Name of School: Sciences

Name of Program: Ph.D Chemistry

Program Structure

Program Description

The Department of Chemistry offers a Doctor of Philosophy (Ph.D.) degree in Chemistry. The Ph.D. degree in chemistry requires evidences of high quality scientific research leading to peer reviewed publications with classroom teaching, laboratory supervision, and proposal and manuscript writing experiences. The program covers all modern aspects of chemistry like analytical, biochemistry, computational, environmental, inorganic, organic, and physical chemistry, Polymer Science and interdisciplinary areas in material, energy, environmental, and biomedical research. The intensive graduate training includes formal lecture courses, hands-on laboratory and theoretical research experiences, teaching experiences, independent proposal development, preparation of manuscripts, and preparation of a research thesis or dissertation for publication.

Programme Objectives:

1. To prepare students for development of methods of independent and systematic investigations leading to scientific discoveries.
2. Students will acquire an in-depth knowledge of the main chemistry field by reading scientific papers and performing original research.
3. To prepare students for a successful career at academic institutions, industrial and business entities, and governmental agencies.
4. To promote professional development and growth of the faculty.
5. Develop and understand the ethical and social dimension of science and the role and responsibility of chemistry for the advancement of the society.
6. The Department also aims at Chemistry outreach in the form of books, online courses, and other Chemistry education activities that showcase the role of Chemistry as a central science.

Programme Outcomes: Students who successfully complete this programme will be able to:

1. Work in the interdisciplinary and multidisciplinary areas of chemical sciences and its applications.
2. Identify and conduct original research, scholarship or creative endeavors.
3. Publish research, extension, or teaching results in peer-reviewed and/or other outlets.
4. A strong appreciation of all aspects of polymer chemistry.
5. The students will be able to analyze the electrochemical data (for example, with respect to mechanisms of redox reactions), design catalysts for electrochemical reactions. Appreciate and know fundamentals of electrochemical phenomena.
6. The students would learn about the importance of metal ions in biological systems and how the metal ions mediate various biological functions such as metal-protein interactions, metal-nucleic acid interactions. They would also learn medicinally important metalloproteins, and development of drugs based on metalloproteins inhibition.
7. The student shall gain a sound understanding of the basics of organic synthesis, methodology development and multi-step synthesis.
8. The students will learn a great deal of physical chemistry principles as applied to organic chemistry. This would enable them to devise experiments to understand new reactions mechanistically

PROGRAMME STRUCTURE- Ph.D CHEMISTRY

S. No.	Name of Programme	Total Numbers of Credits
1.	Ph.D Chemistry	

First Semester

S. No.	Course Title	Lecture (L) Hours Per Week	Tutorial (T) Hours Per Week	Practical (P) Hours Per Week	Total Credits (C)	CBL/ PBL/R BL*
DP-I	Research Methodology	5	0	0	5	CBL
DP-II (A)	Advanced in Inorganic Chemistry-I	5	0	0	5	CBL
DP-II (B)	Advanced in Inorganic Chemistry-II	5	0	0	5	CBL
DP-III (A)	Advanced in Organic Chemistry-I	5	0	0	5	CBL
DP-III (B)	Advanced in Organic Chemistry-II	5	0	0	5	CBL
DP-IV (A)	Advanced in Physical Chemistry-I	5	0	0	5	CBL

DP-IV (B)	**Advanced in Physical Chemistry-II**	**5**	**0**	**0**	**5**	**CBL**
DP-V	**Seminar, Field work & Review Writing**	**5**	**0**	**0**	**5**	**CBL**

***CBL/PBL/RBL: Course Based Learning/Practical Based Learning/Research Based Learning**

COURSE CURRICULUM

Ph.D Chemistry

DP-1	**Research Methodology**	L	T	P	C
Version 1.0	Date of Approval:	5	0	0	5
Pre-requisites					
Co-requisites					

Course Description:

This course introduces and discusses approaches, strategies, and data collection methods relating to research in social sciences. Students will consider how to select the appropriate methodology for use in a study to be performed. Additionally, these students will learn how to collect data based on different data collection methods, construct these tools, and pilot them before they become ready for use. Finally, this course elucidates the requirements for an academic work, considering aspects related to language, writing style, and lay-out. To culminate this final stage, students will learn to write a comprehensive research proposal that may be conducted in the future.

Course Objectives:

1. To develop understanding of the basic framework of research process.
2. Students should know why educational research is undertaken, and the audiences that profit from research studies.
3. Identify appropriate research topics.
4. Identify and discuss the complex issues inherent in selecting a research problem, selecting an appropriate research design, and implementing a research project.
5. To enable the participants in conducting research work and formulating research synopsis and report

6. Identify and discuss the concepts and procedures of sampling, data collection, analysis and reporting.
7. Students should be familiar with ethical issues in educational research, including those issues that arise in using quantitative and qualitative research.

Course Outcomes:

Students who successfully complete this course will be able to:

1. Develop understanding on various kinds of research, objectives of doing research, research process, research designs and sampling.
2. Have basic knowledge on qualitative research techniques.
3. Read, comprehend, and explain research articles in their academic discipline.
4. Apply the understanding of feasibility and practicality of research methodology for a proposed project.
5. Propose and distinguish appropriate research designs and methodologies to apply to a specific research project.

Fundamental Laboratory Techniques : Basic principles, Health and safety, workingwith liquids, Basic laboratory procedures I, Basic laboratory procedures II, Principles of solution chemistry, pH and buffer solutions (Ref. 1. Chapters 1 to 7: pages 03 to 62)

The investigative approach : Making and recording measurements, SI units and theiruse, Scientific method and design of experiments, Project work (Ref. 1. Chapters 8 to 11: pages 65 to 83)

Analysis and presentation data : Using graphs, Presenting data in tables, Hints for solving numerical problems, Descriptive statistics, choosing and using statistical tests, drawing chemical structures, chemometrics, computational chemistry (Ref. 1. Chapters 37 to 44: pages 251 to 295)

Information technology and library resources : The Internet and World Wide Web, internet resources for chemistry, using spreadsheets, word processors, databases and other packages, finding and citing information (Ref. 1. Chapters 45 to 49: pages 299 to 321)

Communicating information : General aspects of scientific writing, writing essays, reporting practical and project work, writing literature surveys and reviews, organizing a poster display, giving an oral presentation examinations (Ref. 1. Chapters 50 to 56: pages 325 to 354)

Chemical safety and Disaster Management:

(a) Emergency response: chemical spills, radiation spills, biohazard spills, leaking compressed gas cylinders, fires, medical emergency accident reporting

(b) General safety : General safety and operational rules, safety equipments, personal protective equipments, compressed gas safety, safety practices for disposal of broken glass wares, centrifuge safety, treated biomedical wastes and scientific ethics.

Research problem : meaning of research problems, sources of research problems, criteria /characteristics of a good research problem, errors in selecting a research problem.

Hypothesis: Meaning, types of hypothesis.

Developing a Research Proposal : Format of research proposal, individual research proposal and institutional proposal.

Research Report: Format of the research report, style of writing the report, references and bibliography.

Books:

1. Practical Skills in Chemistry, J. R. Dean, A. M. Jones, D. Holmes, R. Reed, J. Weyers and A Jones, Pearson Education Ltd. [Prentice Hall] (2002)

2. Creswell, J. (2014). Research Design: Qualitative, Quantitative, and Mixed Methods Approaches (Vol: SAGE Publications.

3. Research Methodology. Methods and Techniques: C. R. Kothari,

4. Tests, Measurements and Research Methods in Behavioural Sciences: A. K. Singh.

DP-II (A)	**Advanced in Inorganic Chemistry-I**	L	T	P	C
Version 1.0	Date of Approval:	5	0	0	5
Pre-requisites					
Co-requisites					

Course Objectives:

1. To introduce concepts of various analytical and spectroscopic techniques.
2. Fundamental understanding on the principle of operation and interpretation of spectra of inorganic compounds for their structural characterization.
3. To develop the understanding of various separations techniques.

Course Outcome: The students will acquire knowledge of

1. Applications of various spectroscopic techniques will be learnt by the students to handle molecular structures during their higher studies or industrial applications.
2. Have basic knowledge on qualitative of various analytical, spectroscopic and separations techniques.

UNIT- I

(a) Thermogravimatric analysis: Introduction, Factors affecting thermogravimetric curves, instrumentation, applications to inorganic compounds (analysis of binary mixtures i.e. Ca and Mg, TG curves of calcium oxalate, determination of Ca, Sr & Ba ions in the mixture, drying of sodium carbonate, decomposition of potassium hydrogen phthalate).

(b) Differential thermal analysis: Introduction, Factors effecting DTA curves, instrumentation, applications, to inorganic compounds (thermal decomposition of mixtures of lanthanum-cerium and praseodymium oxalate, DTA curves for $CuSO_4.5H_2O$, sulphur, detection of organic contamination in ammonium nitrate.

UNIT- II

Nuclear Magnetic Resonance Spectroscopy:- Introduction to Nuclear Magnetic Resonance, Chemical shift, Mechanism of electron shielding and factors contributing to the magnitude of chemical shift, Nuclear overhausser effect, Double resonance, Chemical exchange, Lanthanide shift reagents and NMR spectra of paramagnetic complexes. Experimental technique (CW and FT).

Stereochemical non-rigidity and fluxionality: Introduction, use of NMR in its detection, its presence in trigonal bipyramidal molecules(PF5), Systems with coordination number six ($Ti(acac)_2C_{l2}$, $Ti(acac)_2Br_2$, $Ta_2(OMe)10$,).

UNIT -III

Mossbauer Spectroscopy: Introduction, Principle, Conditions for Mossbauer Spectroscopy, parameters from Mossbauer Spectra, Isomer shift, Electric Quadrupole Interactions, Magnetic Interactions MB experiment, Application of MB spectroscopy in structural determination of the following:

i) High spin Fe (II) and Fe (III) halides FeF2, FeCl2.2H2O, FeF3, FeCl3.6H2O. Low

spin Fe(II) and Fe(III) Complexes-Ferrocyanides, Ferricyanides, Prussian Blue.

ii) Iron carbonyls. $Fe(CO)_5$, $Fe_2(CO)_9$ and $Fe_3(CO)_{12}$

iii) Inorganic Sn(II) and Sn(IV) halides.

UNIT -IV

Electron Spin Resonance Spectroscopy:-. Introduction, Similarities between ESR and NMR, Behaviour of a free electron in an external Magnetic Field, Basic Principle of an Electron Spin Resonance Spectrometer, Presentation of the spectrum, Hyperfine coupling in Isotropic Systems (methyl, benzene and Naphthalene radicals). Factors affecting the magnitude of g-values. Zero field splitting and Kramer's Degeneracy, Line width in solid state ESR, Double resonance technique in e.s.r. (ENDOR) Experimental method. Applications of ESR to the following:

1. Bis-Salicylaldiimine-Copper –II

2. CuSiF6.6H2O & (NH3)5Co-O.Co(NH3)5

UNIT -V

Separation Techniques in Analysis:-Ion exchange Chromatography, types of ion-exchangers, ion exchange equillibria and factors affecting it, cation and anion exchange resins, ion-chromatography, instrumentation, detectors and methods of analysis. Solvent extraction, theory and mechanism of solvent extraction, synergistic extraction, solvent extraction with macromolecules (crown ethers, cryptands, calyx, arenes etc.) solid phase extraction and solid phase micro-extraction.
Modern Analytical Methods:

(b) Advanced separation techniques:

i. High performance liquid chromatography

ii. Gas chromatography for separation and Mass Spectrometry (GC/MS)

DP-II (B)	**Advanced in Inorganic Chemistry-I I**	L	T	P	C
Version 1.0	Date of Approval:	5	0	0	5
Pre-requisites					
Co-requisites					

Course Objectives:

1. To understand the concept of chirality in transition metal complexes.
2. To give a systematic introductory treatment of organometallic compounds, emphasising synthesis, properties, structure and reactivity.

3. The students should be able to describe various types of isomerism which can occur in coordination complexes.
4. To develop the understanding of metal ions in biological systems and how the metal ions mediate various biological functions such as metal-protein interactions, metal-nucleic acid interactions.
5. To develop the understanding of Supramolecular Reactions and Catalysis.

Course Outcome: The students will acquire knowledge of

1. The importance of metal ions in biological systems and how the metal ions mediate various biological functions such as metal-protein interactions, metal-nucleic acid interactions.
2. Students should be able to explain selected crystal structures explain what kind of parameters that affect the crystal structure of a compound.
3. Be able to describe some of the applications of supramolecular chemistry including industrial applications and supramolecular catalysis.
4. Have a good overview of the core concepts in supramolecular chemistry and explain non covalent interactions, molecular recoginition and self-assembly.
5. Have a good overview of the fundamental principles of organotransition-metal chemistry and know how chemical properties are affected by metals and ligands.

UNIT-I

Chirality in transition metal complexes: Chirality and enantiomers, enantiomers and racemic compounds, physical properties of enantiomers and racemics, principles of resolution and preparations of enantiomers, Chirality at metal half-sandwich compounds, asymmetric catalysis by chiral complexes, Chiral recognition in organometallic complexes and asymmetric catalysis, chiral enantiopure molecular materials.

UNIT -II

Catalysis Involving Organometallic compounds: Homogeneous hydrogenation and hydroformylation of unsaturated compounds (Olefins). Asymmetric hydrogenation, hydroformylation, hydrosilylation of unsaturated compounds, hydrocyanation of alkenes; alkenes and alkynes metathesis.

UNIT -III

a) Supramolecular Reactions and Catalysis: Introduction, Catalysis by reactive macrocyclic cation receptor molecule, by reactive macrocyclic anion receptor molecule Supramolecular metallo catalysis.

b) Supramolecular Assemblies: Introduction, Supramolecular solid materials, Molecular recognition at surfaces (Endoreceptors vs Exoreceptors), Molecular and Supramolecular Devices, Photonic, electronic and Ionic Devices

UNIT -IV

a) Role of Metal-ions in Biological Systems: Metal-ion-interactions with Nucleosides and Nucleotides, Metal-ion-interactions with DNA, Metal-ion-interactions with RNA.
b) Electron-Transfer Agents in Biological Systems: Cytochromes, Iron sulphur proteins, Vitamin B12and B12Coenzymes Xanthane oxidase and Superoxide dismutase.

UNIT-V

a) Surface Reactions: Mechanism of surface reactions, unimolecular and bimolecular surface reactions, Langmuir – Hinshelwood mechanism for gases only.

b) Co-ordination Addition Polymerisation: Zeigler Natta catalysts, composition, nature and mechanism of stereo specific placement in polymerisation, bimetallic and monometallic mechanism, stereoregulation, Supported metal oxide catalysts, polymerisation mechanism, bound-ion radical mechanism and bound-ion co-ordination mechanism.

Books:

1. Comprehensive Inorganic chemistry, J. C. Bailar, H. J. Emeleus, Sir R. Nyholm, R. F. Tortman-Dickenson (Pergamon Press, 1973) Volume 1to 5.
2. Chirality in transition metal Chemistry, Hani Amouri and Michel Gruselle (Wiley, 2008)
3. Biological Inorganic Chemistry, Robert R. Crichton
4. Bioorganometallic chemistry, Volume Editor G. Simonneaux (Springer, 2009)
5. Inorganic Material Chemistry, M. T. weller (oxford, 1994)
6. Catalysis: Principles & Applications, B. Vishvanathan, S. Sivasankar and A.V. Ramaswamy (Narosa Publication House, New Delhi 2004)
7. Inductively coupled plasma spectrometry and its applications, Steve J. Hill (Sheffield Academic Press, 1999)
8. High Performance liquid chromatography Principles and Methods, Elena D. Katz (John Wiley & Sons Ltd. 2009)
9. Fundamentals of Molecular Spectroscopy, C. N. Banwel
10. Spectroscopy in Inorganic Chemistry - Rao & Ferraro Vol I & II

DP-III (A)	Advanced in organic Chemistry-I	L	T	P	C
Version 1.0	Date of Approval:	5	0	0	5
Pre-requisites					
Co-requisites					

Course objectives:

1. To understand the principles used in asymmetric synthesis.
2. To understand the stereochemistry of sugar conformations.
3. To learn various organic reactions and reagents used in them as tools applied in the art of organic synthesis.
4. The course aims to provide a sound understanding of the fundamentals of the chemistry of carbohydrates that will enable the student to carry forward.
5. To develop the understanding of peptide synthesis.
6. Students will be introduced to the field of polymer chemistry, synthetic methods and characterization.

Course outcomes: Students who successfully complete this course will be able to:

1. Use various reagents and organic reactions in organic synthesis.
2. To understand the impotence of carbohydrate chemistry in research and their applications in biomedical field.
3. The student shall gain a sound understanding of the basics of organic synthesis, methodology development and multi-step synthesis.
4. To explain the importance of peptide synthesis and their applications in various field of chemistry.
5. Students will be able to use the understanding gained for the synthesis and characterization of polymer materials for designing novel polymeric materials for applications

UNIT-I

Reagents in Organic Synthesis: Reagents in organic synthesis: Willkinson catalyst, Triphenylphosphine-alkyl halide reagent, Lithium dialkylcuprates (Gilman's reagents), Lithium diisopropylamide (LDA), Dicyclohexylcarbobiimide (DCC), Tri-n-butyltinhydride. Nickel tetracarbonyl, Trimethylchlorosilane.

UNIT-II

Asymmetric Synthesis: Principle and categories with specific examples of asymmetric synthesis including newer methods involving enzymatic and catalytic reactions, enantio and diastereoselective synthesis. Stereoselective Reactions: Cyclopropanation, hydroboration, catalytic hydrogenation, and metal ammonia reduction, stereoselective synthesis of (-) ephedrine and (+) ϕ- ephedrine. Stereospecific Reactions: Elimination of 2, 3-dibromobutanedensyl chloride (1,2-diphenyl-1-chloroethane), SN2reactions at chiral carbon.

UNIT-III

Carbohydrates: Types of naturally occurring sugars: Deoxy-sugars, amino sugars, branched chain sugars. General methods of structure and ring size determination with particular reference to maltose, lactose, sucrose, pectin, starch and cellulose, photosynthesis of carbohydrates, metabolism of glucose, Glycoside- (amygdalin).

UNIT-IV

Amino acid, peptides and proteins: General methods of peptide synthesis, sequence determination. Chemistry of insulin and oxytocin. Purines and nucleic acid. Chemistry of uric acid, adenine, protein synthesis.

UNIT-V

Vitamins: A general study, detailed study of chemistry of thiamine (Vitamin B1), Ascorbic acid (Vitamin C), Pantothenic acid, biotin (Vitamin H), α-tocopherol (Vitamin E), Biological importance of vitamins.

Books:

1. M. B. Smith and J. March, *March's Advanced Organic Chemistry, Reactions, Mechanism and Structure*, Sixth Ed., John Wiley & Sons, 2007.
2. J. Clayden, N. Greeves, and S. Warren, *Organic Chemistry*, 2nd Edition, Oxford University Press, 2012.
3. J. March, *Advanced Organic Chemistry*, John Wiley & Sons, 1992.
4. Peter Sykes, *A Guidebook to Mechanism in Organic Chemistry,* Pearson Education India, 1986.

DP-III (B)	**Advanced in organic Chemistry-II**	L	T	P	C
Version 1.0	Date of Approval:	5	0	0	5
Pre-requisites					
Co-requisites					

Course objectives:

1. To learn and apply various concepts such as stereochemistry and fundamental principles of stereoselectivity in organic chemistry.
2. To learn basic principles of NMR, IR, UV-Vis spectroscopy and mass spectrometry and to use these spectroscopic methods for organic structure elucidation and understand how spectroscopic techniques can be used to delineate a molecule's structure.

3. Identify and describe different diffraction methods.

Course Outcomes: At the end of course the students will be able to:

1. Predict number of signals, splitting patterns in the proton NMR of a compound given its structure and use this knowledge to interpret NMR spectra of simple molecules.
2. Identify the absorption frequencies of major functional groups, understand the factors that govern electronic absorption and use this knowledge to interpret IR and UV-Vis spectra of simple organic molecules.
3. Develop ability in the combined use of mass spectrometry and spectroscopic techniques for structure elucidation.
4. Understand and apply the various types of powder diffraction experiment and appreciate the importance of sample preparation.

UNIT-I

Stereochemistry; Stereoselective and stereospecific reactions: Stereoselective reactions: Hydride reduction of cyclic ketones, catalytic hydrogenation, Stereoselective nucleophilic addition to acyclic carbonyl groups. Stereospecific reactions: Bromination of alkenes, Epoxidation and dihydroxylation of alkenes, Hydroboration oxidation. Analysis and separation of enantiomeric mixture: Chiral shift reagent and chiral solvating agents, Separation of enantiomers by chromatography. Enzymatic separation and desymmetrization using lipasases, proteases, Acylases and epoxide hydrolases.

Reaction–Mechanism: Reaction and mechanism of following organic reactions: Stevens rearrangement, Cope rearrangement, Claisen rearrangement, Metathesis of olefins, Di-πmethane rearrangement, Hofmann-Loffler reaction, Sharpless assymetric epoxidation and Stork-enamine reaction

UNIT-II

(A) Ultra Violet and Visible Spectroscopy: Electronic transitions (185-800 nm), Beer- Lambert Law, Effect of solvent on electronic transitions, Ultra Violet bands of carbonyl compounds, unsaturated carbonyl compounds, dienes, conjugated polyenes. Fieser-Woodward rules for conjugated dienes and carbonyl compounds, Ultra- Violet spectra of aromatic and heterocyclic compounds. Steric effect in biphenyls. Applications of UV- visible spectroscopy in organic chemistry.

(B) Infrared Spectroscopy: Instrumentation and sample handling, Characteristic vibrational frequencies of common organic compounds. Effect of hydrogen bonding and solvent effect on vibrational frequencies, overtones, combination bands and Fermi resonance. Introduction to Raman spectroscopy. Applications of IR and Raman Spectroscopy in organic chemistry.

UNIT-III

Nuclear Magnetic Resonance (NMR) Spectroscopy: General introduction, chemical shift, spin-spin interaction, shielding mechanism, chemical shift values and correlation of protons present in different groups in organic compounds. chemical exchange, effect of deuteration, complex spin-spin interaction between two, three, four and five nuclei, virtual coupling. Stereochemistry, hindered rotation, Karplus-relationship of coupling constant with dihedral angle. Simplification of complex spectra-nuclear magnetic double resonance, spin tickling, INDOR, contact shift reagents, solvent effects. Fourier transforms technique, Nuclear Overhauser Effect (NOE). Introduction to resonance of other nuclei –F, P, Principle and introduction to C13NMR, 2-D and 3-D NMR, Applications of NMR in organic chemistry.

UNIT-IV

Mass Spectrometry: Introduction, ion production—EI, CI, FD and FAB, factors affecting fragmentation, ion analysis, and ion abundance. Mass spectral fragmentation of organic compounds, common functional groups, Molecular ion peak, Meta-stable peak, Mc-Lafferty rearrangement. Nitrogen Rule. High-resolution mass spectrometry. Examples of mass spectral fragmentation of organic compounds with respect to their structure determination. Introduction to negative ion Mass spectrometry, TOF-MALDI. Problems based upon IR, UV, NMR and mass spectroscopy.

UNIT-V

X- ray diffraction: Indexing of powder and crystal photographs. Determination of Bravais lattice, point group and space group. Determination of space group with examples. Electron diffraction: The scattering of electron by gases (Wierl equation), visual method, radial distribution method and applications. Neutron diffraction: Introduction, differences between neutron and X- ray diffraction. Application to structure modification and magnetic compounds.

Books:

1. Advanced Organic Chemistry, Fourth Edition, Part A and B F. A. Carey and R. J. Sundberg.
2. Organic Chemistry, Clayden, Greeves, Warren and Wothers
3. Advanced organic chemistry by J. March, 6th Ed.
4. C. Hammond, The Basics of Crystallography and Diffraction, Oxford University Press, 2009

DP-IV (A)	**Advances in physical chemistry -I**	L	T	P	C
Version 1.0	Date of Approval:	5	0	0	5
Pre-requisites					
Co-requisites					

Course objectives:

1. Identify and describe different diffraction methods.
2. To understand the fundamental aspects of spectroscopy with special emphasis on the rotational, vibrational, Raman and electronic spectroscopies. Students will also be introduced to fundamental and application aspects mass spectrometry.
3. To understand the concept of Thermogravimatric analysis and Differential thermal analysis.
4. This course on spectroscopy, aimed at introducing students to the fundamental principles of magnetic resonance spectroscopy –NMR and ESR. Students will learn to solve composite problems using UV, IR, NMR and mass spectrometry in organic, inorganic and organometallic compounds.

Course Outcomes:

At end of the course the students will be able to:

1. Understand and apply the various types of powder diffraction experiment and appreciate the importance of sample preparation.
2. Students will be able to understand and explain the theoretical basis of different spectroscopic techniques.
3. Students will be able to apply the principles of magnetic resonance and other spectroscopic techniques in elucidation of organic, inorganic and organometallic compounds.

UNIT – I

X- ray diffraction: Indexing of powder and crystal photographs. Determination of Bravais lattice, point group and space group. Determination of space group with examples. Electron diffraction: The scattering of electron by gases (Wierl equation), visual method, radial distribution method and applications. Neutron diffraction: Introduction, differences between neutron and X- ray diffraction. Application to structure modification and magnetic compounds.

UNIT – II

Spectroscopy – I: Theory of nuclear magnetic resonance NMR phenomenon, the chemical shift and its measurement. The fine structure (spin – spin coupling). Factors influencing chemical – shift and spin – spin coupling. Non - first – order spectra. Relaxation phenomena in NMR: spin – spin and spin – lattice relaxation processes. Line –width and rate processes. The nuclear Overhauser effect. An introduction to Fourier Transform NMR (FTNMR).

UNIT -III

Theory of Electron Spin Resonance (ESR) phenomenon. Fine and hyper fine structure of ESR. Zero – field splitting of ESR signal. Mapping of charge density on molecule (McConnell relation). Mossbaur spectroscopy: a brief introduction (isomer – shift, quadrupole interaction and magnetic hyperfine interaction).

UNIT -IV

Spectroscopy – II: Rotational and vibrational spectra. Moment of inertia and rotational spectra of rigid and non – rigid diatomic molecules. Vibrational excitation effect. Rotational spectra of symmetric-top molecules. Strak effect. Vibrational energy of diatomic molecules. Anharmonic oscillator, overtones and hot bands. Diatomic vibrator–rotator (P, Q and R – branches of diatomic vibrator – rotator). Rotational – vibrational spectra of symmetric–top molecules. Raman Spectroscopy: qualitative quantum theory of Raman scattering. Rotational Raman spectra of linear and symmetric – top molecules.Vibrational Raman spectra and mutual exclusion principle.

Unit -V

(a) Thermogravimatric analysis: Introduction, Factors affecting thermogravimetric curves, instrumentation, applications to inorganic compounds (analysis of binary mixtures i.e. Ca and Mg, TG curves of calcium oxalate, determination of Ca, Sr& Ba ions in the mixture, drying of sodium carbonate, decomposition of potassium hydrogen phthalate).

(b) Differential thermal analysis: Introduction, Factors effecting DTA curves, instrumentation, applications, to inorganic compounds (thermal decomposition of mixtures of lanthanum-cerium and praseodymium oxalate, DTA curves for $CuSO_4.5H_2O$, sulphur, detection of organic contamination in ammonium nitrate.

Books:

1. Banwell C. N.; McCash, E. M., Fundamentals of Molecular Spectroscopy, 4thEd., Tata McGraw Hill, New Delhi (2017).
2. Lampman, G. M.; Pavia, D. L.; Kriz, G. S.; Vyvyan, J.R., Introduction to Spectroscopy, 5thEd., Cengage Learning India, New Delhi (2015).
3. Silverstein, R. M.; Webster, F. X.; Kiemle, D. J.; Bryce, D. L., Spectrometric Identification of Organic Compounds, 8th Ed., Wiley India, New Delhi (2015).

DP-IV (B)	**Advances in physical chemistry -I I**	L	T	P	C
Version 1.0	Date of Approval:	5	0	0	5
Pre-requisites					
Co-requisites					

Course Objectives:

1. To understand the concept of various parameters involved in electrochemistry and their applications.
2. To understand the concept of surface electrochemistry.
3. To understand the principle of Chemical Relaxation Techniques.

Course Outcomes:

At end of the course the students will be able to:

1. To develop the understanding of electrochemistry and their application in the field of research.
2. Have a good knowledge of surface chemistry.
3. To develop the understanding of chemical relaxation techniques and how do apply the chemical relaxation techniques in the field of research.

UNIT -I

Physical Chemistry of Ionic Solution: Ion –Solvent and Ion –Ion interactions: Ion –quadrupole model of ion –solvent interactions, ion –induced dipole interactions in primary salvation sheath. Heats and entropy changes accompanying hydration. Hydrophobic effect in salvation. Debye–Huckel Theory of ion –ion interactions. Poisson's equation and Debye –Huckel Theory of charge distribution around ions (Linearzation of Boltzmann equation), and linearized Poisson – Boltzmann equation and its solution. Debye–Huckel ionic–cloud model and Debye –Huckel length.

UNIT-II

Surface Electrochemistry: The electrified interface, introduction and basic facts of electro capillarity, thermodynamics of the electrocapillary effect. Thermodynamic treatment of polarizable interface, determination of charge density on the electrode (Lippmann equation), and determination of surface excess (variation of surface tension with solvent composition of electrochemical system) .The structure of electrified surfaces.The Helmholtz –Perrin theory, the Gouy–Chapman Diffuse–Charge Model of double layer and Stern Model. Isotherms of adsorption in electrochemical systems. The Temkin isotherm, ionic isotherm for heterogeneous surfaces and thermodynamic analysis of adsorption isotherm.

UNIT -III

Basic Principles of Chemical Relaxation Techniques: Relaxation time and its significance, determination of rate constants from relaxation data. Evaluation of relaxation time form a relaxation oscillogram. Relaxation time in multi step systems. Chemical relaxation in two and multi step systems. Thermodynamic aspects in relation to chemical relaxation; Gibbs free energy, affinity of a reaction and advancement of a reaction.

UNIT -IV

Experimenta l Techniques for the Study of Relaxation Kinetics (Theory and Applications):∑Pressure Jump Technique: Application to mechanistic investigation of relaxation behaviour in Beryllium Sulphate solution and determination of thermodynamic quantities from amplitude data of relaxation oscillogram. ∑Temperature Jump Technique: Application to mechanism of water addition to carbonyl functional group of organic carbonyl compounds. ∑Electric Field Jump Technique: Application to neutralization reaction. ∑Ultrasonic Relaxation Technique: Application to ion –association (ultrasonic absorption in aqueous solutions of $MnSO_4$), and inter and intra molecular proton transfer reaction.

UNIT –V

Surface Electrochemistry: The electrified interface, introduction and basic facts of electrocapillarity, thermodynamics of the electrocapillary effect. Thermodynamic treatment of polarizable interface, determination of charge density on the electrode (Lippmann equation), and determination of surface excess (variation of surface tension with solvent composition of electrochemical system) .The structure of electrified surfaces.The Helmholtz –Perrin theory, the Gouy–Chapman Diffuse–Charge Model of double layer and Stern Model. Isotherms of adsorption in electrochemical systems. The Temkin isotherm, ionic isotherm for heterogeneous surfaces and thermodynamic analysis of adsorption isotherm.

References:

1. Principles of Instrumental Analysis, 5th edition- D.A. Skoog, F.J. Holler, T.A. Nieman, hiladelphia Saunders College Publishing (1988)
2. Principles of activation analysis - P. Kruger , John Wiley (1971)
3. Modern Electrochemistry, Volume 1 and 2, J.O.M Bokris and A.K.N, Reddy Plenum Press N.Y. (1970)
4. Electrochemical Methods second edition, A. J. Bard and L.R. Faulkner, John Wiley and Son (2001).
5. Bard, A. J. Faulkner, L. R. Electrochemical Methods: Fundamentals and Applications, 2nd Ed., John Wiley & Sons: New York, 2002.
6. Modern Electrochemistry, Volume 1 and 2, J.O.M Bokris and A.K.N, Reddy Plenum Press N.Y. (1970)
7. Antropov, L. I. Theoretical Electrochemistry Physical Principles of Electron Microscopy: An Introduction to TEM, SEM and AEM by Ray F. Egerton Springer

DP-V	**Seminar, Field work & Review Writing**	L	T	P	C
Version 1.0	Date of Approval:	5	0	0	5
Pre-requisites					
Co-requisites					

1. Seminar: Seminar to be delivered on a relevant theme **(01 credits)**
2. Field Work: Visit to industry/National institutes and interaction with experts. (Report to be submitted) **(01 credits)**
3. Review : Preparation and submission of review article based on research papers addressing a contemporary research problem. **(02 credits)**
4. Other activities: Attending National / International workshop/Symposium/ Conferences or participation for oral / poster presentation or interaction with M.Sc. students for problem solving approaches / Work of Nobel laureates in last ten years in Science.
(01 credits)

*** Above topics shall be prepared in consultation with research guide**