Semester-III

Third Semester
Core Course
Course Title: Organometallic Chemistry
Course code: CHM601C

Credits = 4
M.M. = 100
L T P=3 1 0

Course Learning Outcomes: After completion of this course, the students will be able to:

CLO 1:	Understand the fundamental principles of organotransition-metal chemistry and know how chemical properties are affected by metals and ligands
CLO 2:	Learn about the structure and bonding of simple organometallic complexes to understand their stability and reactivity. Learn about metallocenes and metal carbon multiple bonding in complexes
CLO 3:	Understand fundamental reaction types and mechanisms involved in organometallic chemistry and how to combine these for applications of organometallic chemistry in catalysis
CLO 4:	Learn about the fluxionality in organometallic compounds and utilizing multinuclear NMR spectroscopy to study their dynamic behavior

Unit I: Sigma bonded Organometallic Compounds **(Contact hours: 16)**

Classification, Stability, Routes of synthesis, Reactions, Structure and bonding. Decomposition pathways: α and β hydrogen transfer. Intramolecular elimination of alkane, Stability from bulky substituents, Agostic interactions
Metal hydride complexes: Synthesis, Characterization and Chemical reactions.

Unit II: Pi-bonded Organometallic Compounds **(Contact hours: 16)**

Synthesis, Structure and bonding in Metal-alkene, alkyne, allyl and diene complexes
Sandwich compounds: General characteristics, Classification, Synthesis, Reactions, Structure and bonding of Cyclopentadienyl complexes with special reference to ferrocene. Arene complexes
Compounds with transition metal carbon multiple bonds, Alkylidene (carbenes) and alkylidyne (carbynes) Synthesis, Structural characteristics, Nature of bonding.

Unit III: Catalytic Processes Involving Transition Metal Organometallic Compounds **(Contact hours: 16)**

Catalysis, terminology of catalysis and Tolman catalytic loop
Mechanistic aspects: Oxidative addition, reductive elimination, Insertion reactions, Hydrogenation, Hydroformylation, Oxidation, Isomerization and Zeigler–Natta polymerization of alkenes, Monsanto acetic acid reaction
C-C coupling reactions- Suzuki, Heck, Sonogashira and Stille coupling, Buchwald Hartwig amination
.

Unit IV: Fluxional Organometallic Compounds **(Contact hours: 16)**

General characteristics, Rates of rearrangement and techniques of study, Classification of fluxional organometallic compounds, Some simple examples of non-rigid molecules in 4 and 5 coordination geometries, Fluxionality and dynamic equilibria in compounds such as 2-olefin, 3-allyl and dienyl complexes

Books Recommended:

1. The Organometallic chemistry of the transition metals, R. H. Crabtree, John Wiley; 2014.
2. Organometallics; Christoph Elschenbroich, Wiley VCH, 3rd Edn, 2006.
3. Basic organometallic Chemistry; B. D. Gupta, A J Elias; University Press; 2nd Edn; 2013.
4. Organotransition metal chemistry: A. F. Hill, Tutorial chemistry text, RSC, 2002.

Reference Books:

5. Basic organometallic Chemistry; Ionel Haiduc, J. J. Zukerman; Walder de Gruyter, Berlin, New York 1985.
6. Organometallic chemistry, Mehrotra R. C. and Singh A., New Age International; 2007.
7. Inorganic Chemistry; G.L. Miessler & D. A. Tarr; Pearson Edn. Inc; 3rd Edn; 2004.
8. Inorganic Chemistry; Shriver & Atkins; Oxford University Press; 5th Edn; 2010.
9. Inorganic Chemistry; Huheey; Harper & Row; 4th Edn; 1990.
10. Metallo-organic chemistry, Pearson A.J., Wiley; 1994.

Third Semester

Core Course

Course Title: Pericyclic Reactions and Organic Photochemistry

Course Code: CHM602C

Credits = 4
M.M = 100
L T P=3 1 0

Course Learning Outcomes: After completion of this course, the students will be able to:

CLO 1:	Learn about basic concepts pertaining to pericyclic reactions and their various classes.
CLO 2:	Acquire knowledge about mechanism and applications of various pericyclic reactions like cycloadditions, electrocyclic reactions and sigmatropic rearrangements.
CLO 3:	Learn about the basics of photochemistry of organic compounds like electronic transitions, fates of excited molecule through Jablonski diagram.
CLO 4:	Learn about various photochemical reactions like Norrish type-I and Norrish type-II, Paterno-Buchi reaction as well as various photochemical reactions of aromatic systems.

Unit I: Pericyclic Reactions-I **(Contact hours: 10)**

General introduction, Definition and classification of pericyclic reactions. Molecular orbital symmetry, Frontier molecular orbital concept (FMO), HOMO, LUMO and SOMO: Frontier molecular orbitals of various π-electron systems including ethene, 1, 3-butadiene, 1,3,5-hexatriene and allylic systems. Woodward Hoffman rules for pericyclic reactions.

Unit II: Pericyclic Reactions-II **(Contact hours: 14)**

Cycloadditions: Thermal and photochemical 2+2 and 4+2 cycloadditions, Suprafacial and antrafacial cycloadditions.

Electrocyclic reactions: Thermal and photochemical electrocyclic reactions of 4n and 4n+2 systems and their stereochemical aspects, Conrotatory and disrotatory motions.

Sigmatropic rearrangements: Classification, [1,3], [1,5] and [3,3] sigmatropic shifts, Cope and Claisen rearrangements, Suprafacial and antrafacial shifts of hydrogen, Biological pericyclic reactions.

Unit III: Photochemistry-I **(Contact hours: 16)**

Types of photochemical excitations, Direct and indirect excitations, The fate of excited molecule, Singlet and triplet states and their lifetimes, Jablonski diagram, Transfer of excitation energy: sensitization and quenching, quantum yield, Different types of photochemical reactions,

Photochemical reactions of alkenes: Geometrical isomerization reactions, Dimerization and cyclization reactions, Photochemical reactions of 1,3-butadiene, Rearrangements of 1,4 and 1,5-dienes, Photochemistry of vision.

Unit IV: Photochemistry-II **(Contact hours: 12)**

Photochemical reactions of saturated cyclic and acyclic carbonyl compounds, Norrish type-I and Norrish type-II reactions, Paterno-Buchi reaction.

Photochemical reactions of α, β-unsaturated carbonyl compounds (H-abstraction and isomerization to β, γ-unsaturated carbonyl compounds). Photochemistry of enones and para-benzoquinones, Di π – methane rearrangement.

Light induced isomerization of benzene and its alkyl derivatives, Nucleophilic photosubstitution reactions of aromatic compounds, Photo-Fries rearrangement of aryl esters and anilides. Photolysis of organic nitrites.

Books Recommended:

1. Pericyclic Reactions, Ian Fleming, Oxford University Press, 2nd Edn;, 2015.
2. Essentials of Pericyclic and Photochemical Reactions, Biswanath Dinda, 1st Edn;, 2016.
3. Fundamentals of photochemistry, Rohatgi & Mukherjee Wiley Eastern-1992.
4. Advanced Organic Chemistry, Reactions, Mechanism and Structure, Jerry March 4th Edn., (Wiley, 1999).

Reference Books

5. Organic Chemistry, John McMurry. 5th Ed., (Brooks/Cole, 2000).
6. Organic Chemistry, J. Clayden, N. Greeves and S. Warren. Oxford University Press, 2nd Edn;, 2016.
7. Introductory Photochemistry, A. Cox and T. Kemp McGraw Hall-1971.
8. Organic Photochemistry, 2nd Ed., J. Coxon, and B. Halton. Cambridge University press-2nd Edn; 1987

Third Semester
Core Course
Course Title: Electrochemistry and Solid-State Chemistry
Course code: CHM603C

Credits = 4
M.M. = 100
L T P=3 1 0

Course Learning Outcomes: After completion of this course, the students will be able to:

CLO 1:	Understand the changes of metal-electrolyte interfaces through different mathematical models and equations
CLO 2:	Understand and apply the electrochemistry of redox enzymes and about solar cells
CLO 3:	Acquire the knowledge of crystal structures with some basic examples and theories of solids
CLO 4:	Understand basics of semiconductors, superconductors and magnetic properties of solid-state materials

Unit I: Electrochemistry-I (Contact hours: 16)

Metal-electrolyte electrified interfaces, Concept of surface excess, Thermodynamics of electrified interface, Lippmann equation, Electrocapillary curves, Methods for determination of surface excess. Structural models of metal-electrolyte interface: Helmholtz-Perrin, Gouy-Chapman and Stern models, Semiconductor electrodes: Structure of semiconductor/electrolyte interface, Theories of heterogeneous electron transfer: Electron transfer at electrified interface at and away from equilibrium, Butler-Volmer Equation, Low and high field approximations, Significance of transference-coefficient. Marcus theory of charge transfer.

Unit II: Electrochemistry-II (Contact hours: 16)

Electrochemistry of redox enzymes: Direct and mediated electron transfer, Enzyme modified electrodes-challenges and applications. Mechanism and approach to bio-electrosynthesis, examples of bio-electrosynthesis-oxidation of alcohols, synthesis of dihydroxy acetone phosphate, site specific oxidation of sugars, reduction of carbonyl compounds, hydrogenation.

Solar Cells: Principles of Operation and Energetics of Conversion, Photoelectrochemical splitting of water, Photoelectrochemical reduction of CO_2 and N_2.

Unit III: Solid State Chemistry-I (Contact hours: 16)

Point groups, Space groups, Lattice Planes and Miller indices, Bragg's equation, Debye-Scherrer method of X-ray structural analysis, Identification of cubic unit cells from systematic absences in diffraction pattern, Structure factor and its relation to intensity and electron density. Crystal structure of Perovskite ($SrTiO_3$) and Rutile (TiO_2).

Thermodynamics of Schottky and Frenkel defect formation.

Theories of bonding in solids: Somerfield's model, Density of states and its significance. Band theory of solids in light of Kroning-Penny model.

Unit IV: Solid State Chemistry-II (Contact hours: 16)

Semiconductors: Intrinsic and extrinsic semiconductor (n-type and p-type), Temperature dependence of charge carriers, p-n junction- devices based on p-n junction (tunnel diode, injection laser).

Magnetism in solids: Origin of Magnetism, Diamagnetism, paramagnetism (classical and quantum mechanical treatment), ferromagnetism, ferrimagnetism and anti-ferromagnetism in solids.

Super conductors: Characteristic properties- Zero resistance, Meissner effect, Heat capacity, Thermal conductivity, Absorption of electromagnetic radiations and Josephson effect. BCS theory of superconductivity, Applications.

Books Recommended:

1. Modern Electrochemistry 1, 2A, J. O. Bockris and A. K. Reddy, Kluwer Academic/plenum Publishers, New York. 2nd Edn.; 2002.
2. Electrochemical methods, Fundamentals and Methods, A. J. Bard, L. R. Faulkner, Wiley, 2nd Edn.; 2002.
3. Introduction to Solids, Azaroff, Tata McGraw,1993.
4. Solid State Chemistry and its Applications, A R West, Wiley,1989.

Reference Books:

5. Physical Chemistry - P. W. Atkins, Oxford, 2010.
6. Physical Electrochemistry-Fundamentals, Techniques and Applications, E. Gileadi, Wiley-VCH, 2011.
7. Electrochemistry, Carl H. Hamann, Andrew Hammett, Wolf Vielstich, Wiley-VCH. 2nd Edn.; 2007.
8. An Introduction to Aqueous Electrolyte Solutions, Margaret Robson Wright, Wiley, 1st Edn.; 2007.
9. Solid State Physics, N. W. Ashcroft and N. D. Mermin, Saunders College, 2001.
10. Elements of Solid-State Physics, J.P. Srivastava, Prentice Hall of India, 2003.

Third Semester
Core Course
Course Title: Analytical Methods
Course code: CHM604C

Credits = 4
M.M. = 100
L T P=3 1 0

Course Learning Outcomes: After completion of this course, the students will be able to:

CLO 1:	Interpret the complexometric titrations, precipitation titrations along with titrimetric analytical methods
CLO 2:	Illustrate the basic principle and applications of TGA as an essential technique to characterize materials
CLO 3:	Illustrate the basic principle and applications of modern electro-analytical methods as an essential technique to characterize materials used in various environmental, food, pharmaceutical and petrochemical applications.
CLO 4:	Provide detailed information about principle, instrumentation, and application for detection and determination of fluorescent compound at ng or lower levels

Unit I: Complexometric Titrations (Contact hours: 20)

Titrations in non-aqueous solvents: Introduction, Solvents for non-aqueous titrations, characteristics of amphiprotic solvents-Autoprotolysis, Aprotic solvents, choosing a solvent. indicators for non-aqueous titrations.
Amino Carboxylic acid (EDTA) Titrations: EDTA as a titrant and stability of Metal EDTA complexes and factors affecting the stability of EDTA complexes, Conditional formation constant. Types of EDTA Titrations (Direct, Back, Displacement, Indirect), Use of masking agents in EDTA titrations. EDTA titration curves and factors affecting their shape. Using excel spreadsheets for computing and plotting EDTA titration curves. Indicators for EDTA titrations Precipitation titrations: Volhard, Mohr and Fajan's methods. Typical applications.

Unit II: Thermal Methods of Analysis (Contact hours: 12)

Introduction to thermal methods of analysis, Thermogravimetric analysis (TGA), Apparatus, Methodology, Factors effecting TGA curve, Applications of TGA for quantitative analysis, thermal stability of materials, mixture analysis, Kinetic studies, (TG analysis of $CaC_2O_4.H2O$, $CuSO4.5H2O$, problems based on TGA)
Differential thermal analysis (DTA), Apparatus, Methodology, simultaneous DTA and TGA curves, Interpretation of TGA and DTA curves of compounds e.g., Calcium oxalate monohydrate, Magnesium oxalate monohydrate,
Differential Scanning Calorimetry (DSC) Apparatus, Methodology, and Interpretation.
Brief introduction to Thermometric titrimetric and applications to acid-base and complexometric titrations.

Unit III: Electrochemical Methods (Contact hours: 16)

Voltammetry and polarographic analysis: Principle of polarography, residual current, migration current, diffusion current, half wave potential, Ilkovic equation, instrumentation, Dropping mercury electrode (DME), Advantages and dis-advantages of DME, Qualitative and quantitative analysis of inorganic ions Cu, Bi, Pb, Cd, Zn, AC polarography, Pulse polarography
Anode stripping voltametry: Principle, instrumentation, Hanging mercury drop electrode, Application in the analysis of Pb and Cd in environmental samples, Principle of cathode stripping voltammetry

Unit IV: Spectrofluorimetry (Contact hours: 16)

Molecular Luminescence Spectrometry Theory of fluorescence and phosphorescence, variables that affect fluorescence and phosphorescence, emission and excitation spectra, photoluminescence intensity as related to concentration, Instruments for measuring fluorescence and phosphorescence, determination of inorganic and organic species. Applications of fluorometry and phosphorimetry, problems.

Books Recommended:

1. Principles of Instrumental Analysis, Skoog, Holler, Crouch, Brooks 6thEdn: 2007
2. Analytical Chemistry, Seamus P. J. Higson, Oxford University Press, 2004.
3. Instrumental Methods of Analysis by G.D. Christian and C.N. Reilly. 2nd Edn; 1986.
4. Principles of fluorescence spectroscopy: Joseph R Lakowich, Springer. 3rd Edn: 2006

Reference Books:

5. Handbook of Thermal Analysis and Calorimetry, Recent Advances, Techniques and Applications, S. Vyazovkin N Koga and C Schick ,2ndEdn: 2018
6. Instrumental Methods of Analysis, Willard,Merritt, Dean and Settle,CBS Publishers, 7th Edn: 2004
7. Thermal methods of analysis, principals, applications and problems, Peter J. Haines. Blackie Academic and Professional, 1995
8. Ionic Equilibria in Analytical Chemistry; Freiser and Fernando, Wiley, 1963
9. Instrumental methods of Chemical Analysis, G.W. Ewig, McGraw Hill Book Co. 5th Edn., 1962

Third Semester
Core Course
Course Title: Advanced Laboratory Course
Course Code: CHM605C

Credits = 4
M.M. = 100
L T P=0 0 4

Course Learning Outcomes: After completion of this course, the students will be able to

CLO 1:	Acquire practical skills and hands-on experience on high-end analytical instruments
CLO 2:	Know and use of the sophisticated techniques and instruments like spectrophotometry, fluorescence spectrophotometry, Bookfield viscometer, surface tensiometry and Refratometry
CLO 3:	Synthesize inorganic compounds and their characterization
CLO 4:	Acquire practical skills in organic chemistry such as purification, isolation, and synthesis of important organic compounds

Spectrophotometry

1. To study the complexation reaction between Fe(III) & salicylic acid.
2. Determine the dissociation constant of an indicator by spectrophotometric method.
3. Determination of Iron (II) with 1,10-Phenanthroline.
4. Theoretical and experimental comparison of HOMO-LUMO gaps of some organic molecules.
5. Determination of Phosphate by Molybdenum blue method.
6. Estimation of aspirin from given tablet by Spectrophotometry
7. Determination of complex ion composition by jobs method of continuous Variation.
8. Interpretation of IR spectrum of alcohols, ketones, aldehydes and other standard material

Potentiometry

9. Precipitation titration of KCl, KBr, KI and their mixture with $AgNO_3$
10. Determination of formation constant of Ag-NH_3 complex and activity coefficient estimation.
11. Standardization of an Fe(II) solution with a standard dichromate solution over Pt & Calomel assembly.
12. Estimation of iodide with Standard $AgNO_3$ over Pt and Calomel assembly using I^-/I_2 redox couple.
13. Simultaneous determinations of chloride and iodide ions with Standard $AgNO_3$ over Ag-Glass electrode assembly
14. To determine chloride and iodide from a given mixture by potentiometry.

Conductometry

15. Verification of Debye-Huckel-Onsagar law.
16. Estimation of the concentrations of H_2SO_4, CH_3COOH and $CuSO_4$ in a mixture.
17. To determine the solubility and solubility product of a sparingly soluble salt ($BaSO_4$) in water.

Kinetics

18. Study the kinetics of reaction between potassium persulphate and potassium iodide:
    a) Determine the rate constant and order of reaction.
    b) Study the influence of ionic strength on the rate constant.

Viscometry

19. Determination of Mol. Mass of a Polymer (Polyvinyl alcohol) using viscosity method **(Using Brook Field Viscometer)**.
20. Visco-elastic properties of poly allyl amide gel by rheology.

Fluorescence Spectroscopy

20. Determination of absorption and emission spectra of a dye.
21. Fluorescence study of dye-amphiphile interactions.

Surface Tensiometry

22. Determination of critical micellar concentration (CMC) of a surface-active agent in aqueous solution.
23. Determination of thermodynamic parameters from surface tension curves.

Polarimetry

18. Determination of specific, molecular, and intrinsic rotation of an optically active compound
19. Study of inversion of cane sugar in presence of acid.

pH-metric Titrations

24. Purity of Acetyl Salicylic acid (Aspirin) in a commercial tablet by pH Titration.
25. Quantitative analysis of chromate dichromate mixture by pH titration.

Flame Photometry

26. Simultaneous determination of sodium and potassium in a given mixture
27. Determination of cadmium and magnesium in tap water.
28. Estimation of micronutrients from food by AAS (any two elements Fe, Cu, Zn, Mo, B , Mn)

Chromatography

29. Separation of some organic compounds by column chromatography
30. Analysis of Paracetamol from given unknown sample by HPLC
31. Separation of Cobalt (II) and Nickel (II) on anion exchange column followed by estimation through EDTA titrations.
32. Separation of MnO_4^- and $Cr_2O_7^{2-}$ on Alumina column and their estimation from Beer-Lambert plots.
33. Determination of pesticides (Organophosphate) in soil sample using HPLC.

Synthetic Preparations

34. Preparation of tetraamminecarbonatocobalt(III) nitrate and its conversion to pentaamminecholorocobalt(III) chloride.
35. Preparation of trans dicholoro bis (ethylenediamine)cobalt(III) chloride and its conversion to cis-isomer.
36. Preparation and applications of metal organic frameworks (MOFs): MOF−5, ZIF−8, MIL−101 (Fe)
37. Reaction of Cr(III) with a multidentate ligand; a kinetic experiment (visible spectra Cr-EDTA complex)
38. Synthesis of aspirin and its characterization by physical and spectroscopic methods.
39. Synthesis of paracetamol and its characterization by physical and spectroscopic methods.
40. Beckmann rearrangement.

Extraction/Estimation of Organic compounds from natural sources

41. Isolation of lycopene and beta-carotene from tomato, Characterization of lycopene/P-carotene by UV -absorption process.
42. Isolation of caffeine from cold drinks and its physicochemical analysis.
43. Estimation of ascorbic acid in Vitamin C tablet by titration with potassium bromate
44. Estimation of phosphoric acid in soft drink by molybdenum blue method.

Books Recommended:

1. Practical Physical Chemistry, Findley revised by Kitchner. (Longman, 1971)
2. Experimental Physical Chemistry, A. M. Halpern, G. C. McBane, (Freeman, 2006)
3. Experiments in Physical Chemistry, Schoemaker et al. 5th Edn;. (MGH, 2003)
4. Synthesis and Technique in Inorganic chemistry, G. S. Girlomi; R.J. Angleci 3rd edn.; University Science Books.
5. Quantitative Chemical Analysis; Harris; Freeman; 5th Edn.; 1999.
6. Advanced Practical Inorganic Chemistry; Adams; Raynor, Wiley; 1995.
7. Advanced Experimental Inorganic Chemistry; Ayodha Singh; Campus Books 2002.
8. Practical Clinical biochemistry methods and interpretations, R. Chawla, J.P. Bothers Medical Publishers (P) ltd., 1995.
9. Laboratory manual in biochemistry, J. Jayaraman, New Age International Publishers, New Delhi, 1981.
10. Yoshie Sakamaki et al., J. Chem. Educ. 2020, 97, 1109−1116
11. Practical clinical Biochemistry-Harold Varley and Arnold. Heinmann, 4th Edn;
12. Vogel's Textbook of Quantitative Chemical Analysis, J. Mendham, R.C. Denney, J.D. Barnes and M.J.K. Thomas, Third Indian Reprint, 2003 Pearson Education Pvt. Ltd., New Delhi, 6th Edn.
13. Quantitative Analysis, R.A. Day and A.L. Underwood, 1993 Prentice Hall, Inc. 6th Edn; New Delhi.
14. Quantitative Chemical Analysis; Kolthoff, sandell Meehan and Bruckestein; Mcmillan Co., London, 1969

Third Semester
Discipline Centric Course
Course Title: Spectroscopy of Organic Compounds
Course Code: CHM606E

Credits = 3
M.M = 100
L T P=3 1 0

Course Learning Outcomes: After completion of this course, the students will be able to:

CLO 1:	Learn about various concepts related to the topics of UV-visible spectroscopy like electronic transitions, effect of solvent on transitions, Woodward-Hoffmann rules for calculating λ-max for organic compounds. Students will also learn about applications of IR spectroscopy in structure elucidation of organic compounds.
CLO 2:	Learn about various concepts related to mass spectrometry and its applications in structure elucidation of organic compounds.
CLO 3:	Learn about proton NMR spectroscopy and its applications in elucidating molecular structure.
CLO 4:	Learn about carbon NMR spectroscopy and how it can be used to elucidate molecular structure of organic compounds.

Unit I: Ultraviolet and Infrared Spectroscopy (Contact hours: 16)

Ultraviolet absorption spectra of dienes (homo and heteroannular), Enones, Carbonyl compounds, Unsaturated carbonyl compounds, Aromatic and heteroaromatic compounds, Woodward-Fieser rules, Applications and limitations, Kuhn's rule, Application to conjugated polyenes. General applications of ultraviolet spectroscopy.
Characteristic vibrational frequencies of Alkanes, Alkenes, Alkynes, Alcohols, Ethers, Phenols, Amines, Aldehydes, Ketones, Acids, Anhydrides, Esters, Lactones, Amides and conjugated carbonyl compounds, Effect of hydrogen bonding and solvent on vibrational frequencies in IR spectra. General applications of Infra-red spectroscopy.

Unit II: Mass Spectrometry (Contact hours: 16)
Introduction, Instrumentation, A typical mass spectra, molecular ion peak, Ion production, EI, CI, FD, FAB, ESI and MS/MS methods, Role of isotopes in mass spectrometry, Fragmentation pattern of various classes of organic compounds, Metastable peak, Nitrogen rule, High resolution mass spectrometery. Fragmentation pattern, Initial ionization event, α-cleavage, Inductive cleavage, two bond cleavage, Retro-Diels Alder cleavage and McLafferty rearrangement.

Unit III: Proton Nuclear Magnetic Resonance Spectroscopy (^{1}H-NMR) (Contact hours: 16)
Shielding effect, Chemical shift values and correlation for protons bonded to carbon (aliphatic, olefinic, aldehydic and aromatic) and other nuclei (Alcohols, Phenols, Enols, Carboxylic acids, Amines, Amides and mercapto). Chemical exchange, Effect of deuteration, Complex spin-spin interactions between two three, four and five nuclei (first order spectra) virtual coupling, Stereochemistry. Simplification of complex spectra, Nuclear magnetic double resonance, contact shift reagents, Solvent effect, Fourier transform technique, Nuclear overhauser effect (NOE). Bio-chemical applications of NMR (examples).

Unit IV: Carbon-13 NMR Spectroscopy (Contact hours: 14)
General considerations, Chemical shift (aliphatic, olefinic, alkyne, aromatic, heteroaromtic and carbonyl carbon), Coupling constant, Two-dimensional NMR spectroscopy (brief idea)- COSY, NOESY, DEPT, INEPT, APT and INADEQUATE techniques. Problems on structure elucidation based on the data from different spectroscopic techniques.

Books recommended:

1. Spectroscopy of Organic Compounds, P.S. Kalsi, New Age International Private Limited (1 January 2016).
2. Introduction to Spectroscopy. Donald L. Pavia, Gary M. Lampman, George S. Kriz, James A. Vyvyan. Cengage Learning, 2008.
3. Spectrometric identification of Organic Compounds.5th Ed., R. M. Silverstein, G. C. Bassler and T. C. Morill. (Jhon Wiley-1991).

Reference Books:

4. Introduction to NMR Spectroscopy, R. J. Abraham. J. Fisher and P. Loftus (Wiley- 1991)
5. Applications of absorption spectroscopy of Organic Compounds, J. R. Dyer (Prentice Hall-1991).
6. Spectroscopic Methods in organic Chemistry, D. H. Williams; I. Fleming (Tata- McGraw Hill-1988).

Third Semester
Discipline Centric Course
Course Title: Spectroscopy of Inorganic Compounds
Course Code: CHM607E

Credits = 3
M.M. = 100
L T P=3 1 0

Course Learning Outcomes: After completion of this course, the students will be able to

CLO 1:	Learn about the principle and instrumentation of nuclear magnetic resonance spectroscopy and apply the knowledge in characterizing the coordination/organometallic complexes and inorganic compounds containing different sort of NMR active nuclei
CLO 2:	Learn about the principle and instrumentation of NQR spectroscopy and analyze the NQR data for chemical analysis
CLO 3:	Learn about the principle and instrumentation of Mossbauer spectroscopy and analyze the Mossbauer spectrum to obtain information about oxidation state as well as spin state of metal ion
CLO 4:	Learn about the principle and instrumentation of electron spin resonance spectroscopy and apply the knowledge in characterizing inorganic/organic compounds and coordination/organometallic complexes (obtain the idea about oxidation state of metal ion and ligand field)

Unit I: Multinuclear NMR Spectroscopy **(Contact hours: 16)**

Multinuclear NMR spectroscopy in inorganic chemistry, Paramagnetic shift in ^{1}H NMR spectra, ^{31}P NMR, ^{11}B NMR ^{19}F NMR (Splitting pattern and spectrum). Spin dilute systems-satellites in Pt, Sn and Se compounds, Exchange process in solution, Spin-spin coupling, Magnetic resonance imaging (MRI), MRI contrast agents, Applications of ^{1}H, ^{13}C, ^{19}F, ^{31}P, ^{11}B and ^{15}N to simple inorganic and Coordination/organometallic Compounds

Unit II: Nuclear Quadrupole Spectroscopy **(Contact hours: 16)**

NQR Isotopes, Basic theory of quadrupole spectroscopy, Quadrupole nuclei, Nuclear quadrupole moment, Electric field gradient (EFG), Quadrupole Coupling constant (QCC), Effect of applied magnetic field (Zeeman effect), Towns-Dailey Theory, Applications of NQR and NQR spectra of $^{14}N_7$, $^{11}B_5$

Unit III: Mossbauer Spectroscopy **(Contact hours: 16**

Technique of Mossbauer Spectroscopy, Gamma-ray fluorescence, Gamma radiation source, Doppler effect, Isomer shift, Quadrupole splitting, Magnetic hyperfine splitting, Applications; Iron compounds: low-spin and high-spin Fe(II) and Fe(III) complexes, π-bonding effects in iron complexes, structural aspects of iron carbonyls and iron-sulfur proteins. Tin compounds: Tin halides and organotin compounds.

Unit IV: Electron Spin Resonance (ESR/EPR) Spectroscopy **(Contact hours: 16)**

Principle of ESR spectroscopy, Hyperfine structure in ESR spectra, Hydrogen atom, Methyl radical, $(SO_3)_2NO^{\cdot}$ anion, Fermi-contact interaction, *g*-factor: $g_{\parallel}$ *and* $g_{\perp}$, Applications of ESR, Spin labels, McConnell equation, Isotropic and anisotropic systems, Hyperfine splitting, Spin Hamiltonian, Kramer's degeneracy and Zero field splitting, ESR Spectra of d1-d9 Transition Metal Complexes with examples, Interpretation of g in cubic, axial and rhombohedral geometries.

Books Recommended:

1. NMR, NQR and EPR and Mossbauer Spectroscopy in Inorganic Chemistry; Parish and Elis, H; 1990.
2. Physical methods in inorganic chemistry; Russel S. Drago; East West Press Private Ltd.; 2017.
3. Nuclear Quadrupole Resonance Spectroscopy, Das, T. P. and Hahn, E. L. Academic Press; 1958.
4. Spectroscopy of Inorganic Compounds, Jagdamba Singh, Mrituanjay D Pandey and Jaya singh; New Age International (P) Ltd. 1st Edn; 2021

Reference Books:

5. Introduction to ligand fields; B. N. Figgis; Interscience Publishers, John Wiley & Sons; 1967.
6. Molecular structure and spectroscopy, Aruldhas, G.; 2nd Edn., PHI; 2008.
7. Inorganic Chemistry; Catherine, E. H and Sharpe, A. G; 2nd Edn., Pearson.
8. Principles of Physical Chemistry; Puri, B. R.; Sharma, L. R.; Pathiana, M. S.; 4th Edition.
9. Spectroscopy in Inorganic Chemistry; Vol I and II; Rao, Ferraro; Academic Press; 1970.
10. Structural Methods in Inorganic Chemistry; 2nd edn; Ebsworth, E. A. V and Rankin, D. W. H; ELBS; 1991.

Third Semester
Discipline Centric Course
Course Title: Chemo-informatics
Course code:CHM608E

Credits = 3
M.M. = 100

Course Learning Outcomes: After completion of this course, the students will be able to:

CLO 1:	Learn representations of molecules and their classification by their chemical reaction
CLO 2:	Gain the knowledge of searching chemical structure through chemical databases
CLO 3:	Learn computer-assisted virtual screening to design drug like molecules and to predict their pharmacokinetics such as adsorption, distribution, metabolism, excretion, and toxicity (ADMET)
CLO 4:	Acquire the knowledge of importance of chem-informatics in drug discovery

Unit I: Representation of Molecules and Chemical Reactions **(Contact hours: 16)**

Nomenclature, Different types of notations, SMILES coding, Matrix representations, Structure of Molfiles and Sdfiles, Libraries and toolkits, Different electronic effects, Reaction classification.

Unit II: Searching Chemical Structure **(Contact hours: 16)**

Full structure search, sub structure search, basic ideas, similarity search, Three-dimensional search methods, Basics of computation of physical and chemical data and structure descriptors, Data visualization.

Unit III: Computer Assisted Virtual Screening Design **(Contact hours: 16)**

Structure based virtual screening- Protein ligand docking, scoring functions for protein ligand docking, Practical aspects of structure based virtual screening, Prediction of ADMET properties, 2D and 3D data searching, Chemical databases, Role of computers in chemical research.

Unit IV: Application of Cheminformatics in Drug Design **(Contact hours: 16)**

Quantitative structure-property relations,
Descriptor analysis, Computer assisted structure elucidations, Target identification and validation, Lead finding and optimization, Analysis of HTS data, Design of combinatorial libraries, Ligand and structure-based drug design

Books Recommended:

1. Andrew R. Leach, Valerie J. Gillet, Cluwer , Introduction to Chem-informatics, Academic Publisher, Netherlands, 2003
2. Lisa B. English (Editor), Combinatorial Library Methods and Protocols, Humana Press Inc, Volume:201, 2002
3. Frank Jensen, Introduction to Computational Chemistry, Wiley Publisher, 2nd Edn;, 2006
4. The Organic Chemistry of Drug Design and Drug Action, R.B. Silverman, Academic Press.

Reference Books:

5. P. Shanmughavel, "Trends in Bioinformatics", Pointer publishers, 2006
6. Francis A. Carey and Richard J. Sundberg, "Advanced Organic Chemistry-Part A & B" Third Edition, 1990