PERIYAR UNIVERSITY

Salem-636 011, Tamil Nadu, India

NAAC A Grade – State University- NIRF Rank 63-ARIIA Rank-10

M.PHIL. DEGREE

[Choice Based Credit System (CBCS)]

Branch IV (M) CHEMISTRY

Programme Code : CHE02

REGULATIONS AND SYLLABUS

[For the Candidates admitted from the academic year 2021 – 2022 and onwards]

CONTENTS

I. Programme Outcomes (POs)

PO1. Scholars will be trained to adopt a new paradigm of self-learning in the form of review of earlier knowledge acquired.

PO2. Scholars will be brought to light from the previous investigation completed to the newer thrusts of knowledge and implementation in research.

PO3. Scholars will be trained to design, implement and evaluate secured information (hard and soft) systems with assured quality and efficiency.

PO4. Scholars are to be oriented towards becoming globally competent.

II. Programme Specific Outcomes (PSOs)

PSO1. Scholars will learn the techniques of teaching and research in chemistry.

PSDO2. Scholars will be able to explore and expedite the recent avenues in chemistry research

PSO3. Scholars will get experience in the synthetic strategies and analytical instrumentation skills by doing active research.

PSO4. Scholars become globally competent to publish their research articles.

III. Program Objectives

Chemistry is a part of a larger body of knowledge called Science. Although Chemistry is concerned with only a part of the scientific knowledge that has been accumulated, it is in itself an enormous and broad field. Chemistry touches all parts of our lives. The scope of chemistry is extremely broad and it touches every aspect of our lives. The principles of chemistry are fundamental to an understanding of all processes of the living state.

The major objectives of M.Phil. Chemistry course are:

1. To impart knowledge in advanced aspects of all branches of chemistry
2. To acquire deep knowledge in the survey of literature.
3. To acquire specific knowledge in the specialized research area of chemistry.
4. To train the students in various analytical techniques.
5. To train the students with latest teaching and research methodologies

IV. Eligibility:

Candidates who have qualified for M.Sc. Chemistry degree or M.Sc. Chemistry with specialization in Organic/Inorganic/Physical chemistry (CBCS) or M.Sc. Analytical Chemistry of this University or M.Sc. Chemistry of any other University recognized by the Syndicate as equivalent thereto shall be eligible to register for the Degree of Master of Philosophy (M.Phil.) in Chemistry and undergo the prescribed course of study in an approved institution or department of this University.

Candidates who have qualified their postgraduate degree on or after Ist January 1991 shall be required to have obtained a minimum of 55% of marks in their respective postgraduate degrees to become eligible to register for the Degree of Master of Philosophy (M.Phil.) and undergo the prescribed course of study in an approved institution or department of this University.

In the case of teachers registering for M.Phil. degree under FIP/QIP programmes, the minimum percentage of marks for registration is 50%.

For the candidates belonging to SC/ST community, and those who have qualified for the Master's degree before 01.01.1991, the minimum eligibility marks shall be 50% in their Master's Degree.

III. Duration:

The duration of the M.Phil. Course shall extend over a period of one year from the commencement of the course. The one year period consists of two semesters.

IV. Course of Study:

The course of study for the degree shall consist of (a) Part-I comprising three written papers according to the Syllabus prescribed from time to time; and (b) Part-II Dissertation.

Part-I shall consist of a core paper, Paper-I Scientific Research and Methodology and an elective paper, Paper-II an advanced paper in the main subject. The candidates can opt this paper II from the elective papers float by the department time to time. A minimum of 5 students has to opt a particular paper at a time. These two papers will be dealt in the first semester of the course.

There shall also be a third paper which shall be the background paper relating to the proposed dissertation conducted internally by the Department. This syllabus of the paper will be framed by the Guide or Supervisor and handed over to the students by the end of first semester itself. This paper will be dealt in the second semester.

Structure of the Course

S.No	Paper Code	Title of the paper	Hours	L	T	P	C
FIRST SEMESTER							
Core Courses							
1.	21UPCHE2C01	Research methodology	72	3	1	0	4
2.	21UPCHE2C02	Applications of Spectroscopic Methods	72	3	1	0	4
3.	21UPCHE2E--	Elective Course	72	3	1	0	4
SECOND SEMESTER							
4.	21UPCHE2C03	Project Dissertation Viva	1500	-	-	-	12

Elective Courses (Any one)							
1.	21UPCHE2E01	Synthetic Organic Chemistry	72	4	1	0	4
2.	21UPCHE2E02	Coordination Chemistry	72	4	1	0	4
3.	21UPCHE2E03	Organometallic Chemistry	72	4	1	0	4
4.	21UPCHE2E04	Corrosion Chemistry	72	4	1	0	4
5.	21UPCHE2E05	Nanomaterials Chemistry	72	4	1	0	4
6.	21UPCHE2E06	Biomaterials Chemistry	72	4	1	0	4
7.	21UPCHE2E07	Environmental Chemistry	72	4	1	0	4
8.	21UPCHE2E08	Polymer Chemistry	72	4	1	0	4
9.	21UPCHE2E09	Computational Chemistry	72	4	1	0	4
10.	21UPCHE2E10	Surface Chemistry	72	4	1	0	4

V. Scheme of Examinations:

Part-I Written Examination: Course I, II & III

The examination of courses I, II and III shall be held at the end of the first semester. The duration for each paper shall be 3 hours carrying a maximum of 75 marks apart from internal (25 marks).

Part-II - Course IV - Project Dissertation Viva

Course IV examination will be conducted by the Department at the end of second semester. The duration for each paper V also shall be of 3 hours

carrying a maximum of 200 marks (150 marks for dissertation and 50 marks for viva Voce taking the average of marks given by both internal and external examiners).

The examiners will be appointed from the panel of four names of each paper (I and II) submitted by the College/Departments concerned. If one examiner awards a pass mark and the other fail mark the, paper will be valued by a third examiner whose award of marks will be final.

VI.Pattern of Question paper

Time: 3 Hours Max.Marks - 75

PART-A: 5x5=25

(Answer all questions)

(One question from each unit with internal choice)

1. (a) or (b)
2. (a) or (b)
3. (a) or (b)
4. (a) or (b)
5. (a) or (b)

PAPER-B: 5x10=50

(Answer all questions)

(One question from each unit with internal choice)

6. (a) or (b)
7. (a) or (b)
8. (a) or (b)
9. (a) or (b)
10. (a) or (b)

VII. Dissertation / Project Work:

Part-II – Dissertation

The exact title of the Dissertation shall be intimated one month before the end of second semester. Candidates shall submit the Dissertation to the

University through the Supervisor and Head of the Department at the end of the year from the commencement of the course which shall be valued by internal examiner (supervisor) and one external examiner appointed by the University from a panel of four names sent by the Supervisor through the Head of the Department at the time of submitting the dissertation.

The examiners who value the dissertation shall report on the merit of candidates as "Highly Commended" (75% and above) or "Commended" (50% and above and below 75%) or "Not Commended" (below 50%).

If one examiner commends the dissertation and the other examiner, does not commend, the dissertation will be referred to a third examiner and the third valuation shall be final. Submission or re submission of the dissertation will be allowed twice a year.

VIII. Passing Minimum:

A candidate shall be declared to have passed Part-I of the examination if he/she secures not less than 50% of the marks in each paper including Paper – III for which examination is conducted internally.

A candidate shall be declared to have passed Part-II of the examination if his/her dissertation is atleast commended.

All other candidates shall be declared to have failed in the examination.

IX. Restriction in number of chances:

No candidate shall be permitted to reappear for the written examination in any paper on more than two occasions or to resubmit a dissertation more than once. Candidates shall have to qualify for the degree passing all the written papers and dissertation within a period of three years from the date of commencement of the course.

X. Conferment of Degree:

No candidate shall be eligible for conferment of the M.Phil. degree unless he/she is declared to have passed both the parts of the examination as per the Regulations.

XI. Qualifications for persons conducting the M.Phil. Course:

No teacher shall be recognised as a Supervisor unless he possesses a Ph.D. degree or two years of PG teaching experience after qualifying for M.Phil. Degree.

XII Syllabus

SEMESTER -I

CORE PAPERS

PAPER-I

21UPCHE2C01 RESEARCH METHODOLOGY

Objectives

- To perceive knowledge on basic research, scientific literature searching, and scientific documentation
- To gain some knowledge about the statistical analysis of data this will be highly helpful for research
- To create the awareness on laboratory hygiene and safety
- To acquire from nature to research laboratory and perceive fundamentals of isolation and purification techniques
- To gain an idea about digital electronics and computer package

Expected Course Outcomes:		
On the successful completion of the course, student will be able to:		
1	The scholars will know the different routes to design a research problem	K2
2	To improve the numerical aptitude and computational knowledge in the basic of collection and presentation of data.	K3
3	The scholars will acquire knowledge of safe laboratory practices by handling laboratory glassware, equipment, and chemical reagents	K2
4	To idea about digital electronics and computer package	K4
5	General terminology including various methods for the research shall be the outcome of the course	K6
K1 - Remember; K2 - Understand; K3 - Apply; K4 - Analyze; K5 - Evaluate; K6 - Create		

UNIT – I Need for literature survey, Art of thesis and article writing

Introduction:

Nature and importance of research - aims, objective, principles and problems – selection of research problem - survey of scientific literature - primary and secondary sources - citation index for scientific papers and journals - patents.

Dissertation:

Nature and purpose, components and preparation- Writing techniques: Introduction, word processing and page layout, writing and formatting with a computer - Figures: general considerations, line art, drawing with a computer and halftones- Tables: logic behind a table, significance of a table, form of a table, components of a table - Worksheets, lists and databases. Plagiarism.

Collection and Citation of Literature:

Acquisition of information, building up of own literature collection, citation techniques, forms of citation, web of science, SCI, Scopus, H index and I10 index.

Publication of Journal Articles:

Concept, electronic publication, types of journals, impact factor, decision prior to publication, components of a journal article, preparation of the manuscript, from manuscript to publication and online submission.

Submission of Research Proposals:

Leading funding agencies in India, Submission of research project proposals with prescribed formats.

UNIT - II Data Analysis

Errors – classification of errors - precision - accuracy – improving accuracy of analysis – significant figures – mean, standard deviation – comparison of results: “t”test, “f” test and “chi” square test –rejection of results – presentation of data.

Sampling – introduction – definitions – theory of sampling – techniques of sampling – statistical

criteria of good sampling and required size – stratified sampling vs random sampling – minimization of variance in stratified sampling –transmission and storage of samples.

UNIT - III Chemical Safety and Ethical Handling of Chemicals

Safe working procedure and protective environment, protective apparel, emergency procedure and first aid, laboratory ventilation, Safe storage and use of hazardous

chemicals, procedure for working with substances that pose hazards, flammable or explosive hazards, procedures for working with gases at above or below atmospheric pressures – safe storage and disposal of waste chemicals , recovery , recycling and reuse of laboratory chemicals, procedure for laboratory disposal of explosives , identification , verification and segregation of laboratory waste , disposal of chemicals in the sanitary sewage system , incineration and transportation of hazardous chemicals .

Unit - IV Isolation and purification techniques

Methods of isolating natural products from plant sources – Solvent purification techniques – Purification of solid / liquid samples from the crude reaction mixture – vacuum distillation – the use of TLC in monitoring the course of the reaction and that of column chromatography in separating the mixture – Liquid-liquid isolation techniques SFE, PLE, MAE and brief comparison of SFE, PLE and MAE with soxhlet extraction - The principle, working and applications of GC, HPLC and other hyphenated techniques

UNIT - V Electronics and Computer Packages

Basic aspects of electronic circuits and their components used in common instruments like spectrophotometers and electrochemical instruments like cyclic voltammeter. Elementary aspects of digital electronics.

Applications of some computer packages like MS office–Word, Excel, Power Point, Origin, ChemDraw, Sciplot, ISIS draw, ChemSketch and SPSS.

References:

1.Santiago Ramon y Cajol, (translated by Neely S Wanson and Larry WSwanson) ‘Advice for a young Investigator’ A Bradford Book, The MIY Press, Massachusetts, London, England 1999.

2. Maeve O’Connor, ‘Writing successfully in science’ Chapman and Hall, London, 1995.

3. Chemical safety matters–IUPAC –IPCS, Cambridge Univ. Press, 1992.

4. D. B. Hibbert and J. J. Gooding, ‘Data Analysis for Chemistry’, Oxford University press, 2006.

5. J. Topping, ‘Errors of Observation and Their Treatment’, Fourth Edn., Chapman Hall, London, 1984

6. S. C. Gupta, ‘Fundamentals of Statistics’, Sixth Edn., Himalaya publ.House’, Delhi, 2006

7. H. E. Solbers, ‘Inaccuracies in Computer Calculation in Standard Deviation’,Anal. Chem. 55, 1611 (1983)

8. P. M. Wanek et al., ‘Inaccuracies in the Calculation of Standard Deviation with Electronic Calculators’, Anal. Chem. 54, 1877 (1982).

9.R. L. Tokheim, ‘Digital Electronics–Principles and Applications’, 5th Edn., Tata Mc Graw–Hill, New Delhi, 1999.

10. Alan Jhonson, ‘Electronics, A Systems Approach’ Hodder and Stoughton,London, 1987.

11. Robert Boylested, Louis Nashelsky, ‘Electronic Devices and Circuit Theory’,Prentice Hall, 9th Edn., May 2005.

12. Thomas L Floyd, ‘Principles of Electric Circuits: Conventional Current Version’, Prentice Hall, 7th Edn., Jan 2006.

13. For computer applications any commonly available books as well as Common materials available in the web.

14. The art of Scientific Writing – H.F. Ebel, C. Bliefert and W.E. Russey 2nd ed Weinheim; Wiley-VCH (2004).

COs	PO1	PO 2	PO 3	PO4	PO 5
CO1	S	M	S	M	S
CO2	M	S	M	S	M
CO3	S	M	S	M	M
CO4	M	S	M	S	S
CO5	S	M	S	M	M

S-Strong;M - Medium

PAPER –II

21UPCHE2C02 APPLICATIONS OF SPECTROSCOPIC METHODS

Hours	L	T	P	C
72	4	0	0	4

Course Objectives

1. To understand the theory and principles of various spectroscopic techniques.
2. To get an idea on the instrumentation of various spectral analysis.
3. To predict the structure of molecules from the spectral data.
4. To get an insight into various other applications of spectroscopy
5. To get knowledge on the electro analytical techniques

Course Outcomes

On the successful completion of the course, students will be able to

CO Number	CO Statement	Knowledge Level
CO1	Get basic knowledge on the principle, instrumentation and applications of rotational, vibrational and electronic spectroscopy.	K4
CO2	Elucidate the structure of the compounds more precisely with NMR spectral data and also able to use ESR spectra for the effective detection of free radicals.	K4
CO3	To determine nuclear transition frequencies and relaxation times and then to relate those to a property of a material using NQR as well as to use Mossbauer spectroscopy to get an idea on the magnetic properties.	K4
CO4	Using the absorption and diffraction spectroscopy for the structure elucidation of inorganic complexes.	K3
CO5	Understand the principles and applications of electro analytical techniques in the studies of properties of	K2

	materials.	

UNIT-I Rotational and Vibrational and Electronic Spectroscopy

Rotational Spectroscopy: Molecular rotations, Nuclear Quadrupole effects, Stark effect, selection rules, Instrumentation, applications.

Vibrational Spectroscopy - Molecular vibrations - IR and Raman Techniques - Vibrational Spectra and Symmetry, Assignment of bands - Structural informations Group frequencies - use of isotopes - resonance Raman spectroscopy.

Electronic Spectroscopy - principles, theory, instrumentation and applications of UV-Visible Spectroscopy.

UNIT-II NMR and Mass Spectrometry

^{1}H and ^{13}C NMR Spectroscopy:

Proton chemical shifts – anisotropic effects – ^{13}Carbon chemical shifts. Pulse fourier transform techniques. Accumulation of spectra by the pulsed NMR technique – nuclear relaxation – fourier transformation - the pulsed FT NMR spectrometer. Double resonance technique and relaxation mechanisms: Homonuclear decoupling – heteronuclear decoupling – proton decoupling technique. INDOR and nuclear overhauser effect (NOE). 2D-NMR –COSY, HETCOR, NOESY, ROESY-DEPT.

Mass Spectrometry:

Presentation and analysis of spectra - determination of molecular formula - nitrogen rule - isotopic abundance analysis - metastable ions and peaks - the molecular ion peak. Fragmentation process - even and odd electron ions - scission with rearrangement - Retro Diels-Alder rearrangement - McLafferty rearrangement. Fragmentation associated with functional groups - aliphatic compounds - aldehydes - ketones - carboxylic compounds - esters - amides - alcohols - thiols - amines - ethers - sulphides and halides - aromatic compounds - eliminations due to ortho group.

UNIT-III ESR Spectroscopy

Electron Spin Resonance Spectroscopy - Principles, Instrumentation, Hyperfine splittings. Interpretation of spectra, solid, liquid and solution state spectral studies; Anisotropic system - the triplet state; Theory of G-tensor, ESR of transition metal ions and complexes; ENDOR and ELDOR techniques.

UNIT-IV Absorption and Diffraction Spectroscopy

Atomic absorption Spectroscopy - Theory, Forbidden transitions and Selections, space quantisation, Zeeman effect, the Paschen-Back effect, the Stark effect, spectral line width, the Back-Goudsmith effect, applications.

Electronic and Photoelectron Spectroscopy - Excitation and ejection of electrons, electronic energy levels, core n level PES, Symmetry of molecular orbitals, valence levels PES, Applications - transition metal complexes.

X-ray photoelectron Spectroscopy - Principles, instrumentation, X-ray fluorescence and absorption; Electron microscopy - SEM, TEM and AFM.

X-ray diffraction methods - Characterization of XRD patterns, Structure and particle size determination.

UNIT-V Combined Problems in Spectroscopy

Applications of MW, IR, UV-Visible, NMR, ESR, Mass spectra in structural elucidation of organic compounds and inorganic molecules. Problems in Electronic, Photoelectron Spectroscopy and XRD.

REFERENCE BOOKS:

1. William Kemp, NMR in Chemistry, Mac Millan, 1986.
2. A.Carrington, A.D. Melahlam, Introduction to Magnetic Resonance, Harper and Row, New York, 1967.
3. E.A.V. Ebsworth, David, W.H. Ranklin and Stephen Cradock, Structural methods in inorganic chemistry, Black well Scientific Publ., 1987.
4. R. Drago, Physical methods in chemistry, Reinhold, New York, 1968.
5. C.N.Banwell, Fundamentals of molecular spectroscopy, McGraw Hill, New York,1966.
6. J.R.Dyer, Applications of absorption spectroscopy of organic compounds, Prentice Hall of India Pvt. Ltd., New Delhi, 1974.
7. G.W.Ewing, Instrumental methods of chemical analysis, McGraw Hill Pub, 1975.
8. Doughlas. A.Skoog, Principles of instrumental analysis, Saunders College Pub.Co, III Edn., 1985
9. R.C. Kappor and B.S. Agarwal, Principles of polarography, Wiley Eastern Ltd., 1991.

Mapping with Programme Outcomes

COs	PO1	PO2	PO3	PO4	PO5
CO1	M	M	S	S	S
CO2	M	S	S	S	M
CO3	S	S	S	M	S
CO4	S	S	S	S	M
CO5	M	S	M	S	S

S- Strong; M-Medium.

PAPER III

ELECTIVE COURSES

21UPCHE2E01 SYNTHETIC ORGANIC CHEMISTRY

Hours	L	T	P	C
72	4	1	0	4

Course Objectives:

1. To understand the retrosynthetic analysis for successful synthesis of organic molecules
2. To learn variety of organic reactions leading to the formation of C-C as well as C-N bonds.
3. To learn the applications of important oxidizing and reducing agents in organic synthesis.
4. To understand the theory, principles and applications of green chemistry and to get ideas on the green practices in the laboratory
5. To obtain expertise in clean practices in the synthetic laboratory

Course outcomes

On the successful completion of the course, students will be able to

CO Number	CO Statement	Knowledge Level
CO1	Design the syntheses of organic molecules by employing the fundamental organic reactions by retrosynthetic approach.	K4, K5
CO2	Predict the suitable reaction for the formation of C-C and C-N bonds	K4
CO3	Predict the reagents and products of important organic oxidation and reduction reactions and to understand the mechanisms involved.	K4
CO4	Plan synthesis of required molecules using green chemistry principles	K5
CO5	Plan the synthesis of novel molecules employing greener synthetic methods avoiding conventional procedures	K5

UNIT - I Disconnection Approach

Importance of organic synthesis, comparison between linear and convergent syntheses. Retrosynthesis: Introduction to disconnection approach: Basic principles and terminologies used in disconnection approach. One group C-X and C-C disconnections. Retrosynthesis and synthesis of benzofurans, p-methoxy acetophenone and ibuprofen. Functional group transformations in organic synthesis - nitro to keto, nitro to amine and acid to alcohol.

UNIT - II C-C and C-N bond forming reactions

Darzen's reaction, Use of acetylides in C-C bond formation reactions. Acid-catalyzed self condensation of olefins, Prins reaction, Shapiro reaction, Dieckmann cyclization, Robinson annulations, Hofmann-Loeffler-Freytag reaction. Hofmann-Martius reaction. Acyloin condensation. Houben-Hoesch reaction. Stork-enamine synthesis. Use of nucleophilic nitrogen and electrophilic carbon (NH_3, amines and nitrite as nucleophiles in substitution, NH_3 and amines in addition to ketones and aldehydes) and electrophilic nitrogen and nucleophilic carbon (nitration, nitrosation) for the bond formation reactions (Chichibabin reaction, Skraup synthesis).

UNIT - III Oxidation, reduction and asymmetric synthesis

Cr (VI) oxidants, Mn (VII) oxidants, OsO_4, SeO_2, Pb $(OAc)_4$, HIO_4, Ag_2O, DMSO. Ozone, peroxides (H_2O_2, *t*-BuOOH, dibenzoylperoxide) and peracids (CF_3COOOH, *m*-CPBA) as oxidizing agents.

Complex metal hydrides, dissolving metal reductions (including Birch, Benkeser, Clemmensen reductions), catalytic hydrogenation (homogeneous and heterogeneous), organoboranes as reducing agents. Wolf-Kishner reduction, McMurry reaction.

'*ee'* and methods of determination of '*ee'*. Stereoselectivity: classification, terminology and principle. Asymmetric synthesis and asymmetric induction.

UNIT - IV Green organic synthesis I

Introduction and need for green synthesis, basic principles of green chemistry. Green reagents-polymer supported reagents. Green catalysts, polymer supported catalysts, crown ethers. Biocatalysts – enzyme catalysed reactions – Bakers yeast. Green Chemistry for sustainable development. Green solvents, ionic solvents as green solvents, water as green solvent. Microwave assisted organic synthesis – principle, conventional Vs microwave heating, advantages-microwave assisted reactions-solvent free reactions-

microwave assisted synthesis of heterocyclic compounds (synthesis of pyrimidine and pyridine derivatives)

UNIT - V Green organic synthesis II

Ultrasound assisted green synthesis - Introduction, instrumentation, the phenomenon of cavitation. Sonochemical esterification, substitution, addition, alkylation, oxidation, reduction and coupling reactions.

Multicomponent reactions – Introduction, Ugi reaction, Biginelli condensation, Mannich reaction, Hantzsch reaction, Passerini reaction, Strecker reaction, Nef reaction, Perkin reaction, Bischler Napieralski reaction, Friedlander reaction, Paul-Knorr reaction and Michael addition.

References:

1. Advanced organic chemistry, Jerry March, 4th Edn. John Wiley, 2008.
2. Designing organic synthesis: A disconnection approach, S. Warren, John Wiley & Sons, New York, 2nd Edn. 1987.
3. Introduction to organic chemistry, A. Streitweiser, Jr and C. H. Heathcock, Macmillan, 1985.
4. Modern synthetic reactions, H. O. House, W. A. Benjamin, California, 2nd Edn. 1972.
5. Some modern methods of organic synthesis, W. Carruthurs, Cambridge Univ. Press, London, 2nd Edn. 1978.
6. Organic reaction Mechanisms, 3rd Edn., V. K. Ahluwalia and R. K. Prashar, Narosa, New Delhi, 2005.
7. Paul Anastas and John Warner, Green Chemistry: Theory and Practice, Oxford University Press (2000)
8. V.K. Ahluwalia, Green Chemistry: Environmentally Benign Reaction, Third Ed., Ane Books Pvt. Ltd.
9. V.K. Ahluwalia, M. Kidwai, New Trends in Green Chemistry, Second Ed., Anamaya Publishers, New Delhi.
10. D. Nasipuri, Stereochemistry of Organic Compounds: Principles and Applications, New Age International, 1994

Mapping with Programme Outcomes

COs	PO1	PO2	PO3	PO4	PO5
CO1	S	S	M	S	M
CO2	M	S	S	S	M
CO3	S	S	S	M	S
CO4	S	S	S	S	M
CO5	M	S	S	S	S

S- Strong; **M**-Medium

21UPCHE2E02 COORDINATION CHEMISTRY

Hours	L	T	P	C
72	4	1	0	4

Course Objectives

1. To understand the bonding, electron transfer, geometry of coordination compounds
2. To study characterization techniques for coordination compounds.
3. To study the metal complexes in life processes.

Course Outcomes

After the successful completion of the course, students will be able to

CO Number	**CO Statement**	**Knowledge Level**
CO1	Learn the selected crystal structures and to explain what kind of parameters that affects the crystal structure of a compound and understand the electronic spectra and the magnetic properties of complexes	K1, K2
CO2	Know about various possible geometries in coordination compounds	K2, K3
CO3	Learn about utilization of various spectral methods to characterize the compounds.	K2, K3, K4
CO4	Study about functions of metal complexes and enzymes in life process	K2, K3
CO5	Learn about functions of metal complexes as drugs	K2, K3, K4

Unit - I Basics of Coordination chemistry

Bonding theories of Coordination complexes**:** Crystal field theory – tetrahedral, square planar, square pyramidal, trigonal bipyrimidal, octahedral - applications and limitations; Spectrochemical series; Effect of ligand field strength on the colour of the complexes; John-Teller distortion; Molecular orbital theory – sigma and pi-bonding in metal complexes.

Electronic spectra and Magnetic Properties of metal complexes:

Ligand Field Spectra - Calculation of ligand field parameter, Russell-Saunders states, spin orbit coupling, Orgel diagram; Nephelauxetic effect; Charge transfer spectra -

LMCT and MLCT; Magnetic properties of complexes; Optical properties - Luminescence and Phosphorescence.

Unit - II Geometries of Metal complexes

Complexes with coordination number two, three, four (tetrahedral and square planar complexes), five (trigonal bipyramidal and square pyramidal), six (octahedral and trigonal prism) and higher coordination numbers; Factors affecting the coordination numbers; Site preference in square planar and trigonal bipyramidal complexes; Isomerism in four and six coordination complexes.

Unit - III Characterization techniques

IR Spectroscopy: Identification of various functional groups in metal complexes; NMR Spectroscopy: Identification of protons or carbons in different environments; Mass spectrometry: Fragmentation pattern in complexes; ESR: Identification of geometry and coordination number; Thermal studies: Uses of DTA and TGA in the stability of metal complexes; Single crystal XRD: Uses in the structural elucidation of metal complexes; Application of ORD and CD in the identification of complexes; Basic Computational studies: Gaussian for theoretical structural studies.

Unit - IV Metal complexes in biological systems - I

Porphyrin Systems: Structure and functions of Hemoglobin, Myoglobin and Chlorophyll; Metalloenzymes: Structure and functions of Blue copper proteins, oxidase, reductase, Superoxide dismutase (SOD), Carboxy peptidase-A, Carbonic anhydrase and Nitrogenase; Non-Heme iron-sulphur proteins: Ferridoxins, Rubredoxins and Cytochrome C.

Unit - V Metal complexes in biological systems - II

Nucleic acid structures: Types of binding modes of nucleic acids with metal complexes; Chemotherapy - Chelating Agents (with special reference to EDTA) and therapy based on in vivo chelation of radio nucleotides - Dosage and toxicity; Cis-platin and its mode of action, side effects; Radio diagnostic agents - MRI scanning, Gold containing Rheumatic agents and their mode of action – Lithium in Pschycopharmocoloical drugs.

References

1. Inorganic Chemistry - Principles of structure and reactivity, Fourth Edition, J. E. Huheey, E. A. Keiter and R. L. Keiter - Addition Wesley Publishing Co, NY, 1993.
2. Advanced Inorganic Chemistry - F. A. Cotton and G. Wilkinson

3. Mechanism of Inorganic reactions - F. Basolo and R. G. Pearson

4. Inorganic Chemistry - R. B. Heslop and P. L. Robinson

5. Introduction to Ligand Fields - B. N. Figgis - Wiley Eastern Ltd, New Delhi, 1976.

6. Bioinorganic Chemistry - I. Bertini, H.B. Gray, S.J. Lippard and J.S. Valentine; University Science Books.

7. Dr Asim R Dass, Bioinorganic Chemistry 2007. Books and Allied (P) Limited.

8. Physical Methods in Bioinorganic Chemsitry - Lawrence Que,Jr.

9. Bioinorganic Chemistry: Inorganic elements in the chemistry of lie – Wolfgang Kaim, B. Schwederski.

10. Lawrence Que, Jr, Physical Methods in Bioinorganic Chemistry – Spectroscopy and Magnetism.

Mapping with Programme Outcomes

COs	PO1	PO2	PO3	PO4	PO5
CO1	S	S	M	S	M
CO2	M	M	M	S	S
CO3	S	M	S	M	M
CO4	S	S	M	M	M
CO5	M	S	M	S	M

S- Strong; **M**-Medium.

21UPCHE2E03 **ORGANOMETALLIC CHEMISTRY**

Hours	L	T	P	C
72	4	1	0	4

Course Objectives

1. To study the synthesis, structure, bonding and reactions of metal carbonyls and nitrosyls.
2. To understand the chemistry of metal alkyl, metal allyl, metal alkene, metal alkyne complexes.
3. To study the utility of organometallic complexes as catalyst in various organic transformations

Course Outcomes

After the successful completion of the course, students will be able to

CO Number	CO Statement	Knowledge Level
CO1	Know about the synthesis, structure, bonding in carbonyl and nitrosyl.	K2, K3
CO2	Understand the concepts of Bonding of alkenes and Alkyne Complexes.	K2, K3
CO3	Learn about types of carbenes and their reactions	K2, K3
CO4	Know about the bonding and reactivity of Allyl, Arene and cyclopentadienyl complexes.	K2, K3
CO5	Understand about various organic transformations catalyzed by organometallic compounds.	K2, K3, K4

UNIT - I

Classification of organometallic compounds – the metal carbon bond types –ionic bond – sigma covalent bond – electron deficient bond – delocalised bond –dative bond – metal carbonyl complexes – synthesis, structure and reactions – the nature of M-CO

bonding – binding mode of CO and IR spectra of metal carbonyls – metal carbonyl anions – metal carbonyl hydrides– metal carbonyl halides – metal carbonyl clusters – Wades rule and isolobal relationship – metal nitrosyls – dinitrogen complexes – dioxygen complexes.

UNIT - II

Metal alkyl complexes – stability and structure – synthesis by alkylation of metal halides, by oxidative addition, by nucleophilic attack on coordinated ligands – metal alkyl and 18 electron rule – reactivity of metal alkyls – M-C bond cleavage reactions– insertion of CO to M-C bonds – double carbonylation – insertions of alkenes and alkynes – insertions of metals with C-H bonds – alkylidene and alkylidyne complexes - reactivity of alkylidene and alkylidyne complexes. Alkene complexes – synthesis of alkene complexes by ligand substitution, by reduction and by metal atom synthesis – bonding of alkenes to transition metals – bonding in diene complexes – reactivity of alkene complexes – ligand substitution –reactions with nucleophiles – olefin hydrogenation – hydrosilation – Wacker process– C-H activation of alkenes – alkyne complexes – bonding in alkyne complexes – reactivity of alkynes – alkyne complexes in synthesis – cobalt catalysed alkyne cycloaddition.

UNIT - III

Carbenes – carbene tranisition metal complexes – classification of carbene complexes – Fisher carbene complexes – structure and bonding in Fisher carbene complexes – Schrock carbenes – structure and bonding in Schrock carbine complexes transition metal complexes – N-heterocyclic carbenes – pincer N-hereocyclic carbenes activation – bond activation and catalysis of pincer NHC complexes — bridging carbenes – carbynes – Fisher carbynes complexes – structure and bonding in Fisher carbine complexes – Schrock carbynes – structure and bonding in Schrock carbynes complexes - nucleophilic and electrophilic attack on coordinated ligands – dehydrogenation reactions – amidation reactions – alkane activation – intramolecular and intermolecular C–H activation

UNIT - IV

Cyclopentadienyl complexes – metallocenes – synthesis of metallocenes – bonding in metallocenes – reactions of metallocenes – CpFe/Cp2Fe+ couples in biosensors – bent

sandwich complexes – bonding in bent sandwich complexes – metallocene halides and hydrides – metallocene and stereospecific polymerization of 1-alkenes – cyclopentadiene as a non-spectator ligand – monocyclopentadienyl (half-sandwich) complexes – synthesis and structures of allyl complexes – arene complexes – synthesis, structure and reactivity of arene complexes – multidecker complexes.

UNIT - V

Homogeneous catalysis by transition metal complexes-Hydrogenation reactions – reversible cis-dihydro catalysts – monohydride catalysts –hydrogenation of alk-1-ene – asymmetric hydrogenation –role of metal complexes in Nobel Prize in chemistry- transfer hydrogenations – hydrosilation and hydroboration reactions – water gas shift reaction – reduction of carbon monoxide by hydrogen – hydroformylation of alkenes – alcohol carbonylation – decarbonylation reactions – C-C cross coupling and related reactions – alkene oligomerisations and polymerizations – Zeigler-Natta polymerization – alkene dimerisation and oligomerisations – valence isomerisation of strained hydrocarbons – alkene and alkyne metathesis – oxidations of alkanes and alkenes – oxygen transfer reactions –supported homogeneous and phase transfer catalysis.

References

1. Organometallics I, Complexes with transition metal-carbon s-bonds, M. Bockmann, Oxford science publications, Oxford, 1996.
2. Organometallics II, complexes with transition metal-carbon p-bonds, M. Bockmann, Oxford science publications, Oxford, 1996.
3. Inorganic chemistry – Principles of structure and reactivity, J. E. Huheey, E.A.Keiter and R.L. Keiter, Addison-Wesley Publishing Company, New York, 2000.
4. Advanced Inorganic Chemistry, Sixth Edition, F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann, John Wiley and sons, Inc, New York, 1999
5. Organometallic compounds, Indrajeet Kumar, Pragati edition, Meerut, 2010.
6. Organometallic Chemistry, R.C. Mehrotra, A. Singh, New Age International (P) Ltd, Publishers, Second Edition, 2000.

Mapping with Programme Outcomes

COs	PO1	PO2	PO3	PO4	PO5
CO1	S	S	M	M	M
CO2	M	S	S	S	M
CO3	S	M	S	S	M
CO4	M	M	S	S	S
CO5	M	S	M	M	S

S- Strong; **M**-Medium.

21UPCHE2E04 CORROSION CHEMISTRY

Hours	L	T	P	C
72	4	1	0	4

Course Objectives

1. To acquire knowledge about the basic concept of corrosion.
2. To evaluate the different types of corrosion in materials.
3. To study the concept of kinetics of passivity.
4. To learn the various types of inhibitors and coating techniques.
5. To understand the necessary concepts of analytical techniques.

Course Outcomes

After the successful completion of the course, students will be able to

CO Number	CO Statement	Knowledge Level
CO1	In depth knowledge and understanding the concepts and basic principles of corrosion.	K2 & K3
CO2	Get the knowledge of various types of corrosion and enlighten the effect of corrosion.	K1 &K3
CO3	Describe the metals exhibiting passivity and understand the effect of various factors on electrochemical behavior and corrosion.	K1 & K4
CO4	Distinguish the types of inhibitors and acquire knowledge about the polymer coating through electrochemical deposition.	K1& K2
CO5	Understand and get the knowledge on various electroanalytical and surface characterization techniques.	K4

UNIT – I Introduction to Corrosion

Corrosion – Introduction – definition – cost of corrosion – importance of corrosion studies – classification of corrosion – expressions for corrosion rate. Corrosion principles – Electrochemical and thermodynamic principles.

Corrosion and its control- Introduction-Electrochemical theory of corrosion with respect to iron- Factors influencing the corrosion rate- physical state of the metal- nature of the metal- area effect- over voltage- pH- temperature and nature of the corrosion product.

UNIT – II Types of Corrosion

Different forms of corrosion – Introduction – Atmospheric corrosion, corrosion by mineral acids, Intergranular corrosion, pitting corrosion. Exfoliation, Dealloying, Galvanic corrosion, Crevice corrosion, Filiform corrosion, water line attack metal ion concentration cell corrosion, soil corrosion, stress corrosion cracking, erosion corrosion, cavitation corrosion, oxidation of metals.

UNIT – III Electrochemical Passivity

Kinetics of passivity - Introduction - Electrochemical behavior of active/passive metals - Criteria for selecting a metal exhibiting passivity - Effect of various factors on electrochemical behavior and corrosion rate of metals exhibiting passivity - theoretical anodic polarization behavior-Theories of passivity.

UNIT – IV Electrochemical Coatings

Inhibitors-Types of Inhibitors-Anodic inhibitors-cathodic inhibitors-mixed type inhibitors-classification of inhibitors-organic inhibitors-inorganic inhibitors.

Conducting Polymers-Heterocyclic Polymers–Synthesis and applications-Photoconductive polymers-light sensitive polymers and their applications-Coatings-Introduction-Electrodeposition and its types- Fluidized bed coating- Electrostatic fluidized bed coatings- Electrostatic Spray coating-Flame spray coating-Hot dipping coating-Metal spraying- Chemical conversion coating.

UNIT –V Characterization Techniques

Electroanalytical techniques-Voltammetry and its advanced techniques, Potentiometric Polarization Techniques, Cyclic voltammetry, Weight loss method, Open Circuit Potential Method.

Corrosion characterization techniques- Applications of Fourier Transform infrared spectroscopy (FTIR)-X-ray spectroscopy- Scanning electron microscope (SEM) and Energy dispersive X-ray analysis (EDAX).

Books/References

1. Raj Narayanan, An introduction to metallic corrosion and its prevention, Oxford & IBH publishing Co. New Delhi (1983).
2. M. G. Fontana, and N.D. Greene, corrosion engineering, McGraw- Hill, New York (1978).
3. S. Glasstone, An introduction to electrochemistry, Van Nostrand, Princeton, Princeton (1942).
4. J. O. M. Bockris, and K.A.N. Reddy, Modern electrochemistry, Macdonald, London (1970).
5. U. R. Evans, The corrosion and oxidation of metals, Edward Arnold, London (1977).
6. C. N. Banwell, Molecular Spectroscopy, Tata Mc-graw hill, New Delhi-2004.
7. D. A. Skoog, F. J. Holler, T. A. Nieman, Principle of instrumental analysis Thomson learning, Brooks/Cole – 2004.

Mapping with Programme Outcomes

Cos	PO1	PO2	PO3	PO4	PO5
CO1	M	S	M	S	S
CO2	S	M	M	S	M
CO3	M	S	S	M	S
CO4	S	M	S	S	S
CO5	S	S	M	M	M

S- Strong; M-Medium.

21UPCHE2E05 **NANOMATERIALS CHEMISTRY**

Hours	L	T	P	C
72	4	1	0	4

Course Objectives

1. To understand the introduction and importance of nanotechnology
2. To study the various fabrication techniques of nanoparticles
3. To understand the physicochemical properties of the nanoparticles and the tools used in nanotechnology
4. To gain knowledge on the application of nanoparticles

Course Outcomes

After the successful completion of the course, students will be able to

CO Number	CO Statement	Knowledge Level
CO1	Understand the importance of nanotechnology and its fabrication techniques.	K1
CO2	Learn the different processing techniques of nanoparticles. Knowledge on green and biological synthesis of metal nanoparticles.	K2 & K3
CO3	Learn the spectroscopic, microscopic and analytical tools used in nanotechnology	K2
CO4	To get an insight into various physicochemical, optical and thermal properties of nanoparticles	K2
CO5	In depth knowledge about the application of nanoparticles in agricultural, textiles, food, energy, environmental and biomedical field.	K2, K3

UNIT – I

Nanotechnology – Introduction- Importance- various stages of nanotechnology- nanostructures and nonmaterials. Techniques used in nanotechnology- Bottom up- self assembly- Top down fabrication techniques – EBL, DPN, NIL, UV lithography.

UNIT – II

Fabrication of nanoparticles – Grinding with ion balls-Gas condensation-Laser ablation-Thermal and ultrasonic decomposition-Reduction methods-Sol gel synthesis-Ceramic processing-Green and biological synthesis of metal nanoparticles- gold, silver and copper.

UNIT – III

Tools used in Nanotechnology – UV -Visible spectroscopy , FT-IR spectroscopy , Electron microscopy – SEM, TEM, AFM – dynamic light scattering, powder X-ray diffractometry and particle size analyser.

UNIT – IV

Properties of nanoparticles– physicochemical properties – aggregation and disaggregation – surface properties – zeta potential – surface plasmon resonance – optical, thermal, mechanical, properties –quantum confinement – superparamagnetism.

UNIT – V

Application of nanoparticles: Agricultural, textiles, food, energy, environmental and biomedical applications. Nanoenergy devices – carbon nanotubes – nanofibres – nanocages – nanosensors.

REFERENCE BOOKS

1. W.R.Fahrner, Nanotechnology and Nanoelectronics, Springer (India) Private Ltd, 2006.
2. ManasiKarkare, Fundamentals and applications of Nanotechnology, I. K. International, 2008.
3. Y.S. Raghavan, Nanostructures and Nanomaterials, Arise Publishers & Distributors, 1st Editon2010.

4. T.Pradeep, Nano: The Essentials 8th reprint Tata-McGraw Hill Education Private Limited, 2012.
5. Aparna Bhattacharya, Nanomedicine, Rajat Publications, 2008.

Mapping with Programme Outcomes

COs	PO1	PO2	PO3	PO4	PO5
CO1	S	M	S	S	M
CO2	M	S	S	M	M
CO3	S	M	M	M	M
CO4	S	S	M	M	M
CO5	S	S	M	M	M

S- Strong; **M**-Medium.

21UPCHE2E06 BIOMATERIALS CHEMISTRY

Hours	L	T	P	C
72	3	1	0	4

Course Objectives

1. To demonstrate the basics of biomaterials – classification, properties and applications.
2. To explain the importance of metallic implants in hard tissue replacement.
3. To study the usage of polymers in biological applications.
4. To learn the fundamentals and concepts of drug delivery.
5. To get adequate knowledge of materials in biomedical field.

Course Outcomes

After the successful completion of the course, students will be able to

CO Number	CO Statement	Knowledge Level
CO1	Explore the definition and classification of biomaterials. Understand the importance surface properties.	K1
CO2	Gain knowledge about various types of metallic implants and their significance in medicine.	K2& K4
CO3	Understand the basics of biopolymers and get adequate knowledge of biopolymers in medical applications.	K1 & K3
CO4	Recognize and get knowledge on the classification, properties and advantages various biomaterials in drug delivery applications.	K2 & K3
CO5	Get in depth knowledge on application of biomaterials in hard and soft tissue replacement in medical science.	K2

Unit – I Introduction to Biomaterials

Introduction: Definition and requirements of biomaterials. Classification of biomaterials, Comparison of biomaterials properties. Surface properties of materials, physical properties of materials, mechanical properties. Bioinert, biodegradable or

bioresorbable, bioactive ceramics, nanostructured bio ceramics. Mechanical properties, surface chemistry of materials, surface modification, tissue reaction.

Unit – II Materials in Medical Devices

Metallic implants – Stainless steels, Co-based alloys, Ti-based alloys, nanostructured metallic implants. Polymer, Ceramics in implant devices. Importance of stress-corrosion – pitting and uniform corrosion, cracking and degradation. Material preparation, chemical composition. Properties, uses in medicine and biosciences.

Unit – III Polymeric Materials in Medicine

Polymer – Natural and synthetic polymer. Factors influencing the properties of polymers, polymers as biomaterials. Biodegradable polymers, Bio polymers: Collagen, Elastin and Chitin. Materials for ophthalmology: contact lens, intraocular lens. Membranes for plasma separation and Blood oxygenation, electro spinning: a new approach. Physiochemical characteristics of biopolymers. Synthetic polymeric membranes and their biological applications.

Unit - IV Biomaterials in Drug Delivery

Introduction, classification, properties, advantages and application of biomaterials in formulation of controlled release drug delivery systems. Structure –Limitations - Anisotropy of composites - Porous materials. Drug carriers – Types, properties and applications. Targeted drug delivery – application and advantages.

Unit – V Application of Biomaterials

In-vitro Applications, *in-vivo* applications, Biomedical application: Hard and soft tissue replacement - Cardiovascular, Dental implants, Orthopedic application, Skin, Ophthalmologic applications, Tissue engineering application - Wound healing, Biomedical and Biosensor applications.

Text Books

1. J. H. U. Brown (Ed), Advances in Bio Medical Engineering, Academic Press 1975.

2. A. F. Von Racum, Hand Book of Bio Medical Evaluation, Mc-Millan Publishers, 1980.
3. Jacob Cline, Hand Book of Bio Medical Engineering, Academic Press in Sandiego, 1988.
4. J. Black, Biological Performance of Materials- Fundamentals of bio compatibility, 4th Edn., CRC Press 2005.
5. Larry L. Hench and Julian R. Jones, Biomaterials, Artificial organs and Tissue Engineering, 2005.
6. B. D. Ratner, A. S. Hoffman, F.J. Schoen, J. E. Lemons, Biomaterial Science; An Introduction to Materials in Medicine,2nd Edn., Elsevier Academic Press, San Diego, 2004.
7. S.V. Bhatt, Biomaterials, Second Edition, Narosa Publishing House, 2005.

Reference Books

1. M. Kutz, Standard Handbook of Biomedical Engineering and Design, McGraw Hill, 2003
2. J. Enderle, J. D. Bronzino, S. M. Blanchard, Introduction to Biomedical Engineering, Elsevier, 2005.
3. J. B. Park, Biomaterials Science and Engineering, Plenum Press, 1984.
4. A. C. Anand, J. F. Kennedy, M. Miraftab, S. Rajendran, Wood head Medical Textiles and Biomaterials for Healthcare, Publishing Ltd., 2006.
5. D. F. Williams, Materials Science and Technology: Volume 14, Medical and Dental Materials: A comprehensive Treatment Volume, VCH Publishers 1992.
6. M. Saini, Y. Singh, P. Arora, V. Arora, and K. Jain. Implant Biomaterials: A Comprehensive Review, World Journal of Clinical Cases, 2015.

Mapping with Programme Outcomes

COs	PO1	PO2	PO3	PO4	PO5
CO1	S	M	M	S	S
CO2	M	S	S	S	M
CO3	S	M	M	M	S
CO4	M	S	S	S	S

CO5	S	S	M	M	M

S- Strong; M-Medium.

21UPCHE2E07 **ENVIRONMENTAL CHEMISTRY**

Hours	L	T	P	C
72	4	1	0	4

Course Objectives

1. To understand the fundamentals and scope of environmental chemistry.
2. To study the water pollution, aquatic chemical reactions and water sampling techniques.
3. To understand the various stages in the waste water treatment.
4. To understand the industrial waste water treatment and the types of plants.
5. To gain knowledge on the treatment plants for the nitrification, denitrification and technologies used in advanced treatments.

Course Outcomes

After the successful completion of the course, students will be able to

CO Number	CO Statement	Knowledge Level
CO13	Understand the scope of environmental chemistry, various natural cycles and various disasters.	K2
CO2	Learn the water pollution, various aquatic chemical reactions, water pollution and the types of water sampling techniques.	K2
CO3	Understand the different stages in the waste water treatment and various processes to improve the performance of the water treatment plant.	K2 & K3
CO4	Understand the industrial waste water treatment and the different types of plants.	K3
CO5	Get in depth knowledge on the nitrification, denitrification, aerobic, anaerobic and advanced oxidation processes in the waste water treatment.	K3

UNIT I Fundamentals

Concept and Scope of Environmental Chemistry; Origin and development of elements; Natural Cycles – Hydrological Cycle, Carbon Cycle, Oxygen Cycle, Nitrogen Cycle, Phosphorus Cycle, Sulphur Cycle; Natural and Man-made Disasters – Recent Natural Disasters; Anthropogenic Effects.

UNIT II Water Chemistry

Water chemistry- properties of water, nature of metal ions in water, solubility of gases in water, occurrence of chelating agents in water; Redox potential, Significance of redox equilibiria in natural and waste water; microorganisms; The catalyst of aquatic chemical reactions, water pollution and its effects, eutrophication concept of DO, BOD, COD, Sedimentation. Coagulation and filtration. Sampling techniques for water.

Unit III Wastewater Treatment

Wastewater treatment: Pretreatment – screening, grit removal and pre-chlorination; Primary treatment – settling and sedimentation; Secondary treatment – trickling filter process, activated sludge process; Aeration. Role of unit processes in waste water treatment chemical coagulation – Chemical precipitation for improved plant performance chemical oxidation – Neutralization – Chemical Storage.

Unit IV Industrial Wastewater Treatment

Industrial wastewater treatment: Activated sludge treatment plants – mass balances, with and without recycle plants; Types of plants – single tank, contact stabilization, biosorption plants. Biofilters: Hydraulic film diffusion, two component diffusion; Types of plants – trickling filters, submerged filters, rotating biological contractors and rotating disc; removal of particulate organic matter.

Unit V Treatment Plants

Treatment plants for nitrification – mass balances, nitrifying plants and types of plants. Treatment plant for denitrification - mass balances, denitrifying plants and types of plants; redox zones in the biomass. . – Microbial metabolism – Bacterial growth and energetics – Aerobic biological oxidation – Anaerobic fermentation and oxidation – Trickling filters –Combined aerobic processes – Activated sludge film packing .Plant types

– pretreatment, plant with suspended sludge and filter process. Technologies used in advanced treatment – Removal of Colloids and suspended particles – Depth Filtration – Surface Filtration – Membrane Filtration Absorption – Ion Exchange – Advanced oxidation process.

REFERENCES

1. Sharma and Kaur, **Environmental Chemistry,** Krishna Publishers, New Delhi, 2000.
2. A.K. De, **Environmental Chemistry**, Wiley Eastern Ltd, New Delhi, 2014.
3. S.E Manahan, **Environmental Chemistry**, Lewis Publishers, London, 2001.
4. S.K. Banerji, **Environmental Chemistry**, Prentice Hall of India, New Delhi, 2005.
5. S.C.Bhatia, Environmental Chemistry, CBS Publishers, 2003.
6. J.Rose, **Environmental Toxicology**, Gordon and Breach Science Publication, New York, 1998.
7. S.M. Khopkar, **Environmental Pollution analysis**, Wiley Eastern, New Delhi, 1994.

Mapping with Programme Outcomes

COs	PO1	PO2	PO3	PO4	PO5
CO1	S	M	S	M	S
CO2	S	S	M	S	M
CO3	S	S	M	S	M
CO4	S	S	M	S	S
CO5	S	S	M	S	S

S- Strong; **M**-Medium.

21UPCHE2E08 POLYMER CHEMISTRY

Hours	L	T	P	C
72	4	1	0	4

Course Objectives

1. To understand the introduction and importance of advanced nanomaterials
2. To study the various fabrication techniques of advanced nanomaterials
3. To understand the fundamental principles of various characterization techniques
4. To understand the physicochemical properties of the nanomaterials
5. To gain knowledge on the various applications of nanomaterials

Course Outcomes

After the successful completion of the course, students will be able to

CO Number	CO Statement	Knowledge Level
CO1	Understand the fundamental aspects of various polymers and polymerization reactions.	K2
CO2	Learn the different processing techniques of polymers & prepare the polymers.	K2 & K3
CO3	Understand the fundamental principles, instrumentation and applications of various characterization techniques & Characterize a polymer using these techniques.	K2 & K3
CO4	Understand the physicochemical, thermal, mechanical electrical and optical properties of polymers.	K2
CO5	Get in depth knowledge on application of polymers in the fields of medicine, energy and environment.	K2, K3

Unit - I Fundamentals

Basic concepts - classification, nomenclature, molecular weights, molecular weight distribution, glass transition, degree of crystallinity, morphology, and viscosity - molecular weight, mechanical property - molecular weight relationships Importance, polymerization

reactions (polyadditions, polycondensations), configuration and conformation of polymers, coil formation, mobility in polymers, rubber elasticity.

Unit - II Techniques of polymerizations:

Methods of Polymerization - Bulk, solution, suspension and emulsion polymerization techniques, melt polymerization, solid-state polymerization. Step (condensation) polymerization Chain polymerization, controlled radical polymerizations (INIFERTER, ATRP, RAFT, SET). Living Polymerizations, Ziegler-Natta and metathesis polymerizations. Chemical Modification of Polymers: Cellulose modification- esterification, natural rubber modification, cyclisation, hydrogenation and epoxidation of natural rubber. Polystyrene modification- hydrogenation, sulphonation, grafting and crosslinking of polymers.

Unit - III Characterization techniques:

Characterization of polymers by the following techniques: UV-visible, IR, Raman, NMR (proton, carbon), 2D-NMR spectroscopy, pyrolysis, GC-MS, XRD, SEM, TEM, TGA, DTA, DSC, Dynamic mechanical analysis (DMA), electron spectroscopy for chemical analysis (ESCA).

Unit - IV Polymer properties:

Electrical and optical properties: Dielectric strength, dielectric constant, volume resistivity, dissipation factor and loss factor. Optical properties: gloss, haze, yellowness index, transmittance and photoelastic Properties. Thermophysical properties of polymers. Tg, Tm and relationships between Tg and Tm of polymer. Glass transition temperature - elementary theories and methods of determination. Variation of glass transition with structure. Rubber elasticity – concepts, thermodynamic equation of state. Elementary theories of viscoelasticity (Maxwell, Voight). Crystallinity of polymers.

Unit - V Application of Functional Polymers:

Conducting polymers, polymeric reagents, polymer supports and catalysts, Photoresponsive Polymers, polymers in lithography, Immobilization of Enzymes.

Polymeric Materials for biomedical, engineering, agriculture, textiles, energy, environment, electronics, and defence applications

References

1. H.R. Alcock and F.W. Lamber, Contemporary Polymer Chemistry, Prentice Hall, 1981.
2. P.J. Flory, Principles of Polymer Chemistry, Cornell University press, New York, 1953.
3. G. Odian, Principles of Polymerization, 2nd Edition, John Wiley & Sons, New York, 1981.
4. Jean-Pierre Farges, Organic Conductors, Marcel Dekkar, 1994
5. David B Cotts, Z Reyes, Electrically Conductive Organic Polymers for Advanced Applications, William Andrew Inc,1987
6. Larry Rupprecht, Conductive Polymers and Plastics, William Andrew Inc, 1999.
7. Raymond B Seymour, New Concepts in Polymer Science, Polymeric Composites, VSP, 1990.
8. Wallace Gordon, Gordon G Wallace, Geoffrey M Spinks, Conductive Electroactive Polymers, CRC Press, 2002

Text Books:

1. J. Young and P. A. Lovell, Introduction to Polymers, 2nd Edition, Chapman and Hall, 2002.
2. V. R. Gowariker, N.V. Viswanathan and J. Sreedhar, Polymer Science, New Age Int., 1986.
3. W. Billmeyer, Textbook of Polymer Science, 3rd Edition, John Wiley, 1994.
4. R. Gowariker, N. V. Viswanathan, Jayadev Sreedhar, New Age International (P) Ltd, 2005.
5. Odian, Principles of Polymerization, Fourth edition, Wiley-Interscience, 2004.
6. H. Sperling, Introduction to Physical Polymer Science, Wiley- Interscience, 1986.
7. Rubinstein and R. A. Colby, Polymer Physics, Oxford University Press, 2003.

Mapping with Programme Outcomes

COs	PO1	PO2	PO3	PO4	PO5
CO1	S	S	S	M	M
CO2	S	S	S	S	M
CO3	S	S	M	M	M
CO4	S	S	M	M	M
CO5	S	S	S	M	M

S- Strong; **M**-Medium.

21UPCHE2E09 COMPUTATIONAL CHEMISTRY

Hours	L	T	P	C
72	4	1	0	4

Course Objectives

1. To understand the fundamentals of computational chemistry.
2. To study the various computational methods.
3. To study the various applications of computational methods to chemical structures.

Course Outcomes

After the successful completion of the course, students will be able to

CO Number	CO Statement	Knowledge Level
CO1	Understand the fundamental aspects of computational chemistry.	K2
CO2	Understand the fundamentals of different computational methods.	K2 & K3
CO3	Understand the principles of DFT.	K2 & K3
CO4	Understand the fundamentals of various computational analyses.	K2
CO5	Apply the QM and MM to various chemical systems.	K3

UNIT - I Introduction

Computational chemistry - its benefits and applications, Numerical methods: Newton - Raphson method. Matrix diagonalization and Householder algorithm. Numerical quadrature (Gaussian and Gauss - Hermite). Elementary concepts in parallel computing/programming.

UNIT - II Methods of Computational Chemistry

Monte Carlo Method, sampling, Metropolis Algorithm, trial moves, energy expression, force field parameters. Simple molecular mechanics and molecular dynamics computations using force fields. AMBER, GROMACS and LAMMPS. Semi empirical, *ab*

inito, Hartree- Fock and Post Hartree-Fock methods. Basis sets, Slater orbitals, Gaussian orbitals and contraction.

UNIT - III Density Functional Theory

Definition of electron density, Thomas - Fermi Model. Hohenberg-Kohn theorem, Kohn-Sham method, Fermi and Coulomb Holes. Introduction to local density and X-α method, Quest for approximate exchange-correlation functional. LDA-GGA-Meta GGA-Hybrid DFT and their implementation in Gaussian using a few sample molecules.

UNIT - IV Computational Analysis

Geometry optimization, calculation of thermodynamic parameters, vibrational frequencies and intensities, NMR and ESR parameters using elementary examples and a few representative molecules using Gaussian 16. Writing a Z - matrix - basis sets and types - vibrational analysis - Finding TS, NMR analysis software's used in computation, Natural Bond Orbital analysis - current trends in computational chemistry, Output analysis.

UNIT - V Applications

Combined QM/MM methods: Implications of the choice of QM and MM methods; Application of QM/MM methods in organic, inorganic and organometallic systems. Quantitative structure activity relation (QSAR): Early approaches, topological indices, fragmental models; quantum mechanical descriptors. Application to Benzenoid and Non-Benzenoid Aromatic compounds.

References

1. Understanding Molecular Simulations, D. Frenkel and B. Smit, second edition, Elsevier, 2001.
2. Computer Simulation of Liquids, M. P. Allen and D. J. Tildesley, second edition, Oxford University Press, 2017.
3. Exploring Chemistry with Electronic Structure Methods, J. B. Foresman and Aeleen Frisch, Gaussian Inc., 2015
4. A Chemists' Guide to Density Functional Theory, W. Koch & M. C. Holthausen, Wiley-VCH, 2001.

Text Books

1. Frank Jensen (1999). Introduction to Computational Chemistry. England: John Wiley and Sons Ltd.

2. David Young ,Computational Chemistry , Wiley-Interscience, 2001

3. Jerry March, Advanced Organic Chemistry

4. Introduction to Computational Chemistry, Frank Jensen, third edition, Wiley, 2017.

5. Modern Quantum chemistry, A. Szabo & N. S. Ostlund, McGraw-Hill, 1961 edition reprinted by Dover Publications, 1989.

Mapping with Programme Outcomes

COs	PO1	PO2	PO3	PO4	PO5
CO1	S	S	S	M	M
CO2	S	S	M	S	M
CO3	S	S	M	M	M
CO4	S	M	M	M	M
CO5	S	M	M	M	M

S- Strong; **M**-Medium.

21UPCHE2E10 SURFACE CHEMISTRY

Hours	L	T	P	C
72	4	1	0	4

Course Objectives

1. To understand the types of adsorption and isotherm.
2. To understand the adsorption in solution.
3. To understand the micelles and micellar catalysis.
4. To study and understand the various techniques to examine the surfaces.
5. To expand the knowledge on catalysis and characterization techniques.

Course Outcomes

After the successful completion of the course, students will be able to

CO Number	CO Statement	Knowledge Level
CO1	Understand the Chemisorption, Physisorption and various adsorption theories, derivation.	K3
CO2	Learn the adsorption in solution and understand the types, thermodynamics of surface, surfactants.	K2 & K3
CO3	Understand the classification, affecting factors, thermodynamics of surfactans and micellar catalysis.	K2 & K3
CO4	Understand the examination techniques of surfaces and applications of various adsorption isotherms.	K3
CO5	Get in depth knowledge on the examination of different types of catalysis and instrumental methods of characterization techniques.	K3

Unit - I

The Gas- solid inter phase,-types of adsorption. Heat of adsorption and its determination, differences between chemisorption and physisorption. Adsorption isotherms-classical, Freundlich and Langmuir isotherms. Thermodynamic and statistical derivation of Langmuir adsorption isotherm. Multilayer adsorption- the BET theory and Harkins- Jura theory.

Unit - II

Adsorption from solutions: Gibb's adsorption equation and its verification. Adsorption with dissociation. Adsorption with interaction between adsorbate molecules. Different types of surfaces, Properties of surface phase. Thermodynamics of surface. Surface tension of solutions. Surfactants andmiscelles.

UNIT - III

Micelles: Classification of surface active agents, micellization, hydrophobic interaction, critical micellar concentration (CMC), factors affecting the CMC of Surfactants. Thermodynamics of micellization - phase separation and mass action models. Reverse micells, micro-emulsion. Micellar Catalysis, Surface tension capillary action, pressure difference across curved surface (Laplace equation), vapour pressure of droplets(Kelvin equation), Gibbs adsorption isotherm.

Unit - IV

Examination of surfaces using low energy electron diffraction, photoelectron spectroscopy, ESCA, scanning probe microscopy, Auger electron spectroscopy , SEM and TEM. Surface films-different types, surface pressure and its measurement, surface potential and its measurements and interpretation. Measurement of surface area of solids - Harkins – Jura absolute method, entropy method . Use of Langmuir, BET and Harkins – Jura isotherms for surface area determination.

Unit - V

Catalysis: Mechanism and theories of homogeneous and heterogeneous catalysis. Enzyme catalysis, bimolecular surface reactions. Langmuir – Hinshelwood mechanism, instrumental methods of catalyst characterization- diffraction and thermal methods, spectroscopic and microscopic techniques.

References

1. A.W.Adamson, "Physical Chemistry of Surfaces", 5th edition Wiley India, 1990.

2. D.K.Chakrabarty and B. Viswanathan, Heterogeneous catalysis, New Age Publications, 2009.
3. G.A.Somorjai, Y.Li, Introduction to Surface Chemistry and Catalysis.International, 2nd edn., 2010.
4. Gurdeep Raj "Advanced Physical Chemistry" GOEL Publishing House, Meerut, 2004.
5. W.J. Moore, Physical Chemistry, Orient Longman, London, 1972.

Mapping with Programme Outcomes

COs	PO1	PO2	PO3	PO4	PO5
CO1	S	M	M	S	M
CO2	S	S	M	M	S
CO3	S	S	S	M	S
CO4	S	M	S	S	S
CO5	S	S	S	S	M

S- Strong; **M**-Medium.

SEMESTER - II

PART II

21UPCHE2C03 PROJECT DISSERTATION VIVA

Candidates shall carry out research work in consultation with the guide/supervisor and submit the dissertation to the University through the Supervisor and Head of the Department at the end of the year from the commencement of the course which shall be valued by internal examiner (supervisor) and one external examiner appointed by the University from a panel of four names sent by the Supervisor through the Head of the Department at the time of submitting the dissertation.

RESEARCH METHODOLOGY

Time: Three Hours Maximum:75 marks

All questions carry equal marks

Part - A Answer All Questions (5x5=25 marks)

1. (a) How will you carry out literature survey using computer?

(or)

(b) How will you write a research proposal?

2. (a) Explain various types of errors in analyzing the research data.

(or)

(b) Write notes on linear regression and Multiple linear regression.

3. (a) Distinguish between separation and purification methods

(or)

(b) How will you select column for HPLC

4. (a) How will you create management documents.

(or)

(b) What are the latest strategies to be followed in chemistry teaching

5. (a) What are the search engines used in chemistry research

(or)

(b) How internet is used for chemists?

Part-B Answer All Questions (5x10=50 Marks)

1. (a) Discuss various types of primary sources in surveying the literature.

(or)

(b) Write an essay on Rough drafting of a research paper.

2. (a) i) Explain various statistical tests on the accuracy of results.
ii) Discuss Gaussian distribution with deviations from Gaussian law of error

(or)

(b) Write notes on
i. Normal distribution of random errors.
ii. Gross errors iii. Elimination of outlying results

8. (a) Discuss the theory and applications of GCMS

(or)

(b) How will you isolate a compound from a mixture

9. (a) Discuss the recent methodologies used in chemistry teaching

(or)

(b) How will you improve the quality of chemistry education

10. (a) Discuss the use of computer languages used in chemistry research

(or)

(b) Discuss various chemistry databases and e-journals.

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List of Question Setters / Examiners

From Periyar University & Affiliated Colleges		Outside Periyar University	
S.No.	**Name and Address**	**S.No.**	**Name and Address**
01.	Dr. V. Raj Professor and Head Department of Chemistry Periyar University, Salem – 636 011	**01.**	Dr. A.Ilangovan Professor of Chemistry School of Chemistry Department of Chemistry Bharathidasan University Tiruchirapalli – 24
02.	Dr.P.Viswanathamu rthi Professor Department of Chemistry Periyar University, Salem – 636 011	**02.**	Dr. M.G.Sethuraman. Professor Department of Chemistry Gandhigram Rural University Gandhigram - 624 302, Dindigul District
03.	Dr. D. Gopi Professor Department of Chemistry Periyar University, Salem – 636 011	**03.**	Dr.C.R.Ramanathan Associate Professor Department of Chemistry Pomdicherry University Pondicherry-605014
04.	Dr. A. Lalitha Associate Professor Department of Chemistry Periyar University, Salem – 636 011	**04.**	Dr. R. Karvembu Professor Department of Chemistry National Institute of Technology Tiruchirapalli - 620015
05.	Dr. R. Rajavel Associate Professor Department of Chemistry Periyar University, Salem – 636 011	**05.**	Dr.K.P.Elango Professor Department ofChemistry Gandhigram Rural University Gandhigram - 624 302,Dindigul District
06.	Dr. V. Sujatha Assistant Professor Department of Chemistry Periyar University, Salem – 636 011	**06.**	Dr.R.Ramesh Professor of Chemistry School of Chemistry Department of Chemistry Bharathidasan University Tiruchirapalli – 24
07.	Dr. K. Shanmuga Bharathi Assistant Professor Department of Chemistry Periyar University, Salem – 636 011	**07.**	Dr. S. Abraham John Professor Department of Chemistry Gandhigram Rural University Gandhigram, Dindigul - 624 302

08.	Dr. K.Bharathi Assoc. Prof.& Head Department of Chemistry Sri Sarada College, Salem - 636 016	**08.**	Dr.M.Ilanchelian Associate Professor Department of Chemistry Bharathiar University Coimbatore - 46
09.	Dr.S.Malathi Assoc. Professor and Head Department of Chemistry JKK Natraja College, Komarapalayam Salem - 638183	**09.**	Dr.T.M.Sridhar Professor of Analytical Chemistry School of Chemical Sciences University of Madras Chennai-25