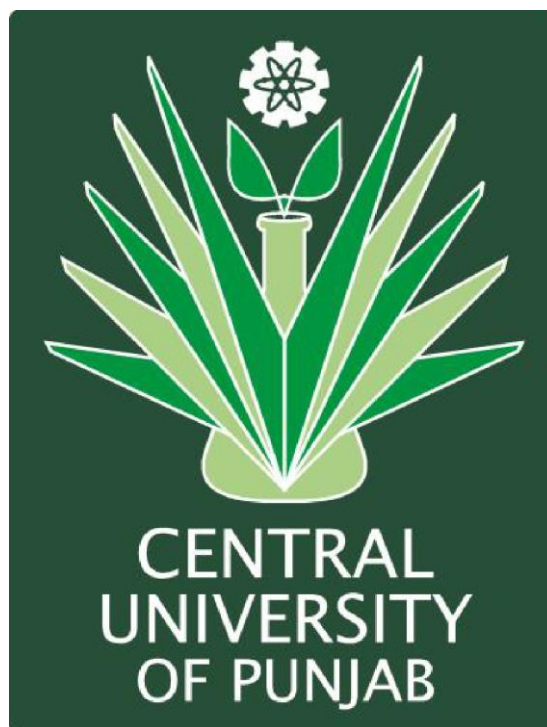


Central University of Punjab, Bathinda



Ph.D. Chemistry

Session: 2020

Department of Chemistry

School of Basic and Applied Sciences

Program Outcomes:

After completion of PhD, student will be able to

- focus on working independently on research problems and solutions of chemical sciences and also disseminating the knowledge and information related to chemistry
- communicate its finding and writing the manuscripts independently and assembling sophisticate analytical instruments as per requirement of research problems.

Course Structure and Syllabus

S. No.	Paper Code	Course Title	L	T	P	Cr
1.	CHM.701	Research Methodology	4	0	0	4
2.	CHM.702	Biostatistics	2	0	0	2
3.	CHM.703	Computer Applications	2	0	0	2
4.	CHM.751	Research and Publication Ethics	2	0	0	2
5.	CHM.799	Seminar	0	0	0	2
Opt any one of the following Elective Courses Offered:						
6.	CHM.705	Advances in Chemistry of Molecular Clusters	4	0	0	4
7.	CHM.706	Recent Trends in Synthetic Strategies and Green Catalysis	4	0	0	4
8.	CHM.707	Chemistry of Nanoscience and Technology	4	0	0	4
9.	CHM.708	Emerging Aspects in Supramolecular Chemistry	4	0	0	4
10.	CHM.709	Advanced Bioinorganic and Biophysical Chemistry	4	0	0	4
11.	CHM.710	Applied Material Chemistry	4	0	0	4
12.	CHM.711	Advanced Organotransition Metal Chemistry	4	0	0	4
13.	CHM. 712	Advanced Organic Synthesis and Catalysis	4	0	0	4
14.	CHM.713	Advanced Analytical Chemistry and Instrumental Methods of Analysis	4	0	0	4
15.	CHM.714	Emerging Trends in Green Synthesis and Drug Discovery	4	0	0	4
16.	CHM 715	Advanced Spectroscopy	4	0	0	4
		Total	14	0	0	16

L: Lectures T: Tutorial P: Practical Cr: Credits

Criteria for evaluation of theory exams: EST = 100%

Criteria for evaluation of Seminar: Report & presentation= 100%

Course Title: Research Methodology

Paper Code: CHM.701

Total Lecture: 60

L	T	P	Cr
4	0	0	4

Learning Outcome: At the end of this course student will be able to

- Design research problem.
- Know why educational research is undertaken, and the audiences that profit from research studies.
- Identify the overall process of designing a research study
- Familiar with ethical issues in educational research, including those issues that arise in using quantitative and qualitative research.

Unit-I

15 Hrs

General principles of research: Meaning and importance of research, Critical thinking, Formulating hypothesis and development of research plan, Review of literature, Interpretation of results and discussion.

Bibliographic index and research quality parameters- citation index, impact factor, *h* index, i10 index, etc. Research engines such as google scholar, Scopus, web of science, etc

Unit-II

15 Hrs

Technical & scientific writing: Technical & Scientific writing - theses, technical papers, reviews, electronic communication, research papers, etc., Poster preparation and Presentation and Dissertation. Reference Management using various softwares such as Endnote, reference manager, Refworks, etc. Communication skills—defining communication; type of communication; techniques of communication, etc.

Unit-III

15 Hrs

Library: Classification systems, e-Library, Reference management, Web-based literature search engines.

Plagiarism: Plagiarism, definition, Search engines, regulations, policies and documents/thesis/manuscripts checking through softwares, Knowing and Avoiding Plagiarism during documents/thesis/manuscripts/ scientific writing.

Unit-IV

15 Hrs

Intellectual Property Rights: Intellectual Property, intellectual property protection (IPP) and intellectual property rights (IPR), WTO (World Trade Organization), WIPO (World Intellectual Property Organization), GATT (General Agreement on Tariff and Trade), TRIPs (Trade Related Intellectual Property Rights), TRIMS (Trade Related Investment Measures) and GATS (General Agreement on Trades in Services), Nuts and Bolts of Patenting, Technology Development/Transfer Commercialization Related Aspects, Ethics and Values in IP.

Mode of Transaction: Lecture, Demonstration, Lecture cum demonstration, Dialogue Mode, Experimentation, Problem solving, Seminar.

Suggested Readings:

1. Gupta, S. (2002). *Research methodology and statistical techniques*. Deep and Deep Publications.
2. Kothari, C. R. (2008.) *Research methodology(s)*, New Age International (p) Limited. New Delhi
3. Best J. W., Khan J. V. (Latest Edition) *Research in Education*, Prentice Hall of India Pvt. Ltd.
4. *Safe science: promoting a culture of safety in academic chemical research*; National Academic Press, www.nap.edu.
5. Copyright Protection in India [website: <http://copyright.gov.in>].
6. World Trade Organization [website: www.wto.org].
7. Wadedhra B.L. *Law Relating to Patents, Trademarks, Copyright Design and Geographical Indications*. Universal Law Publishing, New Delhi. Latest Edition.

Course Title: Biostatistics
Paper Code: CHM.702

L	T	P	Cr
2	0	0	2

Total Lecture: 30

Learning Outcome: At the end of this course student will be able to

- Identify, demonstrate and apply various statistical parameters for the research data collected and infer the results statistically.

Unit I**8 Hrs**

Overview of biostatistics: Difference between parametric and non-parametric statistics, Univariate and multivariate analysis, Confidence interval, Errors, Levels of significance, Hypothesis testing.

Descriptive statistics: Measures of central tendency and dispersal, Histograms, Probability distributions (Binomial, Poisson and Normal), Sampling distribution, Kurtosis and Skewness.

Unit II**7 Hrs**

Experimental design and analysis: Sampling techniques, Sampling theory, Various steps in sampling, collection of data-types and methods.

Unit III**8 Hrs**

Comparing means of two or more groups: Student's t-test, Paired t-test, Mann-Whitney U-test, Wilcoxon signed-rank, One-way and two-way analysis of variance (ANOVA), Critical difference (CD), Least Significant Difference (LSD), Kruskal-Wallis one-way ANOVA by ranks, Friedman two-way ANOVA by ranks, χ^2 test.

Unit IV**7 Hrs**

Regression and correlation: Standard errors of regression coefficients, Comparing two regression lines, Pearson Product-Moment Correlation Coefficient, Spearman Rank Correlation Coefficient, Power and sampling size in correlation and regression.

Mode of Transactions: Lecture, Demonstration, Presentation, Group Discussion, Lecture cum demonstration, Problem solving, Brain storming

Suggested Readings:

1. Norman, G. and Streiner, D. (3rd edn) (2008). *Biostatistics: The Bare Essentials*. Decker Inc., Canada.
2. Sokal, R.R. and Rohlf, F.J. (1994). *Biometry: The Principles and Practices of Statistics in Biological Research*, W.H. Freeman and Company, New York.
3. Skoog, D. A., West, D. M., Holler, F. J., & Crouch, S. R. (2013). *Fundamentals of Analytical Chemistry*. Nelson Education.
4. Danzer, K. (2007). *Analytical Chemistry: Theoretical and Metrological Fundamentals*. Springer Science & Business Media.

Course Title: Computer Applications**Paper Code: CHM.703****Total Lecture: 30**

L	T	P	Cr
2	0	0	2

Learning Outcome:

At the end of this course student will be able to

- Apply various softwares such as Reference Management, Image processing applications for preparation of research reports and papers.
- Identify various computer commands and their application for their research/writing work.

Unit I**15 Hrs**

Fundamentals of computers: Parts of computers, Hardware, BIOS, Operating systems, Binary system, Logic gates and Boolean algebra.

Application software: Spreadsheet applications, Word-processing applications, Presentation applications, Internet browsers, Reference Management and Image processing applications.

Unit II**15 Hrs**

Computer language: Basic DOS commands, AutoHotKey scripting language, HTML and basic structure of a webpage.

World wide web: Origin and concepts, Latency and bandwidth, Searching the internet, Advanced web-search using Boolean logic, Cloud computing.

Mode of Transactions: Lecture, Demonstration, Presentation, Group Discussion, Lecture cum demonstration, Problem solving, Brain storming

Suggested Readings:

1. Gookin, D. (2007). *MS Word 2007 for Dummies*. Wiley.
2. Harvey, G. (2007). *MS Excel 2007 for Dummies*. Wiley.
3. Johnson, S. (2009). *Windows 7 on demand*. Perspiration Inc.
4. Thurrott, P. and Rivera, R. (2009). *Windows 7 Secrets*. Wiley.

Course Title: Research and Publication Ethics (RPE)**Paper Code: CHM 751****Total Contact Hours: 30**

L	T	P	Cr
2	0	0	2

Learning Outcome: After this course completion, students will be able to

- Identify publication ethics.
- Interpret intellectual honesty and research integrity
- Evaluate predatory publications and journals.
- Familiar with philosophy of science and ethical issues in research.
- Analyze indexing and citation databases, research metrics and plagiarism tools

Unit I**3 Hrs****Philosophy and Ethics:**

Introduction to Philosophy: definition, nature and scope, content, branches

Ethics: definition, moral philosophy, nature of moral judgements and reactions

Unit II**5 Hrs****Scientific Conduct:**

Ethics with respect to science and research, Intellectual honesty and research integrity, Scientific misconducts: Falsification, Fabrication, and Plagiarism (FFP)

Redundant publications: duplicate and overlapping publications, salami slicing
Selective reporting and misrepresentation of data**Unit III****11 Hrs****Publication Ethics:**

Publication ethics: definition, introduction and importance, Best practices/ standards setting initiatives and guidelines: COPE, WAME, etc. Conflicts of interest, Publication misconduct: definition, concept, problems that lead to unethical behaviour and vice versa, types, Violation of publication ethics, authorship and contributorship, Identification of publication misconduct, complaints and appeals, Predatory publishers and journals

Open Access Publishing:

Open access publications and initiatives

SHERPA/RoMEO online resource to check publisher copyright & self-archiving policies

Software tool to identify predatory publication developed by SPPU

Journal finder/journal suggestion tools viz. JANE, Elsevier Journal Finder, Springer, Journal Suggester, Etc.

Unit IV**11 Hrs****Publication Misconduct:**

Group Discussions: Subject specific ethical issues, FFP, authorship; conflicts of interest; complaints and appeals: examples and fraud from India and abroad

Software tools: Use of plagiarism software like Turnitin, Urkund and other open source software tools

Databases and Research Metrics:

Databases: Indexing databases; Citation database: Web of Science, Scopus etc.

Research Metrics: Impact Factor of journal as per Journal Citation Report, SNIP, SJR, IPP, Cite Score; Metrics : h-index, g-index, i10 index, almetrics

Mode of Transactions: Lecture, Demonstration, Lecture cum demonstration, Experimentation, group discussions, Problem solving, Brain storming, Tutorial, Case study, Dialogue Mode, practical sessions.

Criteria of Evaluation: Continuous assessment will be done through tutorials, assignments, quizzes and group discussions. Weightage will be given for active participation. Final written examination will be conducted at the end of the course.

Mode of Transactions: Lecture, Demonstration, Presentation, Group Discussion, Lecture cum demonstration, Problem solving, Brain storming

Suggested Readings:

1. Ian Gregory, Textbook of Research Ethics- Theory and Practice, Continuum, London, 2003
2. Paul Oliver, The student's guide to research ethics, Open University Press, 2003
3. Adil E. Shamoo; David B. Resnik, Responsible conduct of research, Oxford University Press, 2003
4. Barbara H. Stanley; Joan E. Sieber; Gary B. Melton, Research Ethics: A Psychological approach, University of Nebraska, 1996

Course Title: Seminar
Paper Code: CHM.799

L	T	P	Cr
0	0	0	2

Total Contact Hours: 30

Learning Outcome: The student will be able to

- Elucidate and demonstrate the technical writing and present the problem in hand highlighting the various ways the problem is addressed in the literature.

The seminar must include discussion on topics such as awareness about weapons of mass destruction (chemical, biological, radiological, and nuclear weapons), disarmament, peaceful uses of chemistry, International Regulation of Biological and Chemical or Weapons of Mass Destruction.

Course Title: Advances in Chemistry of Molecular Clusters
Paper Code: CHM.705
Total Lectures: 60

L	T	P	Cr
4	0	0	4

Learning Outcomes: At the end of this course students will be able to

- Geometrical prediction of a cluster following the certain electron counting rules
- Basic for metallaborane chemistry handling
- Catalytically applications in absence of transition metals

Unit I **15 Hrs**
Main-group clusters: Geometric and electronic structure, three-, four- and higher connect clusters, the *closo*-, *nido*-, *arachno*-borane structural paradigm, Wade-Mingos and Jemmis electron counting rules, clusters with nuclearity 4-12 and beyond 12. Structure, synthesis and reactivity.

Unit II **15 Hrs**
Transition-metal clusters: Low nuclearity metal-carbonyl clusters and $14n+2$ rule, high nuclearity metal-carbonyl clusters with internal atoms. Structure, synthesis and reactivity. Capping rules, isolobal relationships between main-group and transition metal fragments, metal-ligand complexes vs heteronuclear cluster.

Unit III **15 Hrs**
Main-group Transition-metal clusters: Isolobal analogs of p-block and d-block clusters, limitations and exceptions. Clusters having interstitial main group elements, cubane clusters and naked or Zintl clusters.

Unit IV **15 Hrs**
Clusters Applications: Molecular clusters in catalysis, clusters to materials, boron-carbides and metal-borides. Illustrative examples from recent literature.

Mode of Transactions: Lecture, Demonstration, Lecture cum demonstration, Problem solving, Brain storming, Tutorial

Text Books:

1. Mingos, D. M. P. & Wales, D. J. (1990). *Introduction to Cluster Chemistry*, Prentice Hall.
2. Greenwood, N. N. & Earnshaw, E. A. (1997). *Chemistry of elements*, Second Edition, Butterworth-Heinemann.
3. Fehlner, T. P., Halet J. F. & Saillard, J.-Y. (2007) *Molecular Clusters: A Bridge to solid-state Chemistry*, Cambridge University press.
4. Gupta, B. D. & Elias, A. J. (2010). *Basic Organometallic Chemistry: Concepts, Synthesis, and Applications*, Universities Press (India).
5. Mingos, D. M. P. (1998). *Essential Trends in Inorganic Chemistry*, Oxford, University Press.
6. Housecroft, C. E. (1996). *Metal-Metal Bonded Carbonyl Dimers and Clusters*, Oxford Chemistry Primers (44), Oxford, University Press.

Course Title: Recent Trends in Synthetic Strategies and Green Catalysis

Paper Code: CHM.706

Total Lectures: 60

L	T	P	Cr
4	0	0	4

Learning Outcomes: At the end of this course students will be able to

- Implement various modern cross-coupling strategies for the synthesis of value added chemicals.
- Design chemical reactions using various benign tool of Green Chemistry such as ionic liquids, heterogeneous catalysts etc.

Unit I**15 Hours****Synthetic coupling strategies:**

Metal mediated coupling strategies: Mizoroki-Heck Reaction, Suzuki, Stille, Sonogashira, Buchwald-Hartwig reaction. Recent approaches for C-C bond formation, use of abundantly available/cheaper precursors: *N*-tosylarylhydrazones and arylalcohols as coupling partners, decarboxylative coupling, arylalcohols as in situ source of arylalkenes in coupling reactions.

Unit II**15 Hours****C-H bond functionalization:**

Concept of C-H bond activation, replacement of preactivation requirements, arylation of C-H bond, Functional group directed C-H bond activation, amide as directing group, Carboxylic acid as traceless directing group. Cross coupling of C-H substrates/oxidative coupling.

Dehydrative coupling (Direct coupling of a C-H bond with C-OH bond), scope and limitations.

Unit III**15 Hours****Modern Concept of Green Chemistry:**

Green Chemistry and principles, Tandem synthesis designing and challenges, multicomponent reactions (MCRs), Microwave Assisted Organic Synthesis (MAOS), Solid phase synthesis under microwave, aqueous media reactions, Ultrasound assisted Organic synthesis. Ionic liquids and their advantages. Biodegradable ionic liquids, supercritical fluids.

Unit IV**15 Hours****Green Catalysis:**

Types of ionic liquids: acidic, basic and neutral, Ionic liquid catalyzed reactions, Ionic liquids as organocatalysts, Dual role of ionic liquids: solvent as well as catalyst, *in situ* formation of palladium NHC complexes in imidazolium based ionic liquids, Supported ionic liquid catalysts, chiral ionic liquids and their role in asymmetric synthesis.

Recent achievements using catalytic oxidations with H₂O₂ as green oxidant. Solid acid catalysts.

Mode of Transactions: Lecture, Demonstration, Presentation, Group Discussion, Lecture cum demonstration, Problem solving, Brain storming

References:

1. Li, J. J. (2015). *CH bond activation in organic synthesis*. CRC press.
2. Diederich, F., & Stang, P. J. (Eds.). (2008). *Metal-catalyzed cross-coupling reactions*. John Wiley & Sons.
3. Anastas, P.T., Warner, J. C., (2000). *Green chemistry, Theory and Practical*. Oxford University Press, 1st edition.
4. Malhotra, S. V., (2007). *Ionic Liquids in Organic Synthesis*, Oxford University Press.
5. Rodriguez, N., & Goossen, L. J. (2011). Decarboxylative coupling reactions: a modern strategy for C-C-bond formation. *Chemical Society Reviews*, 40(10), 5030-5048.

6. Kumar, R., & Van der Eycken, E. V. (2013). Recent approaches for C–C bond formation via direct dehydrative coupling strategies. *Chemical Society Reviews*, 42(3), 1121-1146.
7. Shao, Z., & Zhang, H. (2012). *N-Tosylhydrazones: versatile reagents for metal-catalyzed and metal-free cross-coupling reactions*. *Chemical Society Reviews*, 41(2), 560-572.
8. Daugulis, O., Do, H. Q., & Shabashov, D. (2009). Palladium- and copper-catalyzed arylation of carbon–hydrogen bonds. *Accounts of chemical research*, 42(8), 1074-1086.
9. Mundy, B. P., Ellerd, M. G., & Favaloro Jr, F. G. (2005). *Name reactions and reagents in organic synthesis*. John Wiley & Sons.

Course Title: Chemistry of Nanoscience and Technology

Paper Code: CHM.707

Total Lectures: 60

L	T	P	Cr
4	0	0	4

Learning Outcomes: After completing this course students will be able to

- Learn about the background on Nanoscience
- Synthesis of nanomaterials and their characterization tools
- Apply their learned knowledge to application and the impact of nanomaterials on environment.

Unit I

15 Hrs

Introduction to Nanotechnology:

Scientific revolution- Atomic Structures-Molecular and atomic size-Bohr radius – Emergence of Nanotechnology –Definition of a Nano system - Types of Nanocrystals-One Dimensional (1D)-Two Dimensional (2D) -Three Dimensional (3D) nanostructured materials - Quantum dots - Quantum wire- Multifunctional nanostructures.

Unit II

15 Hrs

Synthesis of Nanomaterials:

Bulk Synthesis: Synthesis of bulk nanostructured materials - Sol Gel processing-Mechanical alloying and milling-inert gas condensation technique-bulk and nano composite materials - Grinding – high energy ball milling-types of balls-WC and ZrO₂-materials –ball ratio-limitations- melt quenching and annealing.

Physical and Chemical approaches: Self-assembly-Self Assembled Monolayers (SAM) - Vapour Liquid Solid (VLS) approach- Chemical Vapour Deposition (CVD) - Langmuir-Blodgett (LB) films - Spin coating – Templated self-assembly Electrochemical approaches: Anodic oxidation of alumina films, porous silicon and pulsed electrochemical deposition - Spray pyrolysis - Flame pyrolysis - Thin films – Epitaxy -Lithography.

Unit III

15 Hrs

Characterization Techniques for Nanomaterials:

Diffraction analyses :X-ray diffraction – powder diffraction–single crystal XRD –thin film analyses – determination of lattice parameters-structure analyses-rocking curve-strain analyses-phase identification-particle size analyses using Scherer's formula - X-ray photoelectron spectroscopy (XPS)- Auger electron spectroscopy (AES)- low energy electron diffraction and reflection high energy electron diffraction (LEED, RHEED).

Imaging techniques: Scanning Electron Microscope (SEM) – Field Emission scanning Electron microscope (FESEM)-Atomic force microscopy (AFM), scanning tunneling microscopy (STM), scanning near field optical microscopy (SNOM) – Transmission Electron Microscopy (TEM).

Spectroscopic techniques: Infra red spectroscopy (IR)- UV-visible-Absorption and reflection-Raman Scattering -Micro- Raman-tip enhanced Raman-Surface Enhanced Raman scattering (SERS) - Photoluminescence (PL) - Cathodeluminescence (CL).

Unit IV

15 Hrs

Applications of Nanomaterials: Photocatalysis- Solar cell-Water splitting-Energy Harvesting-Molecular electronics and nanoelectronics- LED- Quantum electronic devices - CNT based transistor and Field Emission Display - Biological applications - Biochemical sensor - Biological system - DNA and RNA - Lipids- Membrane based water purification.

Mode of Transaction: Lecture, Demonstration, Lecture cum demonstration, Dialogue Mode, Experimentation.

REFERENCE BOOKS:

1. Rao, C. N. R., Müller, A., & Cheetham, A. K. (Eds.). (2006). *The chemistry of nanomaterials: synthesis, properties and applications*. John Wiley & Sons.
2. BARIĆ, G. (2003). Charles P. Poole Jr. i Frank J. Owens: Introduction to Nanotechnology. Polimeri: časopis za plastiku i gumu, 24(2-4), 134-135.
3. Mukhopadhyay, S. M. (Ed.). (2011). *Nanoscale multifunctional materials: science and applications*. John Wiley & Sons.
4. Kelsall, R., Hamley, I. W., & Geoghegan, M. (Eds.). (2005). *Nanoscale science and technology*. John Wiley & Sons.

Course Title: Emerging Aspects in Supramolecular Chemistry

Paper Code: CHM.708

Total Lectures: 60

L	T	P	Cr
4	0	0	4

Learning Outcome: The students will acquire knowledge of

- Various supramolecular aspects of interaction between two chemical systems.
- Devising supramolecular systems based on complementarily and preorganizational requirements of host.

Unit I

15 Hrs

Introduction: Definition and development of supramolecular chemistry, nature of binding interactions in supramolecular structures: ion-ion, ion-dipole, dipole-dipole, h-bonding, cation- π , anion- π and van der waals interactions, supramolecular chemistry in life, ionophores, porphyrin and other tetrapyrrolic macrocycles, examples from biology and nature.

Host-guest chemistry: Classification of supramolecular host-guest compounds, pre- organization and complementarily, receptors, nature of supramolecular interactions. Synthesis and structure of crown ethers, lariat ether and podands, cryptands, spherands, calixarenes, cyclodextrins, cyclophanes, carcerands and

hemicarcerands. Concepts of selectivity, macrocyclic, macrobicyclic synthesis and template effects,

Unit II

15 Hrs

Cation Binding: Binding Constant and its determination, concept of coordination chemistry, cation complexation using various preorganized host, soft ligands including N, S and P based macrocycles, Schiff's base, proton and ammonium ion complexation, carbon donor and π - acid ligands, siderophores.

Anion Receptor: Anion recognition and its biological relevance, concepts on anion host design, from cation to anion hosts- a simple change in pH, guanidinium- based receptors, neutral receptors, organometallic receptors, coordination interactions. Chromogenic and fluorogenic receptors, dosimeters, ion pair recognition and zwitterion recognition.

Inclusion Complexes: Molecular guests and their inclusion complexation with Cyclodextrin, molecular clefts, tweezers, cryptophanes, cyclophanes, carcerands and hemicarcerands, solid state inclusion including clathrate formation, solid-liquid, solid-gas inclusions.

Unit III

15 Hrs

Molecular Self-assembly: Supramolecular polymers: definition, kinetic and thermodynamic consideration of self-assembly. self-assembly molecules: design, synthesis and properties of the molecules, self-assembly by H-bonding, proteins and foldamers, DNA, catenanes, rotaxanes, molecular knot: topology and examples including trefoil and borromean rings, surfactants self assembly, liquid crystals.

Dendrimers structure and nomenclature, synthesis and characterization, supramolecular chemistry of dendrimers and its assembly, dendritic nanodevices

Supramolecular polymers including amphiphilic block polymers and molecular imprinter polymers, biological self assembly in amyloids, actins and fibrin, Metal organic framework (MOF), covalent organic framework (COF) and supramolecular gels.

Unit IV

15 Hrs

Supramolecular and Molecular Devices: Supramolecular photochemistry and catalysis, molecular electronic devices: molecular electronic devices, molecular wires, molecular rectifiers, molecular switches and molecular logic gates, non-linear optical devices, organics for photonics and electronics.

Molecular Machines: Molecular machine terminology and bio-inspiration, ratchet mechanism including pulsating and tilt mechanism, covalent and supramolecular motors and their controlling mechanisms, machines based on catenanes and rotaxanes. Applications as molecular walkers, switchable catalysts, surface analysis at molecular dimensions.

Mode of Transactions: Lecture, Demonstration, Presentation, Group Discussion, Lecture cum demonstration, Problem solving, Brain storming

Suggested Readings:

1. Steed, J. W., & Atwood, J. L. (2013). *Supramolecular chemistry*. John Wiley & Sons.
2. Lehn, J. M. (1993). *Supramolecular chemistry*. Science, 260(5115), 1762-1764.
3. Beer, P. D., Gale, P. A., & Smith, D. K. (1999). *Supramolecular chemistry*. Oxford University Press
4. Lehn, J. M. (2017). Supramolecular chemistry: Where from? Where to?. *Chemical Society Reviews*, 46(9), 2378-2379.

5. Huang, Z., Qin, K., Deng, G., Wu, G., Bai, Y., Xu, J. F., ... & Zhang, X. (2016). Supramolecular chemistry of cucurbiturils: tuning cooperativity with multiple noncovalent interactions from positive to negative. *Langmuir*, 32(47), 12352-12360.
6. Bruns, C. J., & Stoddart, J. F. (2014). Rotaxane-based molecular muscles. *Accounts of chemical research*, 47(7), 2186-2199.
7. Blanco, V., Carlone, A., Hänni, K. D., Leigh, D. A., & Lewandowski, B. (2012). A rotaxane-based switchable organocatalyst. *Angewandte Chemie International Edition*, 51(21), 5166-5169.
8. Sauvage, J. P. (2017). From chemical topology to molecular machines (Nobel lecture). *Angewandte Chemie International Edition*, 56(37), 11080-11093.
9. Leigh, D. A. (2016). Genesis of the nanomachines: The 2016 Nobel prize in chemistry. *Angewandte Chemie International Edition*, 55(47), 14506-14508.
10. Ogoshi, T., Yamagishi, T. A., & Nakamoto, Y. (2016). Pillar-shaped macrocyclic hosts pillar [n] arenes: new key players for supramolecular chemistry. *Chemical reviews*, 116(14), 7937-8002.
11. Kolesnichenko, I. V., & Anslyn, E. V. (2017). Practical applications of supramolecular chemistry. *Chemical Society Reviews*, 46(9), 2385-2390.
12. Cui, H., & Xu, B. (2017). Supramolecular medicine. *Chemical Society Reviews*, 46(21), 6430-6432.

Course Title: Advanced Bio-inorganic and Biophysical Chemistry

L	T	P	Cr
4	0	0	4

Paper Code: CHM.709

Total Contact Hours: 60

Learning Outcome: At the end of this course student will be able to

- Determined structure and biological functions of metalloproteins and enzymes.
- Classify of metallobiomolecules on the basis of their functional properties.
- Know the role of metals in biology
- Determined the factors that govern the thermodynamic and mechanical stability, folding, and dynamics of proteins.
- Work on the kinetics, thermodynamics, and mechanism of protein folding.

Unit I

15 Hrs

Inorganic Chemistry of Enzymes - I

Metalloporphyrins: hemoglobin and myoglobin, types of hemoglobin, nature of heme-dioxygen binding, model systems, cooperativity in hemoglobin, physiology of myoglobin and hemoglobin, structure and function of haemoglobin and myoglobin. role of distal histidine in haemoglobin and myoglobi, sickle cell hemoglobin and its consequences, Hemoglobin and its allosteric properties, Bohr effect.

Other iron-prophyrin biomolecules, peroxidases and catalases, cytochromes, cytochrome P450 enzymes, other natural oxygen carriers, hemerythrins, electron transfer. Biochemistry of iron, iron storage and transport, ferritin, transferrin, bacterial iron transport.

Unit II**15 Hrs****Inorganic Chemistry of Enzymes - II**

Metallothioneins: ferridoxins, carboxypeptidase, carbonicanhydrase, blue copper proteins, superoxide dismutase, hemocyanines, photosynthesis, respiration and photosynthesis; chlorophyll and photosynthetic reaction center.

Enzymes: Structure and function, inhibition and poisoning vitamin B₁₂ and B₁₂ coenzymes metallothioneins, nitrogen fixation, in-vitro and in-vivo nitrogen fixation, bio-inorganic chemistry of Mo and W.

Metal Ions in Biological Systems

Role of metal ions in replication and transcription process of nucleic acids. Biochemistry of calcium as hormonal messenger, muscle contraction blood clotting, neurotransmitter, calcification reclaiming of barren land. metals in the regulation of biochemical events.

Unit III**15 Hrs**

Biophysical Chemistry: Principles of biophysical chemistry (pH, buffer, reaction kinetics, thermodynamics, colligative properties), structure and physical properties of amino acids, physical principle of structure, function, and folding of proteins, conformations of proteins (Ramachandran plot, secondary, tertiary and quaternary structure; domains; motif and folds), determination of protein structures by spectroscopic methods (CD, FTIR, NMR),

Unit IV**15 Hrs**

Ultrafast reactions and their application in protein chemistry, ultrafast folding dynamics study by laser flash photolysis, photoreduction and photoligand dissociation induced ultrafast folding events, photoreduction-induced metal release studies of metalloproteins, Thermodynamics of protein folding by spectroscopic and calorimetric methods, ultrafast folding dynamics study by laser flash photolysis, protein conformational study by NMR and fluorescence spectroscopy, measurement of hydrodynamic radii by dynamic light scatter and FCS, mechanical unfolding studies by force clamp spectroscopy.

Mode of Transactions: Lecture, Demonstration, Presentation, Group Discussion, Lecture cum demonstration, Problem solving, Brain storming

SUGGESTED READINGS

1. Huheey, J. E., Keiter, E. A., Keiter, R. L., and Medhi, O. K. (2006). *Inorganic chemistry: principles of structure and reactivity*. Pearson Education India.
2. Douglas, B. E., and McDaniel, D. H. (1965). *Concepts and models of inorganic chemistry*. John Wiley and Sons.
3. Cotton, F. A., and Wilkinson, G. (1988). *Advanced inorganic chemistry* (Vol. 545). New York: Wiley.
4. Elschenbroich, C. (2016). *Organometallics*. John Wiley and Sons.
5. Atkins, P., Overton, T., Rourke, J., Weller, J., and Armstrong, F., (2010). *Shriver and Atkins' inorganic chemistry*. Oxford University Press.
6. Cowan, J.A. (1997). *Inorganic Biochemistry: An Introduction*. Wiley – VCH.
7. Lippard, S. J. (1991). *Progress in Inorganic Chemistry*. Vol. 18, Wiley-Interscience.
8. Lippard, S. J. (1991). *Progress in Inorganic Chemistry*. Vols. 38, Wiley-Interscience.

9. Lesk, A.M., (2010). *Introduction to Protein Science: Architecture, Function, and Genomics*. Oxford University Press.
10. Cantor, C.R. and Schimmel, P.R., (1980). *Biophysical Chemistry*. Freeman.
11. Van Holde, K.E., Johnson, W.C., and Ho, P.S., (2006). *Principles of Physical Biochemistry*. Pearson Education.
12. Harding, S.E. and Chowdhry, B. Z. (2001). *Protein-Ligand Interactions*. Oxford University Press.

Course Title: Applied Material Chemistry

Paper Code: CHM.710

Total Contact Hours: 60

L	T	P	Cr
4	0	0	4

Learning Outcome: The students will be able to

- Elucidate the magnetic materials and their properties based on their solid state structures.
- Elucidate and apply various methods of characterizations for the elucidation of the material structure and properties.

Unit I

15 Hrs

Magnetic Materials (Ferrites) Introduction, structure and classification, hard and soft ferrites, synthesis of ferrites by various methods (precursor and combustion method), characterization of ferrites by Mossbauer spectroscopy, significance of hysteresis loop and saturation magnetization in ferrites, magnetic properties of ferrites, applications of ferrites.

Glasses, Ceramics, Composites and Nanomaterials

Glassy state, glass formers and glass modifiers, applications. ceramic structures, mechanical properties, clay products. microscopic composites; dispersion-strengthened and particle-reinforced, fibre-reinforced composites, macroscopic composites, nanocrystalline phase, preparation procedures, special properties, applications.

Unit II

15 Hrs

Mesomorphic behaviour, thermotropic liquid crystals, positional order, bond orientational order, nematic and smectic mesophases; smectic - nematic transition and clearing temperature -homeotropic, planar and schlieren textures, twisted nematics, chiral nematics, molecular arrangement in smectic A and smectic C phases, optical properties of liquid crystals. dielectric susceptibility and dielectric constants. lyotropic phases and their description of ordering in liquid crystals.

Thin Films and Langmuir- Blodgett Films

Preparation techniques; evaporation/sputtering, chemical process, sol gel etc. Langmuir - Blodgett (LB) films, growth technique, photolithography, properties and applications of thin and LB films

Materials for Solid State Devices

Rectifiers, transistors, capacitors -IV-V compounds, low-dimensional quantum structure; optical properties.

Unit III

15 Hrs

Types of ionic conductors, mechanism of ionic conduction, interstitial jumps (Frenkel); vacancy mechanism, diffusion superionic conductors; phase transitions and mechanism of conduction in superionic conductors, examples and applications of ionic conductors.

Molecular Conductor: Oligo (phenylene vinylene)s, oligo(phenylene ethynylene)s, oligo (eneyne)s, oligo(thiophene vinylene), oligo (thiophene ethynylene) etc. and their applications.

Unit IV

15 Hrs

Fullerenes, Carbon Nanotubes and Graphene: Types and Properties, methods of preparation and separation of carbon nanotubes, applications of fullerenes, CNTs and graphene.

Nonlinear optical materials: Non-linear optical effects, second and third order – molecular hyperpolarisability and second order electric susceptibility – materials for second and third harmonic generation.

Mode of Transactions: Lecture, Demonstration, Presentation, Group Discussion, Lecture cum demonstration, Problem solving, Brain storming

SUGGESTED READINGS

1. Ashcroft, N.W. and Mermin, N.D. Solid State Physics, 1976, Saunders College.
2. Callister, W.D. and Rethwisch, D. G. Material Science and Engineering: An Introduction, 9th Edition, 2014, Willey.
3. Anderson, J.C. Leaver, K.D. Alexander J.M. and Rawlings, R.D. Material Science, 5th Edition, 2003, Nelson and Thornes.
4. Keer, H.V. Principle of the Solid State, 1993, New Age International.

Course Title: Advanced Organotransition Metal Chemistry

Paper Code: CHM.711

Total Contact Hours: 60

L	T	P	Cr
4	0	0	4

Learning Outcome: At the end of this course student will be able to

- The chemistry of transition metal complexes and compounds of transition metal-carbon multiple bonds
- Chemistry on alkyls and aryls of transition metals and fluxional organometallic compounds
- Workout on homogeneous catalysis with appropriate planning.

Unit I

15 Hrs

Compounds of Transition Metal-Carbon Multiple Bonds

Alkylidenes, alkylidynes, low valent carbenes and carbynes-synthesis, nature of bond, structural characteristics, nucleophilic and electrophilic reaction on the ligands, role in organic synthesis

Unit II

15 Hrs

Transition Metal Complexes

Transition metal complexes with unsaturated organic molecules, alkenes, alkynes, allyl, diene, dienyl, arene and trienyl complexes, preparations, properties, nature of bonding and structural features important reactions relating to nucleophilic and electrophilic attack on ligands and to organic synthesis, metallocenes.

Unit III

15 Hrs

Alkyls and Aryls of Transition Metals

Types, routes of synthesis, stability and decomposition pathways, organ copper in organic synthesis.

Fluxional organometallic compounds

Fluxionality and dynamic equilibria in compounds such as η^2 olefin, η^2 allyl and dienyl complexes.

Unit IV

15 Hrs

Homogeneous Catalysis

Stoichiometric reaction for catalysis, homogeneous catalytic hydrogenation, Zeigler-Natta polymerization of olefins, catalytic reactions involving carbon monoxide such as hydrocarbonylation of olefins (oxo reaction) oxopalladation reactions, activation of C-H bond.

Mode of Transactions: Lecture, Demonstration, Lecture cum demonstration, Problem solving, Brain storming, Tutorial

SUGGESTED READINGS

1. Collman, J.P.; Norton, J.R.; Hegsdus, L.S.; Finke, R.G. (1987). *Principles and Application of Organotransition Metal Chemistry*, University Science Books.
2. Crabtree, R. G. (2011). *The Organometallic Chemistry of the Transition Metals*, 5th edition, , John Wiley.
3. Mehrotra R. C. & Singh, A. (2005). *Organometallic Chemistry*, 2nd edition, New Age International.
4. Cotton, F.A. and Wilkinson, G. (1999). *Advanced Inorganic Chemistry*, 6th edition, John Wiley.
5. Pearson, A.J. (1985). *Metallo-Organic Chemistry*, Wiley.

Course Title: Advanced Organic Synthesis and Catalysis

Paper Code: CHM.712

Total Contact Hours: 60

L	T	P	Cr
4	0	0	4

Learning Outcomes: At the end of this course students will be able to

- Apply various asymmetric tools for the synthesis of chiral compounds in their research.
- Use various reagents including organometallic compounds, experimental conditions in organic synthesis.
- Design the synthesis of functionalized molecules utilizing phosphorus and sulphur ylides.

Unit I

15 Hours

Organometallic compounds and Coupling reactions:

Organoboranes: Disiamyl borane, thexyl borane, 9-BBN and disopinacamplyel borane, functional group transformations of organo boranes: oxidation, protonolysis and rearrangements. Formation of C-C bonds *viz* organo boranes carbonylation.

Organolithium, organozinc and organocopper and organopalladium compounds.

Palladium catalyzed chemistry for C-C bond formation reaction: Heck coupling, Sonogshira coupling, Suzuki-Miyaura coupling, Negishi coupling.

Unit II**15 Hours**

Asymmetric synthesis and industrial applications: Various tools of asymmetric synthesis: Chiral pools, chiral catalysis: chiral auxiliaries (SAMP/RAMP): Industrial applications of chiral auxiliaries for the synthesis of Tipranavir and Atorvastatin, methods of asymmetric induction—substrate, reagent and catalyst controlled reactions; determination of enantiomeric and diastereomeric excess; enantio-discrimination. resolution – optical and kinetic, chemo- regio- and stereoselective transformations, organocatalysis and biocatalysis

Unit III**15 Hours**

Reaction of ylides: Phosphorus ylide; structure and reactivity, stabilized ylides, effects of ligands on reactivity, Wittig, Wittig-Horner and Wadsworth, Emmons reactions-mechanistic realization; E/Z selectivity for olefin formation, Schlosser modification: Sulphur ylides; stabilized and non-stabilized ylides: thermodynamically and kinetically controlled reactions with carbonyl compounds, regio- and stereo-selective reactions.

Unit IV**15 Hours**

Reagents in organic synthesis: Lithiumdiisopropylamide (LDA) and its use for controlling the stereochemistry of product, Baker's yeast, strategies for reactivity umpolung, Trimethylsilyliodide, Prevost Hydroxylation, Ionic liquids and quaternary ammonium and Phosphonium salts, Merrifield resin, Fenton's reagents, Ziegler-Natta catalyst, Lawesson reagents, applications of K-selectride and L-selectride for selective reduction, IBX, Sodium triacetoxyborohydride for reductive amination, Fetizon reagent, Dioxiranes, Tebbe reagent, Corey-Nicolaou reagent, Mosher's reagent, use of Os, Ru, and Tl reagents.

Mode of Transactions: Lecture, Demonstration, Presentation, Group Discussion, Lecture cum demonstration, Problem solving, Brain storming

Suggested Readings

1. Mundy, B. P., Ellerd, M. G., and Favaloro Jr, F. G., (2005). *Name Reactions And Reagents In Organic Synthesis*. John Wiley and Sons.
2. Claydon, J., Gleeves, N., Warren, S., and Wothers, P., (2001). *Organic Chemistry*. Oxford University Press, UK.
3. Finar, I.L., (2012). *Organic Chemistry*. Pearson Education, UK.
4. Li, J. J., (2014). *Name Reactions: A Collection of Detailed Reaction Mechanism*. Springer-Verlag.
5. Smith, M. B., (2013). *March's Advanced Organic Chemistry: Reactions, Mechanisms, And Structure*. John Wiley and Sons.
6. Corey, E.J. and Cheng, X.-M.(1989). *The Logic of Chemical Synthesis*. John Wiley and Sons.
7. Fuhrhop, J. H., Penzlin, G., and Li, G., (2003). *Organic Synthesis: Concepts And Methods*. John Wiley and Sons.
8. Davies, S. G., (2013). *Organotransition Metal Chemistry: Applications to Organic Synthesis: Applications to Organic Synthesis (Vol. 2)*. Elsevier.

9. Aitken, A., and Kilényi, S. N., (Eds.). (1992). *Asymmetric Synthesis*. CRC Press.
10. Proctor G. (1996). *Asymmetric Synthesis*. Academic Press.

Course Title: Analytical Chemistry and Instrumental Methods

Paper Code: CHM.713

Total Contact Hours: 60

L	T	P	Cr
4	0	0	4

Learning Outcome: The students will be able to

- Choose the method of analysis based on the sample amount/volume, accuracy and precision required for analysis and interference.
- Demonstrate the understanding and application of the principles of instrumental analysis.

Unit I

15 Hrs

Errors in Quantitative Analysis: Accuracy, precision, sensitivity, specificity, mean and standard deviation, classification of errors and their minimization, significant figures, standard reference materials, linear regression, covariance and correlation coefficient.

Quantitative Analysis: Concepts important to quantitative analysis, classification of methods for quantitative analysis, choice of method for analysis, theory of volumetric and gravimetric methods of analysis.

Unit II

15 Hrs

Analytical Spectroscopy: Principle, applications and limitations of spectrophotometry, Beer-Lambert law, analysis of mixtures, sources and treatment of interferences and detection limits to be considered in each of the techniques, fluorescence spectrometry, atomic absorption spectrometry (AAS); flame AAS, electrothermal AAS (ETAAS).

Unit III

15 Hrs

Potentiometry – General principles, calomel electrodes, Ag/AgCl electrodes, membrane electrodes – ion selective electrodes, glass electrodes, liquid membrane electrodes, biosensors.

Amperometry/Coulometry: Basic principles, constant current and constant potential coulometry. coulometric titrations.

Voltammetry: Principles, dropping mercury electrode (DME), polarography, half-wave potential, different wave forms–linear scan, square scan and triangular scan, cyclic voltammetry, voltammograms, and applications of stripping voltametry.

Unit IV

15 Hrs

Chromatography: Partition and distribution, principles of chromatography, plate and rate theory. retention time and retention factor, resolution and separation factor; general idea about adsorption, partition and column chromatography, paper and thin layer chromatography, gas chromatography (GC) and high performance liquid chromatography (HPLC) - instrumentation, methodology and applications. UPLC, SFC LC, hyphenated techniques, LC-MS and LC MS/MS.

Mode of Transactions: Lecture, Demonstration, Presentation, Group Discussion, Lecture cum demonstration, Problem solving, Brain storming

SUGGESTED READINGS

1. Holler, F. J., Skoog, D. A., & Crouch, S. R. (2007). Chapter 1. *Principles of Instrumental Analysis* (6th ed.). Cengage Learning.
2. Willard, H. H., Merritt Jr, L. L., Dean, J. A., & Settle Jr, F. A. (1988). *Instrumental Methods of Analysis*, 7th edition, 2007, CBS Publishers.
3. Mendham, J. Denney, R.C., Jeffery, G.H., and Mendham, J. (2006). *Vogel's Textbook of Quantitative Chemical Analysis*. Pearson Education India.
4. Skoog, D. A., West, D. M., Holler, F. J., & Crouch, S. R. (2013). *Fundamentals of Analytical Chemistry*. Nelson Education.
5. Christian, G. D. (2003). *Analytical Chemistry*, 6th edition. John Wiley and Sons, PA, 1-2.
6. Bard, A. J., Faulkner, L. R., Leddy, J., & Zoski, C. G. (1980). *Electrochemical Methods: Fundamentals and Applications* (Vol. 2, p. 1). New York: Wiley.
7. Rouessac, F., & Rouessac, A. (2013). *Chemical Analysis: Modern Instrumentation Methods and Techniques*. John Wiley & Sons.
8. Danzer, K. (2007). *Analytical Chemistry: Theoretical and Metrological Fundamentals*. Springer Science & Business Media.

Course Title: Emerging Trends in Green Synthesis and Drug Discovery

Paper Code: CHM.714

Total Contact Hours: 60

L	T	P	Cr
4	0	0	4

Learning outcomes:

Students will be able to:

- Elucidated the mechanism of microwave assisted organic transformation
- Conduct ionic liquids, solid supported organic reactions under MW and conventional conditions
- Utilize metal and organocatalysts for various C-C and C-N bond formation reactions
- Apply recent tools in drug discovery and developments

Unit I

15 hours

Microwave Assisted Organic synthesis (MAOS): Heating effects of microwaves: (i) Dipolar polarization and (ii) Ionic conduction, Synthesis of target molecules under solventless conditions and on solid support, Microwave and stereoselectivity, Recent advancement in aqueous reaction conditions and microwave.

Unit II

15 hours

Synthesis of Bioactive molecules using Ionic Liquids: Ionic liquids as green solvents, Replacement of volatile organic solvents and environmental impact, Ionic liquids as catalyst, Designer solvents, Ionic liquids and asymmetric synthesis.

Unit III**15 hours****Developments in metal and catalysis**

New developments in the palladium catalyzed chemistry for C-C bond formation reaction, copper catalyzed C-N bond formation reactions, metal catalyzed reactions under microwave conditions, Solid supported reactions, Organic catalytic systems, Click Chemistry.

Unit IV**15 hours**

Recent Trends in Drug Discovery: Computer in drug designing, Natural product based drug design, Identification of target molecules, Lead candidate and lead optimization, Ligands with multi receptor affinity profile, Diversity oriented synthesis in drug discovery, Nano drug delivery systems.

Mode of Transactions: Lecture, Demonstration, Presentation, Group Discussion, Lecture cum demonstration, Problem solving, Brain storming

Suggested Reading:

1. Mann and Saunders. (2009). *Practical organic chemistry*, Pearson, 4th edition, UK.
2. Anastas, P.T.; Warner J. C. (2000). *Green chemistry, Theory and Practical*. Oxford University Press, 1st edition, US.
3. Paul, M.D. (1997). *Medicinal Natural Products: A Biosynthetic Approach*, John Wiley & Sons., New York.
4. Walton, N.J., Brown, D.E. (1999). *Chemicals from Plants: Perspectives on Plant Secondary Products*, Imperial College Press, London.
5. Gang, D. R., Wang, J., Dudareva, N., Nam, K. H., Simon, J. E., Lewinsohn, E., & Pichersky, E. (2001). An investigation of the storage and biosynthesis of phenylpropenes in sweet basil. *Plant physiology*, 125(2), 539-555.
6. Rubenstein, K., (2009), Medicinal Chemistry for Drug Discovery: Significance of Recent Trends, Insight Pharma Reports.
7. King, F. D. (2003). *Medicinal Chemistry Principles and Practice*, Royale Society of Chemistry, 2nd Edition, London.

Course Title: Advanced Spectroscopy**Paper Code: CHM.715****Contact Hours: 60**

L	T	P	Cr
4	0	0	4

Learning outcomes:

Students will be able to:

- Elucidate the UV-visible spectrum and effect of various factors on UV absorption
- Interpret the IR spectrum having different functional groups and effect of various factors on IR absorption
- Elucidate the structure of simple and complex organic molecules and their stereochemistry
- Elucidate the structure of organic molecules using fragmentation pattern

Unit I**10 hours**

Ultraviolet and Visible Spectroscopy : Various electronic transitions (185-800 nm), Beer- Lambert law, effect of solvent on electronic transitions, ultraviolet bands for carbonyl compounds, unsaturated carbonyl compounds, dienes, conjugated polyenes. Fieser-Woodward rules for conjugated dienes and carbonyl compounds, ultraviolet spectra of aromatic and heterocyclic compounds. Steric effect in biphenyls. Interpretation of UV spectra.

Unit II**10 hours**

Infrared Spectroscopy: Instrumentation and sample handling. Fundamental vibrations, overtones, combination bands and Fermi resonance. Characteristic vibrational frequencies of alkenes, alkynes, aromatic compounds, alcohols, ethers, phenols and amines. Detailed study of Vibrational frequencies of carbonyl compounds (ketones, aldehydes, esters, amides, acids, anhydrides, lactones, lactams and conjugated carbonyl compounds). Effect of hydrogen bonding and solvent effect on vibrational frequencies. Interpretation of IR spectra.

Unit III**20 hours**

Nuclear Magnetic Resonance Spectroscopy: Chemical exchange, effect of deuteration, complex spin-spin interaction between two, three, four and five nuclei (first order spectra), virtual coupling. Stereochemistry, hindered rotation, Karplus curve-variation of coupling constant with dihedral angle. Second order spectra, Simplification of complex spectra-nuclear magnetic double resonance, contact shift reagents, solvent effects. Fourier transform technique, chemical shift reagents, nuclear Overhauser effect (NOE). Resonance of other nuclei-F, P. Carbon-13 NMR Spectroscopy: coupling constants. Two dimension NMR spectroscopy – COSY, NOESY, DEPT, INEPT, APT and INADEQUATE techniques. Interpretation of ^1H and ^{13}C -NMR spectra.

Unit IV**20 hours**

Mass Spectrometry: Introduction, Ion production & detection – EI, CI, FD, FAB, HRMS, factors affecting fragmentation, ion analysis, ion abundance. Mass spectral fragmentation of organic compounds, common functional groups, molecular ion peak, metastable peak, McLafferty rearrangement. Nitrogen rule. High resolution mass spectroscopy. Examples of mass spectral fragmentation of organic compounds with respect of their structure determination, MALDI, APCI & GSI.

Mode of Transactions: Lecture, Demonstration, Presentation, Group Discussion, Lecture cum demonstration, Problem solving, Brain storming

Suggested Readings

1. Pavia, D. L., Lampman, G. M., Kriz, G. S., and Vyvyan, J. A. (2008). *Introduction to Spectroscopy*. Cengage Learning.
2. Gross, J. H. (2006). *Mass Spectrometry: A Textbook*. Springer Science and Business Media.

3. Banwell, C. N., and McCash, E. M. (1994). *Fundamentals of Molecular Spectroscopy* (Vol. 851). New York: McGraw-Hill.
4. Dyer, J. R. (1965). *Applications of Absorption Spectroscopy of Organic Compounds*. Phi Learning.
5. Kalsi, P. S. (2007). *Spectroscopy of Organic Compounds*. New Age International.
6. Kemp, W. (1998). *Organic Spectroscopy*, ELBS.
7. Khopkar, S. M. (1998). *Basic Concepts of Analytical Chemistry*. New Age International.
8. Melinda, J.D. (2010). *Introduction to Solid NMR Spectroscopy*. Wiley India Pvt Ltd.
9. Mendham, J., Denney, R. C., Barnes, J. D., and Thomas, M. J. K. (2008). *Vogel's Textbook of Quantitative Chemical Analysis*, Dorling Kindersley.
10. Silverstein, R. M., Webster, F. X., Kiemle, D. J., and Bryce, D. L. (2014). *Spectrometric Identification of Organic Compounds*. John Wiley and Sons.

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