Course Structure and Syllabus

Ph.D. Chemistry

(SEMESTER: I)

(FOR NEW ADMISSION)

Examinations: 2016-17

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
***Opt any three Elective courses offered**							
4	*CHL.704	Advances in Chemistry of Molecular Clusters	4	1	-	4	100
5	*CHL.705	Recent Trends in Synthetic Strategies and Green Catalysis	4	1	-	4	100
6	*CHL.706	Chemistry of Nanoscience and Technology	4	1	-	4	100
7	*CHL.707	Emerging Aspects in Supramolecular Chemistry	4	1	-	4	100
8	*CHL.708	Biophysical Chemistry	4	1	-	4	100
9.	CHS.799	Seminar	-	-	-	2	50
		Total	**18**	**-**	**-**	**20**	**500**

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	Marks
2	0	0	2	50

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	Marks
4	1	0	4	100

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	Marks
4	1	0	4	100

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	Marks
4	1	0	4	100

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	Marks
4	0	0	4	100

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: Biophysical Chemistry
Paper Code: CHL.708
Total Lectures: 72

L	T	P	Credits	Marks
4	1	0	4	100

Course objective: To explain the fundamental aspects of biomolecular structure, energetics, and structural dynamics of macromolecules.

Unit 1 **18 Hrs**

Interactions in Biological Systems: Intra and inter molecular forces electrostatic interactions and hydrogen bonding interaction, van der Waals and hydrophobic interactions, disulphide bridges, role of water and weak interactions, pH, biological buffers, solution equilibria, Henderson-Hasselbalch equation, Hofmeister series, chaotropic and kosmotropic ions/cosolvents.

Structure of Proteins: Principles of biophysical chemistry (pH, buffer, reaction kinetics, Thermodynamics, **C**olligative 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), structural features of membrane proteins, secondary and tertiary structure prediction of protein conformation.

Unit 2 **18Hrs**

Multiple equilibrium: Titration of proteins to evaluate net and total charge, Scatchard and Hill plots, folding-unfolding equilbrium and denaturation of proteins, effect of temperature and solvent conditions on the thermodynamics of protein folding-unfolding equilibrium, thermodynamic models for reversible and irreversible reactions, conformational stability estimation of proteins, thermodynamics of protein folding by spectroscopic and calorimetric methods, characterization of folding intermediates, spectroscopic/calorimetric/bioinformatics methods to study protein-surfactant/denaturant/drug interactions.

Kinetics of protein folding: Ultrafast biological reactions, methods and techniques of chemical relaxation, effect of denaturants on rates of folding and unfolding, Chevon plots, folding funnels, mechanisms of protein folding, , ultrafast folding dynamics study by laser flash photolysis.

Unit 3 **18 Hrs**

Fluorescence spectroscopy of biomolecules: Fluorescent probes, modification in methionine/ histidine/tryptophan/amine and carboxylic groups, fluorescence life-time and quenching studies, protein conformational study by fluorescence spectroscopy, applications in proteins and membrane studies, energy transfer for distance measurement in proteins and membranes, use of fluorescence polarization and anisotropy, measurement of anisotropy decay, comparative study of rigid proteins, internal flexibility of multidomain proteins, fluorescence dye-nucleic acid complexes.

CD and ORD spectroscopy of biomolecules: Introduction to CD and ORD, relation between CD and ORD, absorption by oriented biomolecules, dichroic ratio of proteins and nucleic acids, comparison of CD and absorption spectra, determination of secondary structures content by CD, determination of pH/temperature/co-solute effects on proteins by CD.

IR and Raman spectroscopy of biomolecules: Comparison of IR and Raman spectroscopy, peptide bond vibrations, conformation (α-helix, β-sheet, β -turns, random coils), quantitative estimation of the structure from amide I, II & III band intensity in proteins.

Unit 4 **18 Hrs**

NMR spectroscopy of biomolecules: NMR spectrometer and concept of FT spectroscopy, nuclear Overhauser effect, 1D and 2D (COSY, NOESY) spectroscopic studies of proteins, protein conformational study by NMR spectroscopy.

ESR and SPR spectroscopy of biomolecules: Introduction of ESR and SPR, applications of ESR and SPR to simple biological systems, identification of high and low spin configurations in metalloproteins by ESR, ligand binding to heme proteins by ESR, spin labelled ligands probe for rigidity of binding sites.

MS: The basic principles of mass spectrometry, applications of mass spectrometry for the analysis of proteins.

DLS: Measurement of hydrodynamic radii by dynamic light scatter.

Course Outcome: After successfully completion of the course**,** the students will get expertise of structural, kinetic, and thermodynamic characterizations of biomolecues using advanced spectroscopic techniques and methods.

Reading Material

1. Proteins: Structure and Molecular Properties by T.E. Creighton
2. Biophysical Chemistry Part I & II by C.R. Cantor and P.R. Schimmel
3. Physical Biochemistry by K.E. van Holde
4. Physical Biochemistry by David Freifelder
5. Introduction to Protein Structure: C. Branden and J. Tooze
6. Protein Physics by A.V. Finkelstein and O.B. Ptitsyn
7. Lakowicz, J., Principles of Fluorescence Spectroscopy, Kluwer Academic and Plenum Publishers (1999)
8. Evans, J.N.S., Biomolecular NMR Spectroscopy, Oxford University Press (1998)
9. Campbell, I.D. and Raymond, A.D., Biological Spectroscopy, Benzamin/Cummings Publishing Company (1984)
10. McCammon, J.A. and Harvey, S.C., Dynamics of Proteins & Nucleic Acids, Cambridge University Press (1988)
11. Friefelder, D., Physical Biochemistry to Biochemistry and Molecular Biology, San Francisco: *W.H. Freeman* (1982)
12. Hinchliffe, A., Molecular Modeling for Beginners, John Wiley (2003)