Program Outcomes (PO) for Science Doctoral Course-work Program

1. **In-depth Knowledge:** Acquire basic in-depth and advance knowledge by critically applying and comprehensive understanding of methodologies to address issue and question of a science discipline and attain specialization in a particular domain.
2. **Research and Scientific Reasoning:** Apply theories, methodologies, knowledge, critical thinking, and inductive and deductive reasoning to design and drive research projects with appropriate hypothesis, experimental design, simulation, etc.
3. **Communication and Digital Skills**: Acquire proficiency in oral and written communication skills to comprehend and write effective reports, design documents, make effective presentation, and give and receive clear instructions,
4. **Professional Ethics:** Acquire the knowledge of ethics and values to inculcate fair practices throughout their professional life.
5. **Project Management:** Develop and apply knowledge of science and technology, project management and finance principles, in a multidisciplinary setting, to carry out meaningful research and project work.
6. **Leadership Readiness**: Interact with people from diverse backgrounds as both leaders/mentors and team members with integrity and professionalism.

Program Specific Outcomes (PSO)

PSO_1 To apply the fundamental knowledge of chemistry and inculcate skill in problem solving, critical thinking and reasoning to seek solutions to complex problems in modern chemistry

PSO_2 Design solutions for complex scientific problems and develop innovative processes that meet the specified needs with appropriate consideration for the public health and safety, and the cultural, societal, and environmental considerations

PSO_3 Independently explore new areas of research in both chemistry and allied fields of science and technology and function effectively as an individual, and as a member or leader in diverse teams, and in multidisciplinary settings

PSO_4 Apply ethical principles in research and commit to professional ethics, responsibilities and norms.

PSO_5 Communicate effectively on complex scientific results with the peers and with the society at large, such as, being able to comprehend and write effective reports and design documentation, make effective presentations, and give and receive clear instructions.

O P JINDAL UNIVERSITY

O P Jindal Knowledge Park, Punjipathra, Raigarh-496109

Department of Chemistry

OPJU

UNIVERSITY OF STEEL TECHNOLOGY AND MANAGEMENT

Programme:	**Ph.D. Course-work Chemistry**	**Semester:**	**I/II**
Course Name:	**Research Methodology**	**Course Code:**	**PCW 101**
Credits :	**5**	**No of Hours :**	**50**
Max Marks:	**100**		

Course Description

Course Outcomes (CO)

Students will be able to	
CO 1	Set a research question or topic in an appropriate scholarly manner;
CO 2	Place a working hypothesis into a real context;
CO 3	Use appropriate tools for data collection and analysis;
CO 4	Match the research method to the research question;
CO 5	Write up research projects using scholarly norms;
CO 6	Communicate efficiently and consistently the outcomes of the research before audience;
CO 7	Critically review a research paper.
CO 8	Manage deadlines in the crafting of a research paper.

Syllabus

UNIT I

Meaning and significance of research; Importance of scientific research in decision making; Types of research and research process; Identification of research problem and formulation of hypothesis

UNIT II

Research Design: Concept and Importance in Research – Features of a good research design – Exploratory Research Design – concept, types and uses, Descriptive Research Designs – concept, types and uses. Experimental Design: Concept of Independent & Dependent variables.

UNIT III

Qualitative and Quantitative Research, Measurement: Concept of measurement, Problems in measurement in research – Validity and Reliability. Levels of measurement – Nominal, Ordinal.

UNIT IV

Factor analysis, Multiple Regressions Analysis. Discriminant Analysis, Use of SPS Package, IPR issues. Factor analysis, Multiple Regressions Analysis. Discriminant Analysis, Use of SPS Package, IPR issues.

UNIT V

Research Report, Types and significance, Structure of research report, Ethical issues in research, Presentation of report. Interpretation of Data and Paper Writing, Journal selection, Impact factor of Journals. Plagiarism and Self-Plagiarism, Software for detection of Plagiarism.

Resources

Name of Text and Reference Books:

- Business Research Methods– Donald Cooper & Pamela Schindler, TMGH, 9th ed.
- Business Research Methods– Alan Bryman & Emma Bell, Oxford University Press.
- Research Methodology – C.R. Kothari.
- Research Methodology, Chawla and Sondhi, Vikas Publication
- Research Methodology, Paneersevam, PHI

CO- PO & PSO Correlation

Course Name	**Seminar Presentation**										
Course Outcomes	**POs**						**PSOs**				
	1	**2**	**3**	**4**	**5**	**6**	**1**	**2**	**3**	**4**	**5**
CO 1											
CO 2											
CO 3											

O P JINDAL UNIVERSITY

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Department of Chemistry

UNIVERSITY OF STEEL TECHNOLOGY AND MANAGEMENT

Programme:	**Ph.D. Course-work Chemistry**	**Semester:**	**I/II**
Course Name:	**Seminar Presentation**	**Course Code:**	**PCH 101**
Credits :	**5**	**No of Hours :**	**50**
Max Marks:	**100**		

Course Description

Course Outcomes (CO)

Students will be able to	
CO 1	
CO 2	
CO 3	

CO- PO & PSO Correlation

Course Name	**Seminar Presentation**										
Course Outcomes	**POs**						**PSOs**				
	1	**2**	**3**	**4**	**5**	**6**	**1**	**2**	**3**	**4**	**5**
CO 1											
CO 2											
CO 3											

Programme:	**Ph.D. Course-work Chemistry**	**Semester:**	**I/II**
Course Name:	**Characterisation Techniques**	**Course Code:**	**PCH 102**
Credits :	**5**	**No of Hours :**	**50**
Max Marks:	**100**		

Course Description

Material Characterization focuses on the theoretical basic knowledge of material synthesis and its application to science and technology. It is an extension and deepening of the prerequisite science concepts at UG & PG level which is one of the core courses for Science graduates. The main objective of this course is to provide students with a systematic and critical study of basic scientific principles for technical problem solving in materials areas and advanced concepts of characterization techniques. Topics include classification of techniques for characterization like thermal analysis techniques, principle, construction and working principles of TEM, SEM, STEM, Atomic absorption spectrometer (AAS), Atomic Emission spectroscopy (AES), XPS (ESCA), Auger Electron Spectroscopy, FTIR, EDS & WDS, Electron Probe Micro Analysis (EPMA), Nuclear Magnetic Resonance (NMR) Techniques, X-ray diffraction and magnetization measurement processes. All these contents provide a foundation for post graduate courses and research.

Course Outcomes (CO)

Students will be able to	
CO 1	Understand the relation between material structure, its properties and methods of determination
CO 2	Learn the principal, instrumentation and applications of thermal, electrochemical & spectroscopic methods for material characterization
CO 3	Analyze the data for predicting the functional groups, structure of organic and inorganic compounds, and other related parameters like bond length, bond angles etc.

Syllabus

UNIT-I

Importance of Material characterization, Classification of techniques for characterization, Differential Thermal Analysis (DTA): Theories of DTA, factors affecting DTA curves, instrumentation and application of DTA. Thermogravimetry (TG): Instrumentation and balances, X'- Y' recorder, thermogram, factors affecting thermogram, correlation of DTA and TGA data. TMA and DSC

UNIT-II

Principle, Construction and Working of TEM, SEM, STEM with their merits, demerit and applications, UV-Visible spectroscopy (UV-VIS), IR & Raman spectroscopy, X-ray Fluoroscopy

(XRF), Atomic absorption spectrometer (AAS), Atomic Emission spectroscopy (AES), XPS (ESCA), Auger Electron Spectroscopy.

UNIT-III

FTIR, EDS & WDS; Electron Probe Micro Analysis (EPMA); Nuclear Magnetic Resonance (1H & C-13 NMR) Technique.

UNIT-IV

Diffraction method; X-ray diffraction, determination of crystal structure, lattice parameter, crystallite size by diffraction techniques / low angle X-ray scattering technique.

UNIT-V

Cyclic voltammetry (CV), potentiodynamic polarization measurement (Tafel plot), electrochemical impedance spectroscopy (EIS), polarography, potentiometry, Coulometry and amperometry, linear sweep voltammetry (LSV), Applications of electrochemical techniques.

Resources

Text and Reference Books:

- F. Weinberg, Editor, Tools & Techniques in Physical Metallurgy, Vol. I & Vol. II, Marcel Dekker, 1970.
- John P. Sibilia, A guide to Material Characterization & Chemical Analysis, VCH Publishers, 1988.
- J.M. Walls, Editor, Methods of Surface Analysis: Techniques & Applications, Cambridge University Press, 1990.
- B.D. Cullity, Elements of X-ray diffraction, Addison-Wesley Publishing Company, INC, 1978.
- Bernhard Wounderlich, Thermal Analysis, Academic Press, INC, 1990.
- B.L. Gabriel, SEM: A user's manual for materials Science, American Society for Metals, 1985.
- An Introduction to Materials Characterization by P. R. Khangaonkar, Penram International Publishing (India) Pvt. Ltd.

CO- PO & PSO Correlation

Course Name	**CHARACTERISATION TECHNIQUES**										
Course Outcomes	**POs**						**PSOs**				
	1	**2**	**3**	**4**	**5**	**6**	**1**	**2**	**3**	**4**	**5**
CO 1	**3**	**2**		**1**		**1**	**2**		**2**	**1**	
CO 2	**3**	**2**	**1**	**2**	**1**		**2**			**2**	
CO 3	**3**	**2**	**1**	**2**		**1**	**2**			**2**	**2**

Programme:	**Ph.D. Course-work Chemistry**	**Semester:**	**I/II**
Course Name:	**Advanced concepts of Chemistry**	**Course Code:**	**PCH 103**
Credits :	**5**	**No of Hours :**	**50**
Max Marks:	**100**		

Course Description

This course aims to understanding of the concepts of periodic properties and chemical bonding and their applications to coordination complexes of transition and inner transition elements along with their synthesis, structures and other applications. The students will acquire the skills for correct stereochemical assignment and interpretation in rather simple organic molecules. They will also be able to learn synthesis and applications of Organometallic and Heterocyclic compounds their synthetic applications. The course also aims to elaborate the solution and colloidal chemistry, symmetry and group theory and brief overview of analytical techniques used in Chemistry.

Course Outcomes (CO)

Students will be able to	
CO 1	Understand the synthesis, properties and applications of inorganic & organic compounds
CO 2	Understand the principal and application of different analytical techniques for purification & characterization of compounds
CO 3	Understand space and point groups in crystals and application of X-ray diffraction technique for crystal structure elucidation

Syllabus

UNIT I: Inorganic Chemistry

Periodic table and periodic properties; chemical bonding, chemistry of coordination complexes; Chemistry of transition and inner transition elements

UNIT II: Organic Chemistry

Stereochemistry- Chirality, Isomerism, Enantiomers, Organometallic chemistry- synthesis of metal alkyls, transition metal compounds and their role, Heterocyclic Chemistry, Mass Spectrometry of Organic compounds

UNIT III: Physical Chemistry

Solution & Colloidal Chemistry, Solid State Chemistry: X-Ray Diffraction, point groups, space groups and crystal structure, Defects in crystals; Various types of defects in crystal; Thermodynamics of Schottky and Frenkel defects formation; Colour centers; Non-stoichiometric defects. Electrochemistry

UNIT IV: Analytical techniques in Chemistry

Purification/ Crystallization: Isolation and purification of organic compounds (solids and liquids) with special emphasis on chromatographic techniques: TLC, column chromatography and HPLC. Drying and dehydrating agents

Resources

Text and Reference Books:

- A Bahl & B S Bahl, Advanced Organic Chemistry, S Chand Publication, 2015
- A R West, Solid State Chemistry and its applications, Wiley, 2013
- J Mendham, R C Denney, J D Barnes, M J K Thomas, Vogel's Textbook of Quantitative Chemical Analysis, 6th Ed., Pearson Education, 2008
- G D Christian, Analytical Chemistry, 6th ED., Wiley, 2013
- W U Malik, G D Tuli, R D Madan, Selected topics in Inorganic Chemistry, S Chand, 2015
- J D Lee, Concise Inorganic Chemistry, 5th Ed., Wiley, 2017
- P Atkin, J De Paula, J Keeler, Atkin's Physical Chemistry, Oxford Univ. Press, 2018
- FA Cotton, G Wilkinson & PL Gaus, Basic Inorganic Chemistry, 3rd Ed., Wiley, 2013
- RT Morrison, Boyd & SK Bhattarjee, Organic Chemistry, 7th Ed., Pearson, 2018

CO- PO & PSO Correlation

Course Name	**ADVANCED CONCEPTS OF CHEMISTRY**										
Course Outcomes	**POs**						**PSOs**				
	1	**2**	**3**	**4**	**5**	**6**	**1**	**2**	**3**	**4**	**5**
CO 1	**3**	**2**			**1**		**1**	**2**		**1**	
CO 2	**3**	**1**		**2**	**1**		**2**			**1**	**1**
CO 3	**3**	**1**	**2**	**2**	**1**		**2**			**1**	**1**

Programme:	**Ph.D. Course-work Chemistry**	**Semester:**	**I/II**
Course Name:	**THRUST AREAS OF CHEMISTRY**	**Course Code:**	**PCH 104**
Credits :	**5**	**No of Hours :**	**50**
Max Marks:	**100**		

Course Description

This course focuses on developing concepts and skills for stereochemical & group assignment and interpretation in rather simple organic molecules, predicting reaction mechanisms and identifying reaction intermediates. Stereo chemical implications of pericyclic reaction in organic synthesis and their mechanistic pathways is also learnt. This course also aims at identification of new avenues of synthesis through Green chemistry and microwave synthesis techniques.

Course Outcomes (CO)

Students will be able to	
CO 1	Learn the different types of reaction mechanism, reaction intermediates, stereochemistry and their spectroscopic identification
CO 2	Understand the concepts and important reactions of photochemistry and pericyclic reactions.
CO 3	Apply the concepts of symmetry and group theory to simple molecules
CO 4	Learn the principles, applications and advantages of green methods for synthesis

Syllabus

UNIT- I: Reaction mechanisms, Intermediates and Stereochemistry

Types of reaction mechanisms, Reaction Intermediates: Generation, structure, stability and reactivity of carbocations, carbanions, free radicals, carbenes, nitrenes, and benzynes

Conformational analysis of cycloalkanes, decalins effect of conformation on reactivity, conformation of sugars, steric strain due to unavoidable crowding.

Elements of symmetry, chirality, molecules with more than one chiral centre, threo and erythro isomers, methods of resolution, optical purity, enantiotopic and diastereotopic atoms, stereospecfic and stereo selective synthesis. Asymmetric synthesis. Optical activity in the absence of chiral carbon (biphenyls. allenes and spiranes).

UNIT II: Pericyclic Reactions & Photochemistry

Molecular orbital symmetry, frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene and allyl system. Classification of pericyclic reactions. Woodward-Hoffmann correlation diagrams, FMO and PMO approach. Electrocyclic reactions- conrotatory and disrotatory motions, 4n, 4n+2 and allyl systems. Cycloadditions - antrafacial and suprafacial additions. 4n, 4n+2 systems, 2+2 addition of ketenes, 1,3dipolar cycloadditions and cheleotropic reactions.

Sigmatropic rearrangements - suprafacial and antrafacial shifts of H, Sigmatropic shifts involving carbon moieties, 3,3- and 5,5- sigmatropic rearrangements, Claisen, Cope and Aza-Cope rearrangements. Fluxional tautomerism, Ene reaction.
Basic of Photochemistry: Absorption, excitation, photochemical laws, quantum yield, electronically excited states- life times-measurements of the times. Flash photolysis, Energy dissipation by radiative and non-radiative processes, Miscellaneous Photochemical Reactions

UNIT III: Symmetry and Group Theory

Symmetry elements and symmetry operation, definitions of group, subgroup, relation between orders of a finite group and its subgroup. Conjugacy relation and classes. Generators, Point symmetry group. Representations of group operators, The great orthogonality theorem (without proof) and its explanation. Irreducible and reducible representation. Bases of representation, Character of a representation. Character table and its meaning.

UNIT IV: Emerging Green Chemistry

Green chemistry, 12 principles, Solvent-free synthesis; Environmentally benign solvents: Water and Ionic liquids as green solvents and catalysts in organic synthesis.
Microwave in chemical synthesis: Basic principles, advantages, and examples.

UNIT V: Organic Spectroscopy

Spectroscopic methods for structure analysis such as mass spectrometry, nuclear magnetic resonance spectroscopy, infrared spectroscopy, and ultraviolet spectroscopy. Fundamentals of the NMR phenomenon, relationship between NMR spectra and molecular structure. Recording of routine spectra (^{1}H and ^{13}C), essentials of data processing.

Resources

Text & Reference Books:

- Physical Methods for Chemistry, R.S. Drago, Saunders Company- Horwood.
- Practical NMR Spectroscopy, M.L. Martin, J.J. Delpeugh and G.J. NBrtin. Heyden.
- Introduction to NMR Spectroscopy, R.J. Abraham, J. Fisher and P.Loftus. Wiley
- Introduction to Organic Photochemistry, John D. Coyle. Wiley.
- Green Chemistry: An Introductory Text, Mike Lancaster, Royal Society of Chemistry, 2002
- Spectroscopy of Organic compounds, P.S. Kalsi, (7th Edition), New Age International Publisher. 2016
- J. Clayden, N. Greeves, S. Warren and P. Wothers, Organic chemistry, Oxford University press INC, New York, 2001
- M.B. Smith & Jerry March, March's Advanced Organic Chemistry, 5th Edition (2001), John Wiley & Sons, New York

- Pericyclic Reactions & Organic Photochemistry, Dr. Satyajit Dey Dr. Nirmal Kr. Hazra. Techno World, 2019
- Symmetry and Group Theory in Chemistry, S. K. Dogra, H. S. Randhawa. New Academic Science Ltd, 2015
- Stereochemistry: Conformation and Mechanism, P.S. Kalsi. New Age Publishers, 2019

CO- PO & PSO Correlation

Course Name	**THRUST AREAS OF CHEMISTRY**										
Course Outcomes	**POs**						**PSOs**				
	1	**2**	**3**	**4**	**5**	**6**	**1**	**2**	**3**	**4**	**5**
CO 1	**3**	**2**		**1**			**2**	**1**	**1**		**1**
CO 2	**3**	**2**					**3**	**2**	**1**		
CO 3	**3**	**1**					**1**				**1**
CO 4	**3**	**3**		**2**			**3**	**2**	**1**		**1**