PERIYAR UNIVERSITY

Salem-636 011, Tamil Nadu, India

NAAC A Grade – State University- NIRF Rank 68

M.PHIL. DEGREE

[Choice Based Credit System (CBCS)]

Branch IV (M) CHEMISTRY

Programme Code : CHE2

REGULATIONS AND SYLLABUS

[For the Candidates admitted from the academic year 2018 – 2019 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	18UPCHE2C01	Research methodology	72	4	1	0	4
Elective Courses							
2	18UPCHE2E01	Spectroscopic and Instrumental methods	72	4	1	0	4
3	18UPCHE2E02	Green Chemistry	72	4	1	0	4
4	18UPCHE2E03	Chemistry of nanomaterials	72	4	1	0	4
5	19UPCHE2 G01 - 10	Background research paper- Guide paper	72	4	1	0	4
SECOND SEMESTER							
6	18UPCHE2C02	Dissertation					

V. Scheme of Examinations:

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

The examination of papers I and II 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).

Paper – III examination will be conducted by the Department at the end of second semester. The duration for each paper III also shall be 3 hours carrying a maximum of 75 marks apart from internal (25 marks).

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.

S.No	Paper Code	Title of the paper	Exam Hours	I	E	T	C
FIRST SEMESTER							
Core Courses							
1	18UPCHE2C01	Research methodology	3	25	75	100	4
2	18UPCHE2E01/ E02/E03	Elective Course	3	25	75	100	4
3	19UPCHE2 G01/02/03/04/05 /06/07/08/09/10	Background research paper- Guide paper	3	25	75	100	4
SECOND SEMESTER							
4	18UPCHE2C02	Dissertation		#50	#150	200	12
		Total				500	24

50 marks : Viva Voce #150 marks : Dissertation

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.

Dissertation / Project Work

Dissertation / Project Work: 200 marks

Concise Dissertation	**150 marks**
Viva-Voce	**50 marks**
Total	**200 marks**

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

I-SEMESTER

CORE PAPERS

PAPER-I

18UPCHE2C01 RESEARCH METHODOLOGY

Hours	L	T	P	C
72	4	0	0	4

Course Objectives

1. To understand the methods of survey of litrature.
2. To understand the Statistical Analysis of Data.
3. To understand the theory and principles of Separation techniques.
4. To understand the basic concepts of Practical training.
5. To study the computer operating skills.

Course Outcomes

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

CO Number	CO Statement	Knowledge Level
CO1	Carry out a thorough literature survey.	K2
CO2	Analyze the statistical data.	K3
CO3	Understand the theory and usage of separation techniques.	K3
CO4	Acquire a complete practical training on effective teaching learning methodologies.	K3
CO5	Understand computer operating skills	K2

UNIT-I Survey of Literature

Primary sources – Journals of different fields of Chemistry - Secondary Sources literature search through loaded CDS. Aids of Computer devices in literature survey. location of journals, e-mail address, specific articles of science citation cards and indices, summarization of works already done and published in the chosen field. Selection of topic and facilities.

Writing and research proposal - Thesis and dissertations, style and conventions in writing, Rough drafting of the article . The general format – page and chapter format – use of quotations – foot note – tables and figures - applicability of the findings to common usage – referencing – abbreviations used etc.

UNIT-II Statistical Analysis of Data

Various types of errors – precision and accuracy – significant figures, various statistical tests on the accuracy of results, positive and negative deviation from accurate results - the Gaussian distribution – the normal distribution of random errors, mean value, variance and standard deviation, reliability interval, deviations from the Gaussian law of error distribution, t-tests-comparison of the mean with the expected value, comparison of the results of two different methods, comparison of the precision of two methods by Ftest, Gross errors and elimination of outlying results, graphical methods – Linear regression, regression line, standard deviation, correlation coefficient – Multiple Linear regression (one variable with two other variables

Unit- III Separation techniques

Methods of separation Distinction between separation and purification – basic principles of separation techniques – filtration, crystallization, fractional crystallization, solvent extraction, distillation Chromatography- Paper, Column, Ion-exchange, GC and HPLC techniques and applications

Unit –IV Practical training

Preparation of charts and models for handling classes of chemistry teacher – Creating management documents e.g. Curriculum Plan, Time Table scheduling, Evaluation – Strategies etc – Learning to write and draw on the blackboard – Preparation of power point/LCD presentations – Preparation of micro-teaching skills- Smart class room teaching.

Unit -V Computer operating skills

Starting a program and opening a document – saving and naming the document – create file and folders – deleting and un-deleting a document – closing a document – renaming and moving a document – finding a document – MS office: Word, Excel, Access, power point, out look, integrated office applications, Chem-draw and its application. internet for chemists – online search of chemistry databases, e-journals, search engines for chemistry, chemweb.

REFERENCE BOOKS

1. J. Anderson, B.H.Durston and M.Poole, "**Thesis and Assignment Writing"**, John Wiley, Sydney 1970.
2. R. **Berry**, "How to Write a **Research Paper",** Pergamon, 1969
3. Ralph Berry , **"The Research Project: How to Write It", Fourth Edition** Routledge (UK), 2000.
4. W.G. Campbell, "Form **and Style in thesis writing**", Boston M.A; Houghton Mifflin Co., 1970.
5. J.Anderson, "**Thesis and Assignment Writing**", Wilely, 1970.
6. Jerry March, "**Advanced Organic Chemistry: Reactions, Mechanisms And Structure,"** 5th ed., Wiley, 1996
7. A.I. Vogel, "**Quantitative Inorganic Analysis**", 3rd Ed., ELBS Longman London.
8. D.A.Skoog and D.M.West, **Fundamentals of Analytical Chemistry**, Holt Rinehart and Winston Publications, IV Edn, 1982.
9. W.L. Cochran, "**Statistical Methods**", Oxford and IBH Publication, New Delhi, (1967).
10. K. Balagurusamy, "**Fortran for Beginners**", Tata McGraw Hill, New Delhi, 1990.
11. K.V. Raman, "**Computer in Chemistry**", Tata McGraw Hill, New Delhi, 1993.
12. K. Balagurusamy C++, Tata McGraw Hill, New Delhi, 1995.
13. Sanjay Saxena, MS OFFICE 2000
14. Manual of MS Office Microsoft inc.
15.

Mapping with Programme Outcomes

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

S- Strong; M-Medium.

PAPER –II ELECTIVE PAPERS

18UPCHE2E01 SPECTROSCOPIC AND INSTRUMENTAL 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 materials	K2

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 ESR Spectroscopy

Nuclear Magnetic Resonance Spectroscopy - Theory, Instrumentation of ^{1}H NMR and ^{13}C NMR - Chemical shift, coupling,; Applications – Nuclear resonance in solids and liquids, resolution – Double resonance methods – spin relaxation modes, etc.

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-III NQR and Mossbauer Spectroscopy

Nuclear Quadrupole Resonance Spectroscopy: Principles, Instrumentation, experimental detection of NQR frequencies; interpretations and chemical applications; solid state applications.

Mossbauer Spectroscopy – The Mossbauer effect, experimental methods, Hyperfine interaction, parameters for Mossbauer spectra, applications, molecular and electronic structures. Solid state chemistry – conversion electron Mossbauer spectroscopy.

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 Electroanalytical Techniques

Polarography – Theory, DME and importance, Current Voltage curves, Diffusion current and its theory, factors affecting it. Polarographic wave and half wave potentials, applications. Oscillographic Polarography, Square wave polarography, Tensimetry. . Chronopotentiometry - Cyclic Voltammetry, Amperometry, theoretical principles, applications in chemical investigations.

Electrogravimetry – Principles and applications.

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.

18UPCHE2E02 **GREEN CHEMISTRY**

Hours	L	T	P	C
72	4	0	0	4

Course Objectives

1. To understand the fundamentals and principles of green chemistry.
2. To understand the concepts, principles and reactions of green synthesis
3. To understand the theory and principles of green synthesis techniques.
4. To understand the basic concepts of and principles of treatment methods
5. To explore the green chemistry techniques to various fields

Course Outcomes

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

CO Number	CO Statement	Knowledge Level
CO1	Understand the fundamentals and principles of green chemistry.	K2
CO2	Understand the concepts, principles and reactions of green synthesis	K3
CO3	Understand the theory and usage of green synthesis techniques.	K3
CO4	Understand the principles of treatment methods	K3
CO5	Explore the green synthesis techniques to various fields	K2

Unit I Introduction

The need for green chemistry – Twelve principles – Atom economy – Scope for green chemistry – Inception and awards.

Unit II Solvent free reactions

Exploration of solvent free reactions – Microwave assisted organic synthesis – Functional group transformations – Protection and deprotection reactions, Condensation reactions, reduction and oxidation. Ionic liquids – Synthesis of ionic liquids – Applications in organic synthesis.

Unit III Eco-friendly green Techniques

Biocatalysts – Modified biocatalysts – Transition metal catalysts – Supported metal catalysts.

Eco-friendly synthesis and reactions of unsaturated nitroalkanes.

Heterogenised reactions – Mineral solid catalysed reactions – Solid supported catalysts – Super critical fluids.

Unit IV Alternative Treatment Technologies

Oxidation at ambient conditions for wastewater treatment – Photocatalytic reactions – Electrocatalytic reactions – Fentons chemistry – Hybrid processes. Chemical methods for dye removal – Oxidative processes – physical treatments – Biological treatments.

Unit V Exploration of Green Chemistry

Trace element speciation by hyphenated techniques – tools for analytical speciation.

Green chemicals – Prospects and future in designing new drugs.

Designing of next generation agrochemicals from nature.

REFERENCE BOOKS:

1. Rashmi Sanghi and M.M.Srivastava (Eds.), **Green Chemistry – Environment friendly alternatives**, Narosa Publishing house, New Delhi, 2003.
2. P.T.Anastas and J.C.Warner, **Green Chemistry: Theory and Practice**, Oxford Science Publications, Oxford, 1998.
3. P.Tundo and P.T.Anastas(Eds.) **Green Chemistry: Challenging Perspectives**, Oxford University Press, Oxford, 2000.
4. P.T.Anastas and T.C.Williamson(Eds.) **Green Chemistry: Frontiers in Chemical Synthesis and processes**, Oxford University Press, Oxford, 1985.
5. A.S.Matlach, **Introduction to Green Chemistry**, Marcel Decker Inc.. New York, 2001.

Mapping with Programme Outcomes

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

S- Strong; M-Medium.

18UPCHE2E03 CHEMISTRY OF NANOMATERIALS

Hours	L	T	P	C
72	4	0	0	4

Course Objectives

1. To understand the fundamentals of nanotechnology.
2. To understand the principles of synthesis of nanomaterials
3. To understand the principles and instrumentation of various characterization techniques.
4. To understand the various applications of nanomaterials
5. To study the sensor applications of nanomaterials

Course Outcomes

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

CO Number	CO Statement	Knowledge Level
CO1	Understand the fundamentals of nanotechnology	K2
CO2	Understand the concepts and principles of synthesis methods	K3
CO3	Characterise a nanomaterial using various characterization techniques.	K3
CO4	Apply the nanomaterials in various fields	K3
CO5	To use the nanomaterials as sensors for environmental applications	K2

Unit I Nanomaterials - An Introduction

Importance and necessity for nanomaterials-Different types of nanomaterialsNanotubes: Single and Multiwalled carbon nanotubes- nanowires, nanorods nanofibres and nanoflowers of polymers, semiconductors, metals and alloysnanocrystalline materials-nanoporous materials-nanothin films-nanocompositesnanoquantum dots.

Unit II Synthesis of Nanomaterials

Wet processes-colloidal chemical method, hydrothermal method, sol-gel method; Precipitation processes-Solid state processes-gas phase synthesis, Dry coatings- PVD, CVD, Electron beem evaporation techniques, RF sputtering-Magnetron sputteringDC and Pulsed electrodeposition-Electrophoretic deposition-Anodic oxidationAutocatalytic deposition and Laser deposition-Arc discharge and plasma polymerization methods.

Unit III Characterization of Nanomaterials

Surface morphology and nanostructure-SEM,TEM,AFM; Structural characterization-UV-Visible and FT-IR spectroscopy, XPS and ESCA; Structure orientation and microtexture-XRD- Mechanism and electrochemical bahaviour-cyclic voltammetry and EQCMB.

Unit IV Application of Nanomaterials:

Photocatalytic applications-applications of carbon nanomaterials in the field of fuel cells, batteries; Energy and environmental applications- Energy production and storage-nanomaterials as actuators and thermal insulators-membranes for chemical processes-Applications of nanomaterials in electronics, biotechnology, medicine.

Unit V Sensor Applications

Application of nanomaterials as chemical sensors-sensing components-enhanced sensing and detection- detection of biomolecules, pollutants and drugs.

References

1. K.L.Choy, **Process principles and applications of novel and cost-effective ESAVD based methods,** World Scientific Publishing, Singapore, 2002.
2. A.Jones and M.Mitchell, **Nanotechnology-Commercial Opportunity,** Evolution Capital Ltd. London, 2001.
3. C.N.R.Rao, A.Muller and A.K.Cheetham (Eds.), **The Chemistry of Nanomaterials** Vol.I & Vol.II., Wiley-VCH, 2004

4. G.Schmid (Eds), **Nanoparticles**, Wiley-VCH, 2004
5. G.Hodes(Eds.), **Electrochemistry of Nanomaterials**, Wiley-VCH, 2001.
6. M.Kohler, W.Fritzsche, **Nanotechnology**, Wiley-VCH, 2004
7. P.Ajayan, L.S.Schadler, P.V.Brawn, **Nanocomposite Science and Technology**, Wiley-VCH, 2003.

Mapping with Programme Outcomes

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

S- Strong; M-Medium.

PAPER –III - (GUIDE PAPER)

19UPCHE2 G01- BACKGROUND RESEARCH PAPER

This background paper should be related to the proposed research work towards the dissertation. The Guide will give the syllabus.

II-SEMESTER

PART II 18UPCHE2C02 DISSERTATION (Project)

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.

M.Phil. CHEMISTRY

CBCS Pattern 2019-2022

SPECIALIZATION PAPERS (ELECTIVE)

19UPCHE2 G01 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.

19UPCHE2 G02 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.

19UPCHE2 G03 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 catalysed 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.

19UPCHE2 G04 CORROSION CHEMISTRY

Hours	L	T	P	C
72	4	1	0	4

Course Objectives

1. To obtain knowledge on the various type of corrosion.
2. To learn the concepts of inorganic and organic electrochemical reaction.
3. To understand the corrosion and corrosion inhibition parameters.
4. To understand the concepts of electrochemical cells.
5. To study the basic concepts of anodic and cathodic protection.

Course Outcomes

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

CO Number	CO Statement	Knowledge Level
CO1	To gain knowledge on the mechanism of electrode reactions principle and applications of Polarography, Amperometry and Cyclic voltametry	K1&K2
CO2	Demonstrate electrochemical reactions of technological interest. Apply the basic techniques on the Corrosion, Passivation and prevention.	K3
CO3	In depth knowledge and understanding about the corrosion, corrosion inhibition parameters and process techniques of electrochemical methods.	K2 &K4
CO4	To gain knowledge on the types of corrosion and the principles of electrochemical cells.	K1&K2
CO5	Understand the prevention strategies for surface engineering. Knowledge on cathodic protection and application of potential theory.	K2

UNIT – I

Mechanism of electrode reactions – Polarisation and Over Potential – the Butler Volmer equation for one step and multi step electron transfer reactions – significance of equilibrium exchange current density and symmetry factor – transfer coefficient and its significance – Theory and applications of dropping mercury electrode – Polarography, Amperometry and Cyclic

voltametry – Principles and applications – mechanism of Hydrogen and Oxygen evolution reactions.

UNIT – II

Electrochemical inorganic and organic reactions of technological interest – Corrosion and Passivation of metals – construction of Pourbaix and Evans diagrams – Prevention of Corrosion. Electrodeposition – Principles and applications.

UNIT III

Determination of corrosion and corrosion inhibition parameters – non-electrochemical methods: coupon – electrochemical resistance – gasometric methods. Electrochemical methods: polarization – galvanostatic-potentiostatic – potentio dynamic- AC impedance- hydrogen permeation.

UNIT – IV Electrochemistry of corrosion

Corrosion – introduction, definitions and types-Electrochemical cells-definitions and principles -Potential measurements - galvanic cells, concentration cells. -EMF and Galvanic series - bimetallic couples-Eh-pH diagrams – fundamental aspects - Construction of Eh – pH diagrams- FeH_2O-O_2 diagram- Copper, Aluminum and general corrosion diagrams.

UNIT – V Methods of corrosion control

Prevention strategies – design and coatings-Prevention strategies – inhibitors and surface engineering - Cathodic protection – principles and classification- Cathodic protection – influencing factors and monitoring - Design aspects for cathodic protection-Stray current corrosion-Passivity – definitions and influencing parameters -Passivity – application of mixed potential theory-Passivity – design of corrosion resistant alloys-Anodic protection.

References

1. S. Glasstone, **Introduction to Electro Chemistry**, Affiliated East West Press, New Delhi, 1960.

2. D.R. Craw, **Principles and applications of Electro chemistry**, Chapman and Hall, 1991.

3. J. Robbins, **Ions in solution – An Introduction to Electro chemistry**, Clarendon Press, Oxford (1972).

4. J.O.M. Bockris and A.K.N. Reddy, **Electrochemistry**, Vols, 1 and 2, Plenum, New York. 1977.

5 R.H. Rieger, **Electrochemistry**, Chapmann and Hall, New York (1994).

6. P. Delahay, **Electrode Kinetics and Structure of Double Layer**, Interscience, 1965.

7. Branko N Popov**,** Corrosion Engneering.

8. Raj **Narayan**, ***Corrosion*** of metals and polymers

Mapping with Programme Outcomes

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

S- Strong; M-Medium.

19UPCHE2 G05 NANOCHEMISTRY

Hours	L	T	P	C
72	4	1	0	4

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	To get an insight into various physicochemical, optical and thermal properties of nanoparticles	K2
CO4	Learn the spectroscopic, microscopic and analytical tools used in nanotechnology	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

Fabricationof 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

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

UNIT – IV

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 – 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.

19UPCHE2 G06 ADVANCED MATERIALS CHEMISTRY

Hours	L	T	P	C
72	4	1	0	4

Course Objectives

5. To understand the introduction and importance of advanced nanomaterials
6. To study the various fabrication techniques of advanced nanomaterials
7. To understand the fundamental principles of various characterization techniques
8. To understand the physicochemical properties of the nanomaterials
9. 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 fundamental aspects of advanced nanomaterials.	K2
CO2	Learn the different processing techniques of advanced nanomaterials..	K2 & K3
CO3	Understand the fundamental principles, instrumentation and applications of various characterization techniques & Characterize a nanomaterial using these techniques	K2 & K3
CO4	Understand the physicochemical, surface, optical, thermal, mechanical and photochemical properties of advanced materials	K2
CO5	Get in depth knowledge on application of nanomaterials inm the fields of medicine and energy.	K2, K3

Unit-1 Fundamentals of Advanced Materials

General introduction about Nano science - Size and Scale, Units, Scaling, atoms, molecules, clusters and supramolecules. Structure and bonding in nanomaterial, chemical bonds (types and strength), intermolecular forces, molecular and crystalline structure, hierarchical structures, bulk to surface transition, surface reconstruction. Definition of nano structures – Emergence of nanotechnology – Historical perspective of nano materials, Classification of nano materials, Challenges in nanotechnology. Special Nanomaterials: Carbon nanotubes, fullerenes, nanowires, porous silicon.

Unit-II Synthesis

Fabrication of nanoparticles - Gas condensation-Thermal and ultrasonic decomposition. Reduction methods-Sol gel synthesis-Ceramic processing, Bio-inspired synthesis: Green and biological synthesis of metal nanoparticles - Gold, silver and copper. Thin films methods: Electrochemical deposition, Chemical vapor deposition, physical vapor deposition (Sputtering, Laser ablation), Galvanic deposition, Spin Coating, Langmuir-Blodgett growth. Mechanical methods: Ball milling, Mechanical attrition, Sol-gel, Microemulsion, Electrochemical, Wet chemical, template synthesis, mechanochemical synthesis and nanolithography. Advantages and Disadvantages of the methods.

Unit-III Characterization

Tools used in nanotechnology- UV- Visible spectroscopy, FT-IR spectroscopy-Electron microscopy- SEM,TEM, AFM, powder X-ray Diffractometry, X-ray Photoelectron Spectroscopy and Particle size analyser and Zeta potential determination, Photo luminescence spectroscopy, TGA/DTA, DSC.

Unit-IV Properties

Properties of Nanoparticles-Physicochemical Properties-Aggregation and disaggregation-Surface Properties-Zeta Potential, Surface Plasma Resonance-Optical Properties-Quantum Confinement, Magnetic, Mechanical, Thermal and Photocatalytic Properties.

Unit-V Applications

Nanotechnology in drug delivery, types of nanocarriers: nanogels, nanoparticles, nanoflims, nanofibres, nanosponges and nanoliposomes. Application of *In vitro* biological evaluation-bioactivity, biodegradation, biocompatibility, hemo biocompatibility, cell proliferation, cell apoptosis, cellular uptake, cell quantification and drug release kinetics. Applications of biomaterials- Fabrication and characterisation-Short term and long term applications in medicine.Nano-electronics, Nano optics, Nanoscale Chemical- Biosensing, Solar cells, Fuel cells, energy storage application.

Books/References:

1. C.N.R. Rao, A. Muller, A.K. Cheetham (eds), The Chemistry of nano materials synthesis, properties and applications, John Wiley- Vch-2001 Vol-2.
2. Challa S.S.R. Kumar Joset Hormes, Carola leuschner, Nano fabrication towards biomedical applications, John Wiley-Vch-2004.
3. Michael Kohler, Wolfgang Fritzsche, Nano Technology an introduction to nano structuring techniques, John Wiley-Vch-2003.
4. M.E. Muller, M. Allgower, R. Schneider, H. Willenegger, Manual of internal fixation techniques, Berlin Heidelberg, New York.
5. J. D. Currey, The mechanical adaptation of bones, Princeton university press, 1984.
6. H. Aoki, Science and medical application of hydroxyapatite, Japanise Associationof apatite science, Tokyo, Japan, 1991.
7. R.Z. Legeros, Calcium phosphates in oral Biology and medicine, karger, Basel, Switzerland, 1991.
8. B. O. Fowler, Structural properties of hydroxyapatites and Related compound, Gaithersburg, 1968.
9. Dr. H. Haur, Spectroscopy- K.K. Mitter, 2004 – 2005.
10. H.S. Randhawa, Modern molecular spectroscopy Rajiv-Beri – 2003.

11. Hobart H. Willard, Cynne C. Mesit Jr John A. Dean Frank, A. Settle Jr. Instrumental methods of analysis, sathish kumar-1986.
12. Robert M. Silverstein Francis X. Webster, Spectometric identification of organic compounds, Dr. G. Clayton Bassler – 1996.
13. C.N. Banwell, Molecular Spectroscopy, Tata Mc-graw hill, New Delhi-2004.
14. Douglas A. Skoog, Donald M. West F. James Holler, Fundamentals of analytical chemistry Harcourt Asia, Replika – 2001.
15. Douglas A. Skoog, F. James Holler, Timothy A. Nieman, Principle of instrumental analysis Thomson learning, Brooks/cole – 2004.
16. Manasi Karkare, Fundamentals and applications of nanotechnology, I.K. International, 2008.
17. Graphene-based materials and their composites: A review on production, applications and product limitations,Velram Balaji Mohanet.al, Composites Part B, (142) 200–220,2018.
18. Recent development of two-dimensional transition metal dichalcogenides and their applications,Wonbong Choiet.al,Materials Today, 20 (3), 116-130, 2017.

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.

19UPCHE2 G07 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
CO1	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.

19UPCHE2 G08 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

Importance, basic concepts, raw materials for polymers, concept of functionality, comparison of chain and step-growth, examples of polymerization reactions (polyadditions, polycondensations) constitution of polymers, homopolymers and copolymers, polymer architectures (graft copolymers, star-branched, hyperbranched and dendrimers), configuration

and conformation of polymers, coil formation, mobility in polymers, glass transition temperature, rubber elasticity, molecular weight distribution,

Unit II Techniques of polymerizations:

Bulk, solution, suspension and emulsion polymerization techniques, melt polymerization, solid-state polymerization. Chemical Modification of Polymers: Cellulose modification- esterification and etherification of cellulose, natural rubber modification, cyclisation, hydrogenation and epoxidation of natural rubber. Polystyrene modification- hydrogenation, sulphonation, grafting and crosslinking of polystyrene.

Unit III Characterization techniques:

Fundamentals, experimental and applications to polymers of the following techniques: UV-visible spectroscopy, IR and Raman spectroscopy, Nuclear Magnetic (proton, carbon), resonance spectroscopy, NMR of polymers in the solid state, two dimensional NMR spectroscopy, pyrolysis GC-MS. X-ray diffraction, Transmission electron microscopy, scanning electron microscopy, thermal analysis (TGA, DTA, DSC), Dynamic mechanical analysis (DMA), electron spectroscopy for chemical analysis (ESCA).

Unit IV Polymer properties:

Approach and concept. Chemical structure of polymers- shapes and energy consideration, copolymers, heteroatomic polymers, molecular weight and distribution of molecular weights. Physical structure of polymers. 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 in relation of chemical structures; Tg, Tm and relationships between Tg and Tm of polymer. The Crystallinity Polymers . Influence of molecular structure on mechanical, electrical, thermal and optical properties of polymers:

Unit V 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. F.W. Billmeyer, TextBook of Polymer Science, 3rd Edition, J.Wiley, 2003.

2. V. R. Gowariker, N.V. Viswanathan and J. Sreedhar, Polymer Science, New Age Int., 1986.

3 H.R. Alcock and F.W. Lamber, Contemporary Polymer Chemistry, Prentice Hall, 1981.

4. P.J. Flory, Principles of Polymer Chemistry, Cornell University press, New York, 1953.

5. G. Odian, Principles of Polymerization, 2nd Edition, John Wiley & Sons, New York, 1981.

6.Jean-Pierre Farges, Organic Conductors, Marcel Dekkar, 1994

7.David B Cotts, Z Reyes, Electrically Conductive Organic Polymers for Advanced Applications, William Andrew Inc,1987

8. Larry Rupprecht, Conductive Polymers and Plastics, William Andrew Inc, 1999.

9. Raymond B Seymour, New Concepts in Polymer Science, Polymeric Composites, VSP, 1990.

10. Wallace Gordon, Gordon G Wallace, Geoffrey M Spinks, Conductive Electroactive Polymers, CRC Press, 2002

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.

19UPCHE2 G09 COMPUTATIONAL CHEMISTRY

Hours	L	T	P	C
72	4	1	0	4

Course Objectives

1. To understand the fundamentals of quantum chemistry
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 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 fundamental aspects of quantum chemistry.	K2
CO2	Learn the fundamentals of computational chemistry and understand the different computational methods	K2 & K3
CO3	Understand the various computational analysis techniques	K2 & K3
CO4	Understand the application of QM and MM in various chemical systems	K2
CO5	Get in depth knowledge on application of computers in the structural elucidation of molecules	K2, K3

UNIT I Quantum Chemistry

Wave particle duality of matter – Louis de Broglie's theory. Heisenberg's uncertainty principle {principle of indeterminacy} – Formation of the New quantum mechanics - postulates

quantum mechanics – simple harmonic Motion (SHM) – Wave mechanics –Schrodinger's wave equation – particle in one dimensional box – particle in three dimensional box

UNIT II Methods of Computational Chemistry

Term "computational chemistry "– its benefits and applications, methods of computational Chemistry-molecular mechanics, semiempirical, ab initio and Density functional theory (DFT) methods, Post Hartree-Fock methods.

UNIT III Computational Analysis

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-IV Application of QM/MM in Chemical systems

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

UNIT V Applications to Chemical structures

Benzenoid and Non-Benzenoid Aromatic compounds:-Introduction - structure of Benzene – Valence bond theory (Resonance theory) – molecular orbital theory – concept of aromatic character (Aromaticity) – theoretical criteria for aromaticity anti aromaticity – aromaticity and nuclear magnetic resonance – Non – benzenoid aromatic compounds

References

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*

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.

19UPCHE2 G10 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.