MSc Syllabus for Chemistry
Program Code: CHE
(Under NEP 2020)

Approved by

BOS, Department of Chemistry	09/04/2025
School Board, School of Physical Sciences	25/04/2025
Academic Council, NEHU (114th Meeting)	16/07/2025

North-Eastern Hill University
Shillong-793022, Meghalaya
2022

PROGRAM OUTCOMES

Knowledge Outcomes:

PO1: Appreciation and application of the fundamental knowledge of the basic principles in various fields of Chemistry.

PO2: Readiness to apply the knowledge capital to build up small scale industry for developing endogenous product.

PO3: Development of awareness and sense of responsibilities towards environment and apply knowledge to solve the issues related to Environmental pollution.

PO4: Readiness to appreciate diverse various aspects of chemistry for benefit of the society in the form of creating sustainable development practices, green energy initiatives, development of smart materials, identification and characterization of natural products and metal complexes.

Skill Outcomes:

PO5: It would help students to collaborate effectively on team-oriented projects in the field of Chemistry or other related fields.

PO6: Communicate scientific information in a clear and concise manner both orally and in writing.

PO7: Inculcate logical thinking to address a problem and become result oriented with a positive attitude.

PO8: Learning to deal with environmental pollution issues and the remedies thereof.

PO9: Understand how to apply the knowledge to develop the sustainable and eco-friendly technology in Industrial Chemistry.

Generic Outcomes:

PO10: Will develop their critical reasoning, judgment, and communication skills.

PO11: Augment the understanding on recent developments in the field of green and eco-friendly reactions, pharmaceutical, Bioinorganic Chemistry and relevant fields of research and development.

PO12: Enhance the scientific temper among the students to develop a research culture and implementation of the policies to tackle the burning issues at global and local level.

PROGRAM STRUCTURE

FIRST SEMESTER		
Paper Code	**Paper**	**Minimum credit reqd**
CHE-CC-500 CHE-CC-501	Physical Chemistry I (Quantum Chemistry & Spectroscopy) (Theory) Organic Chemistry I (LAB)	4 4
CHE-DSEC-502 CHE-DSEC-503	Inorganic Chemistry I /MOOCs (Theory) Physical Chemistry II /MOOCs (Theory)	4 4
CHE-GEC-504	Environmental Chemistry	4
	Total	**20**
SECOND SEMESTER		
CHE-CC-505 CHE-CC-506	Physical Chemistry III (Theory) Inorganic Chemistry II (LAB)	4 4
CHE-DSEC-507 CHE-DSEC-508	Organic Chemistry II /MOOCs (Theory) Interdisciplinary Chemistry/MOOCs (Theory)	4 4
CHE-RM-509	Research Methodology & Proposal writing	4
CHE-DSEC-510	Research Tools in Inorganic Chemistry (Theory)	4
	Total	**24**
THIRD SEMESTER		
CHE-CC-600 CHE-CC-601 CHE-CC-602	Organic Chemistry III (Theory) Physical Chemistry IV (LAB) Inorganic Chemistry III (Theory)	4 4 4
CHE-DSEC-603 CHE-DSEC-604 CHE-DSEC-605	Research Techniques in Chemistry Organic Chemistry IV/MOOCs (Theory) Physical Chemistry V (Research Tools in Physical Chemistry)/MOOCs (Theory)	4 4 4
	Total	**24**
FOURTH SEMESTER		
CHE-CC-606	Research Project	20
	Total	**20**

CC	Core Course
DSEC	Discipline Specific Elective Course
GEC	Generic Elective Course
SEC	Skill Enhancement Course
RM	Research Methodology and proposal writing

FIRST SEMESTER CHE-CC-500 CREDITS: 4

PHYSICAL CHEMISTRY-I

Learning Objectives:

- To understand the principles of Quantum Mechanics, Operator concepts, application to model systems, and approximate methods.
- Application of Quantum Mechanics to chemical bonding, Valence bond and Molecular Orbital Theory, Huckel MO treatment for conjugate pi-electron systems.
- To understand the principles of rotational, vibrational, electronic and magnetic spectroscopy.

Course outcomes:

- Quantum mechanics and spectroscopy are the fundamental part of Physical Chemistry. The student will learn the principles of quantum mechanics and spectroscopy and apply the concepts to all the fields of Chemistry.

Unit 1: ***Principles of Quantum Mechanics, Application to Model Systems and Approximate Methods*** Review of the basic principles of quantum mechanics: Postulates, operators and related theorems, Schrödinger equation, normalization and orthogonalization of wave function. Expectation values, Quantum mechanical operators, Hamiltonian operator, Hermitian operators, angular momentum operator. Exactly solvable problems: Particle in a box, harmonic oscillator, rigid rotator, step potential and tunnelling, hydrogen atom. Approximation methods: Variation and time-independent perturbation methods (up to 2^{nd} order) and simple applications.

Unit 2: ***Chemical Bonding***
Many-electron wave functions and anti-symmetry principle; Born-Oppenheimer approximation; valence bond (VB) and molecular orbital (MO) approaches for diatomic molecules, LCAO-MO treatment of hydrogen molecule ion, hydrogen molecule; bonding and anti-bonding orbital; Comparison of LCAO-MO and VB treatments of H_2 and their limitations; excited states of H_2 - singlet and triplet; term symbols; hybridization; Huckel MO treatment for conjugated π-electron systems.

Unit 3: ***Rotational and Vibrational and Electronic Spectroscopy***
Introduction: Interaction of light with matter, mechanism of absorption and emission of radiation.

(A) Rotational and Vibrational Spectroscopy
Degrees of freedom of molecules; rigid rotor model; rotational spectra of diatomics and polyatomics; effect of isotopic substitution and nonrigidity; selection rules and intensity distribution. Vibrational spectra of diatomics; effect of anharmonicity; Morse potential; Vibration-rotational spectra of diatomics; P, Q, R branches, normal modes of vibration, overtones, hot bands. Raman spectroscopy: Origin; rotational and vibrational Raman spectra of diatomics.

(B) Electronic Spectroscopy
Electronic spectroscopy: Electronic spectra of diatomic molecules, Franck-Condon principle, Vibronic transitions, Spectra of organic compounds, $\pi \rightarrow \pi^*$, $n \rightarrow \pi^*$ transition.

(C) Photochemistry
Types of photophysical pathways, Radiationless transitions, Fluorescence emission, Triplet state and phosphorescence emission.

Unit 4: ***Magnetic Resonance Spectroscopy***

(A) Nuclear Magnetic Resonance: Nuclear spin and nuclear spin states in magnetic field, resonance phenomenon, relaxation processes, NMR line shapes and saturation, shielding and de-shielding of magnetic nuclei, chemical shift, spin-spin interactions, spectra of a two-spin system (A_2, AB and AX cases), ^{13}C, ^{19}F, and ^{31}P NMR spectroscopy.

(B) Electron Spin Resonance: Basic principles, factors affecting g values, hyperfine coupling, spin densities and McConnell relationship. Zero field splitting.

TEXT BOOKS

[1] D. A. McQuarrie, *Quantum Chemistry*, Viva books, 2020.
[2] D. A. McQuarrie and J. D. Simon, *Physical Chemistry*, Viva books, 2020.
[3] C. N. Banwell and E. M. McCash, *Fundamentals of Molecular Spectroscopy*, 5th Ed., Tata McGraw- Hill, New Delhi, 2015.

REFERENCE BOOKS

[1]P. W. Atkins and R. Friedman. *Molecular Quantum Mechanics*, 4th Ed., Oxford University Press, 2005.
[2]R. McWeeny. *Coulson's Valence*, ELBS, 1979.
[3]J. D. Graybeat. *Molecular Spectroscopy*, McGraw-Hill Int. Ed. 1988.

FIRST SEMESTER CHE-CC-501 CREDITS: 4

ORGANIC CHEMISTRY-I (LAB)

Learning Objectives:

- To impart technical skill on separation technologies in organic chemistry
- Application of those skills in extraction of natural products and purification processes.
- To impart hands-on experience on multistep organic synthesis

Course Outcomes:

- Will learn synthesis, separation, purification, and characterization processes

1. Purification Techniques of organic compounds and their spectroscopic identifications.
   a) Purification of binary mixtures by Thin Layer Chromatography (TLC) and Column chromatography (CC).
   b) Purification of tertiary mixtures of amino acids by Paper Chromatography.

2. Extraction of Natural Products: Any one of the following – solasodine, caffeine, nicotine, piperine, rosine, carotenoids, curcumin, citral.

3. Organic Preparations:

   At least eight preparations involving the following representative reactions. Purification will be done by recrystallization technique and structure will be determined by comparing melting points, UV-Vis and IR spectroscopy.

   a) Esterification and saponification
   b) Oxidation (peracid, chromic acid, Mn (Vll)
   c) Hydride reduction or hydrogenation
   d) Nucleophilic substitution
   e) Cycloaddition reaction
   f) Condensation reaction
   g) Preparation of dyes
   h) Aromatic electrophilic substitution
   i) Preparation of oxazoles, isoxazoles, pyrazoles

4. Multicomponent reaction
   a) Synthesis of bisindole, biscoumarin, and bisdimedone
   b) Biginelli reaction and Hantz reaction

5. Qualitative Analysis of organic compounds

Text Books

[1] R. K. Bansal. *Laboratory Manual of Organic Chemistry* (3rd edn.), Wiley-Eastern (1994).
[2] R. G. Brewster & W.E. Mcwedn. *Unitized Experimental Organic Chemistry* (4th edn.), East-West Press (1977).
[3] A. I. Vogel. *Practical Organic Chemistry* (3rd edn.), Longman Group Ltd. (1973).

Reference Books

[1] A. O. Fitton & R. K. Smallery. *Practical Heterocyclic Chemistry* Academic Press (1968)
[2] R. L. Shriner & R. C. Fuson. *Systematic Identification of Organic Compounds* (5th edn.), John Wiley & Sons (1964).

FIRST SEMESTER **CHE-DSEC-502** **CREDIT: 4**

INORGANIC CHEMISTRY – I

Learning Objectives:

- To understand the symmetry and point groups of coordination compounds.
- Learning inorganic reaction mechanism.
- To understand magnetic properties of coordination compounds
- Understanding Electronic Structure of Transition Metal Complexes

Course Outcomes:

- Can gather knowledge on symmetry and point groups of coordination compounds.
- Can gather a fair idea of the reaction mechanism of coordination compounds
- Can gather knowledge on factors affecting magnetic properties of coordination compounds
- Will understand color and various electronic transitions of coordination compounds

Unit 1: *Symmetry and Group Theory:* Symmetry elements and operations; equivalent symmetry elements and equivalent atoms; Identification of symmetry point groups with examples from inorganic compounds; groups of very high symmetry; molecular dissymmetry and optical activity; systematic procedure for symmetry classification of molecules and illustrative examples; molecular symmetry for compounds having co-ordination numbers 2 to 9; Brief review of matrix representation of group, reducible and irreducible representations; Application to molecular vibration.

Unit 2: Structure and mechanism

(a) ***Metal-Ligand Equilibria in Solution***: Stepwise and overall formation constants; trends in stepwise formation constants; determination of binary formation constant by spectrophotometry; factors affecting stability of metal complexes and chelate effect.

(b) ***Reaction Mechanism of Transition Metal Complexes:*** Discussion on general reactivity of metal complexes, Labile and inert complexes; mechanisms of ligand-replacement reactions; ligand displacement reactions in square planar and octahedral complexes; *trans* effect; electron transfer reactions: outer sphere and inner sphere, atom transfer; isomerisation and racemisation of tris-chelate complexes; stereochemical nonrigidity and fluxional molecules.

Unit 3: *Magnetochemistry:* Brief review of different types of magnetic substance and magnetic behaviour, measurement of magnetic susceptibility, Magnetic moment for single and multi-electron system, L-S and j-j coupling, Ground State Term symbols for metal ions; R-S coupling and Lande intervals, Spin-orbit coupling, Thermal energy and magnetic property: temperature-independent paramagnetism, application of crystal field to explain the magnetic properties of coordination compounds: Magnetic moment of first row transition metal ions, spin crossover, quenching of orbital magnetic moment, Magnetic properties of Lanthanides and Actinides, Antiferromagnetic interactions in inorganic compounds: direct interaction and super exchange mechanism.

Unit 4: *Electronic Structure of Transition Metal Complexes:* Electronic absorption spectra and colour of octahedral and tetrahedral complexes, selection rules, Orgel diagrams, Tanabe- Sugano diagrams, calculation of Dq, B and ß values, band intensities and band widths, spectra of high-spin octahedral and tetrahedral complexes of d^1 to d^9 systems, Spectrochemical series; Adjusted crystal field theory, Nephelauxetic series, Molecular orbital theory of complexes, MO diagrams for octahedral and tetrahedral complexes and charge-transfer spectra, optical properties of Lanthanides and Actinides.

TEXT BOOKS

[1] J. E. Huheey, E. A. Keiter, R. L. Keiter & O. K. Medhi *Principles of Structure and Reactivity* (1st impression), Pearson Education (2006).
[2] F. A. Cotton *Chemical Applications of Group Theory*, (3rd edn.), John Wiley & Sons (1999).
[3] R. L. Dutta and A. Syamal, *Elements of Magnetochemistry* (2nd Edn), EWP (2010)
[4] J. D. Lee, *Concise Inorganic Chemistry* (5th Edn) John Wiley & Sons (1996).

REFERENCE BOOKS

[1] P. Atkins, T. Overton, J. Rourke, M. Weller & F. Armstrong. *Shriver and Atkins Inorganic Chemistry*, Oxford University Press (2006).

[2] N. N. Greenwood & A. Earnshaw. *Chemistry of the Elements*, Pergamon Press (1984).

[3] F. Basolo & R. G. Pearson, *Mechanism of Inorganic Reactions*, Wiley Eastern (1967).

[4] S. F. A. Kettle, *Physical Inorganic Chemistry*, Spectrum (1996).

FIRST SEMESTER **CHE-DSEC-503** **CREDIT: 4**

PHYSICAL CHEMISTRY - II

Learning Objectives:

- To understand ion-ion and ion-solvent interactions and their underlying principles.
- To understand the concepts of electrodics, the processes at electrodes, and their applications.
- Solid state chemistry will introduce the students to the world of crystals, their basic concepts, crystal defects, identification of crystal via X-ray diffraction besides some areas such as metals, insulators, and semiconductors.
- Student will learn some important principles of surface chemistry that includes understanding of surfactants and colloids.

Course Outcomes:

- Electrochemistry is fundamental to batteries, fuel cells, and supercapacitors, which are essential for storing and converting energy in devices such as smartphone, electric vehicles, and renewable energy devices. Moreover, they are used for corrosion prevention, electroplating, metal refining, sensing, water purification, electrosynthesis, etc. Understanding the basic principles of electrochemistry will help students to choose career in those fields. The same is true for the rapidly growing field of surface chemistry.
- Similarly, understanding of solid state chemistry in the age of smart materials will help students master the field and has potential to get employment opportunities.

Unit 1: *Electrochemistry*-I

Ion–ion Interaction: Debye-Huckel theory of ion-ion interaction; Poison equation, Linearized Poisson–Boltzmann equation; ionic cloud and chemical potential change; activity coefficients and mean ionic activity coefficients; expression of mean ionic activity coefficients in terms of ionic strength.
Ion-solvent interaction: free energy change due to ion-solvent interactions; Born model; enthalpy and entropy of ion-solvent interactions.

Unit 2: *Electrochemistry*-II

Electrodics: processes at electrodes, electrical double layer; Helmholtz-Perrin model; Gouy-Chapman diffuse charge model and Stern model. The basic electrodic equation: Butler–Volmer equation; overpotential; polarizable and nonpolarizable interfaces, Corrosion.

Unit 3: *Solid State Chemistry*

Review of the basic concepts: Bragg's law, Miller indices, Elements of symmetry (plane, axis and centre of symmetry). X-ray diffraction: powder method, principle and applications.
Crystal Defects: Point defects, Stoichiometric and non-stoichiometric defects, Kroger-Vink notation for crystal defects.
Metals, insulators and semiconductors; intrinsic and extrinsic semiconductors, p-n junction. Solid Solutions: Substitutional, interstitial and subtractional solid solutions & distortions.

Unit 4: *Surface Chemistry*

Surface tension and surface free energy; Pressure across an interface: Laplace equation, Kelvin equation; Wetting: Young-Dupre equation; Adsorption in liquid systems: Gibbs adsorption isotherm. Surfactants, classification of surfactants, hydrophobic interaction, aggregation/micellization of surfactants, critical micelle concentration (cmc), factors affecting the cmc, thermodynamics of micellization: phase separation and mass action models. Sols of surface-active reagents, electrical properties of colloidal systems, size determination of colloidal particles.

TEXT BOOKS

[1] J. O'M Bockris and A. K. N. Reddy. *Modern Electrochemistry*, Plenum, New York, 2007.
[2] D. A. McQuarrie and J.D. Simon –*Physical Chemistry*, VIVA Students Ed., 2003.
[3] A. R. West. *Solid State Chemistry and its Applications,* John Wiley,1998.
[4] Y. Moroi. *Micelles: Theoretical and Applied Aspects*, Plenum, 1992 (Softcover reprint of the original 1^{st} ed. 1992 edition: 20 November 2013).

FIRST SEMESTER | **CHE-GEC-504** | **CREDIT: 4**

ENVIRONMENTAL CHEMISTRY

Learning Objectives:

- This course aims to provide a fundamental understanding of environmental chemistry, focusing on water and air pollution.
- It explores the impact of pollutants on water and air quality, along with wastewater treatment technologies and atmospheric processes.
- It examines pollution control strategies and the environmental and health effects of industrial activities like uranium and coal mining.

Course Outcomes:

- By the end of this course, students will understand global biogeochemical cycles and their relevance to environmental chemistry.
- They will be able to assess water quality, analyse pollutant effects, and evaluate wastewater treatment techniques.
- The course will also equip them with knowledge of atmospheric chemistry, air pollution mechanisms, and pollutant removal processes.
- Lastly, students will gain insight into industrial pollution impacts and advanced environmental remediation strategies.

Unit 1: Water pollution and Remediation

(a) Environmental cycles: Global water, carbon, nitrogen phosphorus cycles

(b) Water Quality parameters: Physico-Chemical Water Quality Indicators (Electrical conductivity, dissolved oxygen, BOD and COD); Effect of inorganic and organometallic compounds; heavy metals and metalloids; and radionuclides on the water quality; nonaqueous-phase liquids (NAPLs) and pesticides as organic water pollutants.

Unit 2: (a) Wastewater Treatment and Related Technologies: Primary, secondary and tertiary treatment process of municipal sewage and water; disinfection by chlorination, ozonation and ultraviolet radiation; Use and disposal of biosolids; Point-of-entry (POE) and point-of use (POU) technologies for water treatment; Advanced Oxidation Processes (AOPs) for wastewater treatment.

(b) Environmental and Health Impacts of Uranium and Coal Mines.

Unit 3: The Atmosphere and Associated Processes

The layers of the atmosphere; atmospheric radiation and photochemical reactions **-** Stratospheric ozone formation and the role of VOCs and NOx, Stratospheric ozone destruction and the role of halogen compounds; Biosphere-Atmosphere interactions (biogenic and anthropogenic emissions);

Unit 4: Air Pollution and its Removal Process: Photochemical smog; greenhouse effect; Peroxyacetyl nitrate (PAN) formation and NOx transport; Aldehydes in the atmosphere; Heterogeneous atmospheric reactions; Atmospheric deposition processes for removal of pollutants.

TEXT BOOKS

[1] G. Hanrahan, Key Concepts in Environmental Chemistry, Elsevier Inc. (2012), ISBN: 978-0-12- 374993-2.

[2] N. Gupta, R. S. Khoiyangbam, and N. Jain, Introduction to Environmental Sciences, Ch. Environmental Chemistry, pp. 15-49, Teri Press (2015).

[3] R. Mahapatra, S. S. Jeevan, S. Das, (Eds); Environment Reader for Universities, Centre for Science and Environment, New Delhi (2017).

SECOND SEMESTER **CHE-CC-505** **CREDIT: 4**

PHYSICAL CHEMISTRY - III

Learning objectives:

- The rate laws, their determinations in different types of reactions, the mechanistic aspects of the reactions, the principles governing reactions rates, effect of surfaces on reaction rates will be learnt.
- Student will learn basic concepts and applications of statistical thermodynamics that bridges atomic and molecular behaviour with macroscopic properties of a system such as temperature, pressure, and entropy.
- To achieve better appreciation from the students on some important topics of non-equilibrium thermodynamics such as entropy of an irreversible process, entropy flow, entropy production, etc.

Course outcomes:

- The student will understand some fundamental principle of physical chemistry such as reaction kinetics and thermodynamics which are integral to understanding molecular behaviour of gases, liquids, and solids.
- The course will give students fair idea on how temperature, pressure, and molecular interactions influence reaction pathways and equilibria.
- Students will be able to appreciate the concepts behind blackbody radiation, specific heat capacities, and the behaviour of quantum gases.

Unit 1: ***Reaction Kinetics-I***

Determination of rate laws: Integral, isolation, half-life and differential methods; comparison of different techniques. Kinetic equations for complex reactions: Chain, parallel, opposing and consecutive reactions; Enzyme catalysis. Enzyme Inhibition reactions, Michaelis-Menten mechanism.

Unit 2: ***Reaction Kinetics-II***

Theory of reaction rates; Temperature effect on reaction rates; Rate constant for simple bimolecular reactions; Collision theory; Activated complex theory, Lindemann, Hinshelwood and the RRKM theories for unimolecular reactions, Reactions in solutions: Diffusion controlled & activation- controlled reactions; Thermodynamic formulation of rate constant: effect of pressure & ionic strength. Reaction in surfaces: Langmuir adsorption isotherm; kinetics of surface catalyzed unimolecular & bimolecular reactions; Concept of potential energy surface for a reaction.

Unit 3: ***Statistical Thermodynamics***

(A) Phase space, ensembles, different types of ensembles, ensemble averaging, concept of distribution, distribution law (Boltzmann statistics), partition function, relation between molecular and molar partition functions, thermodynamic parameters in terms of partition function, equilibrium constant in terms of partition function. Translational partition function, rotational partition function for linear and non-linear molecules; vibrational partition function, electronic partition function, reference state of zero energy for evaluating partition function.

(B) Application of statistical thermodynamics: equipartition theorem, heat capacity behaviour of crystals. Introduction to quantum statistics: Distribution law for fermions (Fermi-Dirac statistics) and for bosons (Bose-Einstein statistics), and its applications.

Unit 4: ***Non-Equilibrium Thermodynamics***

Entropy of irreversible processes – Clausius inequality; entropy production (heat flow, chemical reactions, electrochemical reactions) and entropy flow; Entropy production in open systems; Rate of entropy production – generalized forces and fluxes; Phenomenological equations, Onsager reciprocity relation; Electrokinetic phenomena; Stationary non-equilibrium states -states of minimum entropy production.

TEXT BOOKS

[1] K. J. Laidler, *Chemical Kinetics* (4th Edn.), Pearson Eductions, 2007.
[2] D. A. McQuarrie and J.D. Simon –*Physical Chemistry*, VIVA Students Ed., 2003.
[3] P. W. Atkins & J. de Paula. Physical Chemistry (8th edn.), OUP, 2006.
[4] D. A. McQuarrie. Statistical Mechanics, Viva Books Pvt. Ltd., New Delhi, 2003.
[5] C. Kalidas and M. V. Sanganarayana. *Non-Equilibrium Thermodynamics – Principles and Applications*, Macmillan India, 2002.

REFERENCE BOOK

[1] P. L. Houston, Chemical Kinetics & *Reaction Dynamics*, Dover, NY, 2006.
[2] K Huang, *Statistical Mechanics*, OUP, 2006.
[3] I. Prigogine. *Introduction to Thermodynamics of Irreversible Processes*, Interscience, 1960.

SECOND SEMESTER **CHE-CC-506** **CREDIT: 4**

INORGANIC CHEMISTRY - II (LAB)

Learning Objectives:

- Quantitative estimation of metal ions by volumetric, gravimetric, and spectrophotometric methods
- Learning synthesis of different metal complexes using different ligands
- Characterization of synthesized complexes by different spectroscopic and electrochemical methods.

Course Outcomes:

- Experienced in quantitative analysis of metal ions by volumetric, gravimetric, and spectrophotometric methods
- Can gather a fair idea about metal ligand interactions
- Can gather knowledge on synthesis of ligand and metal complexes.
- Will understand the usefulness of spectroscopic method for compound characterization.

1. Quantitative estimation involving volumetric (redox and complexometry), gravimetric and spectrophotometiric methods of constituents in three component mixtures and alloys.

2. Preparation and Characterization of the following compounds (at least 5 preparations are to be completed by turn):

   I. Tris(acetylacetonato) iron(III)
   II. Reinecke salt
   III. Tris(oxalate) manganese(III)
   IV. Tetrapyridinesilver(II)peroxidisulphate
   V. Bis(*N*,*N*-diethyldithiocarbamato)nitrosyliron(I)
   VI. Optical isomers of tris(ethylenediamine)cobalt(III)chloride
   VII. Linkage isomers of nitro and nitritopentamminecobalt(III) chloride
   VIII. Hydridochlorocarbonyl tris(triphenylphosphine)ruthenium(II)
   IX. $[(p\text{-(cymene)}RuCl_2]_2$

3. Synthesis and characterization of metal Schiff base complex. Characterization includes microanalysis, and conductance measurements and FTIR, UV-Visible, NMR spectroscopy and cyclic voltammetry studies.

TEXT BOOKS

[1] J. Mendham, R. C. Danney, J. D. Barnes & M. Thomas. *Vogel's Textbook of Quanti*-*tative*
[2] *Chemical Analysis*, Peterson Education (2000).
[3] G. Marr & B. W. Rockett. *Practical Inorganic Chemistry*, Van Nostrand (1972).
[4] G. Pass & H. Sutcliffe. *Practical Inorganic Chemistry* (2nd edn.), Chapman & Hill (1974)

REFERENCE BOOKS

[1] J. Basset, R. C. Denney, G.H. Jeffery & J. Mendham. *Vogel's Text Book of Quantitative Analysis*
[2] (4th edn.), English Language Book Society (1978).
[3] H. H. Willard, L. L. Merrit & J. A. Dean. *Instrumental Methods of Analysis* (4th edn.), East-West
[4] Press (1974).
[5] G. W. Parshall (Ed. in Chief). *Inorganic Synthesis*, Vol. 15, McGraw Hill, p. 48 (1974).

SECOND SEMESTER **CHE-DSEC-507** **CREDIT: 4**

ORGANIC CHEMISTRY - II

Learning Objectives:

- To impart knowledge on stereochemistry
- Understanding aromaticity
- Learning organic reactions, reagents, and their mechanism

Course Outcomes:

- Will appreciate stereochemistry, aromaticity, reactions, and reagents
- Student can apply those understandings in professional sphere

Unit 1: Stereochemistry

Axial and planar chirality, helicity; topicity and prostereoisomerism; Racemic modification and optical purity; Conformational analysis of acyclic, cyclic, bicyclic, heterocyclic and steroidal systems; Effects of conformation on reactivity.

Unit 2: Aromaticity and Reaction mechanisms

Concept and application of aromaticity, Aromaticity in benzenoid and non-benzenoid compounds, *n*-annulenes, heteroannulenes, fullerenes, cryptates; Mechanism, stereochemical aspects and application of addition, elimination and substitution reaction. Concept of E, Z geometry of enolates, kinetic vs thermodynamic control of enolates, stereoselective enolate reactions – alkylation and aldol condensation (Zimmerman models). Concept, stereochemical aspect and application of Mukaiyama reaction, Henry reaction, Wittig reaction and Horner-Wordwoth- Emmons reaction; Peterson's olefinantion, Prins reaction,

Unit 3: Reactions and Reagents

(a) Stereochemistry and application of catalytic hydrogenation, hydride reduction, hydroboration, dissolving metal reductions, and carbonyl reduction with hydrazine derivatives; Oxidation of alcohol with PCC, PDC, Collin's reagent, Swern oxidation, IBX, Dess- Martin periodinane, MnO_2, Ag_2CO_3 on celite; oxidation of alkene with peracids, metal/alkyl hydroperoxides, Sharpless asymmetric epoxidation and asymmetric dihydroxylation, dioxiranes, I_2/Ag^+ ; periodates, LTA, SeO_2.

(b) Reactive Intermediates I: Concept, generation, stereochemical aspects, and important name reactions of carbenes, nitrenes, and arynes.

Unit 4: Reactions and Reactive intermediates

(a) Name reactions: Concept, stereochemical aspect and application of Heck reaction, Stille coupling, Suzuki coupling, Chan Lam Coupling, C-H activation reaction, reactions of allylsilane, Biginelli reaction, Hantzsch reaction, Passerini reaction, Ugi reaction, Ring closing metathesis (RCM) - Grubb's reaction, Mitsonobu reaction, Nef reaction, Umpolung effect.

(b) Reactive Intermediates II: Concept, generation, stereochemical aspects, and important name reactions of free radicals.

REFERENCE BOOKS

[1] D. Nasipuri, Stereochemistry of Organic Compounds, 2nd Edn, New Age International (1994).
[2] P. S. Kalsi. Stereochemistry, Conformation and Mechanism (7th edn.), New Age (2008).
[3] March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure (6th edn.), Wiley Student Edition, John Wiley & Sons Asia Pte. Ltd. (2006).
[4] F. A. Carey & R. J. Sundberg. Advanced Organic Chemistry Part B, Plenum Press, 5th edition (2008).
[5] M. B Smith. Organic Synthesis (2nd end.), McGraw-Hill, Inc. (2001).
[6] T. L. Gilchrist & C. W. Rees, Carbenes, Nitrenes and Arynes, Nelson, London (Reprinted 2008).
[8] W. Carruthers, Some Modern Methods of Organic Synthesis (4th edn.), Cambridge University Press (2004).
[9] B. M Trost & I Fleming, Comprehensive Organic Synthesis, Vols 1-9, Pergamon (1991).
[10] M. B Smith, Organic Synthesis (2nd end.), McGraw-Hill, Inc. (2001).

SECOND SEMESTER **CHE-DSEC-508** **CREDIT: 4**

INTERDISCIPLINARY CHEMISTRY

Learning Objectives:

- The knowledge of photochemistry of inorganic complexes and their underlying principles
- Learning practical aspects of various spectroscopic techniques such as IR, NMR, and Mass

Course Outcomes:

- Students familiarize themselves with principles and applications of photochemistry of metal complexes that plays diverse role as catalysts, sensors, biomolecular vectors, etc.
- Learning the spectroscopic techniques will help in analysing data for characterization of organic compounds

Unit 1: *Inorganic photochemistry I*: Introduction to inorganic photochemistry, photophysical and photochemical process, characteristics of the electronically excited states of inorganic compounds, ligand field states, charge transfer states; Photochemical processes: Selection rules, Jablonski diagram, Fluorescence and phosphorescence, delayed fluorescence, Photochromism, Photosensitization, Quantum yield; Photochemical reactions: substitution and redox reactions of Cr(III), Ru(II) and Ru(III) complexes; organometallic photochemistry;

Unit 2: *Inorganic photochemistry II*: Luminescent d^6 and d^{10} complexes; Molecular recognition, Sensing, Bioimaging, Supramolecular chemistry, Photochemical splitting of water, Dye sensitized solar cells, Photoredox catalysis.

Unit 3: Nuclear Magnetic Resonance Spectroscopy:

Revisit of basic concept of NMR spectroscopy. Approximate chemical shift values of carbon- and heteroatom bonded protons; deuterium exchange; chemical and magnetic equivalence; first order and non-first order spectra; Shift reagents; Karplus curve, variation of coupling constant with dihedral angle; Nuclear Overhauser Effect (NOE), ^{13}C-NMR Spectroscopy: Basic concept of ^{13}C-NMR and its chemical shift (aliphatic, olefinic, alkynes, aromatic, hetero-aromatic, carbonyl carbon) values for structure determination.

Basic concept of 2D NMR spectroscopy**,** HETCOR, COSY, NOESY, HMQC, and HSQC**.**

Unit 4: IR and Mass Spectrometry

Infrared Spectroscopy: Identification of organic compounds using characteristic vibrational frequencies of alkanes, alkenes, alkynes, aromatic compounds, alcohols, ethers, phenols, amines and carbonyl compounds (ketones, aldehydes, esters, amides, acid anhydrides, lactones, lactams, conjugated carbonyl compounds); Effects of H-bonding and solvent effect on vibrational frequency.

Mass Spectroscopy: Basic concepts of Mass spectrometry; Structure determination from Mass fragmentation of common organic compounds; McLafferty rearrangements, nitrogen rule, isotope rule.

Structure elucidation of some simple and complex organic molecules by the analysis of FT- IR, ^1H, ^{13}C and mass data.

SUGGESTED BOOKS

[1] D. M. Roundhill. *Photochemistry and Photophysics of Metal Complexes*, Plenum Press (1990). 5.

[2] J. E. Huheey, E. A. Keiter & R. L. Keiter, *Inorganic Chemistry* (4th edn) Prentice Hall (1997)

[3] N. J. Turro, V. Ramamurthy, J. C. Scaiano, *Principles of Molecular Photochemistry: An introduction*, University Science Books (2009).

[4] R. M. Silverstein, G. C. Basseler & T. C. Morill. Spectroscopic Identification of Organic Compounds, 7th Edn., John Wiley (2005).

[5] Donald L. Pavia, Gary M. Lampman, George S. Kriz, James A. Vyvyan, Introduction to Spectroscopy, 5th Edition, Cengage Learning, 2015.

[6] D Williams & I. Fleming. Spectroscopic Methods in Organic Chemistry, McGraw Hill (1989).

[7] W. Kemp, *Organic Spectroscopy*, 3rd Ed, ELBS, 1991

[8] K. Nakamoto, *Infrared and Raman Spectra of Inorganic and Coordination Compounds*, Part A&B; John Wiley and Sons Inc., 6th Ed, 2009.

[9] P. I. Haines, Thermal *Methods of Analysis-Principles, Applications and Problems*, Blackie Academic & Professional, 1st Ed, 1995.

SECOND SEMESTER **CHE-RM-509** **CREDIT: 4**

RESEARCH METHODOLOGY AND PROPOSAL WRITING

Learning Objectives:

This course aims to teach

- Basic understanding of the process of research
- Ethical issues on research publication
- Laboratory safety processes
- The basic data analysis tools and their applications.

Course Outcomes:

- Student will be able to appreciate the process of research
- Will understand the ethical issues in research and publications
- Will generate safety awareness
- Students earn expertise in statistical methods for data authentication and other tools required to pursue research in chemistry.
- Will be able to interpret data

Unit 1: Research methodology: Definitions, Purpose of Research, Types of research, Research approaches, Research Methods, Stages of the research process, Background reading & information gathering: Literature survey, Hypothesis: Identification of Research Problem; Ethical issues in research, Data collection, Data recording and reproducibility, Importance of documentation.

Unit 2: Research ethics and Publication: Presentation of research findings: Elements of research publications; Seminar presentation; Patent; Paper writing; Journal impact factor, h-index; review process.

Unit 3: Laboratory safety: General health and safety concerns; What to do after splash/cut, Chemical hazards, commonly used hazardous laboratory chemicals (azide, perchlorate, nBuLi, acid chlorides, bromine, cyanide, mercury, etc), Personal protective equipment, Environmental safety issues: Fume hood safety, Safety data sheet, Waste handling, Disposal of chemical and plastic-waste; precautionary measure for the maintenance of laboratory equipment.

Unit 4: ***Statistical Methods and Computer Applications in Chemistry*****:** Errors, precision and accuracy; Average Mean Deviation, Standard Deviation, Variance, Chi-square Test. Applications of Curve Fitting, Straight Line Fitting, Interpolation in solving chemical problems. Applications of commonly used Computer Softwares, such as Mercury, Origin, Excel, etc.

REFERENCE BOOKS

[1] National Academy of Sciences, National Academy of Engineering and Institute of Medicine. (2009). *On Being a Scientist: A Guide to Responsible Conduct in Research: Third Edition.* National Academies Press.

[2] K. Prathapan, *Research Methodology for Scientific Research*, Dreamtech Press (2019)

[3] R. Ridley, *Handbook of Good Laboratory Practices*, 2nd Edition, WHO (2009).

[4] Ramesh Kumari, *Computers and their Applications to Chemistry*, 2nd Ed., Narosa Publishing House, 2007.

[5] K. Atkinson, *Elementary Numerical Analysis*, 2nd Ed., John Willy and Sons, 2003.

[6] R. Ridley, *Handbook of Good Laboratory Practices*, 2nd Edition, WHO (2009).

SECOND SEMESTER **CHE-DSEC-510** **CREDIT: 4**

RESEARCH TOOLS IN INORGANIC CHEMISTRY

Learning Objectives:

- To understand basics of spectroscopy and other techniques in inorganic chemistry.
- Learning EPR for the determination of oxidation state and geometry of metal center.
- To understand IR, Raman, electronic and Mössbauer spectroscopy of inorganic compounds.
- Understanding X-ray diffraction for structure elucidation.

Course Outcomes:

- Can gather knowledge on electron paramagnetic resonance spectroscopy.
- Can gather a fair idea of IR, Raman, UV-vis, emission and Mössbauer spectroscopy.
- Can gather knowledge to solve and refine X-ray crystal data.
- Will understand redox and thermal properties of coordination complexes.

Unit 1: ***EPR Spectroscopy:*** Principle, instrumentation, representation of EPR spectrum, line width, hyperfine splitting, magnetically equivalent and nonequivalent sets of nuclei, g-anisotropy, spectra of simple organic free radicals: Spectra of transition metal complexes, zerofield splitting, application: determination of oxidation state of metal ion in samples.

Unit 2: (a) ***IR and Raman spectroscopy:*** Structural studies of coordination compounds using IR and Raman spectroscopy.
(b) ***UV-vis and Emission Spectroscopy:*** Color and spectra of inorganic compounds, selection rules, fluorescence, phosphorescence, application.
(c) ***Mössbauer Spectroscopy:*** Principles, isomer shift, quadrupole effect of magnetic field, applications of Mössbauer Spectroscopy involving iron and tin compounds.

Unit 3: ***X-ray Crystallography*****:** Principle and Instrumentation, Crystal systems, Symmetry-operations, point groups, space groups, Techniques of single Crystal growth. Structure determination by single-crystal X-ray diffraction; X-ray data collection and refinement, Preparation of publication materials. Exercises on the structure elucidation by single crystal X-ray Diffraction data.

Unit 4
(a) ***Electrochemistry*****:** Principles, instrumentation, and applications of cyclic and differential pulse voltammetry.
(b) ***Thermoanalytical Method:*** Principles, instrumentation, and applications of thermoanalytical methods, viz. TGA, DTA and DSC.

TEXT BOOKS

[1] K. Nakamoto, *Infrared and Raman Spectra of Inorganic and Coordination Compounds*, (6^{th} edn.), John Wiley (2008).
[2] R. V. Parish, *NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry*, Ellis Horwood, New York (1990).
[3] J. A. Iggo, *NMR Spectroscopy in Inorganic Chemistry*, OUP Oxford (2000)
[4] G. H. Stout and L. H. Jensen, *X-ray Structure Determination: A Practical Guide*, The McMillan Company, New York (1968)
[5] F. Marken, A. Neudeck A. M. Bond, *Electroanalytical Methods*, Chapter III, 51–97 (2005)

REFERENCE BOOKS

R. S. Drago. *Physical Methods in Chemistry*, Saunders College Publishers (1977).

THIRD SEMESTER	CHE-CC-600	CREDIT: 4

ORGANIC CHEMISTRY – III

Learning Objectives:

- To teach pericyclic reactions and photochemistry, two fundamental aspects of organic reaction
- Learning advances on reagents in organic transformations
- Understanding heterocycles, the core of drug development

Course Outcomes:

- Understanding pericyclic reaction and photochemistry will improve stereochemical aspects of those reactions
- Learn the knowhow of drug development, thereby creating employment opportunities in pharma industries and research
- Knowing more reagents will provide depth on better planning of organic reactions

Unit 1: Pericyclic Reactions

Main features of pericyclic reactions; Woodward-Hoffman rules, correlation diagram and FMO approaches; Electrocyclic reactions – conrotatory and disrotatory motions for 4n and 4n+2 systems; Cycloadditions – antarafacial and suprafacial additions, [2+2] and [4+2] reactions (hν and Δ), 1,3-dipolar cycloadditions and chelotropic reactions; Sigmatropic [i,j] shifts of C-H and C-C bonds; Sommelet-Hauser, Claisen, thio-Claisen, Cope and aza-Cope rearrangements.

Unit 2: Photochemistry

Photochemistry of alkenes and carbonyl compounds; photochemistry of aromatic compounds; concept and applications of photochemical isomerisation, addition, and substitution reactions. di-π-methane rearrangement (DPM), Oxa-di-π-methane (ODPM) aza-di-π-methane (ADPM), Barton reaction, Hofmann-Loeffler-Freytag reaction, Photo-oxidation, photoreduction, photochemistry of imines and enamides and application in natural product syntheses, Visible light photocatalysis in organic syntheses. Photo-Fries rearrangement of ethers and anilides; Photooxygenation - Singlet molecular oxygen reactions.

Unit 3: Reagents

Preparation, structures, reactions involving organocopper, organoborane, organosilicon, organolithium reagents, and reaction intermediates. Reduction of olefin, carbonyl, and other functional groups involving palladium, ruthenium, iridium, rhodium, and aluminum catalysts.

Unit 4: Heterocycles

Hantzsch-Widman nomenclature for monocyclic, fused, and bridged heterocycles; Structure, property, and synthesis of aziranes, oxiranes; azetidines, oxetanes; pyrazole, isoxazole; imidazoles, thiazoles and oxazoles, indole; quinolines, isoquinolines, carbazoles, pteridines, azepines, diazepines.

SUGGESTED BOOKS

[1] J. A. Joule, K. Mills, Heterocyclic Chemistry, John Wiley & Sons (2010)

[2] R. Katritzky & C. W. Rees, Comprehensive Heterocyclic Chemistry, Vols. 1-7, Pergamon Press (1984).

[3] Katritzky, A. R., Ramsden, C. A., Joule, J. A., and V. V. Zhdankin, Handbook of Heterocyclic Chemistry, 3rd edition, Pergamon Press (2010).

[4] T. L. Gilchrist. Heterocyclic Chemistry (2nd edn.), Longman Scientific & Technical Publicns. (1992).

[5] C. Depuy & O. L. Chapman. Molecular Reactions and Photochemistry, Prentice-Hall of India (1975).

[6] Francis A. Carey and Richard J. Sundberg, Advanced Organic Chemistry, 4th Edition, ©2002 Kluwer Academic Publishers

[7] W. Carruthers and Iain Coldham, Modern Methods of Organic Synthesis, 4th Edition, Cambridge University Press

THIRD SEMESTER **CHE-CC-601** **CREDIT: 4**

PHYSICAL CHEMISTRY - IV (LAB)

Learning Objectives:

- To carry out experiments to understand the quantitative aspects of Physical Chemistry.
- To learn how to handle the instrument and apparatus used in laboratory.

Course outcomes:

- Student will learn the techniques and become expert in handling the instruments used in laboratory and for future in the industries and R&D laboratories.

Students are to perform eight experiments from the following list:

1. Determination of order of reaction, rate constant and energy of activation for saponification of an ester by NaOH, conductometrically.
2. Determination of critical micellar concentration (CMC) of sodium lauryl sulphate from the measurement of conductivities at different concentrations.
3. Determination of strengths of halides in a mixture, potentiometrically.
4. Determination of pH of buffer solutions and hence to calculate the E_0 of quinhydrone electrode.
5. Verification of Beer-Lambert's law and determination of pKa of an indicator, spectro-photometrically.
6. Spectrophotometric determination of pKa of an indicator in micellar and microemulsion media.
7. Determination of partial molar volume of a solute in solution.
8. Determination of the stability constant of the complex formed between Cu(II) ions and 5- sulphosalicylic acid between pH 3-5 by colorimetric method and hence to calculate thefree energy of formation of the complex.
9. Determination of specific rotation of sucrose and rate constant of its hydrolysis using a polarimeter.
10. Determination of coordination number of Cu^{2+} in copper-ammonia complex by partition method.
11. To study the kinetics of iodination of acetone.
12. Determination of the acidic and basic dissociation constants of an amino acid and hence its isoelectric point.
13. To study the phase diagram of three component system.
14. Determination of solubility product for sparingly soluble salt.

B. Experiments based on Fluorescence spectroscopy, Dynamic Light Scattering, TGA-DSC.

TEXTBOOKS

[1] D. P. Shoemaker, C. W. Garland & J. W. Nibler. *Experiments in Physical Chemistry,* 5th Ed., McGraw Hill Pub., 1989.

[2] V. D. Athawala & P. Mathur. *Experimental Physical Chemistry*, New Age International. Publishers, 2001.

THIRD SEMESTER **CHE-CC-602** **CREDIT: 4**

INORGANIC CHEMISTRY – III

Learning Objectives:

- To understand the chemistry of organometallic compounds and catalytic processes.
- Learning biomolecules, proteins and enzymes and their functions
- To understand metal-metal multiple bonds and metal carbonyl compounds and clusters.
- Understanding inorganic supramolecular chemistry.

Course Outcomes:

- Can gather knowledge on organometallic compounds and catalysis.
- Can gather a fair idea of biomolecules, proteins and enzymes and their functions
- Can gather knowledge on metal-metal multiple bonds and metal carbonyl compounds and clusters
- Will understand supramolecular interactions and application of supramolecules

Unit 1: *Organometallic Chemistry*

Application of 18-electron and 16-electron rules to transition metal organometallic complexes, Ligands in organometallic chemistry; Synthesis, bonding and reactivity of Metal-alkyl, -alkene, - alkyne, -allyl, -carbene complexes, Agostic interaction, Stereochemical non-rigidity and fluxional behaviour of organometallic compounds with typical examples; Catalytic applications: Oxidative addition, Reductive elimination, Hydroformylation (Oxo process), Wacker oxidation (Pd-catalysed), Polymerization of olefins, Ziegler-Natta catalyst**.**

Unit 2: *Bioinorganic Chemistry*

Essential and trace elements in biological systems, biologically important compounds amino acids, proteins, nucleotides, carbohydrates, and lipids, Bioenergetic principle and role of ATP and ADP; Biological membranes; mechanism of ion transport across membranes, ionophores; channel and pump; O_2-uptake proteins: haemoglobin, myoglobin, hemerythrin and hemocyanin, structure, function, and model study. Electron transport protein: Fe-S proteins (Rubredoxin and ferredoxins), cytochromes, Metal ions transport and storage proteins: ferritin, transferin, ceruloplasmin.

Unit 3: *Metal carbonyls, clusters, and Metal-metal multiple bond*

Synthesis, structure, and reactivity of metal carbonyls; Metal cluster: Low nuclearity and high nuclearity carbonyl clusters; Boron clusters: Structure and bonding of boranes and Lipscomb's topology, styx system of numbering, nomenclature; Synthesis and structure of carboranes, metalloboranes, metallocarboranes; Skeletal electron counting, Wade's rule. Metal-metal multiple bonds, quadruple bond, structures, and bonding (MO).

Unit 4: *Inorganic Supramolecular Chemistry*

Origin of supramolecular chemistry. Concepts and terminology of supramolecular chemistry. Types of supramolecular interactions (Hydrogen bonding, van der Waal's interaction, π-stacking, CH-π, anion-π interaction). Supramolecular chemistry in inorganic perspective: Inorganic crystal engineering and design principle of metal organic framework (MOF) and inorganic-organic hybrid material. Application of supramolecular chemistry in catalysis, drug delivery, and recognition/sensing.

TEXT BOOKS

[1] C. Elschenbroich, *Organometallics* (3rd edn.), Wiley-VCH Publication (2006).
[2] R. C. Mehrotra & A. Singh, *Organometallic Chemistry: A Unified Approach* (2nd edn.), New Age International (2000).
[3] S. J. Lippard & J. M. Berg, *Principles of Bio-Inorganic Chemistry*, Panima Publ. Corpn. (2005).
[4] J. W. Steed & J. L. Atwood. *Supramolecular Chemistry*, John Wiley (2002).

REFERENCE BOOKS

[1] Yamamoto, *Organo Transition Metal Chemistry*, Wiley (1986).
[2] R. H. Crabtree, *The Organometallic Chemistry of the Transition Metals* (4th edn.), John Wiley (2005).
[3] Gautam R Desiraju, J. J Vittal, A. Ramanan, *Crystal Engineering: A Textbook* (1st Edn.) World Scientific Publishing Company (2011)

THIRD SEMESTER **CHE-SEC-603** **CREDIT: 4**

RESEARCH TECHNIQUES IN CHEMISTRY

Learning Objectives:

- This Course will facilitate hands on learning of chemistry techniques

Course Outcomes:

- The experience gained and skill earned in the process will be helpful in opting for a research career or job opportunities in pharmaceutical companies, and other Chemistry related industries.

1. Hands on training on selected areas among the followings:

   DFT Calculations; Computer softwares, such as Mercury, Origin, Excel, etc.; Data manipulation using One-way ANOVA and Prism.

2. Hands on training on selected areas among the followings:

   a) Separation and purification techniques: Distillation, Solvent extraction, Thin layer chromatography, Column chromatography, Flash chromatography, Recrystallization, etc.

   b) Measurement of Chemical Oxygen Demand.

   c) Reaction methods: Reflux, Monowave, Microwave, Sonication, Photolysis/photochemical reactions.

   d) Preparation, characterization, and catalytic applications of organic & inorganic materials.

   e) Spectrophotometric and fluorometric based experiments.

REFERENCE BOOK

[1] BS Furniss, AJ Hannaford, PWG Smith, and AR Tachell, Vogel’s Textbook of Practical Organic Chemistry, Pearson India; 5th edition (2003)

[2] G Svehla, B Sivasankar, Vogel’s Qualitative Inorganic Analysis, Pearson Education India; 7th edition (2012)

[3] Jihad René Albani, Principles and Applications of Fluorescence Spectroscopy, Wiley (2007).

[4] J. B. Foresman and Æ Frisch, Exploring Chemistry with Electronic Structure Methods, 3rd ed., Gaussian, Inc.: Wallingford, CT, 2015.

THIRD SEMESTER **CHE-DSEC-604** **CREDIT: 4**

ORGANIC CHEMISTRY IV

Learning Objectives:

- Understanding the structure and function of biomolecules such as coenzymes and nucleic acids
- Learning structure, synthesis, and function of natural products
- Understanding macromolecules like polymers and supramolecular architecture
- Understanding drugs, their pharmacokinetics, structure, function, and syntheses

Course Outcomes:

- Can appreciate the importance of biomolecules and their roles
- Can gather a fair idea of natural products and develop expertise in synthetic strategies
- Basic polymers and the process involved therein will make students ready for industries
- Understanding supramolecular interactions are key to understand biological processes
- Will understand drugs and the processes involved in drug development

Unit 1: Biomolecules

(a) ***Co-Enzyme****:* Structure & function of coenzyme A, thiamine pyrophosphate, pyridoxal phosphate, NAD^+, $NADP^+$, FMN, FAD, lipoic acid and vitamin B12 in biological processes.

(b) ***Nucleic acids:*** Primary, secondary, and tertiary structure of DNA; Structure and function of *m*RNA, *t*RNA, *r*RNA, Basic concepts of codon, anti-codon, mutation, and wobble hypothesis.

Unit 2: Natural products

(a) ***Terpenoids:*** Classification of terpenoids (with example); structure and synthesis of abietic acid, caryophyllene, isocaryophyllene, and longifolene.

(b) ***Alkaloids:*** Classification of alkaloids (with example); structure and synthesis of strychnine, lysergic acid, nicotine, morphine.

(c) ***Steroids:*** Classification of steroids (with example); structure and synthesis of cholesterol, estrogens, and progesterones.

Unit 3: Macromolecules

(a) ***Polymer chemistry:*** Concept of polymerization, classification, mechanism of polymerization, characterization, co-polymerization, ionic polymerization, thermoplastic, thermosetting polymers, natural and artificial rubber, vulcanization, plasticizer, and elastomers.

(b) ***Supramolecules:*** Concept, nature of supramolecular interactions, host-guest chemistry, crown ethers, cryptands, cyclodextrins, calixarenes, molecular recognition: cations, anions, neutral molecules binding hosts, molecular devices. Supramolecular reactivity and catalysis, Supramolecular sensors, catenanes, rotaxanes, molecular Knots, Borromean ring, Supramolecular machines, switching devices, molecular shuttle, molecular motor, molecular valve, rotary motor.

Unit 4: Introduction to Drugs

Concept of drug, lead compound, prodrugs, and soft drugs; ADME, Factors affecting bioactivity – lipophilicity, partition coefficient, resonance, inductive effect, isosterism, bio-isosterism, spatial considerations; Structure-activity relationship (SAR), quantitative structure-activity relationship (QSAR); Theories of drug action, drug metabolism. concept, classification, SAR and mode of action of Antibiotics (penicillin), Anticancer, Antimalarial, Anti-infective**,** sedatives and Hypnotics drugs. Synthesis of diazepam, barbiturates, thiopental sodium, chloroquine, pamaquine, ciprofloxacin, norfloxacin, penicillin V, 5-fluorouracil and 6-mercaptopurine.

TEXT BOOK

[1] M. S. Bhatnagar. *A textbook of polymer chemistry*, Vol (I-III): S. Chand and Company (2004).
[2] J. W. Steed and J. L. Atwood. *Supramolecular Chemistry*: Willy Reprinted (2002)
[3] I. L. Finar, Organic Chemistry, Vol. II, 5^{th} edition Pearson (2002).
[4] K. Nakanashi, Natural Products Chemistry, Vols. I and II, Academic Press, New York and London (1974).
[5] David Nelson, Lehninger Principles of Biochemistry 8th Edition, W. A. Benjamin (1972)
[6] G. Thomas. Medicinal Chemistry: An Introduction, 2nd Edition, Wiley (2007).

THIRD SEMESTER **CHE-DSEC-605** **CREDIT: 4**

PHYSICAL CHEMISTRY – V

RESEARCH TOOLS IN PHYSICAL CHEMISTRY

Learning Objectives:

- To understand the techniques and tools used in Physical Chemistry research.
- To gather hands on experience on the research tools

Course outcome:

- Student will learn the techniques and tools in Physical chemistry related research. They will learn different software which are used in chemistry research.

Unit 1: Fluorescence Spectroscopy

Basic concept: Origin of molecular fluorescence; intensity and spectra; Quantum yield; Steady state and time-resolved techniques; Experimentally measured parameters; Factors affecting fluorescence spectra; fluorescence quenching and applications; Monitoring excited state properties: Radox behavior and dipole moment; Excited state processes studied through fluorescence - charge transfer, proton transfer, energy transfer etc. Biological applications - some selected examples.

Unit 2: Photoelectron Spectroscopy

Basic principles, photoelectron spectra of simple molecules, X-ray photoelectron spectroscopy (ESCA), Auger electron spectroscopy. Lasers: Laser action, population inversion, properties of laser radiation, examples of simple laser systems. Dynamic Light Scattering: Principles and Applications (determination of Hydrodynamic diameter and ζ-potential.)

Unit 3: Numerical Analysis

Curve fitting by least square principle; Newton–Raphson iterative methods for solving non-linear equations; Interpolation, Numerical differentiation and integration, trapezoidal method, Simpson's 1/3 rule; Runge-Kutta method for solving differential equations.

Unit 4: Computational Chemistry

(a) Ab-initio methods: Hatree-Fock (HF) and post-HF methods; Density functional theory; semi- empirical methods.

(b) Applications of computational chemistry: geometry optimization; energy and frequency calculations; thermochemistry, kinetics, spectroscopic properties; molecular dynamics, etc.
Computational chemistry software: GAUSSIAN, GAMESS, GROMACS, AUTO DOCK.
Visualization softwares: Gaussview, pymol, VMD, Avogadro.

(c) Hands-on training with computers on selected chemical problems related to computational Chemistry.

TEXT BOOKS

[1] J.R. Lakowicz, Principles of Fluorescence Spectroscopy, 3rd ed., Springer, Boston, USA, 2006.
[2] E. Balagurusamy, *Computer Oriented Statistical and Numerical Methods*, Macmillan IndiaLtd. 2000.
[3] Christopher J. Cramer, *Essentials of Computational Chemistry*, 2nd Ed., Wiley, 2002.
[4] K. Atkinson, An introduction to numerical analysis 2nd Ed. Wiley, 2007.

REFERENCE BOOKS

[1] E. Kreyszig. *Advanced Engineering Mathematics*, 5th edn., Wiley Eastern Ltd.,1985.
[2] E.W. Cheney, D.R. Kincaid, *Numerical Mathematics and Computing,* Cengage Learning, 2007.

FOURTH SEMESTER **CHE-DSEC-606** **CREDIT: 20**

RESEARCH PROJECT

Learning objectives

- Working in complete research set-up under supervision of a teacher
- Making hypothesis on a research topic, literature survey, and conducting experiments.
- Giving project seminar, and writing a dissertation.

Course Outcome:

- Students will learn entire gamut of research process and will be able to implement a research idea.