Central University of Punjab

Course Structure and Syllabus

Ph.D. Chemistry

Session: 2023 onwards

Department of Chemistry
School of Basic Sciences

Graduate Attributes:

After completion of the PhD program students will be able to work independently on research problems and solutions. The students will develop ability to identify research problem, propose hypothesis, conduct experiments and analyze the results to propose probable solutions. The students will also able to disseminate the knowledge and information and supervise other researchers in the field of chemical sciences. The students will also be able to write scientific papers and communicate their findings to the scientific community all over the world.

Department of Chemistry, CUP, Bathinda

Semester I

S. No.	Paper Code	Course Title	L	T	P	C
1.	CHM.701	Research Methodology and Computer Applications	4	0	0	4
2.	CHM.751	Research and Publication Ethics	2	0	0	2
3	CHM.752	Teaching Assistantship	0	0	2	1
4.	UNI.753	Curriculum, Pedagogy and Evaluation	1	0	0	1
5.	CHM.799	Seminar	0	2	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
17	CHM.716	Natural Products Based Drug Discovery	4	0	0	4
18.	CHM.717	Molecular Manufacturing Science & Technology	4	0	0	4
		Total	**11**	**2**	**2**	**14**

*To be offered by School of Education

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

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

Course Title: Research Methodology and Computer Applications
Paper Code: CHM.701
Total Lecture: 60

L	T	P	Credits
4	-	-	4

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

CLO1: Review and formulate hypotheses backed with a research plan.
CLO2: Write a technical document.
CLO3: Identify the overall process of designing a research study
CLO4: Familiarize with research laboratory and their practices
CLO5: To understand the protection of innovation and intellectual property rights
CLO6: Acquaint with various software in research

Units/ hours	Content	Mapping with CLOs
Unit-1 **15 Hours**	**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. **Technical Writing:** Scientific writing, writing synopsis, Research paper, Poster preparation, oral presentations and Dissertations. Reference Management using various softwares such as Endnote, reference manager, Refworks, etc. Communication skills: defining communication; type of communication; techniques of communication, etc.	**CLO1, CLO2, CLO3**
Unit-2 **15 Hours**	**Introduction and Principles of Good Lab Practices:** Good laboratory practices: Introduction, History of Good Laboratory Practices, Waste disposal and management, Quality Standards and Quality Assurances, WHO guidelines on GLP and GMP, Chemical Hazards and classification, Radiation hazards and control of exposure to radiation, personal protective equipments, fire prevention methods. Biosafety for human health and environment. Biosafety in Clinical laboratories and biohazard management.	**CLO2**
Unit-3 **15 Hours**	**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), Technology Development/Transfer Commercialization Related Aspects, Ethics and Values in IP.	**CLO5**
Unit-4 **15 Hours**	**Computer Applications:** Parts of computers, Hardware, BIOS, Operating systems, Microsoft Office Application, Literature, Reference and Citation Management, Binary system, Logic gates and Boolean algebra. Image processing applications. Applications of computer in chemical sciences	**CLO6**

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 Tile: Research and Publication Ethics
Paper Code: CHM.751
Total Contact Hours: 30

L	T	P	Credits
2	0	0	2

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

CLO1: Familiar with philosophy of science and ethical issues in research.
CLO2: Interpret intellectual honesty and research integrity.
CLO3: Identify publication ethics.
CLO4: Evaluate predatory publications and journals.
CLO5: Analyze indexing and citation databases, research metrics and plagiarism tools

Units/ hours	Content	Mapping with CLOs
Unit-1 **7 Hours**	**Philosophy and Ethics:** Introduction to Philosophy: definition, nature and scope, content, branches Ethics: definition, moral philosophy, nature of moral judgements and reactions	**CLO1**
Unit-2 **4 Hours**	**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	**CLO2**
Unit-3 **11 Hours**	**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 behavior 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.	**CLO3, CLO4**

Unit-4 **11 Hours**	**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.	**CLO4, CLO5**

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: TEACHING ASSISTANTSHIP
Course Code: CHM.752
Total Hours: 30
Learning Outcome:

L	T	P	Credit
0	0	2	1

At the end of this skill development course, the scholars shall be able to

CLO1: familiarize themselves with the pedagogical practices of effective class room delivery and knowledge evaluation system

CLO2: manage large and small classes using appropriate pedagogical techniques for different types of content

Activities and Evaluation:

- The scholars shall attend Master degree classes of his/her supervisor to observe the various transaction modes that the supervisor follows in the class room delivery or transaction process one period per week.
- The scholars shall be assigned one period per week under the direct supervision of his/her supervisor to teach the Master degree students adopting appropriate teaching strategy(s).
- The scholars shall be involved in examination and evaluation system of the Master degree students such as preparation of questions, conduct of examination and preparation of results under the direction of the supervisor.
- At the end of the semester, the supervisor shall conduct an examination of teaching skills learned by the scholar as per the following **evaluation criteria**:
    - The scholars shall be given a topic relevant to the Master degree course of the current semester as his/her specialization to prepare lessons and deliver in the class room before the master degree students for one hour (45 minutes teaching + 15 minutes interaction).
    - The scholars shall be evaluated for a total of 50 marks comprising *content knowledge* (10 marks), *explanation and demonstration skills* (10 marks), *communication skills* (10 marks), *teaching techniques employed* (10 marks), and classroom interactions (10).

Course Title: CURRICULUM, PEDAGOGY AND EVALUATION
Course Code: **UNI.753**
Total Hours: 15

L	T	P	Credit
1	0	0	1

Learning outcomes:

After completion of the course, scholars shall be able to:

- **CLO1:** analyze the principles and bases of curriculum design and development
- **CLO2:** examine the processes involved in curriculum development
- **CLO3:** develop the skills of adopting innovative pedagogies and conducting students' assessment
- **CLO4:** develop curriculum of a specific course/programme

Units/ hours	Content	Mapping with CLOs
Unit-1 4 Hours	**Bases and Principles of Curriculum** 1. Curriculum: Concept and Principles of curriculum development, Foundations of Curriculum Development. 2. Types of Curriculum Designs- Subject centered, learner centered, experience centered and core curriculum. Designing local, national, regional and global specific curriculum. Choice Based Credit System and its implementation.	**CLO1**
Unit-2 4 Hours	**Curriculum Development** 1. Process of Curriculum Development: Formulation of graduate attributes, course/learning outcomes, content selection, organization of content and learning experiences, transaction process. 2. Comparison among Interdisciplinary, multidisciplinary and trans-disciplinary approaches to curriculum.	**CLO2**
Unit-3 3 Hours	**Curriculum and Pedagogy** 1. Conceptual understanding of Pedagogy. **2.** Pedagogies: Peeragogy, Cybergogy and Heutagogy with special emphasis on Blended learning, Flipped learning, Dialogue, cooperative and collaborative learning **3.** Three e- techniques: Moodle, Edmodo, Google classroom	**CLO3**
Unit-4 4 Hours	**Learners' Assessment** 1. Assessment Preparation: Concept, purpose, and principles of preparing objective and subjective questions. 2. Conducting Assessment: Modes of conducting assessment – offline and online; use of ICT in conducting assessments.	**CLO4**

Transaction Mode

Lecture, dialogue, peer group discussion, workshop

Evaluation criteria

There shall be an end term evaluation of the course for 50 marks for duration of 2 hours. The course coordinator shall conduct the evaluation.

Suggested Readings

- Allyn, B., Beane, J. A., Conrad, E. P., & Samuel J. A., (1986). *Curriculum Planning and Development*. Boston: Allyn & Bacon.
- Brady, L. (1995). *Curriculum Development*. Prentice Hall: Delhi. National Council of Educational Research and Training.
- Deng, Z. (2007). Knowing the subject matter of science curriculum, *Journal of Curriculum Studies*, 39(5), 503-535. https://doi.org/10.1080/00220270701305362
- Gronlund, N. E. & Linn, R. L. (2003). *Measurement and Assessment in teaching*. Singapore: Pearson Education
- McNeil, J. D. (1990). *Curriculum: A Comprehensive Introduction*, London: Scott, Foreman/Little
- Nehru, R. S. S. (2015). *Principles of Curriculum*. New Delhi: APH Publishing Corporation.
- Oliva, P. F. (2001). *Developing the curriculum* (Fifth Ed.). New York, NY: Longman
- Stein, J. and Graham, C. (2014). *Essentials for Blended Learning: A Standards-Based Guide*. New York, NY: Routledge.

Web Resources

- https://www.westernsydney.edu.au/__data/assets/pdf_file/0004/467095/Fundamentals_of_Blended_Learning.pdf
- https://www.uhd.edu/academics/university-college/centers-offices/teaching-learning-excellence/Pages/Principles-of-a-Flipped-Classroom.aspx
- http://leerwegdialoog.nl/wp-content/uploads/2018/06/180621-Article-The-Basic-Principles-of-Dialogue-by-Renate-van-der-Veen-and-Olga-Plokhooij.pdf

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

L	T	P	Credits
4	0	0	4

Course Title: Seminar
Paper Code: CHM.799
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.

Total Lectures: 60

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

CLO1: Geometrical prediction of a cluster following the certain electron counting rules
CLO2: Basic for metallaborane chemistry handling
CLO3: Catalytically applications in absence of transition metals

Units/ hours	Content	Mapping with CLOs
Unit-1 **15 Hours**	**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.	**CLO1**
Unit-2 **15 Hours**	**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.	**CLO2**
Unit-3 **15 Hours**	**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.	**CLO1, CLO2**
Unit-4 **15 Hours**	**Clusters Applications**: Molecular clusters in catalysis, clusters to materials, boron-carbides and metal-borides. Illustrative examples from recent literature.	**CLO3**

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. & Saillar,d 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	Credits
4	0	0	4

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

CLO1: Implement various modern cross-coupling strategies for the synthesis of value-added chemicals.

CLO2: Design new methodologies for concise synthesis of various molecules using concept of C-H bond activation

CLO3: Design chemical reactions using various benign tool of Green Chemistry such as ionic liquids, heterogeneous catalysts etc.

Units/ hours	Content	Mapping with CLOs
Unit-1 15 Hours	**Synthetic coupling strategies:** Metal mediated coupling strategies**:** Mizoroki-Heck Reaction, Suzuki, Stille, Sonoghashira, Buchwald-Hartwig reaction. Recent approaches for C-C bond formation, use of abundantly available/cheaper precursors: *N*-tosylarylhydrazone and arylalcohols as coupling partners, decarboxylative coupling, arylalcohols as in situ source of arylalkenes in coupling reactions.	**CLO1**
Unit-2 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.	**CLO2**
Unit-3 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.	**CLO3**
Unit-4 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 H_2O_2 as green oxidant. Solid acid catalysts.	**CLO3**

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

L	T	P	Credits
4	0	0	4

Paper Code: CHM.707

Total Lectures: 60

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

CLO1: Identification and classification of basic nanomaterials based on their dimensionality

CLO2: Identify and analyze use of physical and chemical methods of synthesis for nanomaterials.

CLO3: Analyze and apply surface to bulk characterization of nanomaterials

CLO4: Apply the properties of organic and inorganic nanomaterials to various application and impact of nanomaterials on the environment.

Units/ hours	Content	Mapping with CLOs
Unit-1 **15 Hours**	**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.	**CLO1**
Unit-2 **15 Hours**	**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 ZrO_2-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.	**CLO2**
Unit-3 **15 Hours**	**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).	**CLO3**

Unit-4 **15 Hours**	**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.	**CLO4**

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

L	T	P	Credits
4	0	0	4

Paper Code: CHM.708

Total Lectures: 60

Learning Outcome: The students will acquire knowledge of

CLO1: To analyze the supramolecular aspects of interaction between two chemical systems.

CLO2: Device and analyze chemosensors for cation and anions

CLO3: Devising supramolecular systems based on complementarity and pre-organizational requirements of the host.

CLO4: Analyze and devise molecular motors and machines

Units/ hours	Content	Mapping with CLOs
Unit-1 **15 Hours**	**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, π − π and van der waals interactions, supramolecular chemistry in life, ionophores, porphyrin and other tetrapyrrollic macrocycles, examples from biology and nature.	**CLO1**
Unit-2 **15 Hours**	**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.	**CLO1, CLO2**
Unit-3 **15 Hours**	**Molecular Self-assembly:** Supramolecular polymers: definition, kineic 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, supramolcular 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.	**CLO1, CLO3**

Unit-4 **15 Hours**	**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.	**CLO4**

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

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
Paper Code: CHM.709
Total Contact Hours: 60

L	T	P	Credits
4	0	0	4

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

CLO1: Know the role of metals in biology
CLO2: Determined structure and biological functions of metalloproteins and enzymes.
CLO3: Classify of metallobiomolecules on the basis of their functional properties
CLO4: Determined the factors that govern the thermodynamic and mechanical stability, folding, and dynamics of proteins.
CLO5: Work on the kinetics, thermodynamics, and mechanism of protein folding.

Units/ hours	Content	Mapping with CLOs
Unit 1 **15 Hours**	**Inorganic Chemistry of Enzymes - I** Metalloporphyrings: 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.	**CLO1, CLO2**
Unit 2 **15 Hours**	**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 B_{12} and B_{12} coenzymes metallothioneins, nitrogen fixation, in-vitro and in-vivo nitrogen fixation, bio-inorganic chemistry of Mo and W.	**CLO1, CLO2, CLO3**
Unit 3 **15 Hours**	**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. **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),	**CLO1, CLO2, CLO3**

Unit 4 **15 Hours**	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.	**CLO4, CLO5**

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., andMedhi, 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., Overtone, 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. andSchimmel, P.R., (980). *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	**L**	**T**	**P**	**Credits**
Paper Code: CHM.710	4	0	0	4

Total Contact Hours: 60

Learning Outcome: The students will be able to

CLO1: Inorganic, organic and mixed materials

CLO2: Characterization of these materials

CLO3: The relationship between material structure and physical attributes associated with them.

CLO4: Interpret and apply the conductivity of ionic and molecular conductors

CLO5: Interpret and analyse the use of materials for NLO, electronics, biomedical and energy applications

Units/ hours	Content	Mapping with CLOs
Unit 1 15 Hours	**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.	**CLO1, CLO2**
Unit 2 15 Hours	Mesmorphic 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** Prepartion 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.	**CLO1, CLO2,**
Unit 3 15 Hours	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 (thiphene ethynylene) etc. and their applications.	**CLO3, CLO4**

Unit 4 **15 Hours**	**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 suspceptibility – materials for second and third harmonic generation.	**CLO5**

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	Credits
4	0	0	4

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

CLO1: The chemistry of transition metal complexes and compounds of transition metal-carbon multiple bonds
CLO2: Chemistry on alkyls and aryls of transition metals and fluxional organometallic compounds
CLO3: Workout on homogeneous catalysis with appropriate planning.

Units/ hours	Content	Mapping with CLOs
Unit 1 **15 Hours**	**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	**CLO1**
Unit 2 **15 Hours**	**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.	**CLO1, CLO2**
Unit 3 **15 Hours**	**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.	**CLO2**
Unit 4 **15 Hours**	**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.	**CLO3**

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	Credits
4	0	0	4

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

CLO1: Use various reagents including organometallic compounds, experimental conditions in organic synthesis.

CLO2: Apply various asymmetric tools for the synthesis of chiral compounds in their research.

CLO3: Design the synthesis of functionalized molecules utilizing phosphorus and Sulphur ylides.

Units/ hours	Content	Mapping with CLOs
Unit 1 **15 Hours**	**Organometallic Compounds and Coupling Reactions:** Organoboranes: Disiamyl borane, thexyl borane, 9-BBN and disopincamphlyel 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, Sonoghshira coupling, Suzuki-Miyaura coupling, Negishi coupling.	**CLO1**
Unit 2 **15 Hours**	**Asymmetric synthesis and industrial applications:** Various tools of asymmetric synthesis: Chiral pools, chiral catalysis: chiral auxiliaries (SAMP/RAMP): Industrial applications of chiral auxillaries 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	**CLO2**
Unit 3 **15 Hours**	**Reaction of ylides:** Phosphorus ylide; structure and reactivity, stabilized ylides, effects of ligands on reactivity, Witting, 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.	**CLO3**
Unit 4 **15 Hours**	**Reagents in organic synthesis:** Lithiumdiisopropylamide (LDA) and its use for controlling the stereochemistry of product, Bakers yeast, strategies for reactivity umpolung, Trimethylsilyliodide, Prevost Hydroxylation, Ionic liquids and quaternary ammonium and Phosphonium salts, Merrifield resin, Fenton's reagents, Ziegler-Natta catalyst, Lawsson reagents, applications of K-selecteride and L-selecteride 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	**CLO1, CLO2**

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 Wother, 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	Credits
4	0	0	4

Learning Outcome: The students will be able to

CLO1: Demonstrate the use of statistics in analysis in chemistry
CLO2: Choose the method of analysis based on the sample amount/volume, accuracy and precision required for analysis and interference.
CLO3: Demonstrate the method of analysis of metal ions using absorption and emission spectroscopy.
CLO4: Demonstrate the understanding and application of the principles of electrochemical methods of analysis.
CLO5: Demonstrate the ability to device a method for analysis of separation method.

Units/ hours	Content	Mapping with CLOs
Unit 1 15 Hours	**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.	**CLO1, CLO2**
Unit 2 15 Hours	**Analytical Spectroscopy:** Principle, applications and limitations of spectrophotometery, 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).	**CLO2, CLO3**
Unit 3 15 Hours	**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 striping voltametry.	**CLO2, CLO4**
Unit 4 15 Hours	**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.	**CLO2, CLO5**

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 Willey 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.

L	T	P	Credits
4	0	0	4

Course Title: Emerging Trends in Green Synthesis and Drug Discovery
Paper Code: CHM.714
Total Contact Hours: 60

Learning outcomes:
Students will be able to:

CLO1: Elucidated the mechanism of microwave assisted organic transformation
CLO2: Conduct ionic liquids, solid supported organic reactions under MW and conventional conditions
CLO3: Utilize metal and organocatalysts for various C-C and C-N bond formation reactions
CLO4: Apply recent tools in drug discovery and developments

Units/ hours	Content	Mapping with CLOs
Unit 1 15 Hours	**Microwave Assisted Organic synthesis (MAOS):** Heating effects of microwaves: (i) Dipolar polarization and (ii) Ionic conduction, Synthesis of target molecules under solvent-less conditions and on solid support, Microwave and stereoselectivity, Recent advancement in aqueous reaction conditions and microwave.	**CLO1**
Unit 2 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.	**CLO2**
Unit 3 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.	**CLO3**
Unit 4 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.	**CLO4**

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

L	T	P	Credits
4	0	0	4

Contact Hours: 60

Learning outcomes:

Students will be able to:

CLO1: Elucidate the UV-visible spectrum and effect of various factors on UV absorption

CLO2: Interpret the IR spectrum having different functional groups and effect of various factors on IR absorption

CLO3: Elucidate the structure of simple and complex organic molecules and their stereochemistry

CLO4: Elucidate the structure of organic molecules using fragmentation pattern

Units/ hours	Content	Mapping with CLOs
Unit 1 15 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.	**CLO1**
Unit 2 15 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.	**CLO2**
Unit 3 15 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 cruve-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 ^{1}H and ^{13}C-NMR spectra.	**CLO3**
Unit 4 15 Hours	**Mass Spectrometry:** Introduction, Ion production & detection – El, Cl, 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.	**CLO4**

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

L	T	P	Credits
4	0	0	4

Suggested Reading:

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.

Course Title: Natural Products Based Drug Discovery

Paper Code: CHM.716

Total Contact Hours: 60

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

CLO1: Rationalize the contribution of natural products in drug discovery.

CLO2: Identify various types of natural products including their properties, occurrence, structure and synthesis.

CLO3: Apply the knowledge of structure-activity relationship studies for natural product-based drug development.

CLO4: Express the challenges encountered in different stages of natural products-based drug discovery.

CLO5: Identify the merits of innovative and multidisciplinary approaches for the discovery of new lead molecules from different sources of natural products.

Units/ hours	Content	Mapping with CLOs
Unit 1 15 Hours	**Importance of Natural Products in Drug Discovery:** Bioactive Compounds from plants and Microorganisms, Antibiotics, non-antibiotic drugs from fungal and other microbial sources, microbial phytotoxins, Chemistry and biology of marine natural products, Case studies of taxol, artemisinin, etc and development of drug from folk medicine: e.g. Withaferin A. Challenges associated with natural product drug discovery and role of advance instrumentations to overcome natural product drug discovery associated challenges; Dereplication, Advancement in NMR, Mass Spectrometry etc.	**CLO1, CLO2**
Unit 2 15 Hours	**New Trends in Field of Natural Product Drug Discovery:** Multidisciplinary approach to natural products drug discovery using innovative technologies. Role of Omics approaches in NP drug discovery; Genomics, Proteomics and Metabolomics. Combinatorial library for constituents obtained from natural resources, extracts used for developing new drugs. Terrestrial, marine and microbial based bioactive scaffolds; role of in silico approaches for finding suitable targets in drug discovery. Advances in screening for bioactive components from medicinal plants; e.g. affinity ultrafiltration mass spectrometry, High throughput screening etc.	**CLO2, CLO3**
Unit 3 15 Hours	**Synthesis and Biological Activities of Natural Products:** Overview of total synthesis and biomimetic synthesis of natural products with importance in drug discovery. Alkaloids: Isolation, structure elucidation, physiological action, of Ephedrine, Nicotine, Morphine, Reserpine etc and general theory of biogenesis. Terpenoids: Isolation, nomenclature, structure determination, isoprene rule, biosynthesis and synthesis of Geraniol, Menthol β-Carotene, Taxol, Podophyllotoxin, Artimisinin and biological activities. Recent developments in medicinal aspects-Antimicrobial activity, antioxidant and anti-inflammatory and anticancer activities of alkaloids and terpenoids.	**CLO3**

Unit 4 **15 Hours**	**Recent development on naturally occurring polyphenolic compounds and Lignans:** Introduction, Recently reported flavonoids, flavonoids as drug candidates, Biological and Pharmacological activities of flavonoids (Antioxidant activity, cyto-toxic activity, anticancer and anti-microbial activity), Biosynthetic pathway. Classification, isolation, biological activity, biosynthesis and synthesis of lignans.	**CLO4, CLO5**

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

Suggested Readings

1. Bhat, S.V., Nagasampagi, B.A., andMeenakshi, S. (2009). *Natural Product Chemistry and Applications*. Narosa Publishing House, New Delhi.
2. Bhat, S.V., Nagasampagi, B.A., and Sivakumar, M. (2005).*Chemistry of Natural Products*. Narosa Publishing House, New Delhi.
3. Cseke, L.J., (2009).*Natural Products from Plants*. CRC Press.
4. Dewick, P.M. (2009). *Medicinal Natural Products: A Biosynthetic Approach*. Wiley and Sons, UK.
5. Finar, I.L., (2006). *Organic Chemistry: Stereochemistry and the Chemistry of Natural Products*. Dorling Kindersley Pvt. Ltd., India.
6. Peterson, F. andAmstutz, R., (2008). *Natural Compounds as Drugs*. Birkhauser-Verlay.
7. Mandal, S. C., Mandal, V., Konishi, T. (2018) Natural Products and Drug Discovery An Integrated Approach. Academic Press.
8. Wolfender J-L, Litaudon M, Touboul D and Queiroz EF. Innovative omics-based approaches for prioritisation and targeted isolation of natural products as new strategies for drug discovery. *Natural Product Reports*, 2019, 36:855-868.
9. Atanasov A. G., Zotchev S. B., Dirsch, V. M. Natural products in drug discovery: advances and opportunities. *Nat Rev Drug Discov.* 2021, 20, 3, 200-216.

Course Title: Molecular Manufacturing Science & Technology
Paper Code: CHM.717
Total Lectures: 60

L	T	P	Credits
4	0	0	4

Learning Outcome: The students will acquire knowledge of

CLO5: Relate the notion of molecular manufacturing with various available science & technologies
CLO6:.Relate and analyze additive manufacturing methods
CLO7: Analyze the protoptypes for innovation
CLO8: Analyze and prototype a theoretical bioinspirational molecular device
CLO9: Analyze and devise molecular motors and machines

Units/ hours	Content	Mapping with CLOs
Unit-1 **15 Hour**	Essentials for Molecular Manufacturing: Supramoelcular Building Blocks for Molecular Manufacturing, proteins and foldamers, DNA, catenanes, rotaxanes, molecular knot: topology and examples including trefoil and borromean rings, surfactants **Tools for Monitoring:** AFM and SPM	**CLO1**
Unit-2 **15 Hour**	**Methods for Molecular Manufacturing:** : Introduction to Additive Manufacturing (AM) - Reverse engineering, Different AM processes and relevant process physics, AM process chain, Application level: Direct processes – Rapid Prototyping, Rapid Tooling. Rapid Manufacturing; Indirect Processes - Indirect Prototyping. Indirect Tooling, Indirect Manufacturing, Materials science for AM - multifunctional and graded materials in AM, 3D printing and injection moulding of polymers, Metal 3D Printing. AM technologies - Powder-based, droplet based, extrusion based, object stereolithography, Micro- and nano-additive processes, Monitoring and control of defects, transformation.	**CLO1, CLO2,** **CLO3**
Unit-3 **15 Hour**	**Bioinspiration for Molecular Manufacturing: Biophysics of Biological Motors and Machines** Case study of (a) Ciliary movements (b) Protein Transduction (c) Protein Engineering **Drug Delivery:** Concept of drug delivery, different architectures involved in drug delivery systems, Approaches for drug delivery for Cancer cure and COVID-19 Black Fungus case study.	**CLO1, CLO4**
Unit-4 **15 Hour**	**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.	**CLO5**

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

Suggested Readings:

14. Steed, J. W., & Atwood, J. L. (2013). *Supramolecular chemistry*. John Wiley & Sons.
15. Lehn, J. M. (1993). *Supramolecular chemistry*. Science, 260 (5115), 1762-1764.

16. Bruns, C. J., & Stoddart, J. F. (2014). Rotaxane-based molecular muscles. *Accounts of chemical research*, *47*(7), 2186-2199.
17. 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.
18. Sauvage, J. P. (2017). From chemical topology to molecular machines (Nobel lecture). *Angewandte Chemie International Edition*, *56*(37), 11080-11093.
19. Leigh, D. A. (2016). Genesis of the nanomachines: The 2016 Nobel Prize in chemistry. *Angewandte Chemie International Edition*, *55*(47), 14506-14508.
20. Ian Gibson, David W. Rosen and Brent Stucker, Additive manufacturing technologies: rapid prototyping to direct digital manufacturing, Springer (2010).
21. Chua C K, Leong K F and Lim C S, Rapid prototyping: Principles and applications, 3rd Edition, World Scientific (2010).
22. Andreas Gebhardt, Understanding additive manufacturing: rapid prototyping, rapid tooling, rapid manufacturing, Hanser Publishers (2011).
23. Zhiqiang Fan and Frank Liou, Numerical modeling of the additive manufacturing (AM) processes of titanium alloy, ln Tech (2012).
24. Nelson, D. L., Lehninger, A. L., & Cox, M. M. (2008). Lehninger principles of biochemistry. Macmillan.
25. Voet, D., Voet, J. G., & Pratt, C. W. (2008). Principles of biochemistry (Vol. 4). New York: Wiley.