Pre-Ph.D. (Chemistry)		Contact Hrs.			Marks			Credits
Subject Code	**Subject Name**	**L**	**T**	**P**	**Int.**	**Ext.**	**Total**	
MREM0-101	Research Methodology	4	0	0	40	60	100	4
PCHM1-101	Requisites of article writing	0	0	2	60	40	100	1
PCHM1-102	Seminar	0	0	2	Satisfactory/Unsatisfactory			1
PREPE0-101	Research and Publication Ethics	2	0	0	40	60	100	2
Departmental Electives (Choose any two subjects)		4x2	0	0	40x2	60x2	100x2	4x2
PCHM1-111	Electroanalytical Chemistry							
PCHM1-112	Supramolecular Chemistry							
PCHM1-113	Chemistry of Organometallic Compounds							
Total		**14**	**0**	**4**	**220**	**280**	**500**	**16**

RESEARCH METHODOLOGY

Subject Code: MREM0-101 **L T PC** **Duration: 60Hrs.**
4 0 0 4

UNIT–I (15 Hrs.)

Introduction to Research: Meaning, Definition, Objective and Process.
Research Design: Meaning, Types - Historical, Descriptive, Exploratory and Experimental.
Research Problem: Necessity of Defined Problem, Problem Formulation, Understanding of Problem, Review of Literature.
Design of Experiment: Basic Principal of Experimental Design, Randomized Block, Completely Randomized Block, Latin Square, Factorial Design.
Hypothesis: Types, Formulation of Hypothesis, Feasibility, Preparation and Presentation of Research Proposal.

UNIT–II (15 Hrs.)

Sources of Data: Primary and Secondary, Validation of Data
Data Collection Methods: Questionnaire Designing, Construction.
Sampling Design & Techniques – Probability Sampling and Non Probability Sampling.
Scaling Techniques: Meaning & Types.
Reliability: Test – Retest Reliability, Alternative Form Reliability, Internal Comparison Reliability and Scorer Reliability.
Validity: Content Validity, Criterion Related Validity and Construct Validity.

UNIT–III (15Hrs)

Data Process Operations: Editing, Sorting, Coding, Classification and Tabulation.
Analysis of Data: Statistical Measure and Their Significance, Central Tendency, Dispersion, Correlation: Linear and Partial, Regression: Simple and Multiple Regression, Skewness, Time series Analysis, Index Number.
Testing of Hypothesis: T-test, Z- test, Chi Square, F-test, ANOVA.

UNIT – IV (15 Hrs.)

Multivariate Analysis: Factor Analysis, Discriminant Analysis, Cluster Analysis, Conjoint Analysis, Multi-Dimensional Scaling.
Report Writing: Essentials of Report Writing, Report Format.
Statistical Software: Application of Statistical Softwares like SPSS, MS Excel, Mini Tab or MATLAB Software in Data Analysis.

*Each Student has to Prepare Mini Research Project on Topic/ Area of their Choice and Make Presentation. The Report Should Consists of Applications of Tests and Techniques Mentioned in The Above UNITs

Recommended Books:

1. R.I. Levin and D.S. Rubin, 'Statistics for Management', 7th Edn. Pearson Education New Delhi.
2. N.K. Malhotra, 'Marketing Research – An Applied Orientation', 4th Edn., Pearson Education NewDelhi.
3. Donald Cooper, 'Business Research Methods', Tata McGraw Hill, NewDelhi.
4. Sadhu Singh, 'Research Methodology in Social Sciences', HimalayaPublishers.
5. Darren George & Paul Mallery, 'SPSS for Windows Step by Step', Pearson Education, New Delhi
6. C.R. Kothari, 'Research Methodology Methods & Techniques', 2nd Edn., New Age InternationalPublishers.

REQUISITES OF ARTICLE WRITING

Subject Code– PCHM1-101 **L T P C** **Duration – 30Hrs**
0 0 2 1

Essentials of Report and article writing: Search Engines, Research/Review paper writing, Introduction to Impact Factor, Indexing, Citations, Peer Review, h-index, i10-index, ISSN, Leading Science Publishers Referencing styles and Process of article submission.

Journal Club – Presentation of research problems and publications. Critical review of published articles.

Working knowledge of softwares like SPSS, Minitab, accelrys Draw, Chem draw, freely available reference management softwares etc.

Recommended Websites

1. www.google.com
2. www.ncbi.nlm.nih.gov/pubmed
3. www.sciencedirect.com
4. www.elsevier.co.in
5. www.wiley.com
6. www.thomsonreuters.com
7. www.benthamscience.com
8. www.scholar.google.co.in

SEMINAR

Subject Code: PCHM1-102 **L T P C** **Duration: 30Hrs.**
0 0 2 1

The Pre-PhD course work candidate will do literature review of minimum 10 research paper of reputed journals related to his/her research field and will finally present the seminar.
The student has to do literature review of minimum 10 research paper of that topic of reputed journals and will finally present the seminar.
Evaluation: Satisfactory/Unsatisfactory by a committee of three faculty member including head of the department.

RESEARCH AND PUBLICATION ETHICS

Subject Code- PREPE0-101 **L T P C** **Duration – 30Hrs**
2 0 0 2

UNIT – I (5 Hrs)

Introduction to Philosophy: Definition, Nature and Scope, Concept and Branches
Ethics – Definition, Moral Philosophy, Nature of Moral Judgements and Reaction, Ethics with respect to Science and Research

UNIT -II (6 Hrs)

Intellectual Honesty and Research integrity
Scientific Misconduct: Falsification, Fabrication and Plagiarism
Redundant Publications: Duplicate and Overlapping Publication, Salami Slicing Selective reporting and misrepresentation of data
Database: Indexing Databases, Citation Databases – Web of Science, Scopus etc.
Research Metrics: Impact Factor of Journal as per journal citation report, SNIP, SJR, IPP, Cite Score
Metrics – H-Index, i10-Index, g-Index, Altmetrics

UNIT -III (9 Hrs)

Publication Ethics- Definition, Introduction and Importance Best Practices/Standard Settings initiatives and guidelines: COPE, WAME etc. Conflict of Interest Software to identify predatory publications developed by SPPU

Journal Finding / Journal Suggester Tools – Elsevier Journal Finder, Springer Journal Suggester etc.SHERPA/RoMEO online resource to check publisher copyright & Self Archiving Policies

UNIT -IV (10 Hrs)

PublicationMisconduct–Definition,Concept,Problemsthatleadtounethicalbehaviour and vice-versa
Violation of Publication ethics and authorship and contributorship, Identification of PublicationMisconduct,ComplaintsandAppeal-ExamplesandFraudfromIndiaandAbroad, Predatory Publishers andJournals
Use of Plagiarism Software like Turnitin, Urkund and other open source software tools

Recommended Books

- Bird A. (2006) Philosophy of Science Roultedge
- MacIntyre Alasdair (1967) A Short History of EthicsLondon
- P. Chaddah (2018) Ethics in competitive Research: Do not get scooped; Donot get plagiarized, ISBN:9789387480865
- National Academy of Sciences, National Academy of Engineering and Institute of Medicine, (2009) On being a scientist: A Guide to Responsible Conduct in research: Third edition, National Academies Press.
- Resnik,D.B.(2011)Whatisethicsinresearchandwhyitissoimportant,NationalInstitute of Environmental Health Sciences,1-10
- Beall, J. (2012) Predatory publishers are corrupting open access, Nature 415 (7415), 179- 179
- Indian National Science Academy (INSA) Ethics in Science Education Research and Governance ISBN: 978-81-939482-1-7

ELECTROANALYTICAL CHEMISTRY

Subject Code: PCHM1-111 **L T P C** 4 0 0 4 **Duration: 60(Hrs.)**

Course Objectives:

1. To introduce the concept of activity and activity coefficient.
2. To introduce various electrochemical theories.
3. To familiarize with the concept of electron transfer.
4. To understand various electrochemical techniques.
5. To introduce various theories of electrolytic solutions and electrolytic conductance.

Course Outcomes:

The students will acquire knowledge of

1. Various electrochemical techniques.
2. Electrochemical theories.
3. Electrolytic solution and conductance.
4. Interfacial electrochemistry

UNIT-I (13 Hours)

Recall: Concept of activity and activity coefficients in electrolytic solutions. The mean ionic activity coefficient. Debye-Huckel theory of electrolytic solutions. Debye-Huckel limiting law (derivation not required). Calculation of mean ionic activity coefficient. Limitations of Debye-Huckeltheory. Extended Debye-Huckellaw. Theory of electrolytic conductance. Nernst equation, redox systems.

UNIT-II (15 Hours)

Transmission of nervous impulse, bioenergetics, electrochemical methods in biology and medicine. Electron transfer in homogeneous systems, theory of electron transfer processes, electron tunneling, electron transfer in heterogeneous systems, electrode-solution interface, rate of charge transfer in electrode reactions, study of kinetics of electrode processes.

UNIT-III (15 Hours)

Potentiometric titrations.Functioning of ion selective electrodes, glass electrodes and pH sensor, ion exchange membrane and neutral carrier membrane electrodes. Sensor selective to dissolved gases, enzyme selective electrodes. Recent developments related to miniaturization, potentiometric sensors in flow system, electroanalysis with potentiometric sensor. Liquid junction potential (LJP) – derivation of the expression for LJP – its determination and elimination**.** Methods of determining structures of electrified interfaces, Guoy-Chapman, Stern.Decomposition potential and its significance. Electrode polarization – its causes and elimination. Concentration over-potential.

UNIT-IV (17 Hours)

Cyclic voltammetry, study of reaction mechanism, spectro electrochemistry, electrochemical quartz crystal microbalance, controlled potential techniques, electrochemical cells, oxygen removal, instrumentation, working electrodes, chemically modified electrodes, microelectrodes.

Recommended Text Books / Reference Books:

1. P. Atkins, J. D. Paula, 'Physical Chemistry', 7th Indian Edn.,Oxford University Press.
2. Ira N. Levine, 'Physical Chemistry', McGraw Hill.
3. D.A. McQuarrie and J.D. Simon, 'Physical Chemistry-A Molecular approach', Viva Books Pvt. Ltd.
4. S. Glasstone, 'Introduction to Electrochemistry', Litton Educational Publishing.
5. J. O. M. Bockris& A. K. N. Reddy, 'Modern Electrochemistry', Plenum.
6. K.L. Kapoor, 'A textbook of Physical Chemistry', Vol.3, Laxmi Publications.

SUPRAMOLECULAR CHEMISTRY

Subject Code: PCHM1-112 **L T P C** 4 0 0 4 **Duration: 60(Hrs.)**

Course Objectives

1. To familiarize the students with the basic concepts of supramolecular chemistry.
2. To make students learn the mechanism of molecular recognition and synthesis & application of supramolecular substrates
3. To understand the supramolecular reactivity and catalysis procedure
4. To acquaint with supramolecular structures.

Course Outcomes:

The students will acquire knowledge of:

1. Fundamental terminology and definitions of supramolecular chemistry
2. Mechanistic aspects of molecular recognition and synthesis & applications of supramolecular reactants
3. Reaction mechanism of supramolecular catalysis
4. Supramolecular structures and their applications

UNIT-I (15 Hours)

Fundamentals of Supramolecular chemistry terminology and definitions in supramolecular chemistry. Intermolecular forces: Ion pairing, ion-dipole and dipole-dipole interactions; hydrogen bonding; cation-pi, anion-pi, pi-pi interactions and Van der Waal forces. Solvent and solution properties, solvation and hydrophobic effect.Binding constants; definition and use, determination of binding constant by physical methods.

UNIT-II (15 Hours)

Molecular Recognition Principle of molecular recognition, host-guest complementarity, preorganisation, chelate effect, cooperativity. Synthesis and applications of supramolecular host (crown ethers, lariat ethers, podands, cryptands, spherands, calix[n]arenes, cyclodextrine) as cation and anion binding receptors and receptors for ion-pair recognition.

UNIT-III (15 Hours)

Supramolecular Reactivity and Catalysis:Organocatalysis mediated through hydrogen bonding, preconcentration, self-assembly of catalysts and preorganisation of catalyst-substrate systems. Influence of organisation (effective molarity) on catalysis, Catalytic acyl transfer, acid-base catalysis, catalysis hydrolysis as ATPase mimic

UNIT-IV (15 Hours)

Supramolecular structures – molecular wires, sensors, switches and logic gate devices, metal-organic frameworks and their applications.

Recommended Books:

1. Supramolecular Chemistry: from Molecules to Nanomaterials Eds. by P.A. Gale and J.W. Steed (2012).
2. Modern Supramolecular Chemistry by F. Diederich, P. J. Stang, R. T. Tykwinski (2008).
3. Core Concepts in Supramolecular Chemistry and Nanochemistry by J. W. Steed, D. R. Turner, K. J. Wallace (2007).
4. Supramolecular Chemistry by J.W. Steed and J.L. Atwood (2011).
5. Supramolecular Chemistry: Concepts and Perspectives by J.-M. Lehn, Wiley VCH, Weinheim (1995).
6. Supramolecular Chemistry by V. Balzani (Editor), L. De Cola, Kluwer, Dordrecht (1992).
7. Introduction to Supramolecular Chemistry by H. Dodziuk, Kluwer Academic Publishers, The Netherlands (2002).
8. Supramolecular Assemblies Y. Murakami (Editor), Mita Press, Tokyo, (1990).
9. Advances in Supramolecular Chemistry, Vol 1 (1990), Vol 2 (1992), Vol 3 (1993) by G. W. Gokel (Editor), JAI Press, Greenwich.
10. Supramolecular Chemistry – Fundamentals and Applications. Advanced Textbook by T. Kunitake, K Ariga, Berlin: Springer-Verlag Heidelberg, 20

CHEMISTRY OF ORGANOMETALLIC COMPOUNDS

Subject Code: PCHM1-113 **L T P C** **Duration: 60Hrs.**

4 0 0 4

Course Objectives

1. To recall classification of ligands and nomenclature of organometallic compounds.
2. To understand structure, bonding and reactivity of organometallic compounds.
3. To familiarize with the role of organometallic compounds in organic syntheses.
4. To understand the applications of organometallic compounds ascatalysts.
5. To understand fluxional behavior in various organometallic compounds.

Course Outcomes:

The students will acquire knowledge of

1. Organometallic compounds and its nomenclature.
2. Bonding and reactivity of metalcomplexes.
3. Fluxional behaviour
4. Role of organometallic complexes in organicsyntheses.
5. Importance of catalyst in syntheses.

UNIT-1 (15 Hrs.)

Nomenclature of organometallic compounds, Classification of Ligands in organo metallic compounds, inert gas rule. Transition Metal compounds with Bonds to hydrogen. Characterization of Hydride complexes, Hydrogen Bridges. Synthetic methods, Chemical behavior of Hydrido Compounds, Mononuclear polyhydrides, Carbonyl hydride & Hydride Anion Molecular Hydrogen compounds, Metal – Hydrogen interactions with C-H groups, Complexes of Borohydrides and AluminohydridesWade's rules, carboranes and other hetro-boranes

UNIT-2 (15 Hrs.)

Energy polarity and reactivity of M-C bond, Stability of Main group organometallics: Methods of preparation in perspective-organolithium compounds: structure and bonding & reaction- carbolithiatic organometallics of group 2 and 12 e.g. Mg and Zn, Cd and Hg: Preparation and structure of organoaluminiumcompounds.Technical applications of Tris (alkyl) aluminium compounds.η 2 - ligands: olefenic and acetylenic complexes, chelating olefenic ligands – synthesis and structure. η 2 – ligands: Allylic and η 4– complexes of cyclopentadiene.

Ferrocenes- Structure & bonding of ferrocenes, basic chemical reactions of ferrocenes, chirality in ferrocene derivatives, ferrocene based condensationpolymers.

UNIT-3 (15 Hrs.)

Transition Metal Carbon Monoxide compounds. Preparation of Metal Carbonyls, Structures of Metal carbonyls Mononuclear, Binuclear, Trinuclear and Tetranuclear and larger Polynuclear carbonyls. Additional structural and Bonding features: Semibridging CO groups, side on Bonding to CO, Oxygen to Metal Bonds, Vibrational Spectra of Metal carbonyls, Detection of Bridging CO groups. Molecular symmetry from the number of Bands, Bond Angles & Relative Intensities, Force constants, Prediction and Assignment of Spectra.Carbonylate Anions, Metal carbonyl, Hydrides, Reactions of Metal Carbonyls; Photochemical Reactions of Metal Carbonyls

:Nucleophilic& electrophilic attacks on CO Metal carbonyl scrambling

Fluxional organometallic compounds: Fluxionality and dynamic equilibria in compounds such as η 2 Allyl, Carbonyl and dienyl Complexes.

UNIT-4 (15 Hrs.)

Applications of organometallic complexes to Catalysis-Basic principles, sequences involved in catalytic reaction, Hydro formylation: Cobalt catalyst & phosphine modified cobalt catalysts, water gas shift reaction, Oxopalladation reactions. Monsato, Cativa&Wackerprocesses, polymerization &oligomerisation of olefins &dienes, Heck reaction and Suzuki-Miyaura Coupling.

Bioorganometallic Chemistry: Role of organometallics in heavy metal poisoning: Mercury and Arsenic poisoning, organometallic compounds as drugs: ruthenium and ferrocene based drugs; Organometallics as radiopharmaceutical, tracers, ionophores and sensors.

Recommended Books

1. 'Basic Organometallic Chemistry: Concepts, Synthesis & Application ofTransition Metals', CRC Press & Univ. Press,**2010**.
2. R.C. Mehrotra& A, Singh, 'Organometallic Chemistry, A Unified Approach', New Age International.
3. B.D. Gupta & A.J. Elias, 'Basic Organometallic Chemistry', UniversitiesPress.
4. F.A. Cotton & G. Wilkinson, 'Advanced Inorg, Chemistry', WileyIntersciences.