatment – Removal of organic and inorganic materials from water and waste water.
Unit 5
Instrumental techniques in environmental analysis – Use of neutron activation analysis – ASV, AAS, GC, HPLC, ion selective electrodes and ion chromatography in environmental chemical analysis.

References:

1. G. W. VanLoon, S. J. Duffy, Environmental Chemistry, Oxford University Press, 2005.
2. J. Girard, Principles of Environmental Chemistry, Jones & Bartlett Learning, 2005.
3. S. E. Manahan, Environmental Chemistry, 7th ed., CRC Press, 2010.
4. E. R. Weiner, Applications of Environmental Chemistry, CRC Press, 2010.
5. I. Williams, Environmental Chemistry, John Wiley, 2001.
6. G. Schwedt, The Essential Guide to Environmental Chemistry, John Wiley, 2001.

ELECTIVE

CHE 2110

Solid State Chemistry

Credit 2 **32 hours**

Course Outcome After completion of the full course the student should be able to	**Cognitive level**
C.O.1: explain the and predict the conductivity of different solids.	Apply
C.O.2: identify the crystal defects and predict the consequences.	Apply
C.O.3: predict the structure-property correlation in crystalline inorganic solids and their probable application.	Apply
C.O.4: provide a comparison of the various synthetic methods for preparation of inorganic solids.	Understand

MAPPING of CO's and PO's

	Programme Outcomes							
Course Outcomes	P.O.1	P.O.2	P.O.3	P.O.4	P.O.5	P.O.6	P.O.7	P.O.8
C.O.1	x	x						x
C.O.2	x	x						x
C.O.3	x	x			x			x
C.O.4	x	x						x

Unit 1

Band theory of solids- energy bands, conductors and non-conductors, intrinsic semiconductors, extrinsic semiconductors, Hall effect.

Unit 2

Crystal structures, crystal defects: point, line and plane defects; vacancies. Stoichiometric Defects: Equilibrium concentration of point defects in crystals - Schottky defects, Frenkel defects; The photographic process - light sensitive crystals, mechanism of latent image formation.

Non-Stoichiometric Defects: Origin of non-stoichiometry, consequences of non-stoichiometry; Equilibria in non-stoichiometric solids, Colorcenters: F-centre, electron and hole centre; Colour centre and information storage.

Unit 3

Electrical properties; conductivity in pure metals; superconductivity; basics, discovery and high Tc superconductors magnetic properties; ferromagnetic and antiferromagnetic materials.

Optical properties; photoconductivity, photovoltaic effect, applications- perovskite solar cell. luminescence. Electrical properties: dielectric properties, piezo-electricity, Ferro electricity. Lasers and their applications in chemistry.

Unit 4

Crystals- Preparation methods: Solid state reaction, chemical precursor method, co-Precipitation, sol-gel, metathesis, self-propagating high temperature synthesis, ion exchange reactions, intercalation/deintercalation reactions; hydrothermal and template synthesis; Microwave Irradiation method, Sonochemical method, preparation of thin films - electrochemical methods, chemical vapour deposition; Crystal growth - Bridgman & Stokbarger methods, zone melting.

References:

1. R. West, Solid State Chemistry and its Applications, John Wiley, 1987.
2. N. B. Hannay, Solid State Chemistry, Prentice Hall of India, 1979.
3. R. J. D. Tiley, Defect Crystal Chemistry and its Applications, Chapman and Hall, NewYork, 1987.
4. L. V. Azaroff, Introduction to Solids, Mc.Graw Hill, New York, 1960.
5. A. K. Galwey, Chemistry of Solids, Chapman and Hall, London, 1967.
6. L. Smart, E. Moore, Solid State Chemistry, Chapman and Hall, 1995.
7. H. V. Keer, Principles of the Solid State, Wiley Eastern Ltd, New Delhi, 1993.

SEMESTER: 2

CORE

CHE 2201

Chemistry of d- and f-block Elements

(Inorganic Chemistry – II)

Credit 3 **48 hours**

Course Outcome After completion of the full course the student should be able to	**Cognitive level**
C.O.1: describe and explain the structure, bonding and magnetism in metal complexes using crystal field theory.	Analyse
C.O.2: describe various metal-ligand interactions in terms of sigma- and pi-bonding.	Analyse
C.O.3: identify various d-d transitions and interpret the electronic spectra of any given transition metal complex.	Evaluate
C.O.4: interpret the ESR spectra of any given transition metal complex.	Evaluate
C.O.5: explain the stability of metal complexes, their reactivity, and the mechanisms of ligand substitution and redox reactions.	Evaluate
C.O.6: interpret the Mossbauer spectra of iron complexes.	Apply

MAPPING of CO's and PO's

	Programme Outcomes							
Course Outcomes	P.O.1	P.O.2	P.O.3	P.O.4	P.O.5	P.O.6	P.O.7	P.O.8
C.O.1	x	x						x
C.O.2	x	x			x			x
C.O.3	x	x				x		x
C.O.4	x	x				x		x
C.O.5	x	x			x			x
C.O.6	x	x				x		x

Unit 1

Bonding in coordination complexes: crystal-field theory, d-orbital splitting in octahedral, tetrahedral, square planar, trigonal bipyramidal, trigonal planar and linear geometries, crystal field stabilization energy, effect of pairing energy, Jahn-Teller effect, tetragonal distortion and square planar complex. Application of crystal filed theory, lattice energies, ionic radii, site preferences in spinels.

Molecular Orbital Theory: construction of molecular orbital diagrams using group theory, qualitative MO diagrams for octahedral, tetrahedral and square planar complexes, effect of π-bonding, experimental evidence for π-bonding, spectrochemical series.

Unit 2

Microstates, Atomic term symbols_Free ion terms for dn configuration, Splitting of terms in octahedral and tetrahedral octahedral fields, Correlation diagram for d^2 configuration in octahedral geometry, d-d transitions, Selection rules for electronic transitions.

Orgel diagram – splittings for d^1, d^9, high spin d^4, d^6, splittings for high spin d^2, d^3, d^8 and d^7

Calculation of Dq, B and β

Tanabe Sugano diagrams – splittings for low spin d^n systems

Electronic Spectral interpretation of some coordination compounds

Consequence of Jahn Teller effect on the electronic spectra of coordination compounds

Charge transfer spectra, Electronic spectra of lanthanide and actinide complexes

Unit 3

Magnetism: brief review of different types of magnetic behaviours, spin-orbit coupling, quenching of orbital angular moments in crystal field, spin-only formula, correlation of μ_s and μ_{eff} values, magnetic moments of T terms and A, E terms, temperature independence paramagnetism, magnetic properties of lanthanides and actinides.

Unit 4

Electronic paramagnetic resonance spectroscopy: Electronic Zeeman effect, Zeeman Hamiltonian and EPR transition energy. Presentation of spectra. The effects of electron Zeeman, nuclear Zeeman and electron nuclear hyperfine terms in the Hamiltonian on the energy of the hydrogen atom. Second order effect. Hyperfine splittings in isotropic systems, spin polarization mechanism and McConnell's relations Anisotropy in g-value, EPR of triplet states, zero field splitting, Kramer's rule, survey of EPR spectra of first row transition metal ion complexes.

Mossbauer spectroscopy- Principles and applications to coordination compounds.

Unit 5

Reaction Mechanism: Thermodynamic and kinetic consideration, formation constant and rate constant, inert and labile complexes, factors affecting the stability and lability of complexes.

Ligand substitution in octahedral complexes, mechanism of substitution reactions in octahedral complexes, dissociative, associative and interchange mechanism, energy profile of reactions, acid and base hydrolysis, factors affecting the rate of substitution reactions in octahedral complexes.

Ligand substitution in square planar complexes, mechanism of substitution reactions in square planar complexes, energy profile of reactions, the trans effect and its applications, theories for explaining trans effect, factors affecting the rate of substitution reactions in square planar complexes.
Electron Transfer Reactions: inner sphere and outer sphere mechanism, Marcus theory, photochemical reactions.

References:

1. G.L. Miessler, P.J. Fischer, D.A. Tarr, Inorganic Chemistry, 5th ed., Pearson, 2014.
2. F. A. Cotton, G. Wilkinson, C. A, Murillo, M. Bochmann Advanced Inorganic Chemistry, 6th ed., Wiley-Interscience: New York, 1999.
3. J.E. Huheey, E. A. Keiter, R. L. Keiter, Inorganic Chemistry: Principles of structure and Reactivity, 4th ed., Harper Collin College Publishers, 1993.
4. J. W. Steed, J. L. Atwood, Supramolecular Chemistry, 2nd ed., John Wiley & Sons Ltd., 2009.
5. D. F. Shriver, P. W. Atkins, C. H. Langford, Inorganic Chemistry, 3rd ed., ELBS, 1999.
6. B. Douglas, D. McDaniel, J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd ed., John Wiley and Sons, 1994.
7. N. N. Greenwood, A. Earnshaw, Chemistry of the Elements, 2nd ed., BH, 1997.
8. R. S.Drago, Physical Methods for Chemists, 2nd ed., Saunders College Publishing, 1992.
9. C. E. Housecroft, A. G. Sharpe, Inorganic Chemistry, 5th ed., Pearson, 2018.
10. W. L. Jolly, Modern Inorganic Chemistry, 2nd ed., McGraw-Hill, New York, 1991.

CORE

CHE 2202

Reactions and Mechanisms

(Organic Chemistry – II)

Credit 2 **32 hours**

Course Outcome After completion of the full course the students should be able to	**Cognitive level**
C.O.1: recognize the mechanistic aspects of substitution, addition and elimination reactions, considering various influencing factors.	Analyse
C.O.2: predict the reactivity of an organic compound from its structure and based on the reaction conditions.	Evaluate
C.O.3: propose a reasonable mechanism for a given organic reaction.	Evaluate
C.O.4: predict the products in a particular reaction considering the stereochemical aspect.	Evaluate
C.O.5 illustrate the mechanistic pathway of different rearrangements reactions and identify the products.	Analyse
C.O.6 identify the mechanism and the product in a given reaction under photochemical condition.	Analyse

MAPPING of CO's and PO's

	Programme Outcomes							
Course Outcomes	P.O.1	P.O.2	P.O.3	P.O.4	P.O.5	P.O.6	P.O.7	P.O.8
C.O.1	x	x			x			x
C.O.2	x	x	x		x			x
C.O.3	x	x			x			x
C.O.4	x	x	x		x			x
C.O.5	x	x			x			x
C.O.6	x	x			x			x

Unit 1

Aliphatic substitution reactions – saturated and unsaturated systems – Mechanism of nucleophilic substitution – SN2, SN1 – ion pairs, SET, Neighbouring group participation – non classical carbocations, SNi, Tetrahedral mechanism. Electrophilic substitution – SE2, SEi, SE1. Free radical substitution.

Reactivity – Effect of substrate structure, nature of reagents, solvents and stereochemistry on the outcome of these reactions. Ambident nucleophiles and substrates. Typical reactions involving substitution.

Unit 2

Mechanisms of polar addition – electrophilic, nucleophilic and free radical addition. Nonpolar additions (excluding pericyclic reactions) - Reactivity and orientation. Eliminations - E2, E1 and E1CB mechanisms, reactivity and orientation. Pyrolytic syn eliminations, α - eliminations, elimination vs. substitution. Typical reactions involving addition and elimination.

Commented [SD1]: Specify reactions

Unit 3

Substitutions on aromatic carbon: Mechanism of electrophilic, nucleophilic and free radical substitutions – orientation and reactivity. Typical reactions involving aromatic substitution.

Unit 4

Rearrangements involving electron deficient carbon and nitrogen. Mechanism of the following rearrangements: Wagner-Meerwein, Pinacol, Demyanov, dienone-phenol, Favorskii, Wolff, Hofmann, Curtius, Lossen, Schmidt, Beckmann, benzidine, and Hofmann-Loffler, Fries, Baeyer-Villiger rearrangements. Fritsch-Buttenberg-Wiechell rearrangement, Corey-Fuchs reaction, Seyferth-Gilbert homologation, Grubbs catalysts and olefin metathesis.

Unit 5

Photochemistry: Unimolecular and bimolecular processes in the excited states, mechanism of important photochemical reactions, Paterno-Buchi reaction, Norrish Type I and Type II fragmentation, di-pi-methane rearrangement, Barton reaction, photochemistry of olefins, arenes, cyclohexadienones; photoreduction and photo-oxygenation.

References:

1. J. March Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 7th ed. Wiley, 2013.
2. T. H.Lowry, K.S.Richardson, Mechanism and Theory in Organic Chemistry, 3rd ed., Benjamin-Cummings Publishing Company, 1997.
3. F. A. Carey, R. J. Sundberg, Advanced Organic Chemistry (parts A and B), 5th ed., Springer, 2008.
4. E. V. Anslyn, D. A. Dougherty, Modern Physical Organic Chemistry. University Science Books, 2006.
5. F. A. Carroll, Perspectives on structure and mechanism in organic chemistry, Wiley, 2011.
6. N. S. Issacs, Physical Organic Chemistry, 2nd ed., Prentice Hall, 1995.
7. A. Pross: Theoretical and Physical Principles of Organic Chemistry, 1st ed., Wiley, 1995.
8. J. Clayden, N. Green, S. Warren, P. Wothers, Organic Chemistry, 2nd ed., Oxford University Press, 2012.

9. I. Flemming, Frontier orbitals and organic chemical reactions, Wiley-Blackwell, 1976.
10. I. Flemming: Molecular orbitals and organic chemical reactions, student ed., Wiley, 2009.
11. J. McMurry, Organic Chemistry, 5th ed., Brooks/Cole, 2000.
12. R. Bruckner, Advanced organic chemistry: Reaction Mechanisms. Academic Press, 2001.
13. P. Sykes, Guidebook to Mechanism in Organic Chemistry, 6th ed., Prentice Hall, 1986.
14. N. J. Turro, Modern Molecular Photochemistry, University Science Books, 1996.
15. N. J. Turro, J. C. Scaiano, V. Ramamurthy, Modern Molecular Photochemistry of Organic Molecules, 1st ed., University Science Books, 2010.

CORE

CHE 2203

Reagents and Synthesis

(Organic Chemistry – III)

Credit 2 **32 hours**

Course Outcome After completion of the full course the students should be able to	**Cognitive level**
C.O.1: compare the differences in reactivity of various reducing and oxidizing agents with mechanistic illustrations.	Analyse
C.O.2: predict the reagents and conditions for the synthesis of specific target molecules.	Apply
C.O.3: explain the reactivity, the stereo chemical aspects and various reactions possible with carbonyl compounds.	Evaluate
C.O.4: demonstrate strategies for the stereospecific/stereo selective organic transformations towards chiral target molecules.	Apply
C.O.5: predict the required protecting groups and functional group equivalents for a particular organic transformation.	Analyse
C.O.6: design a synthetic pathway for simple to complex organic molecules by retrosynthetic approach.	Evaluate

MAPPING of CO's and PO's

	Programme Outcomes							
Course Outcomes	P.O.1	P.O.2	P.O.3	P.O.4	P.O.5	P.O.6	P.O.7	P.O.8
C.O.1	x	x			x			x
C.O.2	x	x			x			x
C.O.3	x	x			x			x
C.O.4	x	x			x	x		x
C.O.5	x	x	x		x			x
C.O.6	x	x	x		x			x

Unit 1

Reagents for oxidation and reduction: Chromium based reagents, activated DMSO oxidations, osmium tetroxide, selenium dioxide, singlet oxygen, peracids, hydrogen peroxide, periodic acid, lead tetraacetate, Woodward and Prevost hydroxylation, Sharpless asymmetric epoxidation. Catalytic hydrogenations (heterogeneous and homogeneous), metal hydride reduction, Birch reduction, hydrazine and diimide reduction.

Unit 2

Synthetic applications of organometallic and organo-nonmetallic reagents: Reagents based on nickel, palladium, silicon, and boron. Gilman's reagent, phase transfer catalysts, hydroboration reactions, synthetic applications of alkylboranes.

Unit 3

Chemistry of carbonyl compounds: Reactivity of carbonyl groups in aldehydes, ketones, carboxylic acids, esters, acyl halides and amides. Substitution at carbonyl carbon, mechanisms of ester hydrolysis. Substitution at α-carbon, aldol and related reactions, stereoselective nucleophilic additions to acyclic carbonyl groups. Cram's Rule. Felkin-Ahn Model. Effect of chelation on selectivity. Claisen, Darzen, Dieckmann, Perkin, Prins, Mannich, Stork-enamine reactions. Conjugate additions, Michael additions and Robinson annulation. Reaction with phosphorous and sulfur ylides.

Unit 4

Protecting groups, functional group equivalents, reversal of reactivity (Umpolung), Chemistry of Nucleophilic Heterocyclic Carbenes (NHCs).

Introduction to Asymmetric Synthesis: Principle, stereospecific and stereoselective synthesis. General strategies-Chiral pool strategy, chiral auxiliaries, chiral reagents and chiral catalysts.

Unit 5

Synthetic strategies: Introduction to retrosynthesis, strategic bond analysis, one group and two group disconnections, synthesis of longifolene, Corey lactone, Djerassi Prelog lactone.

References:

1. M. B. Smith, Organic Synthesis, 2^{nd} ed., McGraw-Hill, 2000.
2. T. W. Greene, P. G. M. Wuts, Protecting Groups in Organic Synthesis, 2^{nd} ed., John Wiley, 1991.
3. J. March, Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 7^{th} ed. Wiley, 2013.
4. P. G. M. Wuts, Greene's Protective Groups in Organic Synthesis, Wiley & Sons, 2014.
5. F. A. Carey, R. J. Sundberg, Advanced Organic Chemistry (Parts A and B), 5^{th} ed., Springer, 2008.
6. S. Warren, Organic Synthesis: The Disconnection Approach, 2^{nd} ed., John Wiley, 2008.
7. H. O. House, Modern Synthetic Reactions, W. A. Benjamin Inc., 1972.

8. W. Carruthers, Some Modern Methods of Organic Synthesis, 4th ed., Cambridge University Press, 2004.
9. I. L. Finar, Organic Chemistry, Volumes 1 & 2, 6th ed., Pearson Education Asia, 2004.
10. J. Clayden, N. Green, S. Warren, P. Wothers, Organic Chemistry, 2nd ed., Oxford University Press, 2012.
11. P. S. Kalsi, Stereochemistry: Conformation and Mechanism, 10th ed., New Age Publications, 2019.
12. E. L. Eliel, S. H. Wilen, Stereochemistry in Organic Compounds, John Wiley, 1994.
13. D. Nasipuri, Stereochemistry of Organic Compounds: Principles and Applications, 2nd ed., Wiley Eastern Limited, New Delhi, 1994.
14. B. P. Mundy, Name Reactions and Reagents in Organic Synthesis, 2nd ed., Wiley, 2005.
15. P. Vogel, K. N. Houk, Organic Chemistry: Theory, Reactivity and Mechanisms in Modern Synthesis, Wiley-VCH, 2019.
16. P. S. Kalsi, Organic Synthesis through Disconnection Approach, 2nd ed., Medtech Publisher, 2019.

CORE

CHE 2204

Spectroscopy of Organic Compounds

(Organic Chemistry – IV)

Credit 2 **32 hours**

Course Outcome After completion of the full course the students should be able to	**Cognitive level**
C.O.1: identify structures of unknown organic compounds using hyphenated techniques and spectral library matching.	Apply
C.O.2: identify structures of unknown organic compounds based on the data from UV-Vis, IR, Mass Spectrometry ^{1}HNMR and ^{13}CNMR spectroscopy.	Apply

MAPPING of CO's and PO's

	Programme Outcomes							
Course Outcomes	P.O.1	P.O.2	P.O.3	P.O.4	P.O.5	P.O.6	P.O.7	P.O.8
C.O.1	x	x						x
C.O.2	x	x						x

Unit 1

Study of Mass Spectrometry applied to organic molecular systems

Elemental analysis, empirical formula, molecular formula, Molecular mass, nominal mass, Exact mass, Index of hydrogen deficiency.

The technique of Mass Spectrometry: Molecular ion, ion production methods (EI). Soft ionization methods: FAB, CA, MALDI, PD, Field desorption electrospray ionization, HRMS and formula mass, LC-MS, GC-MS. MS- MS

Mass spectra of chemical classes and its correlation with structure: Fragmentation patterns, nitrogen and ring rules, Rule of thirteen, McLafferty rearrangement.

Unit 2

Study of Ultraviolet-Visible Absorption and Emission and Chirooptical Spectroscopy applied to organic molecular systems

Energy levels and selection rules, Woodward-Fieser and Fieser-Kuhn rules, estimation of λmax of substituted aromatic ketones, aldehydes and acids. Spectral correlation with structure: Influence of substituents, conjugation, Intramolecular Charge transfer, Solvent effect

Fluorescence Spectroscopy. Excitation and Emission Spectra. Fluorescence Quantum Yield and Lifetime. Spectral correlation with structure: Influence of substituents, ring size, strain and conjugation, Intramolecular Charge transfer, Intramolecular proton transfer, Solvent effect

Chirooptical Spectroscopy: Introduction and applications of ORD, CD, Octant rule, axial haloketone rule, Cotton effect.

Unit 3

Study of Infrared Spectroscopy applied to organic molecular systems

Fundamental vibrations, overtones, Fermi Resonance, Hot bands, combination bands

Spectral correlation with structure: Characteristic regions of the spectrum. Influence of substituents, ring size, hydrogen bonding, vibrational coupling, hybridization and field effect on frequency.

IR spectra of chemical classes including amino acids and its correlation with structure

Unit 4

Study of NMR spectroscopy applied to organic molecular systems

The NMR instrumentation and Experiment: Magnetic nuclei with special reference to 1H and 13C nuclei. Chemical shift and shielding/deshielding, relaxation processes, chemical and magnetic non-equivalence, local diamagnetic shielding and magnetic anisotropy. Proton and 13C NMR scales, characteristics of 13C as a nucleus.

Spin-spin splitting, AX, AX2, AX3, A2X3, AB, ABC, AMX type coupling, First order and non-first order spectra, Pascal's triangle, coupling constant, mechanism of coupling, Karplus curve, quadrupole broadening and decoupling, diastereomeric protons, virtual coupling, long range coupling effects, NOE, coupling with other nuclei.

Simplification non-first order spectra to first order spectra, shift reagents-mechanism of action, spin decoupling and double resonance, Chemical shifts and homonuclear/heteronuclear couplings, the basis of heteronuclear decoupling.

Polarization transfer. Selective Population Inversion (qualitative description only), DEPT, sensitivity enhancement and spectral editing. 2D NMR and COSY, HMQC, HMBC.

Unit 5

Identification of structures of unknown organic compounds using hyphenated techniques and Spectral library matching

Identification of structures of unknown organic compounds based on the data from UV-Vis, IR, Mass, 1HNMR and 13CNMR spectroscopy.

References:

1. D. L. Pavia, G. M. Lampman, G. S. Kriz, J. R. Vyvyan, Introduction to Spectroscopy: A Guide for Students of Organic Chemistry, Indian ed., Brooks/Cole Cengage Learning, 2007.
2. Atta-Ur-Rahman, M. I. Choudhary, Solving Problems with NMR Specroscopy, Academic Press, New York, 1996.
3. L. D. Field; S. Sternhell, J. R. Kalman; Organic Structures from Spectra, 4th ed., Wiley 2008.
4. R. S. Drago, Physical Methods for Chemist, Saunders,1992.
5. C. N. Banwell, E. M. McCash, Fundamentals of Molecular Spectroscopy, 4th ed., McGrawHill, 1994.
6. D. F. Taber, Organic Spectroscopic Structure Determination, A Problem Based Learning Approach, Oxford University Press, 2009.
7. R. M. Silverstein, G. C. Bassler, T. C. Morril, Spectroscopic Identification of Organic Compounds, John Wiley, 1991.
8. D. H. Williams, I. Fleming, Spectroscopic Methods in Organic Chemistry, Tata McGraw Hill, 1988.
9. W. Kemp, Organic Spectroscopy, 2nd ed., ELBS-Macmillan, 1987.
10. F. Bernath, Spectra of Atoms and Molecules, 2nd ed., Oxford University Press, 2005.
11. E. B. Wilson, Jr., J. C. Decius, P. C. Cross, Molecular Vibrations: The Theory of Infrared and Raman Spectra, Dover Publications, 1980.
12. A. Weil, J. R. Bolton, Electron Paramagnetic Resonance: Elementary Theory and Practical Applications, 2nd ed., Wiley Interscience, John Wiley & Sons, Inc., 2007.
13. C. P. Slichter, Principles of Magnetic Resonance, 3rd ed., Springer-Verlag, 1990.
14. H. Gunther, NMR Sprectroscopy: Basic Principles, Concepts and Applications in Chemistry, 3rd ed., Wiley- VCH, 2013.
15. Spectral data bases (RIO DB of AIST, for example).

CORE

CHE 2205

Statistical Thermodynamics

(Physical Chemistry – I)

Credit 2 **32 hours**

Course Outcome At the end of the course student should be able to	**Cognitive level**
C.O.1: explain the different types of statistics and calculate the thermodynamic probability of any given thermodynamic system.	Analyse
C.O.2: calculate the partition function and thermodynamic properties from spectroscopic data.	Apply
C.O.3: apply the principles of statistical thermodynamics to ideal gases, solids and metals.	Apply

MAPPING of CO's and PO's

	Programme Outcomes							
Course Outcomes	P.O.1	P.O.2	P.O.3	P.O.4	P.O.5	P.O.6	P.O.7	P.O.8
C.O.1	x	x						x
C.O.2	x	x			x			x
C.O.3	x	x						x

Unit 1

Kinetic Theory of gases, Distribution of molecular velocities and kinetic energy- Maxwell Boltzmann distribution. Effect of temperature on distribution. Types of molecular velocities- Most Probable Velocity, Mean velocity, r.m.s. velocity.

Transport phenomena- Effusion, diffusion, thermal conductivity and viscosity of gases

Unit 2

Introduction to statistical Thermodynamics, Microstates and Macrostates, Probability, Thermodynamic Probability, Relation between entropy and thermodynamic probability,

Unit 3

Partition Function of noninteracting particles. Molecular partition function. Translational, Rotational and Vibrational Partition Function, Thermodynamic properties in terms of partition function- Ideal monatomic, diatomic and polyatomic gases. Equipartition principle. Partition function and equilibrium constant.

Unit 4

Types of statistics- Maxwell Boltzmann, Bose Einstein and Fermi Dirac Statistics, Comparison of statistics. Dilute system concept.

Applications of B.E and F.D Statistics - Bose-Einstein Condensation, Electron gas concept- Contribution to pressure and heat capacity.

Specific heat capacity of solids- Einstein's and Debye theory.

References:

1. F. W. Sears, Introductions to Thermodynamics, Kinetic Theory of Gases and Statistical Mechanics, Addision Wesley Pub. Cambridge, 1998.
2. F. C. Andrews, Equilibrium to Statistical Mechanics, John Wiley, New York, 2002.
3. L. K. Nash, Statistical Thermodynamics, Addison Wesley, New York, 1999.
4. P. W. Atkins, J. de Paula, Physical Chemistry 8^{th} ed., 9^{th} ed., Wiley, New York, 2006
5. D. A. McQuarrie, Physical Chemistry - A Molecular Approach, South Asian ed., 2008.
6. M. Dole, Introduction to Statistical Thermodynamics, Prentice Hall, London, 1997.
7. J. Kestin, J. R. Dorfman, A Course in Statistical Thermodynamics, Academic press, 1971.

ELECTIVE

CHE 2206

Chemical Bonding and Computational Chemistry

Credit 2 **32 hours**

Course Outcome After completion of the full course the student should be able to	**Cognitive level**
C.O.1: explain the quantum mechanical nature of the chemical bond.	Understand
C.O.2: account for the basic principles and concepts of molecular orbital theory and valence bond theory using quantum mechanical principles.	Apply
C.O.3: describe quantum mechanically the chemical bonding of any given di- and tri- atomic molecules with molecular orbital theory and valence bond theory.	Analyse
C.O.4: describe the main similarities and differences between theoretical approaches and identify advantages and disadvantages for modelling various chemical problems.	Apply
C.O.5: use computational chemistry software to perform and interpret electronic structure calculations.	Evaluate

MAPPING of CO's and PO's

	Programme Outcomes							
Course Outcomes	P.O.1	P.O.2	P.O.3	P.O.4	P.O.5	P.O.6	P.O.7	P.O.8
C.O.1	x	x						x
C.O.2	x	x						x
C.O.3	x	x						x
C.O.4	x	x			x	x	x	x
C.O.5	x	x			x		x	x

Unit 1

Chemical boning, Born Oppenheimer approximation, Valence bond method. Comparison of VB and MO method, LCAO approximation, calculation of energy levels from wave functions, application to diatomic molecules such as, H_2^+, H_2. Concept of σ, σ*, π, π* orbitals and their characteristics, hybrid orbitals, calculation of coefficients of AO used in sp, sp^2 and sp^3 hybrid orbitals, interpretation of geometry, Valence bond model of H_2, Hybridisation of H_2O, BF_3, NH_3 and CH_4

Unit 2

Pi bonding in simple molecules, HMO method for linear conjugated hydrocarbons, linear, cyclic, polycyclic, heterocyclic; ethylene, 1,3-butadiene, allyl radical, cation and anion, aromatic hydrocarbons, cyclopropenyl systems, cyclobutadiene, benzene, naphthalene, thiophene. calculation of charge distribution, bond orders and reactivity.

Unit 3

Tools and philosophy of computational chemistry. potential energy surface - local minima, global minima, saddle point and transition states, geometry optimization- stationary points.

Basis sets, Slater and Gaussian functions, classification of basis sets - minimal, double zeta, triple zeta, split valence, polarization and diffuse basis sets, contracted basis sets, Pople style basis sets and their nomenclature, correlation consistent basis sets.

SCF methods, semiempirical, ab initio, electron correlations, post-Hartree-Fock methods and density functional theory.

Unit 4

molecular structure, internal coordinates, Cartesian coordinates, geometry optimization, frequency analysis, partial charge, MO, Conformational analysis of ethane and butane

calculation of some simple chemical problems using computational chemistry programme packages.

References:

1. J. P. Lowe, Quantum Chemistry, 3rd ed., Academic Press, New York, 2008.
2. F. Jensen, Introduction to Computational Chemistry, 2nd ed., Wiley, New York, 2009.
3. R. Leach, Molecular Modeling, Principles and Applications, 2nd ed., Pearson Education, London, 2001.
4. A. K. Chandra, Introduction to Quantum Chemistry, 4th ed., Tata McGraw-Hill, 1994.
5. L. Pauling, E. B. Wilson, Introduction to Quantum Mechanics, McGraw-Hill, 1935.
6. A. Szabo, N. S. Ostlund, Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory, Dover Book ed., Mc.Graw-Hill, New York, 1982.
7. T. A. Albright, J. K. Burdett, M.-H. Whangbo, Orbital Interactions in Chemistry, 2nd ed., John Wiley and Sons, Inc., Hoboken, New Jersey, 2013.

ELECTIVE

CHE 2207

Bioanalytical Chemistry

Credit 2 **32 hours**

Course Outcome After completion of the full course the student should be able to	**Cognitive level**
C.O.1: demonstrate key features and characteristics of major biomolecules.	Understand
C.O.2: describe and explain the principles and applications of MRI and NMR for bioanalysis.	Understand
C.O.3: outline the principles and theory of major types of electrophoresis and electrophoretic separation.	Apply
C.O.4: explain the theory and applications of biochemical analysis like RIA, ELISA.	Analyze
C.O.5: appreciate the variety of popular methods to separate and isolate biomolecules.	Evaluate

MAPPING of CO's and PO's

	Programme Outcomes							
Course Outcomes	P.O.1	P.O.2	P.O.3	P.O.4	P.O.5	P.O.6	P.O.7	P.O.8
C.O.1	x	x						x
C.O.2	x	x				x		x
C.O.3	x	x				x		x
C.O.4	x	x				x		x
C.O.5	x	x				x		x

Unit 1

Biomolecules- amino acid, protein, nucleic acid –structures, physical and chemical properties, features and characteristics of major biomolecules, structure-function relationship, significance.

Different methods for the estimation of protein.

Transition metals in health and disease - Importance of transition metals in physiological processes, Therapeutic implications of transition metals.

Unit 2

Transmission electron Microscopy (TEM), Scanning electron Microscopy (SEM) – Instrumentation and its biological applications.

Nuclear magnetic resonance (NMR) and magnetic resonance imaging (MRI) technologies: key tools for the life and health sciences. Principles of NMR and the importance of this biomolecular analytical technique. Established and emerging applications of NMR. Principles and uses of MRI. MRI as a principal diagnostic and research tool.

Unit 3

Electrophoretic techniques – Principles of electrophoretic separation. Types of electrophoresis including paper, gel. Electroporation, Pulse field gel electrophoresis- applications in life and health science.

Unit 4

Radio immune assay (RIA) - principle and applications. Enzyme linked immune sorbent assay (ELISA) principle and applications. Biosensors-applications.

Unit 5

principle of centrifugation, concept of RCF, features and component of major types of centrifuge, preparative, differential and density gradient centrifugation, analytical ultra-centrifugation, centrifugation. Flow cytometry: principles and applications of this core method of separation.

References:

1. V. A. Gault, N. H. Mcclenaghan, Understanding bio analytical chemistry - principle and applications, John Wiley and Sons, Ltd Publications, 2009.
2. A. Manz, N. Pamme, D. Iossifidis, Bio-analytical Chemistry, 2004
3. S. R. Mikkelsen, E. Corton, Bio Analytical Chemistry, John Wiley and Sons, Ltd Publications, 2004.
4. K. Wilson, J. Walker, Practical Biochemistry-Principles and techniques, 5th ed., Cambridge University press, 2000.

CORE

CHE 2208

Organic Chemistry Laboratory

Credit 2 **96 hours**

Course Outcome After completion of the full course the students should be able to	**Cognitive level**
C.O.1: acquire knowledge on safe laboratory practices of handling laboratory glassware, equipment and chemical reagents.	Knowledge
C.O.2: plan and perform synthetic procedures, chromatographic separation and purification of organic compounds.	Understand
C.O.3: separate organic compounds from the organic binary mixture and identify the functional group(s) present.	Analysis
C.O.4: use software to Draw the structures and schemes of organic molecules and reactions.	Apply
C.O.5: use Chemical Abstracts, Scopus, Organic Synthesis collective volumes on web etc. to search, analyse and collect chemical information.	Apply

MAPPING of CO's and PO's

	Programme Outcomes							
Course Outcomes	P.O.1	P.O.2	P.O.3	P.O.4	P.O.5	P.O.6	P.O.7	P.O.8
C.O.1	x	x				x		x
C.O.2	x	x	x		x	x		x
C.O.3	x	x		x		x		x
C.O.4	x	x				x	x	x
C.O.5	x	x			x	x		x
C.O.6	x	x				x	x	x

Part I: General methods of separation and purification of Organic compounds such as 1) Solvent extraction 2) Thin layer chromatography and paper chromatography 3) column chromatography

Part II: Separation and identification of the components of organic binary mixtures.

Part III: Preparation of Organic compounds by multistep reactions, purification of products and characterisation using UV-Vis, FTIR and NMR.*

Part IV: Drawing the structures of organic molecules and reaction schemes by Proprietary and open source computer software. Use Chemical Abstracts, Scopus, Organic Synthesis collective volumes on web etc., to search, analyse and collect chemical information.

*Progress of the reactions should be followed by spectroscopic and chromatographic methods (UV-Vis, TLC, GC, HPLC, etc)

References:

1. A. I. Vogel, A. R. Tatchell, B. S. Furnis, A. J. Hannaford, P. W. G. Smith, Vogel's Textbook of Practical Organic Chemistry, 5th ed., John Wiley, 1989.
2. D. L. Pavia, G. M. Lampman, G. S. Kriz, Introduction to Organic laboratory Techniques, 3rd ed., Saunders Golden Sunburst Series.
3. L. W. Harwood, C. J. Moody, Experimental Organic Chemistry-Principles and Practice, Blackwell Science Publications.

CORE

CHE 2209

Open-ended Laboratory – II

Credit 0

Course Outcome After completion of the full course the student should be able to	**Cognitive level**
C.O.: design experiments and validate the hypothesis of an independent research problem.	Evaluate

MAPPING of CO's and PO's

	Programme Outcomes							
Course Outcomes	P.O.1	P.O.2	P.O.3	P.O.4	P.O.5	P.O.6	P.O.7	P.O.8
C.O.	x	x	x	x	x	x	x	x

The students shall perform experiments/analysis for validating the hypothesis.

The students shall submit a project report and appear for viva-voce.

ELECTIVE

CHE 2210

Introduction to Theory of Orbital Interactions in Chemistry

Credit 2 **32 hours**

Course Outcome After completion of the full course the student should be able to	**Cognitive level**
C.O.1: examine the physical properties associated with molecules and the pathways taken by chemical reactions.	Analyse
C.O.2: qualitatively corelate the shape and energy of orbitals and the chemical reaction exhibited by any molecule.	Apply
C.O.3: explore the effects of symmetry, overlap, and electronegativity in the molecular orbital in case of chemical reaction.	Evaluate
C.O. 4: explore the structures and reactivity relationships associated with any molecule.	Evaluate

MAPPING of CO's and PO's

	Programme Outcomes							
Course Outcomes	P.O.1	P.O.2	P.O.3	P.O.4	P.O.5	P.O.6	P.O.7	P.O.8
C.O.1	x	x			x			x
C.O.2	x	x			x			x
C.O.3	x	x			x			x
C.O.4	x	x			x			x

Unit 1

Atomic and Molecular Orbitals, Concepts of Bonding and Orbital Interaction, Orbital Interaction Energy, Molecular Orbital Coefficients, Electron Density Distribution, Perturbational Molecular Orbital Theory, Linear H_3, HF, and the Three-Orbital Problem.

Unit 2

Molecular Orbital Construction from Fragment Orbitals, Triangular H_3, Rectangular and Square Planar H_4, Tetrahedral and Linear H_4, Pentagonal H_5 and Hexagonal H_6, Molecular Orbitals of Diatomic Molecules and Electronegativity Perturbation, Geometrical Perturbation of Molecular orbitals, Molecular Orbitals of AH_2, Walsh Diagrams, Jahn–Teller Distortions.

Unit 3

Molecular Orbitals of Small Building Blocks, AH System, AH_3 Systems, pi-Bonding Effects of Ligands, AH_4 System, Molecules with Two Heavy Atoms, A_2H_6 Systems, Orbital Interactions through Space and through Bonds.

Unit 4

Polyenes and Conjugated Systems, Acyclic Polyenes, Huckel Theory, Cyclic Systems, Conjugation in Three Dimensions, Solids, Energy Bands, Hypervalent Molecules.

Unit 5

Transition Metal Complexes. Octahedral ML_6, pi-Effects in an Octahedron, Distortions from an Octahedral Geometry, Square Planar, Tetrahedral ML_4 Complexes, Five Coordination, Square Pyramidal ML_5 Fragment, ML_3 Fragment, ML_2 and ML_4 Fragments, M_2L_8 Dimers, CpM and Cp_2M, Isolobal Analogy.

References:

1. T. A. Albright, J. K. Burdett, M.-H. Whangbo, Orbital Interactions in Chemistry, 2nd ed., John Wiley and Sons, Inc., Hoboken, New Jersey, 2013.
2. I. Flemming, Molecular Orbitals and Organic Chemical Reactions, Students ed., Wiley, 2009.
3. A. Rauk, Orbital Interaction Theory of Organic Chemistry, 2nd ed., Wiley-Blackwell, 2000.
4. W. L. Jorgensen, L. Salem, The Organic Chemist's Book of Orbitals, Academic Press, 1973.

ELECTIVE

CHE 2211

Nuclear and Radiation Chemistry

Credit 2 **32 hours**

Course Outcome After completion of the full course the student should be able to	**Cognitive level**
C.O.1: analyse the stability and mode of decay for a given nucleus.	Analyse
C.O.2: apply the decay kinetics relations to calculate the rate of radioactive processes.	Apply
C.O.3: identify the type of nuclear reaction and their applications in energy sector.	Understand
C.O.4: describe methods to measure radioactivity and the consequences of interaction radiation with matter.	Understand
C.O.5: study the working principle of isotope dating, labelling, radiation therapy and diagnosis.	Apply

MAPPING of CO's and PO's

	Programme Outcomes							
Course Outcomes	P.O.1	P.O.2	P.O.3	P.O.4	P.O.5	P.O.6	P.O.7	P.O.8
C.O.1	x	x						x
C.O.2	x	x			x			x
C.O.3	x	x			x			x
C.O.4	x	x			x			x
C.O.5	x	x			x			x

Unit 1

Elementary particles, Nuclear Stability- N/P ratio, Even Odd nature, Nuclear potential, Binding energy, Separation energy systematics, abundance systematics, exchange theory, Nuclear models- liquid drop model, shell model, semi-empirical mass equation, Nuclear properties- nuclear radius, mass, dipole moment, nuclear spin, magnetic moment, quadrupole moment and shape of nucleus.

Unit 2

Radioactivity – Types of decay, decay kinetics, kinetics of mixture of unrelated nuclides, parent daughter decay growth relationship, reaction cross section-compound nucleus theory, high energy nuclear, direct nuclear, photonuclear and thermonuclear reactions. Artificial transmutation and artificial radioactivity.

Unit 3

Types of nuclear reactions: Source of nuclear bombarding particles: Charged particle accelerators, gamma ray, X-ray and neutron sources. Fission: Fission products and Fission yield curve, Fission energy, theory of nuclear fission, nuclear reactor, breeder reactor, nuclear fuel, neutron source, chemistry of operating reactor, nuclear power plant – nuclear reactors in India. Fusion reactions, hydrogen bomb and energy of sun, radioactive waste disposal.

Unit 4

Radiation Chemistry, Detection and measurement of activity- Scintillation, semiconductor, thermoluminesence and neutron detector, Isotopes for reactors, preparation of radioisotopes, isotope separation, Transuranium elements, Limits of Stability, Element synthesis, super heavy elements.

Radiation chemistry- interaction of radiation with matter, radiation dosimetry, radiolysis of water, radiation induced damage. Applications of Radioactivity – Carbon dating, rock dating, NAA, Radiopharmaceuticals, RIA, Nuclear Forensics, surface area and solubility determination.

References:

1. H. J. Arnikar, Essentials of Nuclear Chemistry, 4th ed., New Age International, 2011.
2. W. D. Loveland, D. J. Morrissey, G. T. Seaborg, Modern Nuclear Chemistry, 2nd ed., Wiley, 2017.
3. K. H. Lieser, Nuclear and Radiochemistry, 2nd ed., Wiley VCH, 2001.
4. D. I. Coomber, Radiochemical Methods in Analysis, PLENUM PRESS, 1975.
5. J. F. Wishart, B. S. M. Rao, Recent Trends in Radiation Chemistry, World Scientific, 2011.1.

ELECTIVE

CHE 2212

Supramolecular Chemistry

Credit 2 **32 hours**

Course Outcome After completion of the full course the student should be able to	**Cognitive level**
C.O.1: explain the structural features of any given supramolecular system.	Analyse
C.O.2: analyse the type of possible interactions in any given host guest assembly.	Analyse
C.O.3: predict the photochemical and photophysical behaviour in constrained media.	Analyse
C.O.4: analyse the change in electronic structure of the supramolecular systems based on the interaction with the host.	Evaluate
C.O.5: utilize the studied systems for applications for catalysis, solar energy conversions, drug delivery etc.	Evaluate

MAPPING of CO's and PO's

	Programme Outcomes							
Course Outcomes	P.O.1	P.O.2	P.O.3	P.O.4	P.O.5	P.O.6	P.O.7	P.O.8
C.O.1	x	x						x
C.O.2	x	x						x
C.O.3	x	x			x			x
C.O.4	x	x			x			x
C.O.5	x	x			x			x

Unit 1

Structure, Preparation and Properties of: crown ethers, cryptates, cryptands, carcerands, calixarenes, cyclodextrins, fullerenes, dendrimers, rotaxanes, cucurbiturils, COF, MOF.

Unit 2

Noncovalent Interactions–Hydrogen bonding, π Effects, dipole interactions, Induced dipole interactions, Hydrophobic interactions. Solvent Effects, Thermodynamics of binding phenomena.

Unit 3
Molecular Recognition–Host guest interactions, Complementarity and Reorganization, large ion pairing component, hydrophobic component, hydrogen bond, π-component. Complex Architectures–Self-assembly, coordination, hydrogen bonding.
Unit 4
Photochemistry in constrained media- photophysical, photochemical processes, energy transfer, electron transfer. Effect of structural features and interactions on energy levels.
Unit 5
Applications–photocatalysis, water splitting, solar cell, CO_2 reduction, drug delivery, sensors, gas separation and storage.

References:

1. Jonathan W. Steed, Jerry L. Atwood, Supramolecular Chemistry, Wiley, 2013.
2. J. M. Lehn, Supramolecular Chemistry: Concepts and Perspectives, Wiley, 1995.
3. E. V. Ansyln, D. A. Dougherty, Modern Physical Organic Chemistry, University Press, 2006.
4. P. Klán and J. Wirz, Photochemistry of Organic Compounds: From Concepts to Practice, Wiley, 2009.
5. N. J. Turro, V. Ramamurthy, J. C. Scaiano, Modern Molecular Photochemistry of Organic Molecules, University Science Books, 2010.
6. C. S. Diercks, M. J. Kalmutzki, O. M. Yaghi, Introduction to Reticular Chemistry: Metal-Organic Frameworks and Covalent Organic Frameworks, Wiley, 2019.
7. S. Ma, J. A Perman, Elaboration and Applications of Metal-organic Frameworks, World Press, 2018.

SEMESTER: 3

CORE

CHE 2301

Instrumental Methods of Analysis

(Analytical Chemistry – II)

Credit 2 **32 hours**

Course Outcome After the completion of the course, the student will be able to	**Cognitive level**
C.O.1: explain the theory, instrumentation and application of various electroanalytical techniques like coulometry, electrogravimetry, polarography and voltammetry.	Apply
C.O.2: explain the theory, instrumentation and applications of AAS.	Understand
C.O.3: explain the theory, instrumentation and applications of fluorescence spectroscopy.	Apply
C.O.4: explain the instrumentation and applications of various surface characterisation techniques.	Analyze

MAPPING of CO's and PO's

	Programme Outcomes							
Course Outcomes	P.O.1	P.O.2	P.O.3	P.O.4	P.O.5	P.O.6	P.O.7	P.O.8
C.O.1	x	x				x		x
C.O.2	x	x				x		x
C.O.3	x	x				x		x
C.O.4	x	x				x		x

Unit 1

Electrogravimetry- coulometry- constant current and constant potential coulometry applications-primary and secondary coulometry – conductance measurement – conductometric titrations. Ion-selective electrodes, ion-selective FET, immobilized enzyme electrodes construction.

Unit 2

Polarography – current – voltage curve. DME-components of polarographic current – supporting electrolyte – polarographic maxima. Half-wave potential-Instrumentation, Applications of Polarography. Stripping analysis. Amperometric titrations – Different types. Applications, Voltammetry – different types, Cyclic Voltammetry-Theory and applications. Impedance spectroscopy, Voltammetric sensors – individual and simultaneous analysis.

Unit 3

Flame Emission and Atomic Absorption Spectrometer. Instrumentation of AAS, the flame spectra, flame characteristics. Atomizers used in spectroscopy, Hollow cathode lamp – Interference in AAS-applications. Advantages of AAS over AES Atomic emission spectroscopy-flame photometry-ICP – Theory, Instrumentation and Applications.

Unit 4

Fluorescence Spectroscopy- Molecular fluorescence and fluorometers, Jablonski diagram, Quenching, Stern Volmer plot, Fluorescence Sensors, Instrumentation for Fluorescence Spectroscopy.

Unit 5

Chemical Analysis of surfaces: Surface preparations-ion scattering spectrometry secondary ion scattering microscopy (SIMS)-Auger election spectroscopy-ESCA instrumentation and application.

Principles and Applications of SEM, TEM and AFM.

References:

1. D. A. Skoog, D. M. West, F. J. Holler, S. R. Crouch, Fundamentals of Analytical Chemistry, 8th ed., Saunders College Pub., 2007.
2. G. D Christian, Analytical Chemistry, 6th ed., John Wiley & Sons, 2007.
3. J. M. Mermet, M. Otto, R. Kellne, Analytical Chemistry, Wiley-VCH, 2004.
4. H. Gunzler, A. Williams, Handbook of Analytical Techniques, Volume 2, Wiley-VCH, 2001.
5. S. Higson, Analytical Chemistry, OUP Oxford, 2003.
6. A. Zschunke, Reference Materials in Analytical Chemistry, Springer, 2000.
7. K. Wilson, J. Walker, Practical Biochemistry-Principles and techniques, 4th ed., Cambridge University Press, 1997.

CORE

CHE 2302

Organometallic and Bioinorganic Chemistry

(Inorganic Chemistry – III)

Credit 3 **48 hours**

Course Outcome After completion of the full course the students should be able to	**Cognitive level**
C.O.1: distinguish the different types of ligands with respect to the type of interaction with the metal.	Analyse
C.O. 2: evaluate the structure, bonding and reactions of organometallic compounds and metal clusters.	Evaluate
C.O.3: predict the stability of organometallic compounds and metal clusters.	Apply
C.O.4: explain the application of reactions of organometallic complexes in homogeneous catalytic processes.	Apply
C.O.5: identify the role of metals in biological systems.	Apply

MAPPING of CO's and PO's

	Programme Outcomes							
Course Outcomes	P.O.1	P.O.2	P.O.3	P.O.4	P.O.5	P.O.6	P.O.7	P.O.8
C.O.1	x	x						x
C.O.2	x	x			x			x
C.O.3	x	x			x			x
C.O.4	x	x			x			x
C.O.5	x	x						x

Unit 1

Compounds with transition metal to carbon bonds: eighteen electron rule; classification of ligands, nomenclature, σ donor ligands – metal alkyl, aryl complexes; σ donor/π acceptor ligands, – metal alkenyls, alkynyls, carbenes, carbynes, carbonyls, isocyanide, fluxionality of ligands – structure, bonding, spectra, preparation and reactions.

Unit 2

σ, π donor/π acceptor ligands – olefin complexes, alkyne, allyl, enyl complexes, metallocene- ferrocene, titanocene, zircanocene, arene complexes, cycloheptatriene, cyclooctatetraene, cyclobutadiene complexes, fluxionality of ligands – structure, bonding, preparation, reactions and spectroscopy

Unit 3

Metal–Metal bonds and Transition metal clusters; preparation, properties and spectroscopy. Parallels with nonmetal chemistry- isolobal analogy. Application of Wade-Mingos-Lauher rules in predicting the structure of organometallic clusters

Unit 4

Reactions of organometallic complexes – Ligand cone angle, oxidative addition, reductive elimination, insertion, nucleophilic and electrophilic attack of coordinated ligands. Homogeneous catalysis using organometallic compounds: olefin hydrogenation, hydroformylation, Wacker process, Ziegler-Natta polymerisation, cyclo oligomerisation, olefin isomerisation, olefin metathesis, Monsanto acetic acid synthesis, Fischer-Tropsch process, hydrosilylation, coupling reactions in organic chemistry.

Unit 5

Metal ions in biological systems: Heme proteins – hemoglobin, myoglobin

Non-Heme Iron Proteins: Iron storage and transfer – ferritin, transferrin; electron transfer (Iron-sulfur protein) – rubredoxin, ferredoxin; O_2 transport – hemerythrin

Copper proteins and Enzymes – Hemocyanin, superoxide dismutase, ceruloplasmin, cytochrome c oxidase;

Zinc and Cobalt enzymes – carbonic anhydrase, carboxypeptidase, interchangeability of zinc and cobalt enzymes; Vitamin B12 and B12 coenzymes;

Photosynthesis and N_2 fixation

Metals in medicines and therapy

References:

1. Ch. Elschenbroich, A. Salzer, Organometallics – A Concise Introduction, VCH Publishers, 1989.
2. B. D. Gupta, A. J. Elias, “Basic Organometallic Chemistry”, University Press, 2010.
3. P. Powell, Principles of Organometallic Chemistry, 2nd ed., ELBS, 1991.
4. J. E. Huheey, E. A. Keiter, R. L. Keiter, Inorganic Chemistry: Principles of structure and Reactivity, 4th ed., Harper Collin College Publishers, 1993.
5. E.-I. Ochiai. Bioinorganic Chemistry – An Introduction, Allyn and Bacon Inc., 1977.
6. N. Kaim, B. Schwederski. Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life, John Wiley, 1994.

7. I. Bertini, H. B. Gray, S. J. Lippard, J. S. Valentine, Bioinorganic Chemistry, Viva Books, 1998.
8. R. W. Hay, Bio Inorganic Chemistry, Ellis Horwood, 1987.
9. J. A. Cowan, Inorganic Biochemistry – An Introduction, 2nd ed., VCH, 1997.
10. N. S. Hosmane (Ed) Boron Science: New Technologies and Applications, CRC Press, 2011.
11. S. J. Lippard, J. M. Berg. Principles of Bioorganic Chemistry, Panima Publ. Corpn. 2005.
12. M. N. Hughes, The Inorganic Chemistry of Biological Processes, Wiley, 1981.

CORE

CHE 2303

Natural Products

(Organic Chemistry – V)

Credit 3 **48 hours**

Course Outcome After completion of the full course the students should be able to	**Cognitive level**
C.O.1: device synthesis scheme for heterocyclic aromatic and nonaromatic organic compounds.	Analyse
C.O.2: elucidate structure and device synthesis for important natural products.	Apply
C.O.3: describe molecular structure of carbohydrates, proteins, DNA, RNA and synthesis of vitamin C and shikimic acid.	Understand

MAPPING of CO's and PO's

	Programme Outcomes							
Course Outcomes	P.O.1	P.O.2	P.O.3	P.O.4	P.O.5	P.O.6	P.O.7	P.O.8
C.O.1	x	x	x					x
C.O.2	x	x	x					x
C.O.3	x	x	x					x

Unit 1

Nomenclature and general characteristics of heterocyclic compounds. Structure, properties, synthesis and reactivity of three and four-membered ring heterocycles containing one heteroatom.

Unit 2

Heteroaromatic compounds (five and six-membered rings) containing one or two heteroatoms. Fused ring compounds: Synthesis and properties of indole, quinoline, isoquinoline, coumarin, flavone, purine and pyrimidine bases present in nucleosides.

Unit 3

Terpenoids: Classification, biosynthesis. Structure elucidation and synthesis of abietic acid. Steroids: classification, biosynthesis. Structure elucidation of cholesterol, conversion of cholesterol to progesterone, androsterone and testosterone. Fatty acids: structure, biosynthesis. Prostaglandins-classification, structure, biosynthesis and synthesis.

Alkaloids: Classification, isolation, structure elucidation based on degradative reactions (quinine and atropine). Biosynthesis of quinine and papaverine.

Unit 4

Carbohydrates: Structure of ribose, glucose, fructose, maltose, sucrose, lactose, starch cellulose and cyclodextrins. Preparation of alditols, glycosides (O, C, and N), deoxysugars. Synthesis of Vitamin C from glucose. Nucleic acids: Structure and synthesis, genetic code, recombinant DNA, biosynthesis of shikimic acid.

Unit 5

Aminoacids, peptides and enzymes: Synthesis of aminoacids – Strecker and azalactone synthesis, enantioselective synthesis of aminoacids, reactions of aminoacids. Structure of proteins, introduction to enzymes and coenzymes with special reference to the function of chymotrypsin, NAD, thiamine, pyridoxal. In vitro and in vivo synthesis of peptides, solid phase synthesis.

References:

1. F. A. Carey, R. J. Sundberg, Advanced Organic Chemistry (parts A and B), 5th ed., Springer, 2008.
2. I. L. Finar, Organic Chemistry Volumes 1 & 2, 6th ed., Pearson Education Asia, 2004.
3. J. Clayden, N. Green, S. Warren, P. Wothers, Organic Chemistry, 2nd ed., Oxford University Press, 2012.
4. N. R. Krishnaswamy, Chemistry of Natural Products; A Unified Approach, Universities Press, 1999.
5. R. J. Simmonds, Chemistry of Biomolecules: An Introduction, RSC, 1992.
6. R. O. C. Norman, Principles of Organic Synthesis, 2nd ed., Chapman and Hall, 1978.
7. J. A. Joule, K. Mills, Heterocyclic Chemistry, 5th ed., Wiley, 1998.
8. J. J. Li, E. J. Corey, Total Synthesis of Natural Products: At the Frontiers of Organic Chemistry, Springer, 2012.
9. T. Eicher, S. Hauptmann, The Chemistry of Heterocycles, 2nd ed., Wiley, 2003.
10. K. C. Nicolaou, S. A. Snyder, Classics in Total Synthesis II: More Targets, Strategies, Methods, Wiley, 2003.

CORE

CHE 2304

Kinetics, Adsorption and Catalysis

(Physical Chemistry – II)

Credit 3 **48 hours**

Course Outcome At the end of the course student should be able to	**Cognitive level**
C.O.1: apply the laws of chemical kinetics to calculate rate / rate constants of different types of reactions.	Analyse
C.O.2: interpret the basic reaction dynamics and obtain the rate constants in gaseous state and solutions.	Apply
C.O.3: calculate thermodynamic parameters from kinetic data.	Apply
C.O.4: apply the principles of acid and enzyme catalysis to solve any given kinetic data.	Apply
C.O.5: use adsorption isotherms as a tool for obtaining the surface area and rate constants in case of heterogeneous catalysis.	Analyse

MAPPING of CO's and PO's

	Programme Outcomes							
Course Outcomes	P.O.1	P.O.2	P.O.3	P.O.4	P.O.5	P.O.6	P.O.7	P.O.8
C.O.1	x	x						x
C.O.2	x	x			x			x
C.O.3	x	x			x			x
C.O.4	x	x			x			x
C.O.5	x	x			x			x

Unit 1

Rates of reactions- concentration and temperature dependence. Linear and non linear Arrhenius plots. Steady state Approximation. Complex reactions- Concurrent, Consecutive and Reversible Reactions. Pre-equilibria. Theories of Unimolecular reactions Lindemann, Hinshelwood, RRK and RRKM models.

Unit 2

Kinetics of Chain Reactions- Thermal and Photochemical reactions- H_2-Cl_2 and H_2-Br_2, Quantum yield, Branching Chain Reactions- H_2-O_2 reaction. Organic Decomposition Reactions- Rice Herzfeld Mechanism.

Excited state kinetics: Jablonski diagram and photophysical processes – Unimolecular photophysical and photochemical processes. Energy and Electron transfer- Excimers and exciplex. Fluorescence and Phosphorescence. Quenching of fluorescence: Stern Volmer equation.

Unit 3

Reaction Dynamics. Theories of reaction rates. Collision cross section and reaction cross section. Collision theory. Potential energy surfaces and reaction coordinate. Transition state theory. Comparative study of the theories of reaction rates. Thermodynamic treatment of Reaction rates.

Reactions in solution- Cage effect, Transition state theory for reactions in solution. Influence of solvents, Diffusion controlled reactions, Effect ionic strength, dielectric constant and internal pressure- Primary salt effect.

Molecular beam methods: determination of reaction cross section. Stripping and Rebound mechanism. Fast reactions: Flash Photolysis, Flow techniques, Relaxation methods.

Unit 4

Surface Chemistry: Different types of interfaces. Surface free energy and surface tension of solutions, surface excess. Contact angle and wetting. Thermodynamics of surfaces. The Gibbs equation and its derivation. Random walk model.

Adsorption and Desorption. Physisorption. Chemisorption. Adsorption isotherms – Langmuir (kinetic and statistical derivation). Freundlich and BET isotherms (kinetic derivation). Determination of surface area and Heat of adsorption.

Unit 5

Catalysis: Homogeneous and Heterogeneous. Acid-base catalysis. Enzyme catalysis. Inhibition- competitive and non-competitive.

Heterogeneous catalysis: Mechanisms- Hinshelwood and Rideal Eley. Autocatalysis – Oscillatory reactions- Lotka-Volterra, Oregonator, Brussellator.

References:

1. W. J. Moore, R. G. Pearson, Kinetics and Mechanism, Wiley, New York, 1988.
2. K. J. Laidler, Chemical Kinetics, McGraw Hill, New York, 1991.

3. M.R Wright, An Introduction to Chemical Kinetics, Wiley, 2004.
4. P. W. Atkins, Physical Chemistry 8th ed., 10th ed., Wiley, New York, 2006.
5. P.L. Houston, Chemical Kinetics and Reaction Dynamics, Dover Publications, 2006.
6. A. W. Adamson, The Physical Chemistry of Surfaces, 2nd ed., Wiley. New York, 1998.

ELECTIVE

CHE 2305

Electrochemistry and Crystallography

Credit 2 **32 hours**

Course Outcome At the end of the course student should be able to	**Cognitive level**
C.O.1: define the parameters of different crystal systems and apply it to understand crystal structure.	Apply
C.O.2: describe how diffraction patterns can be converted to structural information.	Understand
C.O.3: describe the theories effecting ionic conductance and apply the concepts to calculate conductance behaviour of a given system.	Apply
C.O.4: describe the electronic conductance behaviour in charged interfaces and analyse the catalytic behaviour of a system.	Analyse
C.O.5: learn the working principle and advancement in futuristic electrochemical devices.	Understand

MAPPING of CO's and PO's

	Programme Outcomes							
Course Outcomes	P.O.1	P.O.2	P.O.3	P.O.4	P.O.5	P.O.6	P.O.7	P.O.8
C.O.1	x	x						x
C.O.2	x	x						x
C.O.3	x	x				x		x
C.O.4	x	x						x
C.O.5	x	x				x		x

Unit 1

Electrochemical Cells, Electrodes, Electrolytes, Half Reactions, Electrochemical Work, Nernst Equation, Ionic and Electronic Conductance, Conductance Measurement, Equivalent Conductance, Kohlrausch's Law, Ionic Mobility, Waldens rule, abnormal conductance, Conductometeric titrations.

Variation of Ionic Speeds, Degree of Dissociation, Debye-Huckel Theory, Ionic Atmosphere, time of Relaxation, Mechanism of Electrolytic Conductance, Debye-Huckel-

Onsager Equation, Determination of degree of dissociation, Debye-Falkenhagen Effect, Wien Effect.

Transport Number- Factors Influencing, measurement, in mixtures. Activity and Activity Coefficient of Electrolytes, Debye-Hückel limiting law, Debye-Hückel-Bronsted Equation, Triple Ions, Complex Ions.

Unit 2

Charged Interfaces, Electrode Potential, Factors Influencing electrode potential, Band Bending, electrolytic polarization, dissolution and decomposition potential, concentration polarization.

Concentration cells, liquid junction potential, the electrode double layer, electrode-electrolyte interface, different models of double layer, theory of multilayer capacity, electrocapillary, Lippmann equation, membrane potential.

Overvoltage, theories of overvoltage, Tafel equation, Butler-Volmer equation. Electrocatalyst- Homogeneous, heterogeneous, Randles-Sevcik Equations, Pourbiax diagrams, PCET, bioelectrochemistry.

Molten Electrolyte, Ionic Liquids, Non-Aqueous Systems.

Corrosion, Fuel Cells, M-Ion Batteries.

Unit 3

Crystal Systems, Obtaining and Growing Crystals, Unit Cells, Faces, Crystal Lattice, Crystal Symmetry, Space Group.

Diffraction of Crystals, Bragg's law, Reciprocal lattice. Scattering by one atom, group of Atom, Fourier Synthesis.

Unit 4

Experimental Set Up, Selection of suitable crystal, Source, Detection systems, Data analysis, Data Refinement, Getting Crystal Structure, Important Structural Parameters, Crystal data sources.

Physical Properties – Optical, Electric and Magnetic and Applications.

Liquid Crystals-types, theory and applications.

References:

1. J. Bockris, A. K. N. Reddy, Modern Electrochemistry-1 Ionics, 2^{nd} ed., Springer Science & Business Media, 2018.
2. J. Bockris, A. K. N. Reddy, M. E. Gamboa-Aldeco, Modern Electrochemistry- 2A: Fundamentals of Electrodics, 2^{nd} ed., Springer Science & Business Media, 2018.

3. J. Bockris, A. K. N. Reddy, Modern Electrochemistry 2B: Electrodics in Chemistry, Engineering, Biology and Environmental Science, 2nd ed., Springer Science & Business Media, 2018.
4. R. Crow, Principles and Applications of Electrochemistry, 4th ed., 1994.
5. S. Glasstone, An Introduction to Electrochemistry, Paperback ed., 2007.
6. R. Tilley, Crystals and Crystal Structures, Wiley, 2006.
7. L. E. Smart, E. A. Moore, Solid State Chemistry: An Introduction, Fourth Edition, CRC Press, 2016.
8. P. E. Fanwick, Crystallography for Chemists, Cambridge Scholars Publishing, 2019
9. H. V. Keer, Principles of the Solid State, Wiley Eastern Ltd, New Delhi, 1993.
10. A. Primer, J. P. Glusker, K. N. Trueblood, Crystal Structure Analysis, 3rd ed., Oxford University Press Inc., New York, 2010.

CORE

CHE 2306

Physical Chemistry Laboratory

Credit 2 **96 hours**

Course Outcome After completion of the full course the students should be able to	**Cognitive level**
C.O.1: operate various sophisticated instruments.	Apply
C.O.2: perform experiments based on various laws of physical chemistry.	Apply
C.O.3: interpret the results obtained from various experiments.	Analyse
C.O.4: calculate the unknown concentration of the given solution based on the results obtained from the experiment.	Evaluate

MAPPING of CO's and PO's

	Programme Outcomes							
Course Outcomes	P.O.1	P.O.2	P.O.3	P.O.4	P.O.5	P.O.6	P.O.7	P.O.8
C.O.1	x	x				x	x	x
C.O.2	x	x				x		x
C.O.3	x	x				x		x
C.O.4	x	x		x				x

List of experiments:

1. Molecular weight determination by cryoscopic methods, Formula of complexes.
2. Phase diagrams: Two component liquid–liquid and solid-liquid systems. Three component liquid-liquid systems.
3. Determination of transition temperature, molecular weight determination.
4. Refractometry: Variation of refractive index with composition, formula of complexes.
5. Chemical Kinetics: Acid and base catalysed hydrolysis of esters, Dependence of temperature and ionic strength on the rate of reactions, Hydrolysis of p-nitrophenyl acetate using spectrophotometry.
6. Ostwald Viscometer: Viscosity of liquid and liquid mixtures.

7. Conductometry: Cell constant, conductivity of a weak-acid, solubility of a sparingly soluble salt, conductometric titrations. Determination of critical micelle concentration of colloids.
8. Poteniometry: Measurement of electrode potentials, activity coefficients and potentiometric titrations, pH metric titrations.
9. Adsorption: Checking the validity of Freundlich and Langmuir adsorption and determination of unknown concentration.
10. Spectrophotometry: Checking the validity of beer Lambert's law and determination of unknown concentration.
11. Demonstration of instrumentation of AAS, Flame photometry, Fluorescence spectrometer, GPC, Electrochemical work station etc.

References:

1. A. Findlay, Practical Physical Chemistry, 9th ed., Longman, 1973.
2. D. P. Shoemaker, C.W. Garland, J.W, Nibler, Experiments in Physical Chemistry, 5th ed., McGraw Hill, 1989.
3. J. B. Yadav, Advanced Practical Physical Chemistry, 36th ed., KrishnaPrakashan Media (P) Ltd, 2016.
4. J. N. Gurtu, A.N. Gurtu, Advanced Physical Chemistry Experiments, 6th ed., Pragati, 2014.

ELECTIVE

CHE 2307

Oleochemicals, Nutraceuticals and Surfactant Technology

Credit 2 **32 hours**

Course Outcome After completion of the full course the students should be able to	**Cognitive level**
C.O.1: able to classify and demonstrate the use of oils.	Apply
C.O.2: analyse and characterize oleocemicals, nutraceuticals and surfactants.	Analyse
C.O.3: evaluate the techniques of preparation and purification of oils.	Evaluate
C.O.4: formulation of soaps, detergents and cosmetics.	Create

MAPPING of CO's and PO's

	Programme Outcomes							
Course Outcomes	P.O.1	P.O.2	P.O.3	P.O.4	P.O.5	P.O.6	P.O.7	P.O.8
C.O.1	x	x						x
C.O.2	x	x		x				x
C.O.3	x	x					x	x
C.O.4	x	x	x		x			x

Unit 1

General Introduction, Sources of edible oils and fats, Processing and refining, Stability and Antioxidants, Analysis testing and QC. Introduction to essential oils and comparison with other oils. Raw materials, processing, purification and isolation of essential oil, Conventional and advance methods of production of essential oils, Synthetic Aroma chemicals and aromatherapy, Physicochemical and sensory Analysis and quality control in industry , Detail study of selected essential oils related to production, isolation, applications etc. (3 examples), Applications in soaps, detergents, cosmetics industry, flavors etc. Oleochemical Industry and Market Information.

Unit 2

Introduction to nutraceuticals: definitions, synonymous terms, claims for a compound as nutraceutical, regulatory issues. Study of Properties, structure and functions of various Nutraceuticals (3 examples) formulation of functional food, stability, analysis. Food as remedies, Anti-nutritional Factors present in Foods, Nutraceutical Industry and Market Information.

Unit 3

Soaps and Detergent – Introduction, Chemistry, Classification, Manufacture and Environmental aspects, Analysis of Soaps surfactants and detergents: determination of surface tension, interfacial tension, and CMC, Testing of TFM of soap, % active matter of detergents.

Recent developments- Spray Dried Powdered Detergents, Concept of HLB and other related terms, detersive system, micro emulsion, multiple emulsion system, nanoemulsion system. Disinfectants, Surfactant Industry and Market Information.

Unit 4

Hydraulic expelling, Solvent extraction and separation of oils and fats, Aqueous extraction, Liquid liquid extraction for deacidification, Miscella refining and double solvent refining, High pressure fat splitting, fatty acid distillation, Saponification of Oils, Soap formulation and Plodder Processing, Synthesis various anionic, cationic, nonionic and amphoterric surfactants, Formulation and Processing of Detergent Powder by combined absorption and neutralisation mode, Purification of wax, Formulation and Processing of different Skin and Hair Care Products.

Production Management, Marketing.

References:

1. B.K. Sharma, Industrial Chemistry, GOEL Publishing House, 2000.
2. Mohammad Farhat Ali, Bassam Ali, James Speight, Handbook of Industrial Chemistry Organic Chemicals, McGraw-Hill 2005.
3. O. P. Narula, Treatise on fats, fatty acids and oleochemicals by, Industrial Consultants (India), Vo. I & II, 1994.
4. V. V. S. Mani and A. D. Shitole, Fats, Oleochemicals and surfactants challenges in 21st Century by Oxford and IBH Publishing Co. Pvt. Ltd., 1997.
5. Robert E. C. Wildman, Handbook of Nutraceuticals and Functional Foods, CRC Press 2016.

INTERDEPARTMENTAL ELECTIVE

CHE 2308

Molecular Modeling in Chemistry

Credit 4 **96 hours**

Course Outcome After completion of the full course the students should be able to	**Cognitive level**
C.O.1: describe the basic concepts of the various theoretical models and methods.	Understand
C.O.2: classify the different basis sets used in the computational calculations.	Understand
C.O.3: calculate the geometry of a molecule, its IR and UV spectra, its thermodynamic and kinetic stability, and other information needed for the prediction of the reactivity.	Apply

MAPPING of CO's and PO's

	Programme Outcomes							
Course Outcomes	P.O.1	P.O.2	P.O.3	P.O.4	P.O.5	P.O.6	P.O.7	P.O.8
C.O.1	x	x						x
C.O.2	x	x						x
C.O.3	x	x			x		x	x

Unit 1

The Schrödinger Equation, The Time-Independent Schrödinger Equation, Born-Oppenheimer approximation, The Molecular Potential Energy Surface, Multiple Minima, Saddle Points, Characterization, Finding Minima, LCAO, Hartree-Fock theory, Roothan–Hall equations, Koopmans theorem, HF limit and electron correlation.

Unit 2

Basis sets, basis set approximation, Slater and Gaussian functions, contractions, polarization and diffuse functions, split-valence sets, classification of basis sets – minimal, double zeta, triple zeta, correlation-consistent sets, core-valence sets, general contractions, EMSL basis set exchange.

Unit 3

Semi empirical methods, post Hartree-Fock Method, Configuration interaction, Many-body perturbation theory, Coupled-cluster theory, Nondynamical correlation and multiconfigurational self-consistent-field (MCSCF) theory, Density Functional Theory, Hybrid QM/MM.

Unit 4

Input of molecular structure, Z-matrix construction, single point energy calculations, geometry optimizations, Electronic Energy, Vibrational frequency analysis, symmetry analysis, zero-point vibrational energies (ZPVE's), distinguishing minima from transition states, Intrinsic reaction coordinate (IRC) analysis, transition barrier and activation energy, conformational energetics, reaction energetics, enthalpy of formation, bond dissociation energy, ionization energy, isomerization energy and barrier, potential energy surface, reaction mechanism, enthalpy, entropy and free energy changes for reactions, isodesmic reactions.

Unit 5

Introduction to molecular mechanics; The Force Field Energy, The stretch energy, The bending energy, The out-of-plane bending energy, The torsional energy, The van der Waals energy, The electrostatic energy: charges and dipoles, Force Field Parameterization, Universal force fields, Advantages and Limitations of Force Field Methods, Basics of Molecular Dynamics Simulation, Generating and Analyzing a Molecular Dynamics Trajectory, Methods for Calculation of Free Energy, Application to Intermolecular Interactions and Binding Energies, Solvation Models, Combined QM/MM methods, Application of QM/MM to Enzyme.

References:

1. C. J. Cramer, Essentials of Computational Chemistry: Theories and Models, 2^{nd} ed., John Wiley & Sons, 2004.
2. F. Jensen, Introduction to Computational Chemistry, 3^{rd} ed., Wiley, New York, 2017.
3. A. R. Leach, Molecular Modelling Principles and Applications, 2^{nd} ed., Pearson Education Limited, 2001
4. I. N. Levine, Quantum Chemistry, 7^{th} ed., Pearson, 2013.

INTERDEPARTMENTAL ELECTIVE

CHE 2309

Spectroscopic Techniques

Credit 4 **96 hours**

Course Outcome After completion of the full course the student should be able to	**Cognitive level**
C.O.1: explain the fundamentals of spectroscopy.	Understand
C.O.2: correlate the structure of molecule with UV-Visible and IR spectral data.	Apply
C.O.3: interpret first order NMR spectra.	Analyse
C.O.4: determine the primary structure of peptides based on mass spectra.	Analyse
C.O.5: examine secondary structure of peptides based on IR, NMR and mass spectral data.	Evaluate
C.O. 6: explain the applications of X ray and microscopic techniques.	Understand

MAPPING of CO's and PO's

	Programme Outcomes							
Course Outcomes	P.O.1	P.O.2	P.O.3	P.O.4	P.O.5	P.O.6	P.O.7	P.O.8
C.O.1	x	x						x
C.O.2	x	x				x		x
C.O.3	x	x				x		x
C.O.4	x	x				x		x
C.O.5	x	x				x		x
C.O.6	x	x				x		x

Unit 1

Different regions of electromagnetic spectrum and energy associated with a particular frequency, Types of spectroscopic techniques, Energy levels in molecules. Population of energy levels

basics of light absorption, factors affecting sensitivity, intensity and width of spectral lines, absorption characteristics, structural information based on absorption characteristics

Unit 2

UV-visible spectroscopy – Principle, allowed and forbidden transitions, chromophores, auxochromes, effect of structure on absorption characteristics

Basics of ORD and CD and emission spectroscopy.

IR spectroscopy –Principle, intra and intermolecular hydrogen bonding, effect of concentration and temperature, Fourier transform IR, group frequencies, fundamental frequencies, overtones, Fermi Resonance.

Unit 3

Experimental aspects of FT NMR, factors influencing sensitivity and resolution, Proton NMR, Chemical shift, Applications of chemical shift, spin-spin coupling, Analysis of spin systems, factors affecting coupling constants, NMR of Carbon-13, DEPT analysis and brief introduction to correlation spectroscopy (COSY, HMBC and HSQC). Brief introduction to NMR of other biologically relevant nuclei such as ^{15}N, ^{2}D and ^{31}P.

Unit 4

Mass spectrometry - high resolution mass spectrometry, soft ionization techniques, MS/MS data, application of GC-MS and LC-MS data, introduction to fragmentation modes and determination of primary structure of peptides on the basis of mass spectral data.

Problems based on combined application of various spectroscopic techniques to examine secondary structure of peptides.

Unit 5

Introduction to microscopic and X-ray techniques. Confocal microscopy, fluorescence and radioisotope labeling as diagnostic tools. Basic introduction to Electron microscopy: types, sample preparation and analysis. Powder XRD and single crystal XRD.

References:

1. D. L. Pavia, G. M. Lampman, G. S. Kriz, Introduction to Spectroscopy, A Guide for Students of Organic Chemistry, 3rd ed., Thomson. 2004.
2. Atta-Ur-Rahman, M. I. Choudhary, Solving Problems with NMR Specroscopy, Academic Press, New York, 1996.
3. L. D. Field, S. Sternhell, J. R. Kalman, Organic Structures from Spectra, 4th ed., Wiley, 2008.
4. R. S. Drago, Physical Methods for Chemist, Saunders, 1992.
5. C. N. Banwell, E. M. McCash, Fundamentals of Molecular Spectroscopy, 4th ed., McGrawHill, 1994.
6. D. F. Taber, Organic Spectroscopic Structure Determination, A Problem Based Learning Approach, Oxford University Press, 2009.
7. H. Gunther, NMR Spectroscopy, 2nd ed., John Wiley and Sons, 1995.
8. R. M. Silverstein, G. C. Bassler, T. C. Morril, Spectroscopic identification of organic compounds, John Wiley, 1991.
9. D. H. Williams, I. Fleming, Spectroscopic Methods in Organic Chemistry, Tata McGraw Hill. 1988. 10. W. Kemp, Organic Spectroscopy, 2nd ed., ELBS-Macmillan, 1987.

10. F. Bernath, Spectra of Atoms and Molecules, 2nd ed., Oxford University Press, 2005.
11. E. B. Wilson, Jr., J. C. Decius, P. C. Cross, Molecular Vibrations: The Theory of Infrared and Raman Spectra, Dover Publications, 1980.
12. A. Weil, J. R. Bolton, Electron Paramagnetic Resonance: Elementary Theory and Practical Applications, 2nd ed., Wiley Inter Science, John Wiley & Sons, Inc., 2007.
13. C. P. Slichter, Principles of Magnetic Resonance, 3rd ed., Springer-Verlag, 1990.
14. H. Gunther, NMR Sprectroscopy: Basic principles, Concepts, and Applications in Chemistry, 2nd ed., Wiley 1997.
15. Spectral data bases (RIO DB of AIST, for example).

ELECTIVE

CHE 2310

Advanced Photochemistry

Credit 2 **32 hours**

Course Outcome After completion of the full course the students should be able to	**Cognitive level**
C.O.1: describe various photochemical and photophysical processes and apply established experimental methods for the investigation of these processes.	Apply
C.O.2: explain theories of photoinduced electron transfer and reactivity of excited states and their significance in different fields including biomedical applications and photosynthesis.	Evaluate
C.O.3: apply the knowledge of photochemistry of semiconductors and advanced materials for various applications involving photochemical energy conversions.	Apply
C.O.4: explain theory and application of photocatalysis and explain the environmental impact of atmospheric photochemistry.	Evaluate

MAPPING of CO's and PO's

	Programme Outcomes							
Course Outcomes	P.O.1	P.O.2	P.O.3	P.O.4	P.O.5	P.O.6	P.O.7	P.O.8
C.O.1	x	x						x
C.O.2	x	x						x
C.O.3	x	x			x			x
C.O.4	x	x	x		x			x

Unit 1

Energy Transfer-Theories of Energy Transfer – Photosensitization of Organic and Inorganic Molecules – Singlet Oxygen – Methods of singlet oxygen generation and Detection – Chemistry of Singlet Oxygen – Photodynamic Therapy of Cancer.

Unit 2

Photoinduced Electron Transfer – Theory of Electron transfer – Circumventing Back Electron transfer – Photoinduced Electron transfer reactions of Organic and Inorganic Molecules – Photosynthesis.

Unit 3

Photochemistry and Photophysics of Semiconductors – Semiconductor Photocatalysis and applications. Atmospheric photochemistry.

Unit 4

Photochemistry and Advanced Materials - Artificial Solar Energy Harvesting – Photochemical Splitting of Water – Dye sensitized solar cells - Grätzel Cell - Bulk heterojunction devices for solar energy harvesting - Organic light emitting devices. Photoresists – Photolithography – Photochromism – Photonic Materials and Lasers.

Unit 5

Photochemistry in Practice – Radiometry and Actinometry – Principles of Radiometry and radiometers – Actinometry – Quantum Yields – Light Sources – Optical Materials and Filters – Photochemical Reactors.

References:

1. N. J. Turro, V. Ramamurthy, J. C. Scaiano, Modern Molecular Photochemistry of Organic Molecules, University Science Books, 2010.
2. C.E. Wayne, Photochemistry (Oxford Chemistry Primers), Oxford University Press; 1st ed., 1996.
3. J. R. Lakowicz, Principles of Fluorescence Spectroscopy, Plenum Press, 3rd ed., 2010.
4. A. M. Braun, M.-T. Maurette, Esther Oliveros, Photochemical Technology, John Wiley & Sons, 1991.
5. M. A. Fox, M. Chanon, Photoinduced Electron Transfer Part A, B. C and D, Elsevier Science Publishing Company, 1988.
6. J. Mattay Ed., Photoinduced Electron Transfer 1-5 (Topics in Current Chemistry), Springer, 1st ed., 1990-1993.
7. G. J. Kavarnos, Fundamentals of Photoinduced Electron Transfer, 1st ed., Wiley-VCH, 1993.
8. V. Ramamurthy, K. Schanze, Molecular and Supramolecular Photochemistry, Volume 10, Semiconductor Photochemistry and Photophysics, Marcel Dekker, New York, 2003.
9. V. Ramamurthy, Photochemistry in Organized and Confined Media, VCH Publishers, New York, 1991.

ELECTIVE

CHE 2311

Polymer Chemistry

Credit 2 **32 hours**

Course Outcome After completion of the full course the students should be able to	**Cognitive level**
C.O.1: describe the synthesis and application of different types of polymers in laboratory and in industries.	Understand
C.O.2: apply characterisation techniques to identify polymers.	Apply
C.O.3: illustrate the polymer composites and the additives used in compounding.	Analyse
C.O.4: explain the structure and applications of biopolymers.	Understand

MAPPING of CO's and PO's

	Programme Outcomes							
Course Outcomes	P.O.1	P.O.2	P.O.3	P.O.4	P.O.5	P.O.6	P.O.7	P.O.8
C.O.1	x	x						x
C.O.2	x	x	x					x
C.O.3	x	x						x
C.O.4	x	x						x

Unit 1

Polymerisation processes: Addition, Condensation, cationic and anionic polymerisation, kinetics and mechanism. Important techniques of polymerisation such as emulsion, bulk, solution and suspension.

Unit 2

Industrial polymers: Synthesis, structure and applications. Polyethylene, Polypropylene, Polystyrene, Polyurethane, Polyacrylonitrile, Polyvinylchloride, polyvinylalcohol, Styrene Butadiene Rubber, Chloroprene Rubber, Nitrile Butadiene Rubber and ethylenepropylenediene monomer rubber.

Unit 3

Polymer characterization: concept of average molecular weights, determination of molecular weights, glass transition temperature, thermal analysis of polymers TG/DTG, DTA/DSC, Spectroscopy of polymers IR, UV, NMR and MS techniques.

Unit 4

Polymer composites: Classification of polymer composites- nano, micro and macroscales, reinforcements- short fibre, long fibre and particulate fillers, matrices- thermoplastics, thermosets and rubbers, polymer filler interactions and additives used in rubber compounding.

Unit 5

Biopolymers: Preparation, properties and applications of cellulose derivatives: cotton and rayon: cellulose plastics: cellulose acetate, cellulose nitrate & regenerated cellulose. Structure and applications of starch, shellac, chitin and chitosan.

References:

1. F. W. Billmayer, Text book of polymer science, 3rd ed., Willey, New York, 1991.
2. R. J. Young, Principles of Polymer Science, 3rd ed., Chapman and Hall, New York, 1991.
3. P. J. Flory, A Text Book of Polymer Science, Cornell University of Press, Ithacka, 1953.
4. J. A. Brydson, Polymer chemistry of Plastics and Rubbers, ILIFFE Books Ltd., London.1966.
5. R. J. Brown., Handbook of plastic test methods, the plastic and rubber institute, 1981.
6. P. M. Ajayan, L. Schadler, P. V. Braun Nano Composite Science and Technology, Wiley VCH, 2003.
7. I. Galaev, Bo Mattiasson, Smart Polymers: Applications in Biotechnology and Biomedicine, 2nd ed., CRC Press, 2007.
8. S. Li, A. Tiwari, M. Prabaharan, S. Aryal, Smart Polymer Materials for Biomedical Applications (Materials Science and Technologies), Nova Science Publishers Inc, 2010.
9. I. L. Finar., Organic Chemistry, volumes 1 and 2, Pearson Education India; 6th ed., 2002.
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11. L. A. M. van den Broek, C. G. Boeriu, V. Stevens (Ed.) Chitin and Chitosan: Properties and Applications, John Wiley & Sons Ltd, 2020.
12. V. E. Yarsley, W. Flavell, P. S. Adamson, N. G. Perkins, Cellulosic Plastics. Cellulose Acetate; Cellulose Ethers: Regenerated Cellulose; Cellulose Nitrate, London, 1964.

SEMESTER: 4

CORE

CHE 2401

Project Dissertation

Credit 16

Course Outcome After completion of the full course the student should be able to	**Cognitive level**
C.O.1: identify and hypothesise an advanced level research problem.	Create
C.O.2: design experiments and validate the hypothesis of an advanced level research problem.	Create

MAPPING of CO's and PO's

	Programme Outcomes							
Course Outcomes	P.O.1	P.O.2	P.O.3	P.O.4	P.O.5	P.O.6	P.O.7	P.O.8
C.O.1	x	x	x	x	x	x		x
C.O.2	x	x	x	x	x	x	x	x

The students shall carry out research project in reputed research laboratory for the entire semester.
The students shall submit a project report on the research work carried out.
The students will have to present the results of the research project in a seminar and appear for a comprehensive viva-voce.

Guide lines for setting up Question Papers in Theory Courses

1. The entire syllabus must be covered in the question paper.
2. Each question must be mapped to a specific C.O.
3. All the C.O.s must be reflected in the question paper.
4. The question paper may consist of questions at different cognitive levels such that, 20% of "remember" level, 40% of "understand" level and 40% of "apply and higher" level.

END