Pre Ph.D. (Chemistry)

School of Physical Science

(Chemistry)

DIT University Dehradun

Course Structure & Syllabus for Pre Ph.D. (Chemistry) Course Work

Session: 2020-21

Approved by the Academic Council at its 14th Meeting held on 20.04.2020

Pre Ph.D (Chemistry)

Course Category	Course Code	Course Name	Periods			Credits
			L	T	P	
UC	MB901	Research Methodology	4	0	0	4
	CPE-RPE	Research Publication Ethics	2	0	0	2
DC	CH606	Advanced Chromatographic Techniques	4	0	0	4
DC	CH607	Advanced Spectroscopic Analytical Techniques	4	0	0	4
DC	CH608	Advanced Organic Synthetic Methodology	4	0	0	4
DC	DS001	Seminar	0	0	2	1
		Total				**19**

Note: Apart from above listed Elective courses, Research Scholar may choose any course across departments being offered at PG level, if it is required/suggested by the Research Committee.

Pre Ph.D (Chemistry)

Subject Code	MB901	Subject Title	Research Methodology						
LTP	4 0 0	Credit	4	Subject Category	UC	Year	1st	Semester	I / II

UNIT – I

Fundamentals of Research: Defining research, Objectives of research, types, research process, deductive and inductive reasoning;

Identifying and formulating a research problem, Literature review: Search for existing literature (World Wide Web, Online data bases), Review the literature selected (Case studies, review articles and Meta-analysis), Develop a theoretical and conceptual framework, Writing up the review,

Definition of variables: Concepts, indicators and variables, Types of variables, Types of measurement scales, Constructing the Hypothesis- Null(Research) and alternative, one-tailed and two-tailed testing, errors in testing. Ethical and Moral Issues in Research, Plagiarism, tools to avoid plagiarism – Intellectual Property Rights – Copy right laws – Patent rights

UNIT – II

Research Design: Design of Experiments: Research Designs -Exploratory, Descriptive and Experimental, Experimental designs- Types of Experimental Designs

UNIT – III

Sampling, Sampling distribution, and Data Collection: Sampling distribution, Normal and binomial distribution, Reasons for sampling, sampling technique, sampling errors.Sources of Data-Primary Data, Secondary Data, Data Collection methods

UNIT – IV

Statistical Data Analysis: Descriptive and inferential statistical analysis. Testing of hypothesis with Z-test, T-test and its variants, Chi-square test, ANOVA, Correlation, Regression Analysis, Introduction to data analysis data using SPSS20.0

UNIT – V

Research Report: Writing a research report- Developing an outline, Formats of Report writing, Key elements-Objective, Introduction, Design or Rationale of work, Experimental Methods, Procedures, Measurements, Results, Discussion, Conclusion, Referencing and various formats for reference writing of books and research papers, Writing a Research Proposal.

Books Recommended:

1. Ganesan R, Research Methodology for Engineers , MJP Publishers, Chennai. 2011
2. C.R.Kothari, "Research Methodology", 5th edition, New Age Publication,
3. Cooper, "Business Research Methods", 9th edition, Tata McGraw hills publication
4. Walpole R.A., Myers R.H., Myers S.L. and Ye, King: Probability & Statistics for Engineers and Scientists, Pearson Prentice Hall, Pearson Education, Inc. 2007.
5. Anderson B.H., Dursaton, and Poole M.: Thesis and assignment writing, Wiley Eastern 1997.
6. Bordens K.S. and Abbott, B.b.: Research Design and Methods, McGraw Hill, 2008.
7. Morris R Cohen: An Introduction to logic and Scientific Method (Allied Publishers) – P 197-222; 391–403

Pre Ph.D (Chemistry)

Subject Code	CH606	Subject Title	Advanced Chromatographic Techniques						
LTP	4 0 0	Credit	4	Subject Category	DC	Year	1st	Semester	I / II

COURSE OBJECTIVE:

The basic aim of this course is to enhance the capability of research students on hand on experience. They should understand the fundamentals of different techniques and their applications.

UNIT I: Introduction to Separation Techniques **7 Hours**

Separation Techniques, Classification of chromatographic techniques (Retention mode and sample introduction); fundamentals of paper, TLC and HPTLC chromatography-Mobile phases and Stationary Phases, development of Chromatograms; Detection and Quantitation; Applications in qualitative and quantitative analysis

Unit 2: High Performance Liquid Chromatography **8 Hours**

HPLC: Principle, Retention Parameters in HPLC, resolution and retention Time; Instrumentation; Separation Mechanism in HPLC; Stationary phase effects; Role of HPLC and HPTLC in qualitative and quantitative analysis of bioactive metabolites and some approved drugs and application of LC/MS in analysis.

Unit 3: **Gas Chromatography** **8 Hours**

Gas Chromatography: Principle and theories of separation process; GC-columns, gas chromatographic detectors; Recording and analysis; Resolution; Application of GSC and GLC; Applications of GC/Mass and GC/IR analysis; comparison of GC and HPLC.

Unit 4: Ion Exchange Chromatography **8 Hours**

Ion Exchange Chromatography: Theories, use of synthetic ion exchangers in separation, chelating ion exchange resins, liquid ion exchangers, experimental techniques and applications; Affinity chromatography, Affinity separations and SDS-Gel Electrophoresis-applications in Protein purifications.

References:

1) "Unified Separation Science" by J.C. Giddings
2) "Principles and Practice of Modern Chromatographic Methods" by K. Robards, P.R. Haddad and P. E. Jackson.
3) High Performance liquid chromatography: Principles and Methods, Elena D. Katz(John Wiley & Sons Ltd. 2009)
4) Chromatography and Separation Science Satinder Ahuja, (2003), Academic Press

COURSE OUTCOME:

At the end of the course, the student can:

CO1.A solid theoretical understanding of chromatography and mass spectrometry at an advanced level.

CO2. Some experience in addressing complex analytical problems, and acquaintance with tools to solve them.

CO3. Hands-on experience with advanced and diverse chromatographic systems and mass spectrometers.

CO4. New tools for research processes also studied.

Pre Ph.D (Chemistry)

Subject Code	CH607	Subject Title	Advanced Spectroscopic Analytical Techniques						
LTP	4 0 0	Credit	4	Subject Category	DC	Year	1st	Semester	I / II

COURSE OBJECTIVE:

The basic aim of this course is to enhance the capability of research students for determination of functional group and spectroscopic analysis of organic compounds in chemistry. They should understand the fundamentals of different techniques and their applications.

Unit 1: UV-Vis & IR Spectroscopy **8 Hours**

Introduction, Types of electronic absorption bands, Theory of electronic spectroscopy, Types of electronic transitions, Transition probability, The Chromophore concept, Auxochrome, Absorption and intensity shifts, Types of absorption bands, Solvent effects, Conjugated dienes, Woodward-Fieser rules for calculating absorption maximum in dienes, UV absorption in α, β-unsaturated carbonyl compounds, Applications of UV spectroscopy, Important features in electronic spectroscopy.

IR spectroscopy: principle of IR spectroscopy, Selection rules, Factors influencing vibrational frequencies, Scanning of IR spectrum and application in interpretation of organic functional groups.

Unit 2: ^{1}H NMR Spectroscopy **8 Hours**

Basic theory – phenomenon of energy absorptions (resonance) and relaxation, chemical shift, shielding and deshielding mechanisms, equivalence and nonequivalence of protons, spin-spin coupling – notation for spin systems, coupling constant and its variation with stereochemistry-Karplus equation. Structural application of 1H NMR, aromaticity, antiaromaticity and homoaromaticity of organic molecules and related problems.

^{13}C NMR Spectroscopy: Principles; broad band decoupling, DEPT; structural applications of ^{13}C NMR.

Unit 3: **Mass Spectrometry** **8 Hours**

Types of ionization techniques, basic principles of EI. Fragmentation processes and structural analysis; ESI, GC/MS, LC/MS and MS/MS techniques, fragmentation pattern of small molecules and interpretation of spectroscopic (NMR, IR and mass) data, as applied to organic, inorganic and biological systems Problems incorporating spectroscopic data.

Unit 4: Introduction to 2D NMR **8 Hours**

COSY, NOESY, HSQC, HMBC, HETCOR, HOMCOR, INEPT for simple compounds and problem

REFERENCES

1. Spectroscopic identification of organic compounds by Robert M. Silverstein, Francis X. Webster and David J. Kiemle.
2. Introduction to spectroscopy by Donald L. Pavia, Gary M. Lampman and George S. Kriz.
3. Elementary Organic spectroscopy by Y. R. Sharma.

COURSE OUTCOME:

At the end of the course, the student can:

CO1.A solid theoretical understanding of organic compounds by interpretation through spectroscopic and mass spectrometry at an advanced level.

CO2. *Hands-on experience with advanced and diverse spectroscopy, IR, UV-Vis and mass spectrometer*

Pre Ph.D (Chemistry)

Subject Code	CH608	Subject Title	Advanced Spectroscopic Analytical Techniques						
LTP	4 0 0	Credit	4	Subject Category	DC	Year	1st	Semester	I / II

COURSE OBJECTIVE:

This course provides an introduction to the synthesis of complex organic molecules. Transformations of C-X to C-C bond-formation, functional group reactivity, chemoselectivity, regioselectivity, and the strategy of multistep synthesis will be the core topics that are covered. Concepts include strategy/retrosynthesis, advanced aromatic chemistry, protecting groups, stereochemistry, enolates and other carbonyl chemistry, alkene synthesis, reduction/oxidation (introductory), heterocycles, cross-coupling reactions and other modern methods of synthesis

Unit 1: C-C, C-X and C=C bond forming reactions **8 Hours**

Transition metal complexes in organic synthesis; only Pd, Ni, Co, Fe, Cu (Metal mediated C-C and C-X bond formation reactions: Suzuki, Heck, Sonogashira, Stille, Fukuyama, oxo process etc; C=C formation reactions: Wittig, Horner-Wordworth-Emmons, Shapiro reactions, Mc Murry, Julia-Lythgoe and Peterson olefination reactions etc

Unit 2: Multi-component and Ring forming reactions **8 Hours**

Construction of Ring Systems: Different approaches towards the synthesis of four, five and six-membered rings; photochemical approaches for the synthesis of four membered rings, oxetanes and cyclobutanes. Diels-Alder reaction (inter- and intramolecular); specific examples of Mannich reactions, Ugi, Passerini, Pausan-Khand, Bergman and Biginelli Reactions and Diels-Alder reaction; Click chemistry: criterion for click reaction and Sharpless azides cycloadditions.

Unit 3: **Macro cyclic Compounds** **8 Hours**

Principles in the construction of macrocyclic rings and ring closing metathesis, Grubbs 1st and 2nd generation catalyst; Applications of metallic carbenes in organic synthesis. Use of Boron and Silicon in Industrial organic synthesis, applications and other important reactions like; Baylis Hilman, Eschenmoser-Tanabe fragmentation, Mitsunobu reaction, etc

Unit 4: Chemistry of Protective group **8 Hours**

Protecting groups: Protection and de-protection of hydroxy, carboxyl, carbonyl, carboxy amino groups and carbon-carbon multiple bonds; chemo- and regioselective protection and deprotection; illustration of protection and deprotection in synthesis.

REFERENCES

1. Organic chemistry – J. Clayden, N. Greeves, S. Warren and P. Wothers (Oxford Press)
2. Designing of organic synthesis – S. Warren (Wiley)
3. Some modern methods of organic synthesis – W. Carruthers (Cambridge)
4. Organic synthesis using transition metals-Roderick Bates (Wiley)
5. Organometallics in organic synthesis – J. M. Swan and D. C. Black (Chapman and Hall)
6. Advanced organic chemistry, Part B – F. A Carey and R. J. Sundberg, 5th edition (2007)

COURSE OUTCOME:

At the end of the course, the student can:

CO1.A fundamental and theoretical understanding of organic reactions transformation by mechanistically.

CO2. The knowledge of synthetic organic chemistry is a great demand in pharmacy, medicinal and industrial chemistry.