Scheme of
Ph.D Chemistry
2022-23 (Onwards)

SRI SAI UNIVERSITY
PALAMPUR (H.P.), INDIA

Courses Structure
Ph.D Chemistry

Course Code	Title of Course	Marks				Credits			
		Theory	Practical	Internal Assessment	Total	L	T	P	Total
		Semester –I							
		Compulsory Courses							
CHEM-CC-611	Instrumental Methods	60	…….	40	100	4	0	0	4
RM-CC-023	Scientific Research Methodology	60	….....	40	100	4	0	0	4
RPE-CC-021	Research and Publication Ethics	30	------	20	50	1	2	0	2
		Elective Course							
		(Students have to choose any one from the following Subjects related to Dissertation work)							
CHEM-EC-612	Advanced Inorganic Chemistry-I	60	…….	40	100	4	0	0	4
CHEM-EC-613	Advanced Inorganic Chemistry-II	60	….....	40	100	4	0	0	4
CHEM-EC-614	Organic Synthesis	60	…….	40	100	4	0	0	4
CHEM-EC-615	Polymer Chemistry	60	….....	40	100	4	0	0	4
CHEM-EC-616	Adsorption and Advanced Electrochemistry	60	…….	40	100	4	0	0	4
CHEM-EC-617	Micelle Formation and Nanotechnology	60	….....	40	100	4	0	0	4
		Semester –II-VI							
	Research Work					…	…	8	8*
Thesis Evaluation / Viva Voce Examination after the submission of thesis						…	…	8	8

*If student does satisfactory performance in Thesis work, then He/She will be awarded four 'SSSS' (equal to 8 credits) in respective semester, and if his/her research work found unsatisfactory then he/she may be awarded 'SXXX'/ 'SSXX'/'SSSX' depending upon performance.

Note: Students have to earn minimum 54 credits during the thesis work for the successful award of Ph.D Degree.

Here 'S' carries 2 credits

'X' carries 0 credit

The candidates qualifying the entrance test or those who are exempted from entrance test will have to pass course work before starting their research work. However, they will have to choose supervisor from University for their research. The duration of course work will be one semester and the subjects to be studied shall be decided by the student's supervisor after assessment of his/her already studied courses.

Note: A Ph. D. Scholar will be allowed to undertake creditable research after the completion of course work.

COMPULSORY COURSES

PAPER I

L	T	Credit
4	0	4

CHEM-CC-611: Instrumental Methods

Course Objectives	The primary objective of this course is to acquire basic concepts, principles, and techniques of modern analytical chemistry that would empower students with an analytical mind set and the abilities to solve diverse analytical problems in an efficient and quantitative way that conveys the importance of accuracy and precision of the analytical results. To learn various techniques of spectrometric identification of various compounds. To characterize inorganic compounds by applying various techniques together.
Course Outcomes	On successful completion of this course, students will be able: • to develop an understanding of the range and uses of analytical methods in chemistry. • to establish an appreciation of the role of chemistry in quantitative analysis. • to develop an understanding of the broad role of the chemist in measurement and problem solving for analytical tasks. • to provide an understanding of chemical methods employed for elemental and compound analysis. • to provide experience in some scientific methods employed in analytical chemistry. • to develop some understanding of the professional and safety responsibilities residing in working on chemical analysis.

DETAILED CONTENT

MODULE-1 Advanced Absorption Spectroscopy Techniques.

Ultraviolet and Visible Spectroscopy: Introduction basic principle of absorption spectroscopy (Beer-Lambert law), types of electronic transitions, and effect of solvents.

Infrared (IR) spectroscopy, Fourier Transform (FT) IR spectrophotometer, IR and FTIR spectrophotometers, sampling and sample preparation (Solid, liquid and gaseous samples). Hydrogen bonding and solvent effects, overtones, combination bands and Fermi resonance.

MODULE-2 Nuclear Magnetic Resonance Techniques.

Fundamentals, instrumentation, preparation of sample. Proton spectra and Carbon-13 spectra. Spin-spin interactions, mechanism of measurement, chemical shift values, chemical exchange, effect of deuteration, simplification of complex spectra-nuclear magnetic double resonance, solvent effects, fourier transform technique, nuclear overhauser effect (NOE), structure elucidation. Introduction to fluorescence spectroscopy, instrumentation, applications of fluorescence phenomenon.

MODULE-3 Thermogravimetric Techniques.

Thermal gravimetric analysis (TGA), and Differential thermal analysis (DTA). Instrumentation, techniques. Applications of TGA and DTA. CHN analyzer: basic principle, instrumentation and quantitative analysis

MODULE-4 Chromatographic Techniques.

Fundamentals of chromatography, High-pressure liquid chromatography (HPLC), Gas chromatography and gas chromatography mass spectroscopy (GCMS). Instrumentation and applications.

MODULE-5 Miscellaneous Techniques.

Introduction and applications of Differential scanning calorimetry (DSC), X-ray crystallographic techniques, Tracer technique, Transmission electron microscopy **(**TEM), Scanning electron microscopy (SEM), and small angle X-ray scattering (SAXS) techniques.

Reference Books:

1. Textbook of Quantitative Inorganic Analysis-Vogel A.I.

2. Principles and Practice of Analytical Chemistry-Fifield F.W. and Kealey D, Black well Science

3. Instrumental Analysis R. Braun, Mcgraw Hill, International Edition

4. Instrumental Analysis, Willard Merilt, CBS.

5. Chemical Analysis, Brawn, Mcgraw Hill.

6. Chemical Analysis, Underwood PH Publication Co.

7. Fundamentals of Analytical Chemistry-Skoog D.A and West D.M, Saunders.

8. Analytical Chemistry-Christain G.D, Wiley WSE.

9. Organic Chemistry, Clayden, Greeves, Warren and Wothers, Oxford University Press 2006

10. Textbook of Quantitative Inorganic Analysis, Menohemetal, Pearson

Educatoin

11. Ewings Analytical Instrument hand book – Cazes, Marcel Dekkar

11. Analytical Chemistry, Kellneretal, Wiley VCH

12. Deans Analytical Chemistry Handbook – Patnaik, Mcgraw Hill Co.

13. Instrumental methods of analysis, Willandmerrit and dean, caps publications & Distribution, 1999.

14. Instrumentaiotn methods of analysis, Chatwal&Anand, Himalaya Publications,2003.
15. Principles of Analytical Chemistry by Vacarcel, Springer Publications, 2005

16. R.S. Drago, Physical Methods for Chemistry, Saunders Company

17. R.M. Silverstein, G.C.Bassler, and T.C. Morrill Spectrometric Identification of Organic Compounds John Wiley

18. J.R. Dyer, Application of Spectroscopy of Organic Compounds, Prentice Hall.

19. Pavia, D.L. Lampman, Gary M. George S. Kriz Introduction to Spectroscopy, 3rd ed., Harcourt College Publication (2001)

20. D.H. Williams, I. Fleming Spectroscopic Methods in Organic Chemistry, Tata McGraw-Hill

PAPER II

L	T	Credit
4	0	4

RM-CC-023: Scientific Research Methodology

Course Objectives	This course will help to: understand some basic concepts of research and its methodologies; identify appropriate research topics, select and define appropriate research problem and parameters; prepare a project proposal (to undertake a project), organize and conduct research (advanced project) in a more appropriate manner; write a research report and thesis; write a research proposal (grants); and file their research work for a patent.
Course Outcomes	Upon completion of this course, the students will be able to: • Discuss different methodologies and techniques used in research work. • Explain basic computer skills necessary for the conduct of research. • Assess the basic function and working of analytical instruments used in research • Propose the required numerical skills necessary to carry out research.

DETAILED CONTENT

MODULE-1 Methodology and Literature

Meaning of research, purpose of research, research methods: scientific methods, experimental methods, observational methods, survey and questionnaires methods, role of theory, characteristics of research. Criteria of good research. Need for research design. Types of research: fundamental or pure research, applied research, action research, experimental research. Review of work relevant to the chosen problems, Applied science and technology index. Classical and comprehensive reference works.

MODULE-2: Abstracting and indexing services (A & I)

Current services: CA weekly issues, CA issue indexes-keyword index. General subject index, chemical substance index, formula index, index of ring systems, author index, and patent index. CA Collective indexes: Collective index (CI), volume index, quinquennial index, decennial index (DI).

MODULE-3: Mathematical and Computational Treatment.

Data collection techniques. Classification, analysis and presentation of data. Statistical Arithmetic mean, Geometric mean treatments.

Storage and retrieval of data. Development of database structures, Data processing and basic operation, Sorting. Network protocols. Development of the web page, Use of software in structure elucidation such as MATLAB, MATHEMATICA, STATISTICA, LATEX, CHEMWINDOW, CHEMDRAW, CHEMSKETCH, ORIGIN.

MODULE-4: Scientific Technical Writings

How to present the data in the form of dissertation/thesis, Lab reports, Manuals, Review papers and Research Papers. The use of quotation, footnotes in tables and figures. Referencing, appendixes, editing and evaluating the final report.

MODULE-5 Intellectual Property Rights (IPR)

General introduction to IPR. Approach to securing patent. Protection of IPR. Patent Acts and Treaties. World Trade Organization (WTO). Trade-Related Aspects of Intellectual Property Rights (TRIPS).

Reference Books

1. Thesis and Assignment Writing – J Anderson, B.H. Dursten and M. Poole, Wiley Eastern (1977).
2. Research Methodology (Second Revised Edition) – C.R.Kothari; New Age Publishers, 2004
3. Advanced Organic chemistry- Michael B. Smith and J.March
4. Patents Act.
5. Consumer Protection Act.
6. www.cas.org.
7. How to use chemical abstracts, current abstracts of chemistry and index chemicus- Brian Livesey; Medical information technology and training Ltd., Gover.

PAPER III

L	T	Credit
1	2	2

RPE-CC-021: Research and Publication Ethics

Course Objectives	The main objective of course is to deal with ethical issues associated with the design and conduct of research, the regulation of research, the procedures and process of ethical review and issues related to scientific integrity. It aims to promote, inspire and engage in open and public debate about research ethics on an international scale and to contribute in the area of research.
Course Outcomes	By the end of this course, student should be able to • Have knowledge, general competence, and analytical skills in Research Methodology and Research & Publication Ethics. • Build a strong foundation for future research work in a systematic manner and hands-on experience to carry out research work in all interdisciplinary areas. • Equip themselves with ethical issues related to Research and Publication. • Get familiar with current research trends in various core areas and open access publishing. • Understand Patents and IPR (Intellectual Property Rights). • Write research papers/thesis following publication ethics and to know the ways for avoiding plagiarism.

DETAILED CONTENT

Course structure

- The course comprises of six modules listed in table below. Each module has 4-5 units.

Modules	Unit title	Teaching hours
Theory		
RPE 01	Philosophy and Ethics	4
RPE 02	Scientific Conduct	4
RPE 03	Publication Ethics	7
Practice		
RPE 04	Open Access Publishing	4
RPE 05	Publication Misconduct	4
RPE 06	Databases and Research Metrics	7
	Total	**30**

Syllabus in detail

THEORY

- **RPE 01: PHILOSOPHY AND ETHICS (3 hrs.)**

1. Introduction to philosophy: definition, nature and scope, concept, branches
2. Ethics: definition, moral philosophy, nature of moral judgements and reactions

- **RPE 02: SCIENTIFICCONDUCT (5hrs.)**

1. Ethics with respect to science and research
2. Intellectual honesty and research integrity
3. Scientific misconducts: Falsification, Fabrication, and Plagiarism (FFP)
4. Redundant publications: duplicate and overlapping publications, salami slicing
5. Selective reporting and misrepresentation of data

- **RPE 03: PUBLICATION ETHICS (7 hrs.)**

1. Publication ethics: definition, introduction and importance
2. Best practices / standards setting initiatives and guidelines: COPE, WAME, etc.
3. Conflicts of interest
4. Publication misconduct: definition, concept, problems that lead to unethical behavior and vice versa, types
5. Violation of publication ethics, authorship and contributorship
6. Identification of publication misconduct, complaints and appeals
7. Predatory publishers and journals

PRACTICE

- **RPE 04: OPEN ACCESS PUBLISHING(4 hrs.)**

1. Open access publications and initiatives
2. SHERPA/RoMEO online resource to check publisher copyright & self-archiving policies
3. Software tool to identify predatory publications developed by SPPU
4. Journal finder / journal suggestion tools viz. JANE, Elsevier Journal Finder, Springer Journal Suggester, etc.

- **RPE 05: PUBLICATION MISCONDUCT (4hrs.)**

A. Group Discussions (2 hrs.)

1. Subject specific ethical issues, FFP, authorship
2. Conflicts of interest
3. Complaints and appeals: examples and fraud from India and abroad

B. Software tools (2 hrs.)

Use of plagiarism software like Turnitin, Urkund and other open source software tools

- **RPE 06: DATABASES AND RESEARCH METRICS (7hrs.)**

A. Databases (4 hrs.)

1. Indexing databases
2. Citation databases: Web of Science, Scopus, etc.

B. Research Metrics (3 hrs.)

1. Impact Factor of journal as per Journal Citation Report, SNIP, SJR, IPP, Cite Score
2. Metrics: h-index, g index, i10 index, altmetrics

References

Bird, A. (2006). *Philosophy of Science*. Routledge.

MacIntyre, Alasdair (1967) *A Short History of Ethics*. London.

P. Chaddah, (2018) Ethics in Competitive Research: Do not get scooped; do not get plagiarized, ISBN:978-9387480865

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). What is ethics in research & why is it important. *National Institute of Environmental Health Sciences*, 1–10. Retrieved from https://www.niehs.nih.gov/research/resources/bioethics/whatis/index.cfm

Beall, J. (2012). Predatory publishers are corrupting open access. Nature, 489(7415), 179–179. https://doi.org/10.1038/489179a

Indian National Science Academy (INSA), Ethics in Science Education, Research and Governance(2019), ISBN:978-81-939482-1-7. http://www.insaindia.res.in/pdf/Ethics_Book.pdf

ELECTIVE COURSES:

(PAPER – IV)

A candidate admitted to Ph. D./M. Phil. Programme on the basis of entrance test (after M. Sc. degree) will have to pass one of these elective courses (as per his/her specialization and recommendation of Ph. D. guide)

Elective Course-I

L	T	Credit
4	0	4

CHEM-EC-612: Advanced Inorganic Chemistry -I

Course Objectives	The objectives of the course are that will able student to apply principles of various concepts in understanding, analysis and prediction of scientific problems and to develop human resource with specialization in science along with various experimental techniques required for career in academia and industry.
Course Outcomes	At the end of this course, the students should be able to: • Apply these topics in various fields. • Understand and apply the principles of stability of complexes in synthesis of new molecules. • Relate the structure of complexes to their properties.

DETAILED CONTENT

MODULE-I

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

MODULE-II

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. Metallocene based Zeigler Natta catalysts, catalysts composition, active centre and polymerisation mechanism.

MODULE-III

Synthesis of Coordination compounds:- Theoretical consideration: Labile and Inert Coordination compounds, synthesis of mixed ligand complexes by co-proportionation, chelate effect, trans effect (Peyrone's rule, Jorgensen's rule and Kurnakov's rule), Cis effect, Geometric isomerization of square planer platinum(II) and Palladium(II) complexes, hard-soft acid-base (HSAB) principle, factors affecting the acid base properties of coordination compounds, ligand effects on redox potentials of coordination compounds.

MODULE-IV

Voltammetric methods of analysis: Principle, excitation signals, mass transfer mechanism, instrumentation, methods of analysis and applications of pulse polarography, cyclic voltammetry and anode stripping voltammetry. Use of cyclic voltammetry for the determination of formal reduction potential and number of electron change for ferri/ferrocyanide couple and to study electrode mechanisms of electron reduction of nitrobenzene and voltammetry with microelectrodes.

MODULE-V

Chemistry of High Temperature Solvents– Introduction, structures, solutions of elements (metals and non-metals) in fused salts, reactions in fused salts (acid- base reactions, oxidation-reduction reactions, metathetic reactions), experimental methods (general discussion).

Books Recommended:

1. Homogeneous transition metal catalysis – Christopher Masters
2. Principles and Application of Homogeneous Catalysis – Nakamura and Tsutsui
3. Advanced Polymer Chemistry- Manas Chanda
4. Synthetic Coordination Chemistry: Principles and Practice- J.A. Davies, C.M. Hockensmith, V.Y. Kukushkin and Y.N. Kukushkin.
5. Fundamentals of Analytical Chemistry- Skoog, West, Holler and Crouch
6. Chemistry experiments for Instrumental methods- Sawer, Heineman and Beebe.
7. Electronic absorption spectroscopy and related techniques: D.N. Sathyanaray.
8. The Organometallic Chemistry of Transition metals: R.H. Crabtree.
9. Principles and applications of organotransition metal chemistry by Ccollmen and Hegden

Elective Course-II

L	T	Credit
4	0	4

CHEM-EC-613: Advanced Inorganic Chemistry-II

Course Objectives	The course aims at providing the students with the role of metal ion in biological systems, fundamentals of molecular recognition of the interactions responsible for the formation of supramolecular systems and on the role of metals in biological systems and medicine. The student will be introduced to the principal classes of supramolecular systems (organic / inorganic of biological interest) together with the main techniques currently used for their characterization. Role of various coordinated ligands and electron transfer reactions of complexes.
Course Outcomes	On successful completion of this course, students will be able: • to develop the role of metal ion in biological systems, fundamentals of molecular recognition of the interactions responsible for the formation of supramolecular systems. • To understand the role of metals in biological systems and medicine. • The student will be able to understand the principal classes of supramolecular systems (organic / inorganic of biological interest) together with the main techniques currently used for their characterization. • Role of various coordinated ligands and electron transfer reactions of complexes.

DETAILED CONTENT

MODULE-I

Role of Metal-ions in Biological Systems: Metal-ion-interactions with Nucleosides and Nucleotides, Metal-ion-interactions with DNA, Metal-ion-interactions with RNA.

Electron-Transfer Agents in Biological Systems: Cytochromes, Iron-sulphur proteins, Vitamin B_{12} and B_{12} Coenzymes Xanthane oxidase, Superoxide dismutase.

MODULE-II

Supramolecular Reactions and Catalysis: Introduction, Catalysis by reactive macrocyclic cation receptor molecule, by reactive macrocyclic anion receptor molecule supramolecular metallocatalysis.

Supramolecular Assemblies: Introduction, Supramolecular solid materials, molecular recognition at surfaces (Endoreceptors vs Exoreceptors), Molecular and supramolecular devices, photonic, electronic and ionic devices.

MODULE-III

Reactions at Coordinated Ligands:-Reactions due to metal ion polarization of co-ordinated ligands, Aldol Condensation, Imine formation, hydrolysis and substituent exchange. Template effect and macrocyclic ligands.

MODULE-IV

Electron-Transfer Reactions of Complexes: Electron-transfer theory, Outer-sphere exchange reaction. Bridge mechanism, Two-electron transfers, Non-complementary reactions. Replacement through redox mechanism, photochemical reactions of chromium and ruthenium complexes.

MODULE-V

Reactions of Oxyanions: Factors affecting rates, Oxygen exchange between phosphate and water, Induced reactions, chromate-arsenite reactions, Urea formation reactions.

Books Recommended:

1. Elements of Bioinorganic Chemistry- G.N. Mukherjee and Arabinda Das (1993).
2. Inorganic Chemistry - Purcell and Kotz.
3. The Inorganic Chemistry of Biological Process-M.N. Hughes (2^{nd}Edn.)
4. Inorganic Reaction Mechanism- Edward.
5. Inorganic Reaction Mechanism - Bassolo and Pearson.
6. Supramolecular Chemistry concepts and Perspectives- Jean-Marie Lehn(VCH-1995)

Elective Course-III

L	T	Credit
4	0	4

CHEM-EC-614: Organic Synthesis

Course Objectives	Present course will cover modern theoretical and experimental methods used to study problems of molecular structure and bonding; emphasis on spectroscopic techniques. This course will acquaint the students to concept of synthesis in organic chemistry. This will cover a wide area of synthesis including polynuclear compounds, heterocyclic compounds, reagents in organic synthesis, and new concepts of organic synthesis. Familiarize students with the basic concept of Medicinal Chemistry. Emphasis will be made on the SAR of anti ulcer drugs and their mode of action. Describe the factors that affect its absorption, distribution, metabolism, and excretion, and hence the considerations to be made in drug design. Discuss the stereochemistry of different organic compounds, stereoselective andsterospecific reactions and their role in advanced synthesis.
Course Outcomes	At the end of course students will be able to • perform rigorous characterization of their compound using 1- and 2-dimensional NMR techniques (1 H and 13C), Mass spectrometry, infrared spectroscopy and UV-Vis spectroscopy. • understand the role of reagents and catalysts in organic synthesis. • make a correlation between supramolecular and normal organic synthesis. • Understand the need of Medicinal Chemistry in curing various ailments • implement the concept of stereochemistry in various advanced organic synthesis during research work.

DETAILED CONTENT

MODULE –I

Spectroscopy: Basic theory, Instrumentation and applications of UV spectroscopy, IR Spectroscopy, NMR Spectroscopy and Mass spectrometry in organic compounds. Problems based on IR, UV, NMR and mass spectral data.

MODULE - II

Reaction –Mechanism: Reaction and mechanism of following organic reactions: Stevens rearrangement, Cope rearrangement , Claisen rearrangement, Metathesis of olefins, Di- π methane rearrangement, Hofmann-Loffler reaction, Sharplessassymatricepoxidation and Stork-enamine reaction. Hydrogen spillover.

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

MODULE–III

New Concepts in Organic Chemistry: Green Chemistry:Principles of green chemistry, green reagents , green catalysts: Bio-catalysts PTC and Crown ether, ionic liquids as solvent and catalysts.Organic synthesis in solid state: Michael addition and Aldol condensation, Combinatorial Chemistry: Concepts of Combinatorial chemistry and its use in organicsynthesis,Combinatorial libraries.Click Chemistry: Concepts and uses in organic and polymer synthesis.

MODULE- IV

Stereochemistry; Stereoselective and stereospecific reactions: Stereoselective reactions: Hydride reduction of cyclic ketones, catalytic hydrogenation, Stereoselectivenucliophilic addition to acyclic carbonyl groups stereospecific reactions: Bromination of alkene, 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.

MODULE- V

Drug design and development: Pharmacokinetics and Pharmacodynamics: Introduction to drug absorption, distribution, metabolism, elimination using pharmacokinetics Importance of pharmacokinetics in drug development. Drug design, concepts of lead compound and lead modification, Example: Development of cimetidine-A rational approach to drug design: Anti ulcer therapy, biological activity of cimetidine, structure and activity of cimetidine, metabolism of cimetidine, cimetidine analogues.

Books Recommended:

1. Practical NMR Spectroscopy, M.L.Martin, J.J. delpeuch and G.J.Martin, Heyden.
2. Spectrophotometric Identification of Organic Compounds, R.M. Silverstein, G.C.Bassler and T.C.Morrill, John Wiley.
3. Introduction to NMR Spectroscopy, R.J. Abraham, J. Fischer and P. Loftus, Wiley.
4. Appliation of Spectroscopy of Organic Compounds, J.R. Dyer, Prentice Hall.
5. Spectroscopic Methods in Organic Chemistry, D.H.Williams, I.Fleming, Tata McGraw-Hill.
6. Organic Spectroscopy by Jagmohan.

7. Organic Spectroscopy by W. Kemp.
8. Stereochemistry of Organic Compounds, D.Nasipuri, New Age International.
9. Stereochemistry of Organic Compounds, P.S.Kalsi, New Age International.
10. Organic Synthesis: Jagmohan Singh and Yadav
11. Organic Synthesis: Feiser and Feiser.
12. An Introduction to Medicinal Chemistry, Graham L. Patrick.
13. Medicinal Chemistry: Principles and Practice Edited by F.D. King.
14. Textbook of Organic Medicinal and Pharmaceutical Chemistry, Edited by Charles O. Wilson, et al.
15. Introduction to Medicinal Chemistry, Alex Gringuage.

Elective Course-IV

L	T	Credit
4	0	4

CHEM-EC-615: Polymer Chemistry

Course Objectives	This course aims at acquainting the students: the knowledge of the basic and advanced concepts of polymers. A complete packet of knowledge of the kinetics, thermodynamics of polymerization, various techniques of determination of molecular mass and applications of polymers in various fields of life will be provided to the students; Various factors affecting the structure and properties of polymers will be discussed in detail which makes students aware of the things to be considered while preparing polymers commercially; Different techniques which can be utilized to characterize the polymers such as FTIR, NMR,TGA, GPC, DSC, XRD, SEM; Different types of bio-polymers their surface modification techniques; conducting polymers and environment impact of synthetic polymers; and utilization of conducting polymers
Course Outcomes	This will also help to develop skills to interpret and explain various factors affecting structure and property of macromolecules. The students will be able to pursue their career objectives in scientific research and teaching.

DETAILED CONTENT

MODULE-I

Polymer Synthesis: Kinetic and mechanism of radical, cationic, and anionic addition polymerization, Living polymerization. Significance of chain transfer reactions, Chemistry and kinetics of inhibition and retardation.

Miscellaneous polymerization reactions: Monomers with two different polymerizable groups, Hydrogen transfer polymerization, Polymerization and cyclotrimerization of isocyanates, Monomers with triple bonds, Ring opening polymerization: Scope, polyermerizability, polymerization mechanism and kinetics, examples of cyclic amide and ethers; Monomers containing the same functional groups, Monomers containing different functional groups, Zwitterionic copolymerization.

MODULE –II

Copolymer Synthesis: Principles of polymer reactivity, factors affecting polymer reactivity , Chain transfer copolymerization, Chemistry and methods of graft copolymerization, radical graft copolymerization, ionizing and UV radiation and redox initiation, and other grafting systems.

Block copolymer formation, sequential monomer addition, charge formation reactions, telechelic polymers, Reactions of block copolymers, mechanochemical bond scission, special initiators.

Crosslinking processes, chemical and radiation crosslinking, vulcanization. Halogenations reactions, aromatic substitution and cyclization of aromatic polymers.

MODULE- III

Polymer Characterization: Determination of molecular weight of polymers by colligative properties, viscosity measurement, end group analysis, sedimentation velocity and equilibrium method.

Analysis and Characterization of polymers by chemical analysis, FTIR, NMR, TGA, GPC, DSC, XRD, SEM techniques.

MODULE- IV

Special Polymer Reactions: General introduction to the polymer reactions, Derivatization reactions of biopolymers – cellulose, chitosan, starch and natural gums

Polymer as carriers or supports, polymeric reagents, polymeric substrates, polymeric catalysts, immobilized enzymes, polymeric drugs.

Polymer stability and degradation: Type of degradation, mechanism, ultrasonic, photo, high energy and oxidative degradation, Fire retardants, UV stabilizers and absorbers. Biodegradation by alkali, acid, ionic liquids and enzymes, hydrolytic reactions of biopolymers and their special technological potential with respect to bioethanol and platform molecules, synthesis of speciality chemicals and polymers there from.

MODULE-V

Specialty Polymers: Biodegradable polymers (lactic and glycolic acid based). Conducting polymers, applications of conducting polymers.Hydrogels.Biomedical polymers, contact lenses, dentures, implants, artificial – heart, kidney and blood.

Polymers and environment: Environmental aspects of polymers, energy and feedstock utilization, Problems of non-degradability of synthetic polymers, biomass utilization, bioplastics.

Books Recommended

1. Textbook of Polymer Science, F.W. Billmeyer Jr. Wiley.
2. Polymer Science, V.R. Gowarikar, N.V. Visvanathan and J. Sreedhar, Wiley Eastern.
3. Functional Monomers & Polymers, K. Takemoto, Y. Inaki and R.M. Ottanbrite.

4. Contemporary Polymer Chemistry, H.R. Alcock and F.W. Lambe, Prentice Hall.
5. Physics & Chemistry of Polymers, J.M.G. Cowie, Blakie Academic and Professional.
6. Supramolecular Chemistry , Edited by Alberto Ciferri, Taylor and Francis.
7. The chemistry of Nanomaterials Vol.I and Vol II, Edited by C. N. R. Rao, A Muller, A.K. Cheetham, Wiley VCH. 2005.
8. Metal-Polymer Nanocomposites, Edited L. Nicolais and G Carotenuto, Wiley Interscience 2005.
9. Polymer Chemistry and Physics of Modern Materials, J.M.G. Cowie and V. Arrighi,Taylor and Francis Group 2008.
10. Designing Safer Polymers by P.T.Anastas, P.H. Bickart, M.M. Kirchhoff , Wiley Interscience, 2001.

Elective Course-V

L	T	Credit
4	0	4

CHEM-EC-616: Adsorption and Advanced Electrochemistry

Course Objectives	The learner should be able to learn various aspects of surface chemistry, colloids and electrochemistry. The students will learn about Langmuir and BET theory, Gibbs adsorption theorem and solvent interaction. Moreover, it helps students to learn state diffusion theories and make use of these theories in electrochemistry to analyze electrode kinetics.
Course Outcomes	From this course the students should be able to • Explain importance of adsorption processes, heterogeneous catalysis, Langmuir and BET model. • Learn the adsorption laws, Gibbs adsorption equation and chromatographic adsorption. • Analyze and apply the knowledge acquired to solve problem relating to these topics. • Understand the concept of ion-solvent interactions and ion-ion interactions. • Learn about the Poisson's equation and Debye – Huckel Theory of charge distribution. • Explain Fick's law of diffusion and stern model of double layer.

DETAILED CONTENT

MODULE –I

Adsorption at solid – gas interface: Ideal and non – ideal adsorption. Types of adsorption isotherms. Single – layer and multilayer adsorption. Application of BET theory in the determination of surface area of the solid. Applications of adsorption in water purification, adsorption and catalysis.

MODULE –II

Adsorption at solid – liquid interface: Positive and negative adsorption. Gibb's adsorption equation. Isotherms of concentration and temperature change for the adsorption in solutions. Chromatographic adsorption: column chromatography, its theory and mathematical treatment. Theory of chromatography involving one solute and several solutes.

MODULE - III

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.

Heat and entropy changes accompanying hydration. Hydrophobic effect in salvation. Poisson's equation and Debye – Huckel Theory of charge distribution around ions (Linearization of Boltzmann equation).

MODULE - IV

Physical chemistry of ion – transport in solution: The driving force for diffusion, Fick's law of steady – state diffusion and diffusion – coefficient. The Einstein – Smoluchowski equation. Gross view of non – steady – state diffusion (Fick's second law). Diffusion process stimulated by a constant current (Flux). Einstein relation between absolute ion mobility and diffusion coefficient.

MODULE – 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), determination of surface excess (variation of surface tension with solvent composition of electrochemical system). The structure of electrified surfaces. The Helmholtz – Perrin theory, Gouy – Chapman diffuse – charge model of double layer and Stern model.

Books Recommended:

1. Modren Electrochemistry Vol. 1 & 2: J.O'M Bockris, A.K.N. Reddy and M.G.- Aldeco
2. Physical Chemistry of Surfaces: A.W. Adamson
3. An Introduction to Electrochemistry: S. Glasstone
4. Adsorption from Solutions: J.J. Kipling
5. Principles of Physical Chemistry: B R Puri, L R Sharma, M S Pathania Vishal Publishing Company

Elective Course-VI

L	T	Credit
4	0	4

CHEM-EC-617: Micelle Formation and Nanotechnology

Course Objectives	The objective of this course is to equip students to learn different properties of surface-active agents and their thermodynamics of micellization. Moreover, it helps students to understand different types of nanomaterials their syntheses and characterization and enable them to apply the knowledge of nanomaterials in the research field of science and technology.
Course Outcomes	At the end of this course student will be able to • Explain different applications of surfactants and phenomenon of micellization. • Explain the mechanism of formation of nanomaterials, role of surfactants in the synthesis of nanomaterial by sol- gel and coprecipitation method. • Describe the effects may emerge due to nano-dimensions of particles • Analyze a nanostructured material of a given species through their modified chemical and physical properties. • Propose preparation methods for different nanomaterials and analyze them using various characterization techniques. • Describe applications of Nano chemistry and suggest nanomaterials for specific optical, electronic, medical and energy storage applications.

DETAILED CONTENT

MODULE – I

Micelle formation: Surfactants and their types, micelle and reverse micelle formation, critical micelle concentration (CMC), dependence of CMC on chain length of the surfactant, micelle shape and size, hydrophobic interaction, factors affecting the CMC of surfactants. Monodisperse micelles of ionic and non – ionic surfactants. Thermodynamics and kinetics of micelle formation (Mass Action Model). Counterion binding to micelles (Evan and Ninham - model). Micelle Temperature Range (MTR) or Kraft phenomenon, physicochemical meaning of MTR and effect of salt on MTR.

MODULE – II

Micellar Solubilization & micellar catalysis: Thermodynamics of micellar solubilization, distribution of solubilizate molecules among micelles. Factors affecting solubilization.

Solubilization in micellar liquid chromatography (MLC), partition theory and application of MLC to drug and protein analysis (brief outline only)**.** Effect of micelles on chemical reactions, micelle catalyzed reactions, inhibition in micellar solutions.

MODULE - III

Chemistry of nano – materials: Definition and historical perspective. Fundamentals of nanomaterials and nanostructures. Classification of nanomaterials. Quantum dots and its applications in various fields. Synthesis of nanoparticles, nanoclusters, nanocrystals; top-down approach and bottom-up approach. Chemical and physical methods of synthesis.

MODULE - IV

Characterization techniques: Various characterization techniques for the preparation of nanomaterials and nanostructures. Properties of nanomaterials: electrical, optical, magnetic and chemical properties. Properties of metal nanoclusters, semiconducting nanoparticles and nanotubes.

MODULE - V

Applications of nanomaterials: An overview of applied chemistry of nanomaterials. Applications of nanotechnology in semiconductor devices, energy, sensors, coatings. Importance of nanomaterials in medicines, catalysis, environment and miscellaneous.

Books Recommended:

1. Solubilization in Surfactant Aggregates: Eds S.D. Christian and J.F. Scamehorn (Surfactant Science Series Vol. 55)
2. Polymer – Surfactant System: Ed. J.C.T. Kwak (Surfactant Science Series Vol. 77)
3. Micelles (Theoretical and Applied Aspects): Y. Moroi
4. Introduction to nanotechnology: Charles P.Poole, Jr. Frank, J. Owens: Wiley India
5. Nano Technology: Principles & Practices, Sulabha K. Kulkarni Capital Publishing Company, New Delhi, India.