Course No: CH21401CR
Title: Advanced Inorganic Chemistry (04 Credits)

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

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

- 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
- Understand how atomic arrangement & chemistry of inorganic material can give rise to functional properties and potential applications.

Unit-I OrganoTransition 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.

Compounds with Transition Metal to Carbon multiple bonds: Alkylidene (Schrock and Fischer) Synthesis; Structural characteristics; Nature of bonding. Reactions and their synthetic applications: Dotzreaction and Schrock's Catalyst.

Unit-II Physico Chemical behaviour of OrganoTransition metal Compounds:
(16 Contact hours)

A. Fluxional Organometallic Compounds:

Characteristics; Rates of rearrangement and Techniques of study. NMR study of Fluxional behavior, Classification of Fluxional Organometallic Compounds. Mechanism of Fluxionality in compounds of η^1 Cyclopentadienyls and η^3–allyls. Stereochemical non rigidity in case of coordination numbers- 4 & 5 (cis-trans, atomic inversion, Berry Pseudorotation).

B. 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. Asymmeteric, Photo redox catalysis and supported Organometallic Catalysis (brief idea)

C. Synthetic Reactions involving Organometallics:

Reactions of coordinated ligands, carbon monoxide and alkenes (Green, Mingo's rules).

Role of organo-iron compounds as synthons, Activation of small molecules: prospectus and challenges. Selected reactivities for activation of Carbon monoxide, Carbon dioxide and Alkanes. Carbon-Carbon coupling reactions (Suzuki and Heck).

Unit-III Inorganic Photochemistry; the basics (16 Contact hours)

A. Excited states: Excitation: d-d transition, charge transfer & intra-ligand transitions and selection rules. Excited states; term symbols, splitting of terms in ligand field, Orgel diagram; electrostatic description of spin allowed d-d transitions & energy level diagrams depicting excited states.

Fate of excited states; energy dissipation by radiative and non-radiative processes. Jablonoski diagram.

Molar integrated absorption intensity, natural radiative lifetime & the calculation of life times.

B. Kinetics: Photochemical laws & quantum yield. Kinetics & quantum yield of photo-physical (radiative) and photo-chemical processes. Quantum Yields of a unimolecular and bimolecular photo-chemical reaction; Quenching and Stern-Volmer plots.

C. Tools and Technique: Chemical Actinometry. Time Resolved Spectroscopies: Time correlated Single photon counting technique Time Resolved Transient Absorption Spectroscopies: Flash Photolysis

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

A. 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

B. 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; 2nd and 4thedn; Robert. H . Crabtree; Wiley; 1994, 2004.
2. Fundamental Transition Metal Organometallic Chemistry; Luke hart; Brooks / Cole;1985.
3. Organometallic Chemistry; 2nd edn ; Mehrotra & Singh ; New age international2000
4. Principles and Applications of Organo Transition Metal Chemistry; Collman&
5. Finke; University Science Books;1994.
6. Principles of Organometallic Chemistry; 2nd edn.; P.Powel; Chapman & Hall;1998.
7. Metallo-Organic Chemistry; A.J.Pearson;Wiley.
8. Mechanisms of Inorganic and Organo metallic reactions; Twigg; Plenum press1983.
9. Reaction Mechanism of Inorganic and Organometallic systems; 2nd edn.; Robert .b. Jordan1998.
10. Inorganic Chemistry ; 4th edn.; Huheey ; E. Keiter& R. Keiter; Addison-Wesley;1983
11. Modern Inorganic Chemistry; William. A. Jolly; McGraw Hill;1985.
12. Inorganic Chemistry; 4* edn; Huheey; Harper & Row; 1990.
13. Chemistry of Light; Suppan, Royal Society; 1994.
14. Photochemistry, Carol J. Wayne and Richard P. Wayne; Oxford University Press; 1996.
15. Fundamentals of Photochemistry; C Rohatgi, Mukhergi; Wiley Eastern.; 1992
16. Inorganic Photochemistry; J.ChemEdu.;Vol .60, No.10,1983.
17. Applications of Inorganic Photochemistry; J. Chem. Edu.; Vol.74, No 69. 1997.
18. Principles and applications of Photochemistry, Brian,Wardle, Wiley 2009

Course No: CH21402CR
Title: Advanced Organic Chemistry (4 Credits)

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

Course Outcome: On completion of the course the student should be able to:

- Understandvarious 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.

Unit I Methods in Organic Synthesis (16 Contact hours)

AsymmetricSynthesis: Nature & asymmetry, Chiral pool approach, Chiral auxiliaries and auxillary controlled stereoselection. Chiral reagents. Asymmetric formation of C-C bonds.: Asymmetric aldol, Heck and Baylis-Hillman reactions. Asymmetric hydrogenation and epoxidation of alkenes (Sharpless, Jacobsen and Shi reactions).

Stereoselectivity: Stereochemical control in six-membered rings, Stereoselectivity in bicyclic compounds.

Diastereoselectivity: Addition to carbonyl groups and stereoselective reactions of acyclic alkenes. Stereochemical reactions near a stereocenter.

Racemization & Resolution of enantiomers using chiral molecules.

Chemoselectivity: Selectivity in oxidation and reduction. Competing reactivity.

Methods of multiple bond formations: Carbon-Carbon and carbon heteroatom (N and O) bond formations with special emphasis on Metal catalysed bond formations (Ullmann, Buchwald-Hartwig, Sonogashira, Heck, Suzuki and Stille reactions).

Unit II Reagents in Organic Syntheses (16 Contact hours)

Nature and applications of following reagents in organic syntheses: DABCO, DBU, DDO, Diglyme, DMAP, MCPBA, NCS, PCC, PDC, TBHP, TBAF, Lead Tetraacetate, Osmium Tetroxide, Aluminum isopropoxide, Prevost reagent, Woodward's Reagent, $PdBaSO_4$, DDQ, DCC, SeO_2, $Tl(NO_3)_3$, $NaBH_4$, DIBAL, LAH, diisoamyborane, thexylborane, 9-BBN, $NaIO_4$,Ceric ammonium nitrite, Palladium(II)hydrotalcite, TEMPO, Ceric Ammonium nitrate(CAN), Fatezens reagent,MnO_2. Na/EtOH and Na/liq.NH_3.

UNIT-III PROTECTION AND INTERCONVERSION OF FUNCTIONAL GROUPS (16 Contact hours)

Protection of functional groups: Principle of protection of functional groups and its significance. Protection of carbon-hydrogen bonds (in terminal alkynes and Carbon-hydrogen bond of aldehydes), carbon-carbon double bonds, alcoholic and Phenolic hydroxyl groups, amino groups, carbonyl and carboxyl groups.

Functional Group Interconversion (FGI) / Transformations: Significance of Functional Group Interconversion (FGI) / Transformations in Organic synthesis. Methods of transformation of different functional groups into one another. Chemoselectivity.

Unit-IV Designing Organic Synthesis (16 Contact hours)

The disconnection approach: Introduction to synthons, their types and equivalent reagents. Reversal of Polarity(umpolung). One group, two group and Reteroelectrocyclic disconnections. Reterosynthetic Analysis involving connections and rearrangements. Guidelines for good disconnections.

One group disconnections: Reterosynthetic analysis of alcohols, amines (aliphatic and aromatic), alkenes, carbonyl compounds, carboxylic acids and their derivatives using one group disconnections and FGIs. Use of acetylenes in the syntheses of above mentioned compounds.

Two group disconnections: Reterosynthetic analysis of 1, 2- difunctional compounds (1,2 – diols), 1,3- difunctional compounds (1,3-dioxygenated compounds, α, β-unsaturated carbonyl compounds, 3-amino alcohols and 3- amino ketones), 1,4- and 1,5-difunctional compounds.

Multistep Synthesis: Application of reterosynthetic analysis in designing /achieving syntheses of some complex molecules (for example Brufen, benziodarone, Juvabione, warfarin and brevicomin(Examples other than these may also be included).

Books Recommended

1. Designing Organic Synthesis, S. Warren; Wiley; 2013.
2. Organic Synthesis- concept, methods and Starting Materials, J. Furhop and G. Penzlin;
1. Verlage VCH;1986.
2. Principles of Organic Synthesis2nd edn;. R. O. C. Norman; Chapman and Hall; 1978.
3. Advanced Organic Chemistry Part B, 5th edn.; F. A. Carey and R.J Sundberg ; Springer;
4. 2007.
5. Organic Chemistry, 10th edn;. T. W. G. Solomons and Craig B. Fryhle ; Wiley-2012.
6. Organic Chemistry; Clayden, Greeves, Warren and Wothers ; Oxford University Press-2012.
7. Organic Chemistry, David Klein; John-Wiley-2012.
8. Advanced Organic Chemistry: Reactions, Mechanism and Structure, 6lh Ed., J. March,; Wiley; 2012.
9. Organic Synthesis- The disconnection Approach; Sturat Warren; Wiley; 2013.
10. Reagent Guide, Synthetic Organic Chemistry, & Materials Chemistry, 8th Edition.
11. Modern Methods of Organic Synthesis, Carruthers W. William Caruther and Iain Coldham, 4th edition.
12. A Guide to Reagents in Organic Synthesis., S Gupta, V Gupta, R.S Dhundal, 1st edition 2015
13. Transition Metal Reagents and Catalysts: Innovations in Organic Synthesis, by Jiro Tsuji, published: 17 July 2002.
14. Organic Synthesis, Jagdamba Singh, L.D.S Yadav, 1st Edition, 2006

Course No: CH21403CR
Title: Advanced Physical Chemistry (04 Credits)

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

Course Outcome: 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 co-polymers 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, 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.
Catalysis of Industrial processes: Mechanistic and kinetic aspects of some selected industrial process; Synthesis of methanol, Fischer-Tropsch process, Synthesis of ammonia, Oxidation of ammonia, Photocatalytic breakdown of water. Catalysis and petroleum industry**;** catalytic reforming, catalytic cracking, cracking reactions and cracking catalysts.
Industrial Bio-catalysis: High-Fructose Corn Syrup, The Mitsubishi Rayon Acrylamide Process, The BMS Paclitaxel Process, The Tosoh/DSM Aspartame Process.
An introduction to catalysis in Energy-Related Environmental Technology.

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, thermoreversible, 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. Rheological properties of hydrogels (steady-state, oscillatory and thixotropic behavior). Characterization of hydrogels. 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, thermography, optical imaging and ferroelectric liquid crystals.

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: CH21404CR
Title: Project Seminar and Dissertation (02 Credits)

Max. Marks:50

Course Outcome: On completion of the lab project the students will be required to prepare a dissertation based on their lab project work. The students will also be required to deliver a PowerPoint presentation for evaluation.

Course No: CH21405DCE
Title: Lab Project in Chemistry (04 Credits)

Max. Marks:100 **Duration:** 3 lab session of one hour each per day

Course Outcome: On completion of the lab project the student should be able to:

- Design and setup various kinds of organic reactions in the laboratory.
- Monitor and analyze the progress of the reaction, and take appropriate measures to ensure its successful completion.
- Use catalysts, reagents and substrates keeping in mind the green chemistry practices.
- Separate the mixture of compounds by column chromatography and their analyses.
- Understand and develop the skills for extraction of compounds from plants and evaluation of their biological profile.

Course No: CH21406DCE
Title: Inorganic Materials (02 Credits)

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

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

- 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
- Understand 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.

Synthetic routes, structure and applications of 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: synthesis by Chemical methods: reduction, Solvothermal/hydrothermal route, electrospining. Micro-emulsion method, templating 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/ Research Papers 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. Solid State chemistry, AR West
7. Y. Leng, Materials Characterization-Introduction to microscopic and spectroscopic methods. Second Edn. Wiley-VCH

Course No: CH21407DCE
Title: Supramolecular Chemistry (02 Credits)

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

Course Outcome: The course focus on understanding the nature of intermolecular interactions, responsible for aggregation and consequent material properties and applications. Chemistry behind working and fabrication of molecular devices and sensors is dealt with to provide students an apprehension to understand design, working and fabrication of applied materials.

Unit-I Supramolecular Chemistry (16 Contact hours)

A. Acid-Base Theories-

Overview of Acid-Base theories. Hard Soft Acid Base (HSAB) Concept– Introduction, Classification, Symbiosis, PearsonPauling Paradox.

Utility of HSAB Concept in Drug Design, Quantitative Analyses of Metal Cations and Prediction of Direction of Inorganic Reactions.

B. Supramolecular Chemistry

Definition and Development of Supramolecular Chemistry. History and Genesis of the Nobel Prizes Awarded in the Area. Types and Nature of Supramolecular/Non-Covalent Interactions: Hydrogen Bonding, π-π Interactions, Halogen Bonding, van der Waal Interactions. Quantification of non-covalent interactions through computational method: Electrostatic Potential Maps, de-di and fingerprint Plots.

Unit –II Crystal Engineering (16 Contact hours)

Definition and Development of Crystal Engineering.

Hydrogen bonding: Definition, Nature and Importance. Classification of Hydrogen Interactions.

Identification of Weak, Moderate and Strong Hydrogen Bonds.

Crystal Engineering of organic molecules: Co-crystals and Molecular Salts. Pharmaceutical Co-crystals. Polymorphism. Crystal Engineering of inorganic molecules: Coordination Complexes and Metal Organic Frameworks (MOFs)

Transformation of Molecules into Devices

Supramolecular Sensors and Devices-Thermochromism, Solvatochromism and Photophysics. Charge Transfer Complexes. Theory of π-π Stacking. Degree of Charge Transfer. Organic Conductors and Semiconductors. Organic Light Emitting Diodes (OLEDs) and Transistors. Organic Lasers (Elementary Idea)

Books/Research Articles 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.

Course No: CH21408DCE
Title: Medicinal Chemistry (02 Credits)

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

Course Outcome: On completion of the course the student should be able to:

- Understand types of drugs and drug discovery process.
- Corelate structure with biological activity and quantitative analysis of structure activity relationshipsof drug molecules.
- Comprehend the mechanism of the function of drugs used as antipyretic, analgesic, antibiotic, psychoactive, cardiovascular and antiviral medicines.

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

Drug Design: Classification and sources of drugs, concept of lead compounds and leadmodification. 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.

Antipyretics Analgesics: Paracetamol, Acitaminophin, Asprin, Acetaanalide, Salicalamide, Benorylate, Phenozones, Dipyrones, Mefnanine Acid,

Synthesis of Diuretics, Anti-inflammatory, Muscle relaxants, Antihistaminics drugs, Uricosurics (Anti-gout-Agents), anti-coagulants.

Synthesis of naturally occurring bioactive compounds (Vitamin A, C and D), Prostaglandins.

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

Antibiotics: Pencillins-classification and structures. Synthesis of Pencillins, V, G, chloroamphenicol and ciprofloxacin. Tetracyclins.

Psychoactive Drugs: Introduction, CNS depressants, CNS stimulants, sedatives and hypnotics, barbutirates. Synthesis of diazepam, phenytoins and glutethisimide.

Cardiovascular Drugs: Introduction, cardiovascular diseases, synthesis of Amylnitrate. sorbitrate, quinidine, verapanil, methyl dopa and atenolol.

Antiviral Drugs: Chemistry of Viruses, Mechanism of action, Synthesis of indinavir, Noval Corona Virus; variants and the vaccinations.

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. Chemsitry of Natural Products. S.V. Bhat, B.A. Nagasampagi, M. Siva Kumar. Naroosa

Course No: CH21409DCE
Title: Chemistry of Natural Products (02 Credits)

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

Course Outcome: On completion of the course the student should be able to:

- Understand the role and importance of natural products in medicine and drug discovery.
- Recognise the chemistry and spectroscopic methodsinvolved in structure determination and synthesis of different classes of natural products *viz*terpenoids, steroids, alkaloids and flavonoids.

Unit-I: Terpenoids and Steroids (16 Contact hours)

Terpenoids*:* Introduction and classification. Chemistry of Citral/Geraniol, α-Terpeniol, Camphor, Zingiberene and Vitamin A. Biogenesis of terpenoids.

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

Unit-II ALKALOIDS AND FLAVONOIDS. (16 Contact hours)

Alkaloids: Introduction, qualitative tests and general methods of isolation. Structural elucidation synthesis and biogenesis of Reserpine and Morphine.

Flavonoids: Introduction, qualitative tests and general methods of isolation. Structure and synthesis of Apigenin, Quercetin, Genistein and Anthocyanidin. Antioxidant properties 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: CH21410DCE
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 outcome: After learning the contents of this course, the students shall:

- 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:

(a) Numerical solution of equations

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.

Eigen values and Matrix Diagonalization: Eigen value problem, diagonalization of a matrix, Jacobi and Householder methods.

(b) Numerical differentiation

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

(c) Numerical Integration

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

(d) 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)

***ab initio* Calculations of Electronic Structure**

a) 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^+.

b) 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.

c) Use of Gaussian quantum mechanical packagefor:

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: CH21411DCE
Title: Applied Electrochemistry (02 Credits)

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

Course outcome: After learning the contents of this 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 Applied Electrochemistry-I (16 Contact hours)

Photo- and Environmental Electrochemistry

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 Applied Electrochemistry-II (16 Contact hours)

Electrochemistry for Energy Conversion and Energy Storage

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 (Zinc-Air, 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, EliezerGileadi and Noam Eliaz, 2018, Wiley-VCH.

3. Electrochemistry, 2nd Edition, Carl H. Hamann, Andrew Hammett, Wolf Vielstich, Wiley-VCH.
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.

Course No: CH21004GE
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 will 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 **(08 Contact hours)**

Introduction, Definition, Classification based on source, Structure, Synthesis and Forces of attraction. Thermosetting and Thermosensitive plastics, Types of Monomers,Homopolymers and Copolymers.

Unit-II **(08 Contact hours)**

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-III **(08 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

Unit-IV **(08 Contact hours)**

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 .

Course No: CH21005GE
Title: Novel Materials (02 Credits)

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

Unit-I Block Co-Polymers, Langmuir Blodgett Films and Organic Solids

(16 Contact hours)

Block Copolymers: Introduction: classification, micellization of di block and triblock copolymers. Introduction topH-, thermo-and Photo-responsive block copolymers. Linear–dendrimer block copolymers: introduction, structural peculiarities of their aggregates, potential 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, photo conductivity and sensors.

Organic solids and fullerenes: Organics conductors, organic super conductors. Fullerenes-History, bonding, properties, dopedfullerenes, fullerenes as superconductors. Carbonnanotubes: Types, Properties and Applications.

Unit-II Optical and Nano-materials: **(16 Contact hours)**

Luminesenceand phosphors. Lasers - general principle of lasing action, Rubylaser, semi conducing glasers and quantum cascade lasers.

Nonlinear optical effects, second and third order harmonic generation, nonlinear optical materials.

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

Nanomaterials: Introduction with examples and applications of nanoparticles, nanofibers (nanowires, nanotubes and nanorods) and nanoplates.

Composites: Polymer-nano-object blends, Metal-Matrix composites, self-repairing composites and Nano fluids for Thermal transport.

Books Recommended

1. Solid State Chemistry and its Applications, West, Wiley,2014.
2. The Physical Chemistry of Solids, Borg, Biens, Academic press, 1992.
3. Solid State Physics, N. W. Ashcroft and N. D. Mermin, Saunders college, 2001
4. Principles of Solid State, H. V. Keer, Wiley Eastern; 2008.
5. Thermotropic Liquid Crystals, Ed., G.W. Gray, John Wiley.
6. The Physics and Chemistry of materials, J.I. Gersten, F.W. Smith, John Wiley and sons, Inc. 2001.
7. New directions in solid state chemistry, C.N.R. Rao and J. Gopalakrishnan, Cambridge University Press, 2nd ed.
8. Nanotechnology, An Introduction, J**.** J. Ramsden, Elsevier,1st Edition, 2011.
9. Essentials of Nanotechnology, J**.** J. Ramsden, J. Ramsden and Ventus Publishing ApS, 2009.

Course No: CH21004OE
Title: Food Chemistry (02 Credits)

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

Course outcome: On completion of the course, the students will acquire knowledge of chemistry involved in:

- Different components of food.
- Different Pigments in animal and plant tissues.
- Food colorants & flavorings.
- Food Preservation & food additives.

Unit-I **(16 Contact hours)**

(a) Food Components

Chemistry of different components of food: Composition and functions of Sugars, Polysaccharides, Lipids, Proteins, Vitamins and Minerals.

(b) 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)**

(a) The Chemistry of Food Preservatives:

Introduction. Basis of Food Preservation. Food additives: Sodium Chloride, Nitrites, Smoke, SO_2, Benzoates and other Organic acids.

(b) 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.