Course No: CH24401CR
Title: Advanced Inorganic Chemistry (04 Credits)

Max. Marks: 100 | **Duration: 64 Contact hours**

Continuous Assessment: 20 marks | **End Term Exam: 80 Marks**

Course outcomes: After studying this course, the students will be able to

- correlate the reactivity with bonding in different classes of organometallic systems.
- correlate and interpret transitions with the electronic structure of the metal complexes.
- utilize the transition metal based photocatalysts for applications in organic transformations, energy and allied applications.

Unit-I Sigma and pi bonded Transition metal Compounds (16 Contact hours)

Sigma bonded OTMC: Classification, Mechanistic pathways of kinetic instability, Routes of synthesis and reactions of σ OTMC, Decomposition Pathways: Choice, and mechanisms. Alpha, Beta hydrogen transfer reactions. Intramolecular elimination of alkane, Cyclometallation, Stability from bulky substituents, Agostic alkyls, Umpolung.

Pi-Organometallic Compounds: Comparison of σ and π OTMC, comparative bonding in Metal-alkene, alkyne, allyl, 1,3-butadiene and Cyclobutadiene Pi- systems. Sandwich Compounds: Characteristics; Classification, Reactions and Structure and bonding of Ferrocene.

Unit-II Fluxionality and metal to carbon multiple bonded systems (16 Contact hours)

Classification NMR line shape analysis for mechanistic elucidation of non rigidity. Mechanisms of Fluxionality in compounds of η^1 Cyclopentadienyls (ring Whizzing) and η^3–allyls (syn anti exchange). Energetics of molecular dynamism. Stereochemical non rigidity case studies (cis-trans, atomic inversion, and Berry Pseudo rotation of TBP structures

Schrock and Fischer carbene complexes: Structural characteristics; reactivities and synthetic applications (Dotz reaction and Schrock's Catalyst). Olefin catalysis: Oxidation, Isomerization, and metathesis.

Unit-III Organo Transition metal Compounds in catalysis (16 Contact hours)

Catalytic processes involving OTMC: mechanism of Hydrogenation, Hydroformylation, Oxidation and Isomerization of alkenes; Olefin metathesis. Monsanto acetic acid and Reppe reaction. Fischer-Tropsch Synthesis and Ziegler Natta polymerization of alkenes. Asymmetric, Photo redox catalysis and supported Organometallic Catalysis (brief idea)

Synthetic Reactions involving Organometallics: Reactions of coordinated ligands, carbon monoxide, alkanes and alkenes (Green, Mingo's rules). Role of organo-iron compounds as synthons, Activation of small molecules: prospectus and challenges. Activation of Carbon monoxide, Carbon dioxide and Alkanes. Carbon-Carbon coupling reactions (Suzuki and Heck).

Unit-IV Electron Transfer in Excited Metal Complexes (16 Contact hours)

Marcus-Hush Model: Energy transfer under conditions of weak and strong interaction. Excited state electron transfer. Conditions of the excited states to be useful as redox reactants. Photochemical electron transfer, $[Ru\ (bipy)_3]^{2+}$;Structure, excited state properties and photo chemistry as sensitizers

Inorganic Photochemistry in practice: Applications, Prospects and Challenges Solar energy storage and conversion. Photovoltaic Solar cells, Perovskite Solar cells, Dye sensitized and quantum dot sensitized solar cells. Metal oxide semiconductor based photo-splitting of water. Photochemical supra-molecular devices: devices for photo-induced energy or electron transfer, Devices for information processing, photo-chemically driven molecular machines Supramolecular photochemistry in natural systems: photosynthesis, bacterial photosynthesis and artificial photosynthesis

Books Recommended:

1. The Organometallic Chemistry of Transition Metals; 6th edn; Robert. H . Crabtree; Wiley;2014.
2. Fundamental Transition Metal Organometallic Chemistry; Charles M. Lukehart; Brooks /Cole;1985.
3. Basic Organometallic Chemistry; 2nd edn ; Gupta Elias ; CRC Press, 2010
4. Principles and Applications of Organotransition Metal Chemistry; Collman& Finke; University,
5. Science Books; 1994.
6. Principles of Organometallic Chemistry; 2nd edn.; P.Powel; Chapman & Hall; 1998
7. Principles and Applications of Photochemistry, B. Wardle, John Wiley, 2009
8. Ligand Field Theory and Its Applications; B. A. Figgis and M. A. Hitchman; Wiley India,2000.
9. Reaction Mechanisms of Inorganic and Organometallic Systems; 2nd edn.;Jordon; Oxford; 1998.
10. Inorganic Chemistry; G. Wulfsberg; Viva Books, 2000.
11. Mechanism of Inorganic Reactions; Katakis, Gordon; Wiley; 1987.
12. Fundamentals of Photochemistry; C Rohatgi, Mukhergi; Wiley Eastern.; 1992.
13. G. J. Ferraudi, Elements of Inorganic photochemistry, John Willey and Sons (1988).
14. O. Horvath and K. L. Stevenson, Charge Transfer Photochemistry of Coordination compounds, VCH publishers Inc. (1993).
15. D. M. Roundhill, Photochemistry and photophysics of metal complexes, Plenum Press, New York and London (1994).
16. V. Balazani and V. Carassiti, Photochemistry of coordination compounds, Academic Press, London (1970).
17. Photochemistry and Photophysics of Metal Complexes D. M. Roundhill, 1st edition 1994, Springer Science ISBN 978-1-4899-1497-2 ISBN 978-1-4899-1495-8 (eBook)
18. Biomedical Applications of Inorganic Photochemistry, Peter C. Ford, Rudi van Eldik 1st Edition, Volume 80 – 2022 , Academic Press Hardback ISBN: 9780323991711.

Course No: CH24402CR
Title: Advanced Organic Chemistry (04 Credits)

Max. Marks: 100 | **Duration: 64 Contact hours**
Continuous Assessment: 20 marks | **End Term Exam: 80 Marks**

Course outcomes: On completion of the course, the student should be able to:
- understand various advanced methodologies used in the organic chemistry like asymmetric synthesis, disconnection approach and retrosynthesis.
- understand the functions of various reagents and their applications in organic synthesis.
- recognize the importance of the protection and deprotection of functional groups and their use in organic synthesis.
- design synthetic routes for complex organic molecules using retrosynthetic analysis and disconnection strategies.

Unit-I: Asymmetric Synthesis (16 Contact hours)

Asymmetric Synthesis: Nature & asymmetry, Methods of asymmetric synthesis: Chiral pool approach, Chiral reagents, Chiral auxiliaries and auxiliary controlled stereo-selection.
Asymmetric formation of C-C bonds.: Asymmetric aldol and Diels-Alder reactions. Nayori Asymmetric hydrogenation and epoxidation of alkenes (Sharpless, Jacobsen and Shi reactions). Racemization & Resolution of enantiomers using chiral molecules.

Unit-II: Reagents in Organic Synthesis (16 Contact hours)

Oxidizing Reagents (Preparation and Applications)
PCC (Pyridinium chlorochromate), PDC (Pyridinium dichromate), MCPBA (meta-Chloroperoxybenzoic acid), TBHP (tert-Butyl hydroperoxide), DDQ (2,3-Dichloro-5,6-dicyano-1,4-benzoquinone), MnO_2 (Manganese dioxide), TEMPO (2,2,6,6-Tetramethylpiperidine 1-oxyl), Osmium tetroxide (OsO_4)
Reducing Reagents: (Preparation and Applications)
$NaBH_4$ (Sodium borohydride), DIBAL (Diisobutylaluminum hydride), LAH (Lithium aluminum hydride), Diisoamylborane, Na/EtOH (Sodium in ethanol-dissolving metal reduction), Na/liquid NH_3 (Birch reduction).
Specialized Reagents: ((Preparation and Applications))
DCC (Dicyclohexylcarbodiimide), DABCO (1,4-Diazabicyclo [2.2.2] octane), DBU (1,8-Diazabicyclo [5.4.0] undec-7-ene).

Unit-III: Protection and Interconversion of Functional Groups (16 Contact hours)

Protection of Functional Groups: Principle of protection of functional groups and its significance in multistep synthesis.
Protection of specific functional groups*: Carbon–hydrogen bonds:* Terminal alkynes, Aldehydic C–H bonds, Carbon–carbon double bonds, Alcoholic and phenolic hydroxyl groups, *Amino* groups, Carbonyl groups (aldehydes and ketones), Carboxyl groups.
Functional Group Interconversion (FGI) / Transformations: Significance of FGI in organic synthesis and retrosynthesis.
Common transformations of functional groups: Alcohols ↔ Carbonyl compounds, Carbonyl compounds ↔ Amines (via imines, oximes, reductive amination), Carboxylic acids ↔ Esters ↔ Amides

↔ Acid chlorides, Alkenes ↔ Alcohols ↔ Alkyl halides, **Chemo-selectivity**: Concept, importance in multistep synthesis.

Unit-IV Designing Organic Synthesis (16 Contact hours)

Introduction to the Disconnection Approach: Concept of retrosynthetic analysis. **Synthons**: definition, types (nucleophilic, electrophilic), and equivalent reagents. Reversal of polarity (Umpolung) and its synthetic applications. Guidelines for effective disconnections in synthetic design. Use of connections and rearrangements in retrosynthetic planning.

One-Group Disconnections*:* Retrosynthetic analysis of: Alcohols, Amines (aliphatic and aromatic), Alkenes, Carbonyl compounds, Carboxylic acids and derivatives,

Two-Group Disconnections*:* Retrosynthetic analysis of difunctional compounds: 1,2-difunctional compounds: e.g., 1,2-diols.

1,3-difunctional compounds*:* e.g., 1,3-dioxygenated compounds, α,β-unsaturated carbonyls, 3-amino alcohols, 3-amino ketones.

1,4- and 1,5-difunctional compounds*:* strategies and synthetic significance.

Multistep Synthesis Applications*:* Application of retrosynthetic analysis in the design of complex molecules. Case studies/illustrative examples: Ibuprofen (Brufen), Benziodarone, Juvabione, Warfarin, Brevicomin

Books Recommended:

1. Modern Methods of Organic Synthesis, Carruthers W. William Caruther and Iain Coldham, 4th edition, Cambridge, 2024.
2. A Guide to Reagents in Organic Synthesis., S Gupta, V Gupta, R.S Dhundal, 1st edition, 2015
3. Transition Metal Reagents and Catalysts: Innovations in Organic Synthesis, by Jiro Tsuji, 2002.
4. Organic Synthesis, Jagdamba Singh, L.D.S Yadav, 1st Edition, 2006.
5. Principles of Organic Synthesis 2nd edn;. R. O. C. Norman; Chapman and Hall; 1978.
6. Advanced Organic Chemistry Part B, 5th edn.; F. A. Carey and R.J Sundberg; Springer; 2007.
7. Organic Chemistry, 10th edn;. T. W. G. Solomons and Craig B. Fryhle ; Wiley-2012.
8. Organic Chemistry; 4th Ed., Clayden, Greeves, Warren and Wothers ; Oxford University Press-2012.
9. Advanced Organic Chemistry: Reactions, Mechanism and Structure, 6lh Ed., J. March,; Wiley; 2012
10. Asymmetric Synthesis, Garry Procter, Oxford University Press; 1st edition, 1996.
11. Stereoselectivity in Organic Synthesis, Garry Procter, Oxford University Press, 1996.
12. Principles of Asymmetric Synthesis, Robert E. Gawley and Jeffery Aube, 2nd Edition, 2012.
13. Stereochemistry of Organic Compounds, V.K. Ahluwalia, Springer, 2022.
14. Principles and Applications of Stereochemistry, Michael North, CRC Press-1998.
15. Stereochemistry and Stereoselective synthesis: An Introduction, Laszlo Poppe and Mihaly Nogardi, Wiley-VCH, 2016.
16. Designing Organic Synthesis, S. Warren; Wiley; 2013.
17. Organic Synthesis- concept, methods and Starting Materials, J. Furhop and G. Penzlin; Verlage VCH;1986.

Course No: CH24403CR
Title: Advanced Physical Chemistry (04 Credits)

Max. Marks: 100 **Duration: 64 Contact hours**
Continuous Assessment: 20 marks **End Term Exam: 80 Marks**

Course outcomes: After learning the contents of this course, the students shall:

- appreciate the importance of catalysts for green chemistry and development of sustainable chemicals processes for industrial scale production of various chemicals/materials.
- learn as to how simple kinetic investigations and concepts acquired in the field of inorganic, organic and organometallic chemistry can be employed for the design of effective and stable catalysts for chemical transformations.
- get a knowhow of different types of catalysts, their mode of action, advantages and disadvantages, as well as their principal applications.
- understand the forces involved in the aggregation of molecules for the formation of soft matter relevant for life.
- get familiar with various soft materials formed by surfactants, polymers and block copolymers like hydrogels, liquid crystals and microemulsions
- understand the importance of the soft matter in environmental remediation, health, diagnosis, catalysis, development of smart materials, and fabrication of non-linear optical materials.

Unit-I Catalysis-The Basics (16 Contact hours)

Overview of catalysis, homogeneous, heterogeneous and bio-catalysis, Catalysis and Green Chemistry; Catalysis and Efficiency, E-factors, and Atom Economy, Replacing Stoichiometric Reactions with Catalytic Cycles.
Potential functions of catalysts with examples; reaction initiation, intermediate/transition state stabilization (Sabatier's principle), reactant localization and reactant orientation, bond cleavage facilitation, electronic effect, reaction selectivity enhancement, energy and mass transfer facilitation effects of catalysts. Kinetics of catalytic reactions.
Catalyst deactivation, sintering, thermal degradation, Inhibition, poisoning.
Solvents as catalysts, solvation and its impact on reactant, product and transition state stabilization, impact of solvent on reaction rates, qualitative and semiquantitative predictions of the effect of solvents on reaction rates. Hydrophobic interactions, examples regarding facilitation of reaction kinetics and reaction selectivity via use of hydrophobic interactions.

Unit-II Applied Catalysis (16 Contact hours)

Catalysis by Metals: Elementary reactions on metals, mechanism of metal catalyzed reactions, Trends over the periodic table, Metal Catalysts for specific organic transformations, Blowers-Masel equation for catalyst selection.

Bio-catalysis: Enzyme Catalysis vs Whole-Cell systems, Immobilized Enzymes: design and applications, Developing New Biocatalysts: Better than Nature's Best, Catalytic Antibodies (Abzymes), Catalytic RNA (Ribozymes).

Catalysis of Industrial processes: Mechanistic and kinetic aspects of some selected industrial process; Steam Reforming, Hydrogenation of alkenes and CO, Synthesis of methanol, Fischer-Tropsch process, Synthesis of ammonia, Oxidation of ammonia, Photocatalytic breakdown of water, The BHC Ibuprofen Process.

Unit-III Introduction to Soft Matter, Amphiphiles, block copolymers and microemulsions (16 Contact hours)

Introduction to Soft Matter: Constituents of soft matter, Intermolecular forces: van der waals, electrostatic forces, covalent bond, hydrogen bond and hydrophobic
interactions. viscoelastic response

Amphiphiles: General overview of self-assembly of amphiphiles. Introduction and applications of stimuli-Responsive surfactants: Biosurfactants, redox, photochromic, thermos-reversible, pH-sensitive, cleavable and magnetic surfactants. Lipid bilayer, hydrophobicity: entropy driven interactions, self-assembly. Physics of membranes: elasticity, Helfrich energy. Plasma membrane: architecture, composition, Fluid mosaic model, membrane channels, active pumps, function.

Block Copolymers: Introduction: classification, micellization of diblock and triblock copolymers. Introduction to pH-, thermo- and Photo-responsive block copolymers. Applications.

Microemulsions: Emulsions and microemulsions, Physicochemistry of Microemulsions: Formation, Stability, and Droplet Clustering, Percolation Phenomenon in Microemulsions. Applications of microemulsions in cosmetics and detergency, pharmaceutics, soil decontamination, enhanced oil recovery and biocatalysis.

Unit-IV Hydrogels, Langmuir Blodgett Films and Liquid crystals (16 Contact hours)

Hydrogels: Introduction, Classification of hydrogels based on type of source, crosslinking and composition. Introduction to stimuli responsive hydrogels and their types. Characterization of hydrogels: Rheological (steady-state, oscillatory and thixotropic behavior), spectroscopic (IR only) and microscopic (SEM and EDX only). Applications of Hydrogels in adsorption, 3D printing, shape memory materials, drug release and other biomedical applications.

Langmuir-Blodgett Films: Introduction and general preparative techniques. LB Films of various compounds (hydrocarbon, liquid crystals compounds and polymers), Applications – nonlinear optical effects, conduction, photoconductivity and sensors.

Liquid Crystals: Mesomorphism, types of liquid crystals, molecular structural requirement of mesomorphism, properties of liquid crystals, Applications – Liquid crystal displays, and thermography.

Books Recommended:

1. Chemical Kinetics, K. J. Laidler, 3rd Edition, Pearson, 1987.
2. Chemical Kinetics and Reaction Dynamics, Paul L. Houston, Dover Publications, INC., Mineola, New York, 2001.
3. Chemical Kinetics and Dynamics, J. I. Steinfeld, J. S. Francisco, W.L. Hase, Prentice Hall, 1989
4. Chemical Kinetics and Catalysis, R.I. Masel, Wiley, 2001
5. Chemical Kinetics: From Molecular Structure to Chemical Reactivity, Luis G Arnaut, Sebastiao Jose Formosinho, Hugh Burrows, Elsevier, 2007.

6. M. J. Rosen, J. T. Kunjappu, “Surfactants and Interfacial Phenomena”, John Wiley & Sons, New York, 4th Edition, 2012.
7. D. Fennell Evans, H. Wennerstrom, “The Colloidal Domain where physics, chemistry, biology and technology meet” VCH, New York, 1994.
8. Thermotropic Liquid Crystals, Ed., G.W. Gray, John Wiley.
9. I. W. Hamley, The Physics of Block Copolymers (Oxford University Press, Oxford, 1998.
10. N. Hadijichristidis, S. Pispas and G. A. Floudas Block Copolymers (Wiley, New York, 2003)..

Course No: CH24404CR
Title: Project Seminar and Dissertation (02 Credits)

Max. Marks: 50 | **Duration: 32 Contact hours**
Continuous Assessment: 10 marks | **End Term Exam: 40 Marks**

Course outcomes: The main outcomes of the course are to:

- prepare a structured and well-written dissertation in standard scientific format, ensuring clarity, proper referencing, and academic integrity after completing the lab project.
- present and defend research findings effectively through seminars and viva-voce using suitable visual aids and logical arguments.
- demonstrate professional skills such as independent research ability, teamwork, time management, and ethical conduct in scientific work.

Course Contents:

This course is designed to provide students with the skills required to organize, compile, and present the outcomes of their laboratory-based project work in a professional scientific format. Emphasis is placed on critical analysis of literature, scientific writing, seminar presentation, and defense of research findings, thereby preparing students for advanced research or professional careers in chemistry.

Students will begin by conducting a thorough literature survey to understand the background of their research problem. This will involve reviewing published scientific articles, identifying research gaps, and justifying the objectives of their work. The next stage focuses on the preparation of the dissertation, where students will learn to structure their thesis systematically with sections such as introduction, literature review, objectives, methodology, results and discussion, conclusions, and references. Training will be provided in scientific writing styles, proper use of figures, tables, and graphs, as well as citation practices and maintenance of academic integrity.

In addition, students will prepare a seminar presentation based on their dissertation work. This component will emphasize effective use of visual aids such as PowerPoint slides, charts, and spectra, as well as clear and logical communication of scientific findings. During this seminar, students will participate in a viva-voce or defense, where they will present the key results of their work and respond to critical questions from faculty and peers, thereby strengthening their ability to defend research outcomes.

All these components together ensure that students not only complete their dissertation but also acquire essential skills for higher studies, research, and careers in the chemical sciences.

Course No: CH24405DCE
Title: Lab Project in Chemistry (04 Credits)

Max. Marks: 100 | **Duration: 128 Contact hours**
Continuous Assessment: 20 marks | **End Term Exam: 80 Marks**

Course outcomes: The main outcomes of the course are to:

- identify, formulate, and analyze a research problem in chemistry and design a methodology to address it.
- critically review scientific literature and identify research gaps to frame project objectives.
- demonstrate competence in performing experiments, simulations, or theoretical analysis relevant to the project.
- interpret and analyze results with proper scientific reasoning, supported by evidence.
- develop independent research ability, teamwork skills, time management, and problem-solving aptitude required for advanced research or professional careers.

Course Contents:

The "*Lab Project in Chemistry*" course is designed to provide students with an immersive experience in conducting research, developing practical skills, and apply theoretical knowledge in a laboratory environment. The course emphasizes independent thinking, problem-solving, and scientific reasoning, preparing students for higher research or professional careers in chemistry. The following are the core components:

Identification and Formulation of Research Problem: Students begin by identifying and formulating a suitable research problem in chemistry. This involves selecting a topic under the supervision of a faculty member of their choice that is relevant, feasible, and scientifically significant. They define clear objectives and hypotheses and design a detailed methodology to address the research problem. This stage develops the ability to plan experiments, simulations, or theoretical analyses systematically, ensuring that the research approach is both logical and practical.

Literature Survey and Critical Review: A critical component of the course is the literature survey and review. Students conduct an extensive study of existing research related to their chosen problem, critically evaluating published data and methodologies. Through this process, they identify research gaps, justify the need for their project, and contextualize their objectives within the broader scientific framework. This exercise enhances their analytical skills and strengthens the foundation of their project work.

Experimental or Computational Work: The experimental or computational work forms the core of the course. Students execute their designed methodology in the laboratory or through simulations, applying appropriate techniques, instrumentation, and computational tools with precision and safety. They systematically collect, record, and organize data according to scientific protocols. This hands-on experience develops technical competence, attention to detail, and familiarity with standard laboratory practices and equipment.

Data Analysis and Interpretation: Data analysis and interpretation are crucial aspects of the lab project. Students analyze experimental or simulation results using appropriate statistical or analytical methods, correlating observations with chemical principles and theoretical expectations. They critically evaluate the reliability of their data, discuss deviations, and provide scientifically sound reasoning to support their conclusions. This phase strengthens their ability to think logically and draw evidence-based inferences.

Professional and Research Skill Development: Finally, the course fosters professional and research skills essential for scientific careers. Students develop independent research abilities, effective problem-solving strategies, and collaborative teamwork skills. Emphasis is placed on efficient time management, ethical conduct in the laboratory, proper handling of chemicals, data integrity, and adherence to safety protocols. Together, these experiences prepare students not only to complete their lab project successfully but also to function confidently in research and professional environments.

Course No: CH24406DCE
Title: Inorganic Materials (02 Credits)

Max. Marks: 50 **Duration: 32 Contact hours**

Continuous Assessment: 10 marks **End Term Exam: 40 Marks**

Course outcomes: After studying this course, the students will be able to have:

- an insight into structures of solid state inorganic materials like metal oxides, metal Hydroxides, MXenes, Pervoskites, MOFS, & Zeolites
- conceptual understanding of structure- property relationship in functional inorganic materials by correlating structure with properties.
- knowledge of standard synthesis methods of Inorganic Nanomaterials.
- theoretical knowledge of Techniques & Methods for characterization & Analysis of Inorganic materials at Nano Level.
- understanding how atomic arrangement & chemistry of inorganic material can give rise to functional properties and potential applications.

Unit-I Transition Metal Based Functional Materials (16 Contact hours)

History, development and importance of functional inorganic materials. Transition metal based materials: Synthetic routes, structure and applications of Metal oxides, Metal hydroxides, MXenes and Pervosikites. MXenes - Li and Na ion batteries, Super capacitors and Optoelectronic devices. Pervosikites - Solar cell applications. Zeolite Molecular Sieves: Structure, Chemistry, and applications. Metal Organic Frameworks (MOFs): Synthetic routes, structure and applications of Metal Organic Frameworks (MOFs): Characterization methods, Isoreticular series. Application in gas storage and separation. MOF thin films for separation and catalysis. Medical applications of MOFs.

Unit-II Inorganic Nano Materials (16 contact hours)

Definition, development and importance of Nano materials. Metal and metal-oxide Nanoparticles: Synthetic routes: Chemical methods: reduction, Solvothermal/hydrothermal route, electrospining. Micro-emulsion method, combustion method, microwave synthesis, gas phase method, and conventional Sol-Gel method. Structure and properties. Band structure, Band gaps, Quantum Dots. Nanosize effects. Quantum confinement effect, Size dependent physical phenomenon in nano materials. Optical and mechanical properties of nano materials. Electrical properties, electron transfer and charge transport .
Analysis methods (elementary idea): Powder X-ray diffraction, Electron Microscopy (SEM and TEM), Scanning probe microscopy (AFM, STM) Applications in the fields of solar cells, light-emitting diodes, transistors, optoelectronic packaging, photo-catalysis, sensors and coatings.

Books Recommended

1. G. Cao, Nanostructures and Nanomaterials: Synthesis, properties and applications, Imperial College Press, 2004.
2. C. N. R. Rao, A. Muller, A. K. Cheetham, The chemistry of nanomaterials: Synthesis, properties and applications, Wiley (2004).
3. Hornyak, Dutta, Tibbals and Rao, Introduction to Nanoscience and Nanotechnology, New York, CRC press, 2008
4. J. Goldstein, D. E. Newbury, D.C. Joy, and C.E. Lym, “Scanning Electron Microscopy and X-ray Microanalysis”, 2003.

5. D. Williams and B. Carter, "Transmission Electron Microscopy - A Textbook for Materials Science", Plenum Press, New York, 2nd Edition, 2009
6. AR West, Solid State chemistry and its applications, John Wiley & Sons, Ltd. 2nd Edition, 2014.
7. Y. Leng, Materials Characterization-Introduction to microscopic and spectroscopic methods. Second Edn. Wiley-VCH

Course No: CH24407DCE
Title: Supramolecular chemistry & Crystal Engineering (02 Credits)

Max. Marks: 50 | **Duration: 32 Contact hours**
Continuous Assessment: 10 marks | **End Term Exam: 40 Marks**

Course outcomes: After learning the contents of this course, the students shall have:
- understanding the nature and role of intermolecular interactions, responsible for aggregation their influence on material properties and applications.
- understanding of the structure-property relationships.
- understand design, working and fabrication of applied materials.

Unit-I Supramolecular Chemistry (16 Contact hours)

Definition and Development of Supramolecular Chemistry. Crystal Engineering.
Non-Covalent Interactions: Types and Significance. Hydrogen bond - Definition and classification. Etters' rules and Graph set analyses. Supramolecular synthon concept.
π-π Interactions: Nature and types, Charge transfer (CT) interactions, Arene-perfluoro arene (AP) interactions. Role of π-interactions in biological systems and processes - stability and expression by nucleic acids and proteins. π-Aggregates - H and J type, and their importance in designing of optoelectronic materials.
Halogen bonding: Definition and classification. Comparison with hydrogen bonding, Special features of halogen-boded materials.
Polymorphism, co-crystals and molecular salts. Definition, synthesis, and significance. Applications in Pharmaceutics (pharmaceutical polymorphs and co-crystals) and optics (engineering of luminescent crystals and co-crystals, structure-property correlations)

Unit-II Crystal Design, Growth, Characterization and Applications (16 Contact hours)

Growth and design. Different methods of crystal growth. Correlation between molecular and crystal properties, Tuning of crystal properties through crystallochromism (change in functional group), polymorphism (change in crystal packing), and co-crystallization (change in co-former).
Supramolecular Optical Materials: Aggregation-induced Emission (AIE), Opportunities and Challenges in Solid-State Luminescent Materials. Crystal engineering of organic fluorescent, phosphorescent, and thermally activated delayed fluorescent (TADF) organic materials. TADF materials - Design and applications. Electroluminescence and electroluminescent materials (elementary idea). Multicolor emitters (Hetero-structures and epitaxial growth) and Light-emitting diodes (LEDs/OLEDs).

Books Recommended

1. Supramolecular Chemistry. Jonathan W. Steed and Jerry L. Atwood. Wiley 2nd Edn.
2. Supramolecular Chemistry-Fundamentals and Applications. A. Katsuhiko and K. Toyoki. Springer.
3. Crystal Engineering. G. R. Desiraju, J. J. Vittal and A. Ramanan. World Scientific, IstEdn.
4. Organic Crystal Engineering: Frontiers in Crystal Engineering. E. R. T. Tiekink, J. Vittal and M. Zaworotko. Wiley, 2010.
5. Frontiers in Crystal Engineering. Edward R. T. Tiekink (Editor), JagadeseVittal (Editor). Wiley, 2005.

6. An Introduction to Supramolecular Chemistry. Asim K. Das, Mahua Das, CBS Publishers and Distributors Pvt Ltd. 2005.
7. Introduction: Supramolecular Chemistry. Huang,F.; Anslyn. E. V.Chem. Rev.2015, 115, 6999- 77000.
8. Supramolecular materials. Amabilino, D. B.; Smith, D. K.; Steed. J. W. Chem. Soc. Rev., 2017, 46, 2404-2420.
9. A Bond by Other Name. Desiraju. G. R. Angew. Chem.Int.Ed.2011, 50, 52-59.
10. The Weak Hydrogen Bond: In Structural Chemistry and Biology. Desiraju, G.; Steiner. T.Oxford, IUCr Monograph on Crystallography.
11. Application of the Principle of Hard and Soft Acids and Bases to Organic Chemistry. Pearson, R. G.; Songstad, J. J. Am. Chem. Soc. 1967, 89,1827-1836.
12. Photoluminescent organic crystals and co-crystals, Dar, A. A. and Malik, A. A Journal of Materials Chemistry C, 2024, 12 (27), 9888-9913

Course No: CH24408DCE
Title: Medicinal Chemistry (02 Credits)

Max. Marks: 50 **Duration: 32 Contact hours**

Continuous Assessment: 10 marks **End Term Exam: 40 Marks**

Course outcomes: After learning the contents of this course, the students would be able to:

- understand types of drugs and drug discovery process
- corelate structure with biological activity and quantitative analysis of structure activity relationships of drug molecules
- comprehend the mechanism of the function of drugs used as, antibiotic, psychoactive, cardiovascular and antiviral medicines.

Unit-I Medicinal Chemistry-I (16 contact hours)

Introduction to Drug Design: Classification and sources of drugs, concept of lead compounds and lead modification. Analogues, prodrugs, factors governing drug design.
Structure activity relationship (SAR): Isosterism, bioisosterism, changing the size and shape, changing the number of methylene groups in chain, changing the degree of unsaturation. Effect of introduction of methyl groups, halogens, hydroxyl, carbonylic, thiols, sulphides groups and introdction/removal of ring systems on pharmacological activity.
Quantitative structure activity relationships (QSAR): Theories of drug activity, Clark's occupancy theory, the rate theory, two state theory. Lipophillic constant, Hamett constant, steric parameters and Hansch analysis.

Unit-II Medicinal Chemistry-II (16 Contact hours)

Antibiotics: Pencillins-classification and structures. Synthesis of Pencillins, V, G, ciprofloxacin, Antibiotic resistance.

Psychoactive Drugs: Introduction, CNS depressants, CNS stimulants, sedatives and hypnotics, barbiturates.

Cardiovascular Drugs: Introduction, cardiovascular diseases, synthesis of Amyl-nitrate, verapamil and methyl dopa

***Anti-neoplastic drug**:* Introduction; cancer chemotherapy, carceneolytic antibiotic, plant derived anti-cancer agents (Taxol) role of alkylating agents and antimetabolites in treatment of cancer, mitotic inhibitors (elementary idea).

Antiviral Drugs: Examples and Mode of action

Antidiabetic Drugs: Examples and Mode of action

Books Recommended

1. Introduction to Medicinal Chemistry, Alex Gringauz (Wiley- VCH-1997).
2. Medicinal Chemistry- An Introduction, Gareth Thomas (Wiley-2000). 3rd Edition.
3. Medicinal Chemistry, Ashutosh Kar. (Wiley Eastern-1993).
4. Biochemistry, Biotechonolgy and Clinical Chemistry of Enzmyes. Trevor Palmer (EWP)
5. Organic Chemistry by I. L. Finar Vol. II (ELBSLongamnn)
6. Lehninger's Principles of Bio-chemistry, D.L. Nelson. M.Cox Worth publications,2000.
7. Introduction to nucleic acids and related natural products Ulbight (OldbornPress)
8. Chemistry of Natural Products. S.V. Bhat, B.A. Nagasampagi, M. Siva Kumar. Naroosa.

Course No: CH24409DCE
Title: Chemistry of Natural Products (02 Credits)

Max. Marks: 50 | **Duration: 32 Contact hours**
Continuous Assessment: 10 marks | **End Term Exam: 40 Marks**

Course outcomes: On completion of the course, the students will be able to:

- understand the role and importance of natural products in medicine and drug discovery.
- recognize the chemistry and spectroscopic methods involved in structure determination and synthesis of different classes of natural products viz terpenoids, steroids, alkaloids an flavonoids.

UNIT-I: Terpenoids and Steroids. (16 contact hours)

Terpenoids: Introduction, classification. Chemistry of Geraniol, α-Terpeniol, Camphor, Zingiberene and Vitamin A. Biosynthesis of terpenoids.

Steroids: Introduction and classification. Chemistry of cholesterol, Progesterone, Oestrone, Androsterone, Testosterone and Cortisone. Biosynthesis of cholesterol.

Unit-II: Alkaloids and Flavonoids (16 contact hours)

Alkaloids: Introduction, Qualitative tests and General methods of isolation. Structural Elucidation and synthesis of Reserpine and Morphine.

Flavonoids: Introduction, Qualitative tests, Classification and Structure elucidation. Synthesis of Apigenin, Quercetin, Genistein and Anthocyanidin. Medicinal applications of Flavonoids.

Books Recommended

1. Chemistry of Natural Products; S. V. Bhat, B. A. Nagasampagin. (Narosa 2005).
2. Organic Chemistry, 5th Ed. Vol.2,1. L. Finar (Addison Wisley Longman-2000).
3. Chemistry of Natural Products, N.R. Krishnaswamy (University Press-1999).
4. Flavonoids; Oyvind M. Andersen and Kenneth R. Markhan. (Taylor & Francis -2006)
5. The Flavonoids, Jeffrey B. Harborne, Tom J. Mabry, Helga Mabry, Academic Press 1975

Course No: CH24410DCE
Title: Computational and Advanced Quantum Chemistry (02 Credits)

Max. Marks: 50 **Duration: 32 Contact hours**

Continuous Assessment: 10 marks **End Term Exam: 40 Marks**

Course outcomes: On completion of the course, the students will be able to:

- appreciate the potential of numerical methods to solve the complex mathematical equations like simultaneous equations, integrals, differentials, determinants, eigen value problems etc.
- have in depth understanding of use of MS Excel as easily available tool to solve above equations numerically.
- get knowhow of the Hartree Fock and Density functional theories to evaluate the energy and other properties of multielectron systems using slater and gaussian wave functions.
- get acclimatized with the gaussian software for running HF or DTF methods for evaluating energy, getting optimized geometry, predict NMR, UV-Vis frequency etc.

UNIT-I: Numerical Methods (16 contact hours)

Basic theory, discussion of algorithms and errors for following numerical methods:

Solution of Equations: Bisection, Newton-Raphson method for solving polynomial and transcendental equations. Convergence. Errors and ill-conditioning

Linear Simultaneous equations: Gaussian elimination and Gauss-Siedel method. Errors and ill-conditioning.

Numerical differentiation: Solutions of simple differential equations by Taylor series and Runga-Kutta methods.

Numerical integration: Newton-Cotes formulae, Romberg integration, errors in integration formulae.

Interpolation and Curve Fitting: Lagrange's interpolation method, Newton's divided differences, Cubic spline, piece wise interpolation. Least squares approximation, linear and quadratic.

Unit-II: Advanced Quantum Chemistry (16 contact hours)

Hatree-Fock Self Consistent field method: Hartree-Fock method: Coulomb and exchange operators and integrals, Roothaan equations: the Fock matrix elements, Koopman's theorem. Self-Consistent Field procedure. Slater-type orbitals (STOs), Gaussian type orbitals (GTOs), Basis Sets: minimal basis set, split-valence basis set, Polarization basis sets. Model SCF calculations on H_2 /HeH^+.

***Beyond Hatree-Fock method*:** Electron correlation: configuration state functions, configuration interaction (CI) and its calculations.

Density Functional Theory (DFT): Introduction, electron probability density, Hohenberg-Kohn theorems and Kohn-Sham formulation of DFT.

Use of Gaussian quantum mechanical package for:

1. A single point energy calculation: HCHO /CH_3CHO, HCHO MOs.
2. Geometry Optimization: Input and Output for ethene, fluoroethene, propene conformers. Basis set effect on geometrical parameters on these molecules.
3. NMR properties of ethane, ethene and ethyne.
4. Frequency Calculations: Input, Formaldehyde frequencies, Normal modes, zero point energy, thermodynamic properties, polarizability, hyperpolarazability.

5. Selecting an appropriate theoretical method:
   a) Electron correlation and post SCF methods, limitations of Hartree-Fock theory: HF bond energy, Optimization of O_3.
   b) Density Functional Theory: CO_2 structure and atomization energy.

Books Recommended

1. Data Reduction & Error Analysis, Bevington& Robinson, (McGraw-Hill, 2003)
2. Numerical Methods for Scientists and Engineers, H. M. Antie, (TMH,).
3. Mathematical Methods for Scientists and Engineers, D.A. McQuarie, Viva Books, 1st Ed., 2009.
4. Quantum Chemistry, Ira. N. Levine, (Prentice Hall, 2009).
5. Molecular Quantum Mechanics, P. W. Atkins and R. S. Friedmann, (Oxford, 2008).
6. Quantum Chemistry and spectroscopy, Engel & Reid, Pearson (2007)
7. Modern Quantum Chemistry - Introduction to Advanced electronic structure theory - A. Szabo & N. S. Ostlund, (Macmillan, 1982, Dover 1996).
8. GAUSSIAN Manual, Gaussian Inc
9. Exploring chemistry with electronic structure methods, Foresman J.B., Frisch A., Gaussian Inc.

Course No: CH24411DCE
Title: Applied Electrochemistry (02 Credits)

Max. Marks: 50 | **Duration: 32 Contact hours**
Continuous Assessment: 10 marks | **End Term Exam: 40 Marks**

Course outcomes: On completion of the course, the students shall:

- appreciate the potential utility of electrochemical methods for sensing and detoxification of pollutants, solar energy harvesting, energy generation and storage
- learn about the basic principles, design and applications of photoelectrochemical cells.
- learn about how to use electrochemical methods for detoxification of pollutants especially water contaminants
- learn about the basics of fuel cells and batteries, the design, operation and challenges associated with the different types of such systems in energy applications.

UNIT-I: Photo- and Environmental Electrochemistry (16 contact hours)

Photo-electrochemistry: Semiconductor electrodes, Band bending across Semiconductor/electrolyte solution interface, photo-electrochemistry across semiconductor/electrolyte interfaces, p-type photocathode, n-type-photoanode, surface effects in photo-electrochemistry, Photogalvanic and Photovoltaic Cells, The Efficiency of Solar Energy Conversion in Photoelectrochemical Cells, Liquid-Junction Solar Cells: Principles of Operation and Energetics of Conversion.

Photoelectrochemical splitting of water, Photoelectrochemical reduction of CO_2, Production of solar fuels.

Environmental Electrochemistry: Positive Features of Electrochemical Remediation. Direct Electrolysis of Pollutants. Indirect Electrolysis of Pollutants. Electroremediation of Soils.

Water Disinfection: Background and Principles. Electrochemical Disinfection of Water, electrodialysis, Photoelectrochemical Disinfection of Air and Water.

Unit-II: Electrochemistry for Energy Conversion and Energy Storage (16 contact hours)

Fuel Cell: Basic principles, advantages and limitations, fuel cell performance.

Fuel Cell Thermodynamics: Open circuit voltage, efficiency and efficiency limits, efficiency and fuel cell voltage. Operational fuel cell voltage; fuel cell irreversiblities, causes of voltage drop.

Types of fuel Cells: Alkaline, Phosphoric acid, Polymer Electrolyte membrane and direct MeOH fuel cell, biofuel cells.

Energy storage devices: Desirable characteristics of energy storage devices, Discharge plot, Ragone plot.

Batteries: How batteries work, Battery characteristics, Battery specification, Battery components. Primary and secondary batteries, Measures of battery performance. Classical batteries (Lead Acid, Nickel-Cadmium, Zinc-Mangenese dioxide). Modern batteries (ZincAir, Nickel- Metal Hydride, Lithium Ion Batteries).

Books Recommended

1. Electrochemical Methods Fundamentals and Applications, 2nd Edition, Allen J. Bard, Larry R. Faulkner, John Wiley and Sons, INC.
2. Physical Electrochemistry: Fundamentals, Techniques, and Applications, 2nd Edition, Eliezer Gileadi and Noam Eliaz, 2018, Wiley-VCH.
3. Electrochemistry, 2nd Edition, Carl H. Hamann, Andrew Hammett, Wolf Vielstich, WileyVCH.
4. Modern Electrochemistry 2B, 2nd Edition, J. O`M. Bockris and A. K. Reddy, Kluwer Academic/Plenum Publishers, New York.
5. Fuel Cell Fundamentals, 3rd Edition, Ryan O'Hayre, Suk-Won Cha, Whitney Colella, Fritz B. Prinz, John Wiley & Sons.
6. Understanding Batteries, Ronald Dell, David Anthony James Rand,Royal Society of Chemistry, 2001.
7. Industrial Electrochemistry, 2nd Edition, D. Pletcher, F. C. Walsh, London, GB. Chapman & Hall.
8. Environmental Electrochemistry, 1st Edition, Krishnan Rajeshwar, Jorge Ibanez, Academic Press, 1997.

CH24004GE
Title: Synthetic Polymers and their Applications (02 Credits)

Max. Marks: 50 | **Duration: 32 Contact hours**
Continuous Assessment: 10 marks | **End Term Exam: 40 Marks**

Course outcomes: On completion of the course, the students shall acquire knowledge of:
- Basic concepts about polymers.
- Different types of mechanism involved in polymerization processes.
- Chemistry of commercially important polymers.
- Chemistry of natural rubber and polysaccharides.

UNIT-I: (16 contact hours)

Introduction, Definition, Classification based on source, Structure, Synthesis and Forces of attraction. Thermosetting and Thermosensitive plastics, Types of Monomers,Homopolymers and Copolymers.
Polymerisation processes, Addition polymerization, Free radical, Cationic, Anionic mechanism of addition polymerization Initiators, Inhibitors and Propagators. Stereochemical control of polymerization- Zeiglar Natta catalysts, Poly condensation; Polymerisation.

Unit-II: (16 contact hours)

Commercially important polymers: Polyesters, Polycarbonates, Polyamides, Polyurethanes, Poly sulphides, Resins: Phenol-formaldehyde and Melamine-formaldehyde resins. Conducting Organic Polymer (elementary idea), Biodegradable polymers
Natural polymers: Rubber, Vulcanization, Polysaccharides: Cellulose, Amylopectin and Starch, Proteins: Wool, Silk and Collagen; Regenerated properties.

Books Recommended

1. Organic chemists: Francis . A. Carey, Robert M. Giuliano. 8th ed. Tata Mc Graw Hill. 2010.
2. Polymer chemistry- An introduction. Mallolin. P. Steven, 2nd ed. Oxford University. 1998.
3. Organic chemistry: L. G. Wade, Tr. Maya Shankar Singh. 6th ed., 2005, Pearson.
4. Introduction to polymers: 2nd ed. R.J. Young and P.A. Lovell. Chapman and Hill.
5. Organic chemistry: David Klein; Willey 2012 .

CH24004OE
Title: Food Chemistry (02 Credits)

Max. Marks: 50 **Duration: 32 Contact hours**
Continuous Assessment: 10 marks **End Term Exam: 40 Marks**

Course outcomes: On completion of the course, the students will be able to:
- explain the composition, structure, and functions of major food components, including sugars, lipids, proteins, vitamins, and minerals.
- identify natural and artificial food colorants and flavors and describe the chemical basis of taste and aroma.
- understand food preservation methods, additives, and potential toxins to ensure food safety and quality.

UNIT-I: **(16 contact hours)**

Food Components: Chemistry of different components of food: Composition and functions of Sugars, Polysaccharides, Lipids, Proteins, Vitamins and Minerals.
The Chemistry of Food Colours and flavours : Introduction. Pigments in animal and plant tissues: Chlorophyll, Carotenoids, Anthocyanins and other Phenols. Natural and artificial food colorants. Definition of flavor. Classification of food flavors. Chemical components responsible for the following: Sweetness, Saltiness, Sourness, Bitterness, Astringency, Pungency, Meatiness and Fruitiness. Synthetic flavouring.

Unit-II: **(16 contact hours)**

The Chemistry of Food Preservatives: Introduction. Basis of Food Preservation. Food additives: Sodium Chloride, Nitrites, Smoke, SO2, Benzoates and other Organic acids.
The Undesirables in Food Stuff : Autooxidation and antioxidants. Modified atmosphere and vacuum packaging. Toxins of plant foods. Toxins of animal foods. Toxic agriculture residue Toxic metal residue. Toxins generated during heating and packaging of food. Environmental pollutants of food stuff.

Books Recommended

1. Food Chemistry; Owen R. Fennema; 3rd Ed.; Marcel Dekker, Inc. NY; 2005.
2. Food: The Chemistry of its components; T.P. Coultate; 3rd Ed.; RSC Paperbacks; 1996.
3. Food Flavours; Biology and Chemistry; Carolyn Fisher and Thomas R Scott; RSC Paperbacks; 1997.
4. Food Preservatives; H.J. Russell and G. W. Gould; 2nd ed.; Springer International Edition; 2005.