Course Structure and Syllabus

Ph.D. Chemistry

(SEMESTER: I)

Session: 2018-19

Department of Chemical Sciences
School of Basic and Applied Sciences
Central University of Punjab
Mansa Road
Bathinda – 151001

Department of Chemical Sciences
Ph.D. in Chemical Sciences

SEMESTER 1 (Course work)

S. No.	Paper Code	Course Title	L	T	P	Cr	Total Marks
1.	CHM.701	Research Methodology	4	-	-	4	100
2.	CHM.702	Biostatistics	2	-	-	2	50
3.	CHM.703	Computer Applications	2	-	-	2	50
4.	CHM.799	Seminar	-	2	-	2	50
***Opt any one elective courses offered**							
5.	*CHM.704	Advances in Chemistry of Molecular Clusters	4	-	-	4	100
6.	*CHM.705	Recent Trends in Synthetic Strategies and Green Catalysis	4	-	-	4	100
7.	*CHM.706	Chemistry of Nanoscience and Technology	4	-	-	4	100
8.	*CHM.707	Emerging Aspects in Supramolecular Chemistry	4	-	-	4	100
9.	*CHM.708	Bioinorganic and Biophysical Chemistry	4	-	-	4	100
10.	*CHM.709	Applied Material Chemistry	4	-	-	4	100
11.	*CHM.710	Organotransition Metal Chemistry	4	-	-	4	100
12.	*CHM. 711	Advanced Organic Synthesis	4	-	-	4	100
13	*CHM.712	Analytical Chemistry and Instrumental Methods of Analysis	4	-	-	4	100
		Total	**14**	**2**	**-**	**18**	**450**

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

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

L	T	P	Credits	Marks
4	-	-	4	100

Learning objective: To involve the students in their particular research areas with leaning of search engine, writing articles, critical thinking, ideas, patent files, rule and regulations for submission of articles.

Unit 1 **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-2 **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; technicques of communication, etc.

Unit-3 **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-4 **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.

Course Outcome: The students will acquire knowledge of

1. Improve the skills for writing of research manuscripts with knowing about plagiarism.
2. Potentially be able to run the software's of various search engines
3. Able to understand about the property rights about patents and publications.

SUGGESTED READINGS:

1. Gupta, S. (2005). Research Methodology and Statistical Techniques,Deep and Deep Publications (p) Ltd.New Delhi.
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: Biostatistics
Paper Code: CHM.702
Total Lecture: 30

L	T	P	Credits	Marks
2	-	-	2	50

Learning objective: To impart knowledge of the various statistical tools for presenting and analyzing data and its relevance in the research problems of interest of the students.

Unit 1 **8 Hrs**

Overview of biostatistics: Difference between parametric and non-parametric statistics, Univariant and multivariant 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 2 **7 Hrs**

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

Unit 3 **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 4 **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.

Course Outcome: The students will acquire knowledge of

1. Various methods of presenting data in graphical forms
2. Hypothesis testing for analyzing data
3. Judicious use of statistical tools in chemical problems.

SUGGESTED READINGS:

1. Norman, G. and Streiner, D. (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., Holler, F. J., and Crouch, S. R. (2017). *Principles of Instrumental Analysis*. Cengage learning.
4. Danzer, K. (2007). *Analytical Chemistry: Theoretical and Metrological Fundamentals*. Springer Science and Business Media.

Course Tile: Computer Applications
Paper Code: CHM.703

L	T	P	Credits
2	0	0	2

Total Lecture: 30

Learning objective: To acquaint with various computer based tools for use in research in chemical sciences including report writing, data analysis and presentation softwares.

Unit 1 **7 Hrs**

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

Unit 2 **8 Hrs**

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

Unit 3 **8 Hrs**

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

Unit 4 **7 Hrs**

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

Course Outcome: The students will acquire knowledge of

1. Basic computing methodologies
2. Tools for report writing, data analysis, reference writing and presentation softwares.
3. Webpage designing and basic internet facilities
4. Judicious use of search engines for critical literature search.

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: Advances in Chemistry of Molecular Clusters
Paper Code: CHM.704
Total Lectures: 60

L	T	P	Credits
4	1	0	4

Learning objective: A broad view of the cluster chemistry with front areas of research like synthesis, characterization and current applications.

Unit 1 **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 2 **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 3 **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 4 **15 Hrs**

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

Course Outcome: The students will acquire knowledge of

1. Have a great knowledge about clusters including electron counting rules.
2. Correlation between main group and transition metal fragments including various principles.
3. Cluster to nanomaterials journey.

SUGGESTED READING:

1. Mingos, D. M. P. and Wales, D. J., (1990). *Introduction to Cluster Chemistry*. Prentice Hall.
2. Greenwood N. N. and Earnshaw, E. A. (1997). *Chemistry of Elements*. Butterworth-Heinemann.
3. Fehlner, T. P., Halet, J. F., and Saillard, J-Y. (2007). *Molecular Clusters*: *A Bridge to Solid-State Chemistry*. Cambridge University press,
4. Gupta, B. D. and 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.705
Total Lectures: 60

L	T	P	Credits
4	1	0	4

Learning objective: To get familiar withvariouscross-coupling strategies for C-C and C-N bond formation, C-H and C-OH bond activation strategies/functionalization, various tools of green chemistry for catalysis.

Unit 1 **15 Hrs**

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.

Unit 2 **15 Hrs**

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 3 **15 Hrs**

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 4 **15 Hrs**

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.

Course Outcome: The students will be acquainted with

1. Various cross-coupling strategies for C-C and C-N bond formation and their applications in organic synthesis.
2. The concept of C-H and C-OH bond activation for waste-free synthesis.
3. Modern concepts/tools forGreen catalysis and their importance for sustainable development.

SUGGESTED READINGS:

1. Carey, F. A., and Sundberg, R. J., (2007). *Advanced Organic Chemistry, Part A: Structure and Mechanism.* Springer.
2. Carey, F. A., and Sundberg, R. J., (2008). *Advanced Organic Chemistry, Part B: Reaction and Synthesis.* Springer.
3. de Meijere, A., and Diederich, F.,(2008). *Metal-Catalyzed Cross-Coupling Reactions*. Wiley-VCH.
4. Li, J. J., (2015). *C-H Bond Activation in Organic Synthesis*. CRC Press.
5. Anastas,P.T., and Warner, J. C., (2000). *Green Chemistry*: *Theory and Practical*. Oxford University Press.
6. Malhotra, S. V., (2007). *Ionic Liquids in Organic Synthesis*. Oxford University Press.
7. Rodrıguez, R., and Goossen, L. J., (2011). *Decarboxylative coupling reactions: A Modern Strategy for C-C-bond Formation*. *Chemical Society Reviews*. 40, 5030-5048. doi: 10.1039/C1CS15093F

8. Kumar, R., and Van der Eycken, E. V., (2013). *Recent approaches for C-C Bond Formation via Direct Dehydrative Coupling Strategies*. Chemical Society Reviews, 42, 1121-1146.doi:10.1039/C2CS35397K
9. Shao, Z., and Zhang, H.,(2012). N-Tosylhydrazones: Versatile Reagents for Metal-Catalyzed and Metal-Free Cross-Coupling Reactions. *Chemical Society Reviews*, 41, 560-572. doi: 10.1039/C1CS15127D
10. Daugulis, O., Do, H. Q., and Shabashov, D., (20009). Palladium- and Copper-Catalyzed Arylation of Carbon-Hydrogen Bonds, *Account of Chemical Research*, *42*(8), 1074-1086. doi:10.1021/ar9000058

Course Title: Chemistry of Nanoscience and Technology

Paper Code: CHM.706

L	T	P	Credits
4	1	0	4

Total Lectures: 60

Learning objective: To introduce and provide a broad view of the nascent field of nanoscience and nanotechnology and to introduce students to inter- and multi-disciplinary science and engineering which could be applied as materials, sensors, and devices.

Unit 1: 15 Hrs

Introduction to Nanotechnology:

Scientific revolution- Atomic structures-Molecular and atomic size-Bohr radius – Emergence ofNanotechnology –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 2: 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 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.

Unit 3: 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 4: 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.

Course Outcome: The students will acquire knowledge of

4. Have a working knowledge of nanoscience and nanotechnology, including theory and experiment.
5. Potentially be able to join a research group in nanoscience/nanotechnology as a student researcher.

SUGGESTED READING:

1. Rao, C. N. R, Müller, A., and Cheetham, A. K., (2005). *The Chemistry of Nanomaterials:Synthesis, Properties and Applications*. Wiley-VCH.
2. P,Charles Poole Jr., and J., Frank Owens, (2013). *Introduction to Nanotechnology*. Wiley-VCH
3. Mukhopadhyay S. M., (2011). *Nanoscale Multifunctional Materials*. Wiley-VCH
4. Kelsall, W. R., Hamley I W., and Geoghegan M., (2005). *Nanoscale Science and Technology*. John Wiley and Sons.

Course Title: Emerging Aspects in Supramolecular Chemistry

L	T	P	Credits
4	0	0	4

Paper Code: CHM.707

Total Lectures: 60

Learning objective: To impart knowledge of molecular interactions apart from bonding. Use of such interactions in template host and their designing for complimentary target guest and devising supramolecules which could be applied as organic materials, sensors, and devices.

Unit 1 **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, π - π and van der waals interactions, supramolecular chemistry in life, ionophores, porphyrin and other tetrapyrrollic macrocycles, coenzymes, neurotransmitters, DNA and biochemical self-assembly. Classification of supramolecular host-guest compounds, pre- organization and complementarily, receptors, nature of supramolecular interactions.

Host-guest chemistry: synthesis and structure of crown ethers, lariat ether and podands, cryptands, spherands, calixarenes, cylcodextrins, cyclophanes, carcerands and hemicarcerands. Concepts of selectivity, macrocyclic, macrobicyclic synthesis and template effects,

Unit 2 **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 cluorogenic receptors, dosimeters, ion pair recognition and zwitterion recognition.

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

Unit 3 **15 Hrs**

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, COF and supramolecular gels.

Unit 4 **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.

Course Outcome: The students will acquire knowledge of

1. Various supramolecular aspects of interaction between two chemical systems.
2. Devising supramolecular systems based on complementarity and preorganizational requirements of host.

SUGGESTED READINGS

1. Steed, J. W., and Atwood, J. L. (2013). *Supramolecular chemistry*. John Wiley and Sons.
2. Lehn, J. M., (1995). *Supramolecular Chemistry-Concepts and Perspectives*. Wiley – VCH.
3. Beer, P.D., Gale, P. A., and Smith, D. K., (1999). *Supramolecular Chemistry*. Oxford University Press.
4. Martin, N., and Nierengarten, J.-F., (2012). *Supramolecular Chemistry of Fullerenes and Carbon Nanotubes*. Wiley-VCH.
5. Vicens, J., and Harrowfield, J., (2007). *Calixarenes in the Nanoworld*. Springer.
6. Schalley, C. A., (2012). *Analytical Methods in Supramolecular Chemistry*. Vol. 1 & 2, Wiley-VCH.
7. Erbas-Cakmak, S., Leigh, D. A., McTernan, C. T., and Nussbaumer, A. L., (2015). Artificial molecular machines. *Chem. Rev*, *115*(18), 10081-10206.

Course Title: Bio-inorganic and Biophysical Chemistry
Paper Code: CHM.708
Total Contact Hours: 60

L	T	P	Credits
4	0	0	4

Learning objective: To provide knowledge of structure, function, and physicochemical properties of biomolecules.

Unit 1 **15 Hrs**

Inorganic Chemistry of Enzymes - I

Metalloporphyrings: hemoglobin and myoglobin, nature of heme-dioxygen binding, model systems, cooperativity in hemoglobin, physiology of myoglobin and hemoglobin, structure and function of haemoglobin and myoglobin. 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 2 **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 B_{12} and B_{12} coenzymes metallothioneins, nitrogen fixation, in-vitro and in-vivo nitrogen fixation, bio-inorganic chemistry of Mo and W.

Unit 3 **15 Hr**

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 4 **15 Hr**

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), 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

Course Outcome: The students will acquire knowledge of

1. Structure and biological functions of proteins and enzymes.
2. The role of metals in biology
3. Factors that govern the thermodynamic stability, folding, and dynamics of proteins.
4. Kinetics, thermodynamics, and mechanism of protein folding.

SUGGESTED READINGS

1. Huheey, J. E., Keiter, E. A. and Keiter, R.L. (2006). *Inorganic Chemistry Principles of Structure and Reactivity*. Haper Collins.
2. Douglas, B., McDaniel, D. and Alexander, J. (2006). *Concepts and Models of Inorganic Chemistry*. John Wiley and Sons.
3. Cotton, F.A. and Wilkinson, G. (1998). *Advanced Inorganic Chemistry: A Comprehensive Text*. John Wiley.
4. Elschenbroich, Ch. and Salzer, A. (1992). *Organometallics. A Concise Introduction*. Wiley-VCH.

5. Atkins, P., Overtone, T., Rourke, J., Weller, J.and Armstrong, F. (2010). *Shriver and Atkin's 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*. Vols. 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.709
Total Contact Hours: 60

L	T	P	Credits
4	0	0	4

Learning objective: To impart knowledge of materials, their characteristics and physical functions

Unit 1: 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 2: 15 Hrs

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; opticalproperties.

Unit 3: 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 (thiphene ethynylene) etc. and their applications.

Unit 4: 15 Hrs

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

Nonlinear optical materials: Non-linear optical effects, second and third order – molecularhyperpolarisability and second order electric suspceptibility – materials for second and third harmonic generation.

Course Outcome: The students will acquire knowledge of

1. Inorganic, organic and mixed materials
2. Characterization of these materials
3. The relationship between material structure and physical attributes associated with them.

SUGGESTED READINGS

1. Ashcroft, N. W., and Mermin, N. D. (1976). *Introduction to Solid State Physics*. *Saunders.*.
2. Callister Jr, W. D., and Rethwisch, D. G. (2012). *Fundamentals of Materials Science and Engineering: An Integrated Approach*. John Wiley and Sons.
3. Anderson, J. C., Leaver, K. D., Rawlings, R. D., and Leevers, P. S. (2004). *Materials Science for Engineers*. CRC Press.
4. Keer, H. V. (1993). *Principles of the Solid State*. New Age International.

Course Title: Organotransition Metal Chemistry
Paper Code: CHM.710
Total Contact Hours: 60

L	T	P	Credits
4	0	0	4

Learning objective: The course provides advanced knowledge of organotransition metal chemistry

Unit 1 **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 2 **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 importantreactions relating to nucleophilic and electrophilic attack on ligands and to organic synthesis, metallocenes.

Unit 3 **15 Hrs**

Alkyls and Aryls of Transition Metals

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

Fluxional organometallic compounds

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

Unit 4 **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.

Course Outcome: The students will acquire knowledge of

1. Transition metal complexes and compounds of transition metal-carbon multiple bonds
2. Alkyls and aryls of transition metals and fluxional organometallic compounds
3. Homogeneous catalysis and their applications.

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. and 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
Paper Code: CHM.711
Total Contact Hours: 60

L	T	P	Credits
4	0	0	4

Learning objective: To impart knowledge of various important topics in organic synthesis such as asymmetric synthesis, reagents including organometallic reagents and some important reactions of ylides.

Unit 1 **15 Hrs**

Asymmetric synthesis: Chiral pools, chiral catalysis: chiral auxiliaries, 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 2 **15 Hrs**

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.

Unit 3 **15 Hrs**

Organometallic compounds

Organoboranes: Preparation of organobornaes viz hydroboration with BH_3-THF, dicylohexyl borane, disiamyl borane, thexyl borane, 9-BBN and disopincamphlyel borane, functional group transformations of organo boranes: oxidation, protonolysis and rearrangements. formation of carbon-carbon-bonds *viz*organo boranes carbonylation. Organolithium, organozinc and organocopper compounds, organosilicon compounds for organic synthesis, organopalladium and organostannous (applications in coupling reactions).

Unit 4 **15 Hrs**

Reagents in organic synthesis: Gilman'sreagent,Lithiumdiisopropylamide(LDA), 1,3-Dithiane (Umpolung reagent), Trimethylsilyliodide, Bakersyeast,Prevost Hydroxylation, Phasetransfercatalysts:quaternaryammoniumandPhosphoniumsalts,Crownethers, Merrifield resin, Fenton's reagents, Ziegler-Natta catalyst, Lawsson reagents, K-selecteride and L-selecteride, Sodium cyanoborohydride, IBX, Sodium triacetoxyborohydride, Fetizon reagent, Dioxiranes, Ceric ammonium nitrate, Tebbe reagent, Corey-Nicolaou reagent, Mosher's reagent, use of Os, Ru, and Tl reagents.

Course Outcomes: The students will acquire knowledge of

- Asymmetric synthesis and chiral resolution.
- Various reagents including organomettalic compounds, experimental conditions and their applications in organic synthesis/industry.
- Some important reactions utilizing phosphorus and sulphur ylides.

SUGGESTED READINGS

1. Claydon, J., Gleeves, N., Warren, S., &Wother, P.,(2001). *Organic Chemistry*. Oxford University Press, UK.
2. Finar, I.L., (2012). *Organic Chemistry*. Pearson Education, UK.
3. Li, J. J., (2014). *Name Reactions: A Collection of Detailed Reaction Mechanism*. Springer-Verlag.
4. Smith, M. B., (2013). *March's advanced organic chemistry: reactions, mechanisms, and structure*. John Wiley and Sons.
5. Ho T. L., (2011), *Fieser's Reagents for Organic Synthesis*, Wiley Interscience.
6. Reich, H.J., &Rigby, J. H., (1999). *Handbook of Reagents for Organic Synthesis Acidic and Basic Reagents*. VoI. IV, Wiley-Interscience.
7. Warren, S.,and Wyatt, P., (1989). *Designing Organic synthesis: A Disconnection Approach*. 2nd edition, John Wiley and Sons, New York.

8. Corey, E.J. and Cheng, X.-M.(1989). *The Logic of Chemical Synthesis*. John Wiley and Sons.
9. Fuhrhop, J. H., Penzlin, G., and Li, G., (2003). *Organic synthesis: Concepts and Methods*. John Wiley and Sons
10. Davies, S. G., (2013). *Organotransition Metal Chemistry: Applications to Organic Synthesis: Applications to Organic Synthesis* (Vol. 2). Elsevier.
11. Aitken, A., &Kilényi, S. N., (Eds.). (1992). *Asymmetric Synthesis*.Springer Publishers.
12. Proctor G. (1996). *AsymmetricSynthesis*. Academic Press.
13. Mundy, B. P., Ellerd, M. G., &Favaloro Jr, F. G., (2005). *Name Reactions and Reagents in Organic Synthesis*. John Wiley and Sons.

Course Title: Analytical Chemistry and Instrumental Methods
Paper Code: CHM.712
Total Contact Hours: 60

L	T	P	Credits
4	0	0	4

Learning objective: To impart knowledge of various analytical and instrumental methods for chemical characterization and analysis.

Unit 1 **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.

Thermogravimetry: TGA, DTA, DSC - Instrumentation, methodology, applications.

Unit 2 **15 Hrs**

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).

Unit 3 **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 striping voltametry.

Unit 4 **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.

Course Outcome: The students will acquire knowledge of

1. Various analytical methods and their applications
2. Various instrumental methods and their applications.
3. Further the student should be able to figure out the analytical process and instrumental method to be advised for a particular problem in hand

SUGGESTED READINGS

1. Skoog, D. A., Holler, F. J., and Crouch, S. R. (2017). *Principles of Instrumental Analysis*. Cengage learning.
2. Willard, H. H., Merritt Jr, L. L., Dean, J. A., and Settle Jr, F. A. (1988). *Instrumental Methods of Analysis.*CBS Publishers.
3. Mendham, J., Denney, R. C., Barnes, J. D., and Thomas, M. J. K. (2008). *Vogel's Textbook of Quantitative Chemical Analysis*, Dorling Kindersley.
4. Skoog, D. A., West, D. M., Holler, F. J., and Crouch, S. (2013). *Fundamentals of Analytical Chemistry*. Nelson Education.
5. Christian, G. D. (1994). *Analytical Chemistry*. John Wiley and Sons, USA, 331.

6. Bard, A. J., and Faulkner, L. R. (2001). *Electrochemical Methods*, 2nd. John Wiley New York, *669*.
7. Rouessac, F., and Rouessac, A. (2013). *Chemical analysis: Modern Instrumentation Methods and Techniques*. John Wiley and Sons.
8. Danzer, K. (2007). *Analytical Chemistry: Theoretical and Metrological Fundamentals*. Springer Science and Business Media.