Course Structure and Syllabus

Ph.D. Chemistry

(SEMESTER: I)

Session: 2017-18

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

Centre for Chemical Sciences
Ph.D. in Chemical Sciences

SEMESTER 1 (Course work)

S. No.	Paper Code	Course Title	L	T	P	Cr	Total Marks
1.	CHL.701	Research Methodology	2	-	-	2	50
2.	CHL.702	Biostatistics	2	-	-	2	50
3.	CHL.703	Computer Applications	2	-	-	2	50
4.	CHS.799	Seminar	-	2	-	2	50
***Opt any two Elective courses offered**							
5.	*CHL.704	Advances in Chemistry of Molecular Clusters	4	-	-	4	100
6.	*CHL.705	Recent Trends in Synthetic Strategies and Green Catalysis	4	-	-	4	100
7.	*CHL.706	Chemistry of Nanoscience and Technology	4	-	-	4	100
8.	*CHL.707	Emerging Aspects in Supramolecular Chemistry	4	-	-	4	100
9.	*CHL.708	Bioinorganic and Biophysical Chemistry	4	-	-	4	100
10.	*CHL. 709	Applied Material Chemistry	4	-	-	4	100
11.	*CHL. 710	Organotransition Metal Chemistry	4	-	-	4	100
12.	*CHL. 711	Advanced Organic Synthesis	4	-	-	4	100
		Total	**14**	**2**	**-**	**16**	**400**

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

Course Tile: Research Methodology
Paper Code: CHL.701
Total Lecture: 36

L	T	P	Credits	Marks
2	-	-	2	50

Unit 1 **10 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.

Technical writing: Scientific writing, Writing research paper, Poster preparation and Presentation and Dissertation.

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

Unit-2 **10 Hrs**

Entrepreneurship and business development: Importance of entrepreneurship and its relevance in career growth, Characteristics of entrepreneurs, Developing entrepreneurial competencies, Types of enterprises and ownership (large, medium SSI, tiny and cottage industries, limited, public limited, private limited, partnership, sole proprietorship), Employment, self employment and entrepreneurship, Financial management-importance and techniques, Financial statements- importance and its interpretation,

Good Laboratory Practices: Recent updates on good laboratory practices.

Unit-3 **16 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.

Suggested Readings:

1. Gupta, S. (2005). *Research methodology and statistical techniques*, Deep & 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: CHL.702
Total Lecture: 36

L	T	P	Credits	Marks
2	-	-	2	50

Unit 1 **10 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 **5 Hrs**

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

Unit 3 **12 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 **9 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.

Suggested Readings:

1. Norman, G. and Streiner, D. (3rd edn) (2008). *Biostatistics: The Bare Essentials*. Decker Inc., Canada.
2. Sokal, R.R. and Rohlf, F.J. (1994). *Biometry: The Principles and Practices of Statistics in Biological Research*, W.H. Freeman and Company, New York.

Course Tile: Computer Applications
Paper Code: CHL.703
Total Lecture: 36

L	T	P	Credits
2	0	0	2

Unit 1 **18 Hrs**

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

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

Unit 2 **18 Hrs**

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

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

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. Norman, G. and Streiner, D. (3rd edn) (2008). *Biostatistics: The Bare Essentials*. Decker Inc., Canada.
5. 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.
6. Thurrott, P. and Rivera, R. (2009). *Windows 7 Secrets*. Wiley.

Course Title: Advances in Chemistry of Molecular Clusters
Paper Code: CHL.704
Total Lectures: 72

L	T	P	Credits
4	1	0	4

Unit 1 **20 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 **25 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 **12 Hrs**

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

Text Books:

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

Course Title: Recent Trends in Synthetic Strategies and Green Catalysis
Paper Code: CHL.705

L	T	P	Credits
4	1	0	4

Total Lectures: 72

Unit 1 **18 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 **18 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 **18 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 **18 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.

References:

1. Advanced Organic Chemistry, Part A and Part B, 5th Edition, Springer, 2009
2. Armin de Meijere, François Diederich, Metal-Catalyzed Cross-Coupling Reactions, 2nd Edition, Wiley-VCH, 2008.
3. Jie Jack Li, C-H Bond Activation in Organic Synthesis, CRC Press, 2015.
4. P.T. Anastas, J. C. Warner, Green chemistry, Theory and Practical. Oxford University Press, 1st edition, US, 2000.
5. Sanjay V Malhotra, Ionic Liquids in Organic Synthesis, Oxford University Press, US, 2007.
6. Nuria Rodrıguez, Lukas J. Goossen, Decarboxylative coupling reactions: a modern strategy for C-C-bond formation, *Chem. Soc. Rev*., 2011, 40, 5030.
7. R. Kumar, E. V. Van der Eycken, Recent approaches for C-C bond formation *via* direct dehydrative coupling strategies, *Chem. Soc. Rev.* 2013, 42, 1121.
8. *N*-tosylhydrazones: versatile reagents for metal-catalyzed and metal-free cross-coupling reactions, Z. Shao and H. Zhang, *Chem. Soc. Rev*., 2012, 41, 560.
9. Palladium- and Copper-Catalyzed Arylation of Carbon-Hydrogen Bonds, O. Daugulis, J. Q. Do, D. Shabashov, *Acc. Chem. Res*., 2009, 42, 1074.

Course Title: Chemistry of Nanoscience and Technology
Paper Code: CHL.706
Total Lectures: 72

L	T	P	Credits
4	1	0	4

Unit 1: 12 Hrs

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

Unit 2: 20 Hrs

Synthesis of Nanomaterials:
Bulk Synthesis: Synthesis of bulk nanostructured materials - Sol Gel processing- Mechanical alloying and milling-inert gas condensation technique-bulk and nano composite materials - Grinding – high energy ball milling-types of balls-WC and ZrO2-materials –ball ratio-limitations- melt quenching and annealing.
Physical and Chemical approaches:Self assembly-Self Assembled Monolayers (SAM) - Vapour Liquid Solid (VLS) approach- Chemical Vapour Deposition (CVD) - Langmuir-Blodgett (LB) films - Spin coating – Templated self assembly Electrochemical approaches: Anodic oxidation of alumina films, porous silicon and pulsed electrochemical deposition - Spray pyrolysis - Flame pyrolysis - Thin films –Epitaxy -Lithography.

Unit 3: 20 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: 20 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.

REFERRENCE BOOKS:

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

Course Title: Emerging Aspects in Supramolecular Chemistry
Paper Code: CHL.707
Total Lectures: 72

L	T	P	Credits
4	0	0	4

Unit I: Introduction **18 Hrs**

Definition and Development of Supramolecular Chemistry, Nature of binding interactions in supramolecular structures: ion-ion, ion-dipole, dipole-dipole, H-bonding, cation-p, anion-p, p-p and vander waal 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.

Unit II: Cation and Anion Binding **18 Hrs**

Crown ethers, Lariat ether and Podands, Cryptands, spherands, selectivity, Macrocyclic, Macrobicyclic and Template effects, soft ligands, calixarenes, carbon donor and π- acid ligands, siderophores.

Biological anion receptors, concepts on anion host design, from cation to anion hosts- a simple change in pH, Guanidinium- based receptors, Neutral receptors, organometallic receptors, coordination interactions.

Unit III: Molecular self-assembly **18 Hrs**

Definition, types of intermolecular interactions and their energetics. Synthesis, structure and properties of supramolecular systems - Metal guided self-assembly of nitrogen based ligand systems, molecular knot with double helical Cu(I) complexes - Thermodynamics and kinetic stability of supramolecular systems and their applications.

Fullerness as hosts or guests and as superconducting intercalation compounds and their applications. Dendrimers Structures and methods of synthesis; functionalization at the periphery; applications.

Inorganic light emitting materials and devices - synthesis, properties and their applications.

Unit IV: Supramolecular and Molecular Devices **18 Hrs**

Higher order Supramolecules including Catenanes, Rotaxanes, Knots and Bromenean Rings. Supramolecular photochemistry, molecular electronic devices: Switches Switching Electron- transfer Processes by photon inputs, redox inputs, and acid-base inputs., wires and rectifiers (oligo (phenylene vinylene)s, oligo(phenylene ethynylene)s, oligo (eneyne)s, oligo(thiophene vinylene), oligo (thiphene ethynylene) etc. and their applications) , machines based on catenanes and rotaxanes Organics for photonics and electronics.

Books :

1. J.W Steed and J.L Atwood, Supramolecular chemistry, John Wiley & Sons, Ltd. New York.
2. *J. M., Lehn, Supramolecular Chemistry-Concepts and Perspectives, Wiley –VCH (1995).*
3. *P.D., Beer, P. A., Gale, and D. K., Smith, Supramolecular Chemistry, Oxford University Press (1999).*

Course Title: Bio-inorganic and Biophysical Chemistry

Paper Code: CHL.708

Total Contact Hours: 72

L	T	P	Credits
4	0	0	4

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

Unit 1 **18 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 **18 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 **18 Hrs**

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 **18 Hrs**

Biophysical Chemistry

Principles of biophysical chemistry (pH, buffer, reaction kinetics, thermodynamics, colligative properties), structure and physical properties of amino acids, physical principle of structure, function, and folding of proteins, conformations of proteins (Ramachandran plot, secondary, tertiary and quaternary structure; domains; motif and folds), determination of protein structures by spectroscopic methods (CD, FTIR, NMR), 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. AndKeiter, R.L. Inorganic Chemistry Principles of Structure and Reactivity, 4th edition, 2006, Haper Collins.
2. Douglas, B., McDaniel,D. AndAlexander, J. Concepts and Models of Inorganic Chemistry, 3rd edition, 2006, John Wiley and Sons.
3. Cotton, F.A. andWilkinson, G. Advanced Inorganic Chemistry: A Comprehensive Text, John Wiley, 5th edition.
4. Elschenbroich,Ch. and Salzer,A. Organometallics. A Concise Introduction, 2nd edition, 1992, Wiley-VCH.
5. Atkins, P., Overtone, T., Rourke, J., Weller, J. And Armstrong, F. Shriver and Atkin'sInorganic Chemistry, 5thedition, 2010, Oxford University Press.
6. Cowan, J.A. Inorganic Biochemistry: An Introduction, 2nd edition, 1997, Wiley – VCH,.

7. Lippard,S. J. Progress in Inorganic Chemistry,Vols. 18, 1991, Wiley-Interscience.
8. Lippard,S. J. Progress in Inorganic Chemistry,Vols. 38, 1991, Wiley-Interscience.
9. Lesk, A.M., Introduction to Protein Science: Architecture, Function, and Genomics, 2nd edition, 2010, Oxford University Press.
10. Cantor, C.R. and Schimmel, P.R., Biophysical Chemistry, 1980, Freeman.
11. Van Holde, K.E., Johnson, W.C. and Ho, P.S., Principles of Physical Biochemistry, 2nd Edition, 2006, Pearson Education.
12. Harding, S.E. and Chowdhry, B. Z. Protein-Ligand Interactions, 2001, Oxford University Press.

Course Title: Applied Material Chemistry

Paper Code: CHL.709

Total Contact Hours: 72

L	T	P	Credits
4	0	0	4

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

Unit 1: 18 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: 24 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; optical properties.

Unit 3: 12 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: 18 Hrs

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

Nonlinear optical materials: Non-linear optical effects, second and third order – molecular hyperpolarisability and second order electric 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. 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: Organotransition Metal Chemistry

Paper Code: CHL.710

L	T	P	Credits
4	0	0	4

Total Contact Hours: 72

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

Unit 1 **18 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 **18 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 **18 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 **18 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. Principles and Application of Organotransition Metal Chemistry, 1987, University Science Books.
2. Crabtree, R.G. The Organometallic Chemistry of the Transition Metals, 5th edition, 2011, John Wiley.
3. Mehrotra R. C. and Singh, A. Organometallic Chemistry, 2nd edition, 2005, New Age International.
4. Cotton, F.A. and Wilkinson, G. Advanced Inorganic Chemistry, 6th edition, 1999, John Wiley.
5. Pearson, A.J. Metallo-Organic Chemistry, 1985, Wiley.

Course Title: Advanced Organic Synthesis
Paper Code: CHL.711
Total Contact Hours: 72

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 **14 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 **18 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 **20 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 **20 Hrs**

Reagents in organic synthesis: Gilman'sreagent, Lithiumdiisopropylamide(LDA), 1,3-Dithiane (Umpolung reagent), Trimethylsilyliodide, Bakers yeast, Prevost Hydroxylation, Phase transfer catalysts: quaternary ammonium and Phosphonium salts, Crown ethers, 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. and Wother, P. Organic chemistry, 2001, Oxford University Press, UK.
2. Fieser and Fieser, Reagents for organic synthesis, Vol 1-26, 3rd edition, 2011, Wiley Interscience.
3. Finar, I.L. Organic Chemistry, 6th edition, 2012, Pearson Education, UK.
4. Li, J.J.Name Reactions: A Collection of Detailed Reaction Mechanism 4th edition, 2009 Springer.
5. Smith, M. B. March's advanced organic chemistry: reactions, mechanisms, and structure. 7th Edition, 2013, John Wiley & Sons.
6. Reich, H.J. and Rigby, M.Handbook of Reagents for Organic Synthesis Acidic and Basic Reagents VoI. IV, 1999, Wiley-Interscience.
7. Warren, S. Organic synthesis: The Synthon Approach. 2010, John Wiley & Sons, New York,
8. Warren, S. and Wyatt, P. Designing Organic synthesis: A Disconnection Approach. 2nd Edition, 2010, John Wiley & Sons, New York.
9. Corey E.J. and Cheng, X.-M. The Logic of Chemical Synthesis, 1989, John Wiley & Sons.
10. Fuhrhop J.-H. and Penzlin, G. Organic Synthesis: Concepts methods, StartingMaterials, 2nd edition,1994, Verlag chemie.

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