

**DR. BABASAHEB AMBEDKAR MARATHWADA UNIVERSITY,
CHHATRAPATI SAMBHAJINAGAR.**



CIRCULAR NO.SU/M.Sc./Deptt./NEP/110/2024

It is hereby inform to all concerned that, the syllabi prepared by the Departmental Committee and recommended by the Dean, Faculty of Science & Technology, **Academic Council at its meeting held on 08 April 2024 has accepted the following Syllabi under the Faculty of Science & Technology as per National Education Policy-2020** run at the University Department, Dr.Babasaheb Ambedkar Marathwada University as appended herewith.

Sr.No.	Courses	Semester
1.	M.Sc.Physics	IIIrd & IVth semester
2.	M.Sc.Chemistry with Specializations Inorganic Chemistry, Organic Chemistry & Physical Chemistry.	IIIrd & IVth semester
3.	M.Sc.Zoology	IIIrd & IVth semester

This is effective from the Academic Year 2024-25 and onwards.

All concerned are requested to note the contents of this circular and bring the notice to the students, teachers and staff for their information and necessary action.

University Campus,
Aurangabad-431 004.
REF.NO.SU/2024/ 100-108
Date:- 01.06.2024

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*Deputy Registrar,
Academic Section*

Copy forwarded with compliments to :-

- 1] **Head of the Department, Department of Physics, Chemistry and Zoology Dr.Babasaheb Ambedkar Marathwada University,Chhatrapati Sambhajanagar.**
- 2] **The Director, University Network & Information Centre, UNIC, with a request to upload this Circular on University Website.**

Copy to :-

- 1] **The Director, Board of Examinations & Evaluation, Dr.Babasaheb Ambedkar Marathwada University, Chhatrapati Sambhajanagar.**
- 2] **The Section Officer,[B.Sc.Unit] Examination Branch, Dr.Babasaheb Ambedkar Marathwada University, Chhatrapati Sambhajanagar.**
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- 5] **The In-charge,[E-Suvidha Kendra], Rajarshi Shahu Maharaj Pariksha Bhavan, Dr.Babasaheb Ambedkar Marathwada University, Chhatrapati Sambhajanagar.**
- 6] **The Public Relation Officer, Dr.Babasaheb Ambedkar Marathwada University, Chhatrapati Sambhajanagar.**
- 7] **The Record Keeper, Dr.Babasaheb Ambedkar Marathwada University, Chhatrapati Sambhajanagar.**

**DR. BABASAHEB AMBEDKAR MARATHWADA UNIVERSITY,
CHHATRAPATI SAMBHAJINAGAR**



NAAC Re-accredited 'A' Grade
Department of Chemistry

FACULTY OF SCIENCE & TECHNOLOGY

**Two Years P.G. Programme in Chemistry
(M. Sc. Inorganic Chemistry Semester III&IV)**

As Per National Education Policy-2020

(To be implemented from Academic Year 2023-24)

**Course structure and Curriculum
(OBE with Choice Based Credit System)**

**Subject : Chemistry
Specilization : Inorganic Chemistry**

Effective from 2024-25

**Professor & Head
Department of Chemistry,
Dr. Babasaheb Ambedkar Marathwada University,
Chhatrapati Sambhajinagar - 431004.**

PREFACE

National Education policy 2020 has been intensely debated policies come into existence. In January, 2020 UGC has given the guideline for Learning outcome based curriculum framework (LOCF) work towards more holistic experience for the students. while focussing not just on knowledge delivery in higher education but also on the application of knowledge through field and laboratory work and emphasis on application of knowledge to real life experiences, LOCF is student-centric education in the context of development of personal, social, professional and acquired knowledge requirements in their career and life building, which focuses on measuring student performance through outcomes. It includes the knowledge, skills and attitudes enhancement in the students.

The aspects of LOCF is all-round development of the students, skill acquisition outside chosen subjects and research were undetermined but NEP has changed all of these in one stroke. The prominent features of the NEP framework are:

- Student centric education
- Flexibility in postgraduate programmes
- Multiple entry and exit points
- Skill based & outcome base education
- Credit based evaluation system
- Academic bank credits

It also focuses on evaluation of outcomes of the program by considering the knowledge, skill and behaviour of a students after completion of two year program. The educational triangle of Teaching-Learning and Evaluation process is the unique features of the OBE approach. The curriculum practices such as Competency based curriculum, Tailor-made curriculum development, spades, curriculum principles, Blooms Taxonomy and further use of assessment methodologies like, Norm-reference testing and Criterion reference testing, etc is being practiced since decades. It is also interesting to know that, globally, different countries and universities adopts the curriculum development models/approaches such as, CDIO (Conceive-Design-Implement-Operate), Evidence based education systems approach, etc as the scientific and systematic approaches in curriculum design.

Maharashtra state government and the authorities of Dr. Babasaheb Ambedkar Marathwada University, Chhatrapati Sambhajnagar has decided to implement National Education policies -2020 from the academic year 2023-24 for postgraduate program with outcome based education

As per guideline of OBE the department has prepared curriculum for Master of science in chemistry with specialization Inorganic chemistry, Organic Chemistry, Physical Chemistry and self-supported Analytical Chemistry. The OBE syllabus will help to improve the quality and employability of the Post-graduates of the university department.

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Professor & Head
Department of Chemistry
Dr. Babasaheb Ambedkar
Marathwada University,
Chhatrapati Sambhajnagar

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1. **Vision of Department :**

A respectable teaching- learning and research organization nationally and internationally in the area of chemical sciences by providing competitive trained chemists which will assist the chemical world, industries and stake holders.

2. **Mission Department :**

- To bring sustainable progress of society by nurturing chemistry with responsibilities
- To create and maintain programs of excellence in the areas of research , education and public outreach
- Department will produce students who are knowledge in chemistry and can think critically.
- To develop the researcher and scientist in chemical science through post-graduate education and research programme.
- To develop the competent manpower with technology based experimentation methodologies and value based practices for business and industries.
- To undertake projects to solve field base problems.
- To provide student centric learning facilities for the development of overall personality of learner.

3. **Eligibility Criteria :**

4. **Assessment and Evaluation :**

5. **Duration of Course Programme : Two years**

6. **Credit Allotted for two year master programme in chemistry :88 Credit**
Semester - I : 22

Semester -II : 22

Semester -III : 22

Semester -IV : 22

7. **Program Educational Objectives:**

The program educational objectives (PEO's) are the statement that describes the career and professional achievement after the program of studies (post-graduation). The PEO's are driven from the Mission statement (What is the purpose of organization). The PEO's can be minimum three and maximum five.

PEO1:To have advanced knowledge of chemistry domain.

PEO2:To provide the professional services to industry, Research organization and

institutes.

PEO3: To provide the professional consultancy and research support for the relevant organization in the domain of super specialization.

PEO4: To opt for higher education, disciplinary & multi-disciplinary research and to be a life-long learner.

PEO5: To provide, value based and ethical leadership in the professional and social life.

8. Program Outcomes:

The program outcomes (PO's) are the statement of competencies/ abilities. POs are the statement that describes the knowledge and the abilities the post-graduate will have by the end of program studies.

i). In-depth and detailed functional knowledge of the fundamental theoretical concepts and experimental methods of chemistry.

ii). Apply/implement interface between on the one hand, the history of chemistry and natural science and, on the other hand, issues pertaining to the areas of modern technology, health, and environment.

iii). Skills in planning and conducting advanced chemical experiments and applying structural-chemical characterization techniques.

iv). Skill in examining specific phenomena theoretically and/or experimentally.

v). Generation of new scientific insights or to the innovation of new applications of chemical research.

9. Course Program outcome

Course Program Outcomes are developed through the curriculum (curricular/co-curricular-extra-curricular activities). The program outcomes are attained through the course implementation. As an educator, one must know, **"To which POs his/her course is contributing?"** So that one can design the learning experiences, select teaching method and design the tool for assessment.

M.Sc. Inorganic Chemistry Semester-III Course Structure

Sr. No.	Course Code	Course Name	Teaching (Hr/W)	Credits Assigned	Conti.Int er.Assme n.	End. Sem Exam	Total Marks
Course type :DSC-Major Mandatory							
1.	ICHTC-600	Structural Elucidation by Spectral Methods	4	4	40	60	100
2.	ICHTC-601	Applied Inorganic Chemistry	4	4	40	60	100
3.	ICHTC-602	Chemistry of Material	2	2	20	30	50
4.	ICHLC-603	Inorganic Chemistry Laboratory Course	4	2	20	30	50
5.	ICHLC-604	Inorganic Chemistry Laboratory Course	4	2	20	30	50
Course type : DSE(Choose any two from pool of the course)							
6.	ICHTE -605	Bioinorganic Chemistry	2	2	20	30	50
7.	ICHTE -606	Supramolecular Chemistry	2	2	20	30	50
8.	ICHTE -607	Solid State Chemistry	2	2	20	30	50
9.	ICHTE -608	Environmental Chemistry	2	2	20	30	50
Course type :Research Project							
10.	ICHRP-649	Research Project -I	8	4	40	60	100
Total			32	22	220	330	550

Course code Nomenclature :

DSC-Discipline Specific Core ,**DSE**- Discipline Specific Elective, **T**-Theory, **L**- Laboratory course, **ICHTC**- Inorganic Chemistry Theory Core , **ICHLC**- Inorganic Chemistry Laboratory Core, **ICHTE**- Inorganic Chemistry Theory Elective , **ICHRP**- Inorganic Chemistry Research Project

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Course Name: Structural Elucidation by Spectral Methods Course Code: ICHTC-600
 Course type : DSC-15 4 Hrs/ Week
 Total contact hours : 60 Hrs Theory Credit: 4 Marks : 100

Course outcomes:

On completion of this course, the students will be able:

1. Describe the concept of structural elucidation.
2. Describe spectral methods.
3. Apply the knowledge of the chemistry of terpenes, alkaloids and steroids.
4. Implement structure elucidation of new compound natural or synthetic
5. To know about the Nuclear magnetic resonance spectroscopy. Proton chemical shift, spin-spin coupling, coupling constants and applications to organic structures ¹³C resonance spectroscopy
6. To learn the Mass, ESR, Mössbauerspectroscopy and its applications

Unit-I : Nuclear Magnetic Resonance Spectroscopy (¹H NMR) 12Hrs

Elementary ideas (Recapitulation); Spin-spin couplings, Different types of couplings, factors affecting on coupling constants, Karplus equation, Spin systems (AB, AX, ABX, AMX), Rate processes, spin decoupling, shift reagents, Nuclear Overhauser effect (NOE), INEPT and INADEQUATE.

Unit-II : ¹³C Nuclear Magnetic Resonance Spectroscopy 12Hrs

Elementary ideas, instrumental problems, chemical shifts (aliphatic, olefinic, alkyne, aromatic, heteroaromatic and carbonyl carbons); Effect of substituent's on chemical shifts.

Unit-III : Mass Spectroscopy 12Hrs

Introduction, ion production (EI, CI, FD and FAB), ion analysis, ion abundance, factors affecting on fragmentation, fragmentation of different functional groups, molecular ion peak, isotopic peaks, metastable peak, Nitrogen rule, McLafferty rearrangement, Retro-Diels-Alder reaction.

Unit-IV : 12Hrs

Problems based on joint applications of UV, IR, ¹H NMR, ¹³C NMR and Mass spectroscopy.

Unit- V : Mossbauer & ESR spectroscopy 12Hrs

Mossbauer spectroscopy: Principle, factors affecting the line position and shape, isomer effect and Quadrupole splitting iron salt like compounds, complexes, carbonyl compounds (temperature dependence of isomer shift

and Quadrupole splitting in simple compound and coordination, polynuclear complexes), Numericals.

Electron Spin Resonance Spectroscopy: Introduction, principle of ESR spectroscopy, presentation of spectrum, hyperfine splitting in various structures, hyperfine splitting diagram of representative examples, factors affecting the magnitude of 'g' values, Zero field splitting, Kramer's degeneracy, Anisotropy in the hyperfine coupling constant, electron delocalization, instrumentation and applications

References Books

1. Introduction to Spectroscopy: D. L. Pavia, G. M. Lampman, G. S. Kriz
2. Spectrometric Identification of Organic Compounds: R. M. Silverstein & F. X. Webster
3. ^{13}C NMR Spectroscopy: G. C. Levy, R. L. Lichter, G. L. Nelson
4. Spectroscopic Methods in Organic Chemistry: D. H. Williams & I. Fleming
5. Spectroscopy of Organic Compounds: V. M. Parikh
6. Mass Spectrometry: K. G. Das & James
7. Coordination Chemistry by Experimental Methods: K. Barger
8. Coordination Chemistry vol. 1: E. Martell
9. Physical Methods for Chemistry: R. S. Drago
10. Structural Methods in Inorganic Chemistry: E. A. V. Ebsworth & D. W. H. Rankin
11. Organic Structure Analysis: Philips Crews

Course Name: Applied Inorganic Chemistry

Course Code: ICHTC-601

Course type : DSC-16

4 Hrs/ Week

Total contact hours : 60 Hrs Theory Credit: 4

Marks : 100

Course outcomes:*On completion of this course, the students will be able:*

1. To understand the fundamental concepts of zeolites and their morphology, porous behaviour structures, catalytic active sites and selectivity.
2. To understand the various methods for synthesis of zeolite
3. To understand the factors affecting for the synthesis of zeolite
4. To understand the methods of modification of zeolite to improve reactivity of zeolite
5. To understand the application of different characterization techniques for identification of morphology, structure, active centres, acidity of zeolites.
6. To understand the catalytic applications of zeolites
7. To understand the catalyst and catalysis and their types.
8. To understand factors affecting performance of catalysts and role promoters and their types.
9. To understand the calculation of percent composition, selectivity, conversion and balancing input and output of chemical reactions,
10. To understand the principles of green chemistry, and concepts of atom economy and green metrics.

Unit-I : Unit –I: Basic concept of zeolites**12Hrs**

Introduction, definition, classifications on the basis of morphological appearance, SBU, substitution of other iso-electronic metal ions, types of pore size. Lowenstein's rule. pore and channels, channel dimensions, shape of the pore opening, nomenclature of zeolites, structural aspect of zeolites, acidity of zeolite, identification of acidic sites, nature of active sites, synergetic effects, shape selectivity.

Unit-II : Synthesis of zeolites**12Hrs**

General methods for synthesis of zeolite, hydrothermal treatment, mechanism of aluminosilicate formation during Sol-Gel, co-precipitation process, factors affecting the zeolite formation. Modification of zeolites, Oswald's rules of successive transformation, crystallization and its identification, factors affecting crystallization, template theory, organic additives, crystallizing zeolites, ZSM-5 from an organic free solvent

system, synthesis in nonaqueous solvents.

Unit-III : Characterization and applications of zeolite

12Hrs

General characterization techniques for analysis of zeolites, DetailsonFTIR, Pyridine adsorbed- IR analysis, XRD analysis, ^{27}Al MAS NMR and ^{29}Si MAS NMR analysis, Temperature programmed desorption (TPD), probe molecules for TPD analysis, NH_3 - TPD and CO_2 - TPD .Applications of zeolite. Zeolitecatalysed reactions, water softening .

Unit-IV : Fundamentals of catalysis

12Hrs

Catalysis, types of catalysis, catalyst, properties of catalyst, classification of catalysts, Sabtier's principle, classification of solid catalysis, fundamentals of heterogeneous catalysis, factor affecting the catalyst performance, promoters, types of promoters, Inhibitors, catalyst poisoning, overview on heterogeneously catalyzed process in industry.

Unit-V : Basic Chemical Calculations:

12Hrs

Moles, Mole fraction, percent composition, weight & volume percent analysis of solid in composition, Material balance involving chemical reaction: Introduction, material balances, Concept of Selectivity, Conversion, and numericals. Principle of green chemistry, Atom economy and green metrics, numerical.

References Books

1. Molecular sieves: Principles of synthesis and Identifications R-Szostak.
2. Atlas of zeolite framework type; Ch. Barlocher, W M. Meier, D. H. Olson; 5th rev. Ed. Elsevier Amsterdam 2001
3. Molecular Sieves Science and Technology vol I & II, H G Karge, J Weitkamp- Springer
4. Molecular Sieves Science and technology; H. G. Karge, J Weitkamp Vol I to V, Springer
5. Industrial catalyst- A Practical Approach, Jens Hygen, WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim, Germany
6. Stoichiometry- B.I. Bhatt & S.M. Vora.

Course Name: Chemistry of Materials

Course Code: ICHTC-602

Course type : DSC-17

2 Hrs/ Week

Total contact hours :30 Hrs Theory Credit: 2

Marks :50

Course outcomes:

On completion of this course, the students will be able:

1. To understand the fundamental concepts of nanomaterials.
2. To understand the various methods for synthesis of nanomaterials
3. To understand the colloidal solution and their interaction .
4. To design the experimental procedure for synthesis of metal and semiconductor nanomaterials.
5. To identify the structure, morphological appearance and particle size of nanomaterials by using spectroscopic, diffraction , microscopic techniques
6. To understand the different properties of nanomaterials
7. To understand the various applications of nanomaterials

Unit-I : General introduction & synthesis of nanomaterials by physical method 10Hrs

Objective of study, synthesis of nanoparticles by physical method, mechanical methods- high energy ball milling, melt mixing, method based on evaporation, physical vapour deposition with consolidation. Ionized cluster beam deposition. Laser vaporization, Laser pyrolysis, sputter deposition, electric arc deposition, Chemical Vapour Deposition (CVD).

Unit-II :Synthesisof nanomaterials by chemical methodand characterization of nanomaterials 10Hrs

Introduction, colloids and colloids in solution, interaction of colloids and medium, colloids in vacuum, colloids in medium, effect of charge on colloids, stearic repulsion, synthesis of colloids, growth of nanoparticles, synthesis of metal and semiconductor nanoparticles by colloidal route, Langmuir-Blodgett (L-B) method, sol gel method, electrochemical method.

Characterization techniques: Microscopes, Electron microscopes, SEM, TEM, Scanning probe microscope (SPM), Scanning Tunneling microscope, Atomic force microscope, X-ray diffraction, UV-visible and IR spectroscopy.

Unit-III :Properties, types and application of Nanomaterials

10Hrs

i).Properties of nanomaterials – Mechanical, electrical, optical, magnetic, semiconductor. ii).Some special nanomaterials – Carbon nanotubes, porous silicon, Arogels, Zeolites. iii). Application – Electronic, energy automobiles, sport and toys, textile, cosmetics, domestic appliances, biotechnology, medical, space, defence & environment.

References Books

1. Solid State Chemistry and applications- A.R. West (John Wiley and Sons)
2. Principles of the Solid State- H.V. Keer (Wiley Eastern Limited)
3. Nanotechnology: Principles and practices- Sulabha K. Kulkarni (capital Pub. Co.)
4. NANO- The next revolution –Mohan Surendra Rajan(National book Trust, India)
5. The British Glass Website- Types of Glass://www.britiglass.org.uk.
6. Fundamental of Nanotechnology – Gabor L. Hornyak, John J. Moore, Harry F. Tibbals, Joydeep Dutta.
7. Recent advances in the liquid phase synthesis of Inorganic Nanoparticles- B. L. Cushing
8. V. L. Kolesmichenko&C.J.O. Connor Chem. Review 104, 3893-3946.(2004)

Course Name: Inorganic Chemistry Laboratory Course

Course Code: ICHLC-603

Course type : DSC-18

4 Hrs/ Week

Total contact hours :60 Hrs Lab. Work Credit: 2

Marks : 50

Course outcomes:

On completion of this course, the students will be able:

1. To apply previous knowledge for performing experiment scientifically and safety.
2. To design and development of experimental procedure for the modification of zeolites for specific applications.
3. To understand the analysis of Lewis and Bronsted acidic sites by FTIR techniques.
4. To design the procedure for Pyridine adsorption on active center's of catalytic materials.
5. To synthesize the MgO-Zeolite supported catalyst for base catalyzed reaction.
6. To know the catalytic application of K10, and modified zeolite for synthesis of esters and other derivatives.
7. To utilize XRD software for morphological analysis of zeolite from given data.
8. To understand the synthesis and characterization of ZSM-5 and TS-1 zeolites.
9. To understand how the material is balanced in chemical reaction
10. To understand the separation and estimation metal ion by volumetric analysis .

List of experiments (Any 6)

1. Adsorption of pyridine on active centre of Aluminosilicate zeolite and its identification by FTIR technique.
2. Preparation of ZnO-beta zeolite and adsorption of pyridine for the identification of Lewis and Bronsted acidic site using FTIR technique.
3. Modification of Aluminosilicate zeolite by acid treatment to improve the acidic sites and its application as catalyst in condensation reaction
4. Modification of Aluminosilicate zeolite by Ammonium chloride treatment and its application as catalyst in condensation reaction.
5. Preparation of MgO -Zeolite catalyst and its utilization as catalyst in base catalysed reaction.
6. Modification of zeolite by acid treatment and its utilization as catalyst for the synthesis of esters.
7. Utilization of K10-Montmorillonite catalyst for conversion of diazoaminobenzene into para-aminoazobenzene
8. Utilization of K10-Montmorillonite catalyst for the synthesis of 7-hydroxy-4-methyl coumarin

9. X-ray diffraction analysis of zeolite from given data of zeolite .
10. Synthesis and characterizations of ZSM-5 zeolite by hydrothermal method .
11. Synthesis and characterizations of TS-1 zeolite by hydrothermal method .

Estimation (Any 2)

12. Separation and estimation of Zn(II) and Mg(II) from given mixture using Amberlite IRA 400 anion exchange resin
13. Determine the percentage of chlorine from bleaching powder using Volhard method.
14. Synthesis of magnesium oxalate from Magnesium chloride and Sodium oxalate and Estimation of amount of reacted and unreacted amount of magnesium chloride and sodium oxalate by volumetric method.

References Books

1. Monograph on Green Chemistry Laboratory Experiments, Green Chemistry Task Force Committee, DST
2. A Text book of Quantitative Inorganic Analysis- A. I. Vogel
3. Molecular sieves: Principles of synthesis and Identifications R-Szostak.
4. Molecular Sieves Science and technology ; H. G. Karge, J Weitkamp Vol I to V , Springer
5. Literature search on Internet

Semester : III

Course Name: Inorganic Chemistry Laboratory Course

Course Code: ICHLC-604

Course type : DSC-19

4 Hrs/ Week

Total contact hours :60 Hrs Lab. Work Credit: 2

Marks : 50

Course outcomes:

On completion of this course, the students will be able:

1. To apply previous knowledge for performing experiment scientifically and safety
2. To design experimental procedure for the synthesis and characterization of metal and metal oxide nanoparticles.
3. To understand the synthesis and interpretation of data obtained from spectral/ diffraction / microscopic techniques for nanoparticles.
4. To perform the chemical analysis by using Spectrophotometer, Conductometer, pH meter, Potentiometry.
5. To interpret the experimental results obtained by conductometer, spectrophotometer, pH meter
6. To know the principle of various instrumental techniques.
7. To understand the principles of the experiment performed in the laboratory.

List of experiments

Sr **Synthesis and characterizations of nanoparticles(Any 4)**

No

1. Synthesis and characterization of Cadmium sulphide nanoparticles.
2. Synthesis and characterization of Zinc oxide nanoparticles.
3. Synthesis and characterization of Iron oxide nanoparticles.
4. Synthesis and characterization of Nickel/ Nickel oxide nanoparticles.
5. Synthesis and characterization of Copper/ Copper oxide nanoparticles.
6. Synthesis and characterization of silver nanoparticles.

List of experiments(Any 4)

Potentiometrically :

7. Estimate the amount of copper and bismuth ions using EDTA photometric titration method

P^H metrically

8. Determine the Pk value of Glycine by using irri vaingRossotgiP^H metric technique

Conductometry

9. Analyze the mixture of copper sulphate, hydrochloric acid and acetic acid by conductometric method.

Potentiometry

10. Determine the redox potential of Fe(II)/Fe(III) system and number of electron involved in the system using $K_2Cr_2O_7$ by potentiometric method.

Application of P^Hmeter , conductometer, spectrophotometer for analysis various samples

11. Determination of P^H, Conductance, percent transmittance of Tap water, RO filter water, Industrial waste water, Bore well water and Rain water. Justify the observed results.
12. Measurement of percent transmittance of various glass samples and polymer samples using spectrophotometer.

References Books

1. Nanotechnology : Principles and Practices – Sulbha K Kulkarni
2. Systematic experimental physical chemistry – T. K. Chondhekar & S.W. Rajbhoj
3. Experiments in chemistry – D.V. Jahagirdar

Semester : III

Course Name: Bioinorganic Chemistry

Course Code: ICHTE-605

Course type : DSE-9

2 Hrs/ Week

Total contact hours : 30 Hrs Theory Credit: 2

Marks :50

Course outcomes:

On completion of this course, the students will be able:

1. To understand the different types of bio-molecules and peptides and their linkages
2. To describe the structural and functional relationships, mechanisms and importance of Iron containing enzymes and proteins.
3. To understand the biological importance of Copper & Zinc and its metabolism & structural and functional relationships and mechanisms .
4. To understand the structural features of Vitamin B₁₂ coenzymes.
5. To know the structures of Nucleic acid and binding sites in nitrogen bases
6. To understand the coordination complexes of nucleic acids and their bases with metal ions. Hydrogen bonding, redox reaction and hydrolytic reaction of nucleic acids .
7. To describe the Active and passive transport across the membrane ,
8. To describe the naturally occurring ionophore, antibiotics and its types and mechanism of ion transport
9. To explain the models of active transport of cations across the biological membrane, Na⁺-K⁺ pump, Calcium pump and its functions .

Unit-I :Metalloenzymes :

10Hrs

Biomolecules: Sugars, Organic acids, Amino acids and its types, peptides and peptide linkages, proteins and its structures. Enzymes, nitrogenous base, **Biochemistry of Iron and Iron metabolism:** Fe-containing proteins and enzymes and structural features of different Fe-proteins, Ribonucleotide reductase, and methane monooxygenase, Transport and storage in higher animals and lower organisms. **Cu-containing proteins and enzymes & metabolism:** Cu-containing proteins and enzymes and their structural features, super oxide dismutases, transport and storage of copper, microbial mining of copper. **Zn-containing enzymes,** chemistry behind nature's selection of Zn(II) in enzymatic activity, binding sites of Zn (II) in proteins – catalytic and structural sites. Similarities between Copper and Iron in Biological processes. **Vitamin B₁₂ and Coenzymes :** structural feature;

names of different forms; chemistry of cobalamin, biochemical functions of cobalamins, models of vitamin B₁₂ special characteristics of B₁₂ coenzyme.

Unit-II : Metal Nucleic Acid Interactions

10Hrs

Introduction, Nucleic acid structures, structures and binding sites in nitrogen bases, phosphates and sugar base. Coordination complexes of nucleic acids and their bases with metal ions. Hydrogen bonding, redox reaction and hydrolytic reaction of nucleic acids mechanisms of these reactions, natures role, pharmaceutical role, catalytic role

Unit-III : Transport Across the membrane

10Hrs

Active and passive transport across the membrane, Ion transport, Crown ether and cryptands, Naturally occurring ionophore, antibiotics and their types, mechanism of ion transport, valinomycin, nonactin, gramicidin, Models of active transport of cations across the biological membrane through the ionophores, Sodium-potassium pump and Na⁺-K⁺-ATP-ase and its active transport, nerve impulse, Na⁺ and K⁺ channels, Calcium pump and Ca⁺-ATP-ase,

References Books

- 1 Bioinorganic Chemistry - A. K. Das.
- 2 Principles of Bioinorganic chemistry - S. J Lippard & M. J. Berg
- 3 Inorganic Biochemistry, (Vol.I& II) - G. L. Eicchorh.
- 4 Bioinorganic Chemistry -Bertini Ivano, Gray H. B., Lippard S. J. & Valentine J. S.
- 5 Bioinorganic Chemistry - R. W. Hay.
- 6 Bioinorganic Chemistry - Chatwal G. R. & A. K. Bhagi.
- 7 Supramolecular Chemistry -Lehn J. M.
- 8 Bioinorganic & Supramolecular chemistry - Chatwal G. R. & A. K. Bhagi.
- 9 Bioinorganic, Bioorganic & Supramolecular chemistry-Kalasi P. S.
- 10 Supramolecular Organometallic Chemistry- J. L. Atwood and Jonathava W. steed, Macel Jekkar Publisher
- 11 SupramolecularOrganometallic Chemistry -Jean Marie-Lehn.
- 12 Elements of bioinorganic chemistry - G N Mukharji& Arvind Das

Course Name: Supramolecular Chemistry	Course Code: ICHTE-606
Course type : DSE-10	2 Hrs/ Week
Total contact hours : 30 Hrs Theory Credit: 2	Marks :50

Course outcomes:

On completion of this course, the students will be able:

- 1 To know the basic concepts & principle of supramolecular chemistry.
- 2 To describe the nature of non-covalent interactions on the basis of the formation of supramolecular compounds.
- 3 To understand the receptor, recognition & its types, Co-receptor.
- 4 To understand the reactivity of supramolecules.
- 5 To understand the catalysis by reactive anion receptor molecules, biomolecular and abiotic catalysis., cyclophane type receptors.
- 6 To understand the concept and application of supramolecular devices.

Unit-I : Basic concept of Supramolecular chemistry **10Hrs**

Basic concepts and principles of supramolecular chemistry, Definition, Supramolecular chemistry, Host-guest interactions Classifications, Receptors, Coordination and the Lock and Key Analogy Molecular recognition; Recognition, Information, Complementarity, Molecular Receptors - Design Principles, Spherical recognition- Cryptates of metal cations, Tetrahedral recognition by macrocyclic cryptands. Anion coordination chemistry and the recognition of anionic substrates. Co-receptor molecules and multiple recognition, Dinuclear and polynuclear metal ion Cryptates, Multiple recognition in metalloreceptors, supramolecular dynamics.

Unit-II : Supramolecular reactions and catalysis **10Hrs**

Supramolecular reactivity and catalysis: Catalysis by reactive macrocyclic cation receptor molecules, Catalysis by reactive anion receptor molecules, Catalysis with cyclophane type receptors, Supramolecular metal catalysis, Biomolecular and abiotic catalysis. **Transport process and carrier design :** Carrier mediated transport, Cation and Anion transport process, Coupled transport process. Electron, Proton, Light, coupled process.

Unit-III :Molecular and supramolecular devices **10Hrs**

Molecular recognition, information and signals. Semiochemistry, Supramolecular photochemistry - supramolecular photonic devices, Light conversation and energy transfer devices, Photo sensitive molecular devices,

Photoinduced electron transfer in photoactive devices, NLO properties of supramolecular species. Supramolecular electronic devices, electron conducting devices. Switchable molecular wires. ionic devices, Tubular mesophases, ion and molecular sensors.

References Books

1. Supramolecular Chemistry- concepts and Perspectives – Jean Marie- Lehn – Wiley- VCH
2. Bioinorganic & Supramolecular chemistry - Chatwal G. R. & A. K. Bhagi.
3. Bioinorganic, Bioorganic & Supramolecular chemistry Kalasi P. S.
4. Supramolecular organometallic chemistry J. L. Atwood and Jonathava W. steed, Macel Jekkar Publisher
5. SupramolecularOrganometallicchemistry -Jean Marie-Lehn.
6. Elements of bioinorganic chemistry - G N Mukharji& Arvind Das
7. Bioinorganic & Supramolecular chemistry - Chatwal G. R. & A. K. Bhagi.
8. Supramolecular Chemistry - Jonathan W. Steed, Jerry L. Atwood

Course Name: Solid State Chemistry

Course Code: ICHTE-607

Course type : DSE-11

2 Hrs/ Week

Total contact hours : 30 Hrs Theory Credit: 2

Marks : 50

Course outcomes:*On completion of this course, the students will be able:*

- 1 To understand the various types of defects present in solid
- 2 To understand the Nonstoichiometric defects in solids
- 3 To describe the different theories solid state materials.
- 4 To understand the conductor, semiconductor and superconductor materials.
- 5 To design and development of solid materials with pre-required properties based on the structure of solids.
- 6 To analyze the physical-chemical ,unique optical, electrical, magnetic, thermal, and mechanical properties of solids
- 7 Describe the preparation properties of glasses and ceramics

Unit-I :Imperfections in solids**10Hrs**

Perfect and imperfect crystals, point defects, stoichiometric defects, Schottky and Frenkel defects. Thermodynamics of their formation, colour centres. Nonstoichiometric defects, metal excess and metal deficiency defects. Line imperfections, edge dislocation and screw dislocations, Burgers circuits. Surface imperfections, grain boundaries and stacking faults.

Unit-II :Theories of solid state and electronic properties**10Hrs**

Free electron theory, Conduction by free electrons, Band theory, refinement to simple band theory, band structure of metals, insulators and semiconductors. Intrinsic and extrinsic semiconductors, semiconductor material and their fabrication. **Super conductivity:** conventional super conductors, organic super conductors(organic metals), fullerene, high temperature super conductors, organic charge transfer complexes, Applications

Unit-III :Properties of solid**10Hrs**

Optical properties: Luminescence and phosphors, lasers, photoconduction, photoelectric effects. **Magnetic Properties:**Behaviour of substances in a magnetic field, classification of magnetic materials, effect of temperature, magnetic domains and hysteresis. **Electrical properties:** Thermoelectric effects, Thomson effects, Peltier effect, Seebeck effect, thermocouples, Hall

Effect, Dielectric materials, Ferro, Pyro, Piezo electricity and their relations.
Applications.

References Books

1. Solid state chemistry and its applications – A. R. West (John Wiley and sons)
2. Principles of the solid state – H. V. Keer (Wiley Eastern Limited)
3. Material science and engineering – V. Raghavan (prentice hall of India)
4. Principles of electronics – V. K. Mehta (S. Chand and Co.)
5. Engineering Chemistry - P. C. Jain and M. Jain (Shanpat Rai and Sons)
6. Industrial chemistry – B. K. Sharma (Goel Publishing House)
7. The British Glass Website- Types of Glass: <http://www.britglass.org.uk>.

Course Name: Environmental Chemistry

Course Code: ICHTE-608

Course type : DSE-12

2 Hrs/ Week

Total contact hours : 30 Hrs Theory Credit: 2

Marks : 50

Course outcomes:*On completion of this course, the students will be able:*

- 1 To describe the air, water, pollution by diffract industry, pesticides , microorganism.
- 2 To demonstrate knowledge of chemical and biochemical principles of fundamental environmental processes in air, water, and soil.
- 3 To know e different types of toxic substances & responses and analyze toxicological information
- 4 To know how to control air ,water and pesticidal pollution.
- 5 To describe experimental methods for analysis of water and soil analysis and pollution awareness to society.
- 6 To describe the effect of toxic elements on environmental and biological systems.
- 7 Describe causes and effects of environmental pollution by energy industry and discuss some mitigation strategies
- 8 To know the various types of pesticides, , Insecticides and Herbicides and their effects on environment
- 9 To understand the decomposition of pesticides.

Unit-I : Air Pollution**10Hrs**

Polluted air, Types of pollution and units of measurements. Air quality standards, Sampling, Monitoring, Analysis of CO, Sources and sinks of CO pollution, Effects of CO on plants and humans, Control of CO pollution, Analysis of oxides of nitrogen, NO_x sources and sinks of NO_x pollution, Control of NO_x pollution, Hydrocarbons and photochemical smog and its control, Analysis of hydrocarbon in exhaust gasses, Petrol and air, Sulphur dioxide sources, Analysis and control, Acid rain particulates and their effects on human and climate, Control of particulates.

Unit-II : Water Pollution and Chemical toxicology**10Hrs**

Water Pollution: Aquatic environment, Water pollutants, Sampling of water and its preservation Trace metals in water, Chemical speciation with special reference to Copper, Lead, Mercury and Arsenic. Water quality standards Water quality parameters., pollution by Industrial waste water.

Chemical toxicology :Toxic chemicals in environment, Impact of toxic

chemicals on enzymes, Biochemical effects of Arsenic, Cadmium, Lead, Mercury, Carbon monoxide, Sulphur dioxide, Pesticides and Carcinogens.

Unit-III :Pesticides and Environmental pollution

10Hrs

Types of pesticides, , Insecticides and Herbicides . Effect of pesticides, Insecticides and Herbicides on environment , Physicochemical decomposition of pesticides, Insecticides and Herbicides by soil microorganism and other living organism .

References Books

1. Environmental Chemistry -A. K. De, , Wiley Eastern Ltd. New Delhi.
2. Analytical, Agricultural Chemistry -S. L. Chopra and J. S. Kanwar, , Kalyani Publishers, New Delhi.
3. Environmental chemistry-, V P Kudesia , Pragati prakashan , Meerut.
4. Chemical and biological methods for water pollution studies- R. K. Trivedy and P. K. God, Environmental publications, co. New Delhi.
5. , Diagnosis and improvement of saline and alkali soils- L. A. Richards. Oxford IBH publications co. New Delhi.
6. Environmental Chemistry- S. M. Khopkar
7. Environmental chemical analysis- M. S. Creos and Morr, American publications.
8. Standard methods of water and waste water analysis, American public health association – D. C. Washington
9. Environmental chemistry laboratory manual - R. Gopalan and Amrutha Anand
10. Standards for water for drinking and other purposes, Bureau of Indian Standards India.
11. Guideline for drinking water quality recommendations of world health organization, Geneva.
12. Environmental Chemistry- B. K. Sharma and H. Kaur,

Course Name: Research project-1

Course Code: ICHTE-608

Course type : Research project

8 Hrs/ Week

Total contact hours : 120 Hrs

Theory Credit: 4

Marks : 100

Course outcomes:

On completion of this course, the students will be able:

- 1 To know , how to search literature review on proposed topic
- 2 To able to design research oriented project on particular context
- 3 To able to conduct experiment scientifically with safety
- 4 To characterize the prepared material by using microscopic, spectroscopic, diffraction, adsorption and thermal techniques
- 5 To know the research paper publishing agencies, Impact factor of Journals, Citations etc.
- 6 To develop handling of computer based software such as MS word, Power point presentation, EXCEL, Chem office, XRD analysis Software's etc.
- 7 To demonstrate dissertation writing, communication and presentation skill
- 8 To interpret observed data of samples scientifically
- 9 To know the Project writing framework (Introduction, Experimental, Results, Discussion, Conclusion & References)

Examination: Power point presentation at the time of term end of examination

Tentative topics:

1. Transition/ non-transition metal complexes
2. Application of heterogeneous catalysts
3. Application of metal salts catalyzed reaction
4. Catalytic applications of metal oxide/ mixed metal oxides
5. Agriculture waste biomass transformation into value added product
6. Metal organic framework
7. Utilization of computational software for theoretical studies of chemical compounds
8. Application of Inorganic nano materials for biological & catalytic applications
9. Comparative studies metal salts and their oxides by FTIR technique
10. Watersamples analysis of various places
11. Soil analysis for special application
12. Design & development of ligands for spot test of metal ions

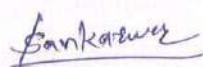
13. Preparation and applications of activated carbons from waste biomass
14. Preparation & application of ionic liquids
15. Isolation of value added product from Agricultural plants / fruit waste / pulp
16. Extraction of oil from specific types of plants
17. Utilization of fly ash
18. Design & development of micro reactor for chemical reactions
19. Preparation & application supported catalyst
20. Photosensitizer molecules
21. Preparation of photo reactive metal oxides & their application for degradation organic pollutant
22. Solvent extraction

M. Sc. Inorganic Chemistry Semester- IV

Sr. No.	Course Code	Course Name	Teaching (Hr/W)	Credits Assigned	Conti.I nter.As smen.	End. Sem Exam	Total Marks
Course type :DSC-Major Mandatory							
1.	ICHTC-650	Organotransition Metal Chemistry	4	4	40	60	100
2.	ICHTC-651	Photoinorganic Chemistry	4	4	40	60	100
3.	ICHTC-652	Nuclear Chemistry	2	2	20	30	50
4.	ICHLC-653	Inorganic Chemistry Laboratory Course	4	2	20	30	50
Course type : DSE(Choose any two from pool of the course)							
5.	ICHTE -654	Therapeutic Bioinorganic and Chemistry of Forensic materials	2	2	20	30	50
6.	ICHTE -655	Analysis of Oils , Fertilizer and Ores	2	2	20	30	50
7.	ICHTE -656	Inorganic Chemistry -III	2	2	20	30	50
8.	ICHTE -657	Technology to Converting Agriculture Waste Biomass in to Energy	2	2	20	30	50
Course type :Research Project							
9.	ICHRP-699	Research Project -2	12	6	60	90	150
Total			32	22	220	330	550

Course code Nomenclature :

DSC-Discipline Specific Core DSE- Discipline Specific Elective, T-Theory, L- Laboratory course, ICHTC- Inorganic Chemistry Theory Core , ICHLC- Inorganic Chemistry Laboratory Core , ICHTE- Inorganic Chemistry Theory Elective , ICHRP- Inorganic Chemistry Research Project


Professor & Head
 Department of Chemistry,
 Dr. Babasaheb Ambedkar Marathwada University,
 Chhatrapati Sambhajnagar - 431004.

Course Name: Organotransition Metal Chemistry

Course Code: ICHTC-650

Course type : DSC-20

4 Hrs/ Week

Total contact hours : 60 Hrs Theory Credit: 4

Marks : 100

Course outcomes:*On completion of this course, the students will be able:*

1. To describe the structure and bonding aspects of simple organometallic compounds
2. To apply different electron counting rules to predict the shape/geometry of organotransition metal compound
3. To understand the methods of synthesis , properties of mono, di, tri, tetra, penta and hexahapto organ transition metal compound.
4. To describe the steps of organotransition metal complex catalyzed reaction for value added chemicals.
5. Identify the different types of organotransition metal complexes catalyzed reactions and apply the above concepts to explain different catalytic reactions

Unit-I : General Properties of Organotransition Metal Compounds**12Hrs**

Definition, Classification based on the number of coordinated carbon (Hapticity), number of electrons donated by ligands, and type of bonding. Nomenclature, 16, 17, 18 Electron complexes and ligand substitutions, electron counting for common ligands and geometry of organo transition metal compounds.

Unit-II : Alkyl, aryl Carbene and carbene transition metal compounds**12Hrs**

General method of synthesis of alkyl and aryl transition metal compounds, (i.e Ti, V, W, Mn, Ir, Co, Fe), Chemical properties, stability and decomposition pathways. **Carbene transition compounds:** Types of carbene compounds, properties of carbene ligands, Synthesis of Fischer type carbene compounds, Chemical reaction on coordinated carbene compounds. **Carbyne transition metal compounds :** Synthesis and chemical properties

Unit-III : Transition metal compounds with Unsaturated organic molecules**12Hrs**

η^2 -Alkene transition metal compounds : General methods of the synthesis, Chemical properties: Reaction with nucleophiles and Electrophiles, Structure and bonding (DCD model) **η^2 -alkyne transition metal compounds:** Introductions, preparation, chemical properties, Structure and bonding. **η^3 -allyl transition metal compounds:** Introduction, Structural verities in allyl transition metal compounds, General methods of preparation, chemical

properties, structure and bonding. η^4 -butadiene transition metal compounds: Introduction, General methods of preparation, reaction on coordinated ligand, structure and bonding. η^4 -Cyclobutadiene transition metal compounds: Preparation and chemical properties of $(C_4H_4)Fe(CO)_3$, structure and bonding. η^5 -Cyclopentadienyl transition metal compounds: Introduction, classification of η^5 -Cyclopentadienyl derivatives, Preparation and chemical properties of $(\eta^5-C_5H_5)_2Mn$, $(\eta^5-C_5H_5)Mn(CO)_3$, structure and bonding in Ferrocene.

Unit-IV : Organotransition metal compound as catalysts and synthetic reagents

12Hrs

Activation process: consequent changes in the coordinated ligand reactivity template effect. **Protection:** Steric control, facilitation of nucleophilic addition reactions. **Product isolation:** Reductive elimination, β -eliminations, radical formation, alkene or arene displacement by competing ligand, electron transfer from metal atom to an oxidant, release of carbenoid ligands.

Unit- V : Catalytic processes involving organotransition metal compound

12Hrs

Hydrogenation of alkene using Wilkinson's catalysts, hydrosilation reaction, hydroformylation of alkene (oxo process) Ziegler Natta polymerizations. Fischer Tropsch process, water gas shift reaction. Monsanto process for acetic acid synthesis., Wacker process of oxidation of alkene.

References Books

1. Organo metallic Chemistry, R. C. Mehrotra, & A. Singh
2. Principal and applications of organotransition metal Chemistry, J. P. Collman, L. S. Hegeudus, J. R. Norton
3. Inorganic Chemistry, Attkin and Shriver
4. Advanced Inorganic Chemistry, Gurdeep Raj.
5. Inorganic Chemistry, J. E. Huhey

Course Name: Photoinorganic Chemistry

Course Code: ICHTC-651

Course type : DSC-21

4 Hrs/ Week

Total contact hours : 60 Hrs

Theory Credit: 4 Marks : 100

Course outcomes:*On completion of this course, the students will be able:*

1. To describe the Laws of photochemistry, life time measurement of quantum yields of inorganic compounds
2. To understand the physical properties of electronic excited states and photophysical processes
3. To identify the photoreactive excited states, charge transfer excitation in transition metal complexes and its MOED and photoredox models.
4. To describe the photochemical properties the selected transition metal complexes and its various photochemical reaction
5. To understand the concept and role of sensitizer molecule and photosensitized reaction
6. To describe the fundamentals of solid inorganic materials and their photoreactivity and applications.

Unit-I : Basic concept of Photo Chemistry**12Hrs**

Introduction to photochemistry, laws of photochemistry, Quantum yield, deviation in quantum yield, Experimental determination of quantum yield, Quantum yield and reactivity, life time of electronically excited state, kinetic aspects of photochemical reactions, temperature dependence of photochemical reaction, Methods used to study the kinetics of photochemical reaction: Flow methods, flash photolysis methods, numerical on quantum yield calculations.

Unit-II : Physical properties of electronically excited molecules**12Hrs**

Nature of changes on electronic excitation, potential energy diagram, shapes of absorption bands and Franck-Condon principle, emission spectra, environmental effect on absorption and emission spectra. **Photo physical process in electronically excited molecule:** Types of physical pathways, Jablonski diagram, theory of radiationless transition, theory of radiative process, bimolecular quenching, experimental results

Unit-III :Excited States of Metal Complexes**12Hrs**

Spectroscopic states of d^1 to d^{10} configurations, Ligand field excited states of Co(II), Cr(III), Ru(II), Ru(III), Fe(II) and Rh(III) in an octahedral complexes. Excited states of organic ligand, Selection rules for electronic transitions. **Charge transfer photochemistry** :Introduction, charge transfer absorption spectra, types of charge transfer excitations and their energy level. Types of reactions observed by CTM, Models of photoredox system.

Unit-IV : Ligand field photo chemistry of transition metal complexes**12Hrs**

Photochemistry Cr(III) of complexes : properties of ligand field excited states, Photo-substitutions reaction ,Photo aquation reactions, photolysis rule , photoisomerization , photo racemization, photoanation reactions, photo reactive excited state, doublet hypothesis, role of quartet excited states. Sensitizer, mechanism of photo sensitization, photosensitized aquation reaction. Photochemistry of Co(III) complexes : Energy level diagram, Photoaquations in Co(III) amine, Co(III) cyanide complexes. Photochemistry of Fe(II) low spin complexes, Ru(II) amine derivative complexes, Photo redox properties of (Ru(III) complexes.

Unit- V : Photochemical reactions on solid surface**12Hrs**

Photo catalysis, photoreactive oxide materials, relation between band gap & energy, wavelength, photo electron transfer mechanism, energy level diagram of solid acceptor and donor levels. Supported photo catalyst: Types of support & need : Semiconductor supported metal oxides for Photolysis of water. Decomposition of organic pollutants, experimental setup and photo degradation end product of organic moieties.

References Books

1. Concepts of Inorganic Photo chemistry, W. Adamson
2. Photochemistry of Coordination Compound – V. Balzani and Carassiti ,AcademicPress London & New York
3. Inorganic spectroscopy - A. B. P. Lever
4. Inorganic Chemistry- J. E. Huhey
5. Fundamental of Photochemistry- Rohatgi Mukherjee
6. Charge Transfer Excitation of Coordination compounds. Generation of reactive intermediate – A Vogler and H Kunkely
7. Metal complex Sensitizers in dye sensitized solar cells, Coord. Chem .Review , Andre Sarto Polo et al , 238, 1343-1361, 2004

8. Metal centered ligand field excited state : Their roles in the design & performance of transition metal based photochemical molecular device , Paul S Wagenkecht and Peter C Ford , Coord. Chem. Review, 255, 591, **2011**.
9. D. Chatterjee , Visible light induced photo degradation of organic pollutants on dye Adsorbed TiO₂ surface : Bull. Cat. Soc. India 2,,56-58, **2004**

Course Name: Nuclear Chemistry

Course Code: ICHTE-652

Course type : DSC-22

2 Hrs/ Week

Total contact hours : 30 Hrs Theory Credit: 2

Marks : 50

Course outcomes:*On completion of this course, the students will be able:*

1. To understand the fundamental nuclear particles , nuclear structure, stable and unstable atomic nuclei, nuclear reactions.
2. To Illustrate different type's nuclear models and their features.
3. To describe the Nuclear Reactions and their energies .
4. To understand the features of nuclear model
5. To understand the characteristics of alpha, beta and gama rays .
6. To know the different applications of radioactive isotopes.

Unit-I :Nuclear particles and its properties**10Hrs**

The fundamental particles, roll call of elementary particles, composition of the nucleus, theories of nuclear composition, nuclear properties, mass defect and binding energy, nuclear stability explained by different factors. Nuclear size and density, mechanical effects due to orbiting and spinning of nucleons, orbital angular momentum of the nucleons, Total angular momentum of the nucleons, magnetic quantum numbers, principal and radial quantum numbers, total angular momentum of nucleus

Unit-II :Nuclear models**10Hrs**

The shell model and its salient features, periodicity in nuclear properties- magic numbers, forces of nuclear potential, energy level in nuclear potential well, the sequence of filling the orbital including models, nuclear configuration. The liquid drop model, and its details and The Fermi gas model.

Unit-III :Radioactivity and its application**10Hrs**

Historical background, Natural radioactive elements, general characteristics of α , β and γ rays, detection and measurement of radioactivity, Theory of radioactive disintegration, decay kinetics, units of radioactivity, parent daughter growth relationship , secular and transit equilibrium , theory of α decay , β decay , energy of β decay numericals . Application of radioisotopes as tracer, chemical investigation, Physiochemical research, Analytical application , Agriculture applications. Industrial applications,

Radioisotopes as a source of electricity

References Books

1. Source of Atomic energy by S.Glasstance, D. Van Nostrand co. INC
2. Essentials of nuclear chemistry by H.J. Arnikar 4thEdn, New Age International(p) Ltd.
3. Introduction to Nuclear By chemistry B. G. Harvey,
4. Nuclear chemistry by M. G. Arora & M. Singh Anmol pub., New Delhi
5. Elements of nuclear chemistry by A. K. Srivastav, P. C. Jain, S. Chand & Co.
6. A text book of Nuclear chemistry by C.V. Shekar Deminant publication & distribution, New Delhi.
7. Radiochemistry & nuclear chemistry, 3rdedn G. chappin, Butterwerth-Heinemann

Course Name: Inorganic Chemistry Laboratory Course

Course Code: ICHLC-653

Course type : DSC-23

4 Hrs/ Week

Total contact hours :60 Hrs Lab. Work Credit: 2

Marks : 50

Course outcomes:*On completion of this course, the students will be able:*

1. To design experimental procedure for the synthesis and spectral analysis of metal complexes .
2. To understand the composition of various alloys and estimation of % metal ions .
3. To understand importance of accuracy and precision in measurement of chemical analysis
4. To understand importance of laboratory skills, precaution, accuracy and precision.
5. To know how to prepare activated carbon and their application
6. To design the procedure for the synthesis of ferrocene as organometallic compound

List of experiments**Synthesis and Spectral / thermal analysis metal complexes. (Any 5)**

- 1 Tris (thiourea) Copper(II) Sulphate
- 2 Bis (thiourea) Zinc (II) sulphate
- 3 $\text{NH}_4[(\text{Cr}(\text{III})(\text{C}_2\text{O}_4)_3]$
- 4 [Copper (II) (Acetyl acetone)₂]
- 5 $[\text{Cu}(\text{NH}_3)_4]\text{SO}_4 \cdot \text{H}_2\text{O}$
- 6 $[\text{Co}(\text{NH}_3)_4\text{CO}_3]\text{NO}_3$
- 7 $\text{K}_3[\text{Cr}(\text{CNS})_6] \cdot 4\text{H}_2\text{O}$
- 8 $\text{K}_3[\text{Cr}(\text{C}_2\text{O}_4)_3]$
- 9 $[\text{Cr}(\text{urea})_6]\text{Cl}_2 \cdot 3\text{H}_2\text{O}$
- 10 Synthesis and characterization of Ferrocene
- 11 Preparation of activated carbon from agriculture waste biomass and their application.

Alloy analysis (Any 3)

- 12 Solder alloy analysis
- 13 Brass alloy analysis
- 14 Bronze alloy analysis
- 15 Copper nickel alloy

References Books

1. Practical Inorganic Chemistry- Pass Geoffrey and Haydn Sutcliffe
2. A Text book of Quantitative Inorganic Analysis- A. I. Vogel
3. Advanced Practical Inorganic Chemistry- Gurudeep Raj

Course Name: Therapeutic Bioinorganic and
Chemistry of Forensic Materials

Course Code: ICHTE-654

Course type : DSE-13

2 Hrs/ Week

Total contact hours : 30 Hrs Theory Credit: 2

Marks : 50

Course outcomes::

On completion of this course, the students will be able:

1. To understand the Biochemical aspects of cancer, carcinogens and anticancer agents.
2. To illustrate the role of Pt(II) and Pt (IV) complex as anticancer agents.
3. To understand the anticancer activity of Rhodium Gold, Copper, and Cobalt complexes in biological system.
4. To understand the Antibacterial, antifungal and antiviral activity of metal complexes.
5. To explain the applications of inorganic materials in toxicology
6. To illustrate the antidots for poisons
7. To describe the metal ion toxicity of Pb(II), Cd(II), and Hg(II) in human and animals
8. To explain the role of chelation theory in detoxification caused due to metals and metal ions in diagnosis.

Unit-I : Metal ions in carcinogenesis

10Hrs

Biochemical aspects of cancer, carcinogens and anticancer agents. Carcinogenesis and its mechanism. Role of metal complexes of Pt(II) and (IV) as anticancer agents. Anticancer activity of Rhodium, Gold, Copper, and Cobalt complexes. Selenium and its biochemical role and its mechanism of cacinostatic actions. Examples of metallodrugs containing arsenic, antimony, gold, mercury and tin metal. Antibacterial, antifungal and antiviral activity of metal complexes.

Unit-II : Chemistry of Forensic Materials

10Hrs

Forensic toxicology, Definition of poison and toxicology, human and cattle poison, and its antidotes. Principle underlying removal of poison from the body and use of antidotes. Corrosive poison and its classification. Common household poisons. Characteristic sign, symptoms, treatment and medicolegal aspects of common household poisons, classifications of poisons according to their mode of action.

Unit-III :Metal ion toxicity, Interactions of metal ions and metal complexes and 10Hrs

Metals in medicine

Metal ion toxicity :Metal ion toxicity in man and animals. general aspects of Pb(II), Cd(II), and Hg(II), biochemical and physiological effects caused due to Pb(II), Cd(II), and Hg(II) ion toxicity. Detoxifications of this metals using chelating agents.**Interactions of metal ions and metal complexes** : :Structure and functions of amino acids, proteins, peptides, enzymes nucleoside, nucleotide and its comparative study. Metal ion binding sites present in amino acids, peptides, proteins, enzymes, nucleoside and nucleotide. **Metals in medicine** :Chelation therapy, Limitation of chelation therapy in metal ion detoxification , Zinc salt in the treatment of sickle cell anaemia. Lithium therapy in psychiatric mind disorder.

References Books

1. Pharmacological basis of therapeutic, 5th& 6thEdn.–Louis S. Goodman, (Macmillan Publishing companyNC, New York, Toronto and London)
2. Inorganic biochemistry-Guther L. Eicchor, Voll&2 (Elsevier, London New York.
3. Metal ions in biological system - Helmut Sigel. Vol. 19 21, 22 - (Marcel Dekker INC, New York and Basel)
4. Metal ions in biological system :Concepts on metal ion toxicity - Helmut Sigel. Vol.7- (Marcel Dekker INC, New York and Basel)
5. Parikh's Textbook of Medical Jurisprudence, Forensic Medicine and Toxicology (Six Edition) By C. K. Prikh. (CBS Publishers New Delhi)
6. Bioinstrumentations – L Veerakumari , MJP publisher Chennai
7. Principles of bioinorganic chemistry – S. J Lippard & J M Berg , Mill Valley California
8. Elements of Bioinorganic - G N Mukherjii, and Arbinda Das U N Dhur and Sons Pvt. Ltd Kolkatta

Course Name: Analysis of Oils , Fertilizer and Ores

Course Code: ICHTE-655

Course type : DSE-14

2 Hrs/ Week

Total contact hours : 30 Hrs

Theory Credit: 2

Marks : 50

Course outcomes:*On completion of this course, the students will be able:*

1. To understand the basic concepts and composition of oils ,fats soap and detergent ,its analysis
2. To understand the composition, types and methods of analysis methods of fertilizers.
3. To know the chemical composition of superphosphate, Lime and Potash fertilizer.
4. To know the Legislation and recent amendments with respect to pesticides materials.
5. To identify the composition and method of analysis of ores and alloys.

Unit-I :Analysis of Oils, Fats Soap and Detergents**10Hrs**

Introduction to natural oils and fats, Analysis of oils and fats, Softing point, Congent point, Titer point, Cloud point, Iodine, Saponification, acid, Hydroxyl,R-M and polenske values, Elaiden test. General concepts on soaps, Analysis of soaps, for saponification, Unsaponifiable and saponified matter in soaps, Estimation of free alkali and phenol in soap, Classification of detergents (in Brief), Analysis of active ingredients from detergents , Estimation of CMC, Chlorides, Total phosphates

Unit-II : Analysis of fertilizers and pesticides**10Hrs**

Analysis of fertilizers. Classification of fertilizer, NPK value, Chemical composition of superphosphate, Lime and Potash fertilizer, Analysis of commercially available fertilizers for N, P & K. **Analysis of pesticides.** :Legislation and recent amendments with respect to pesticides materials. Names of pesticides and their chemical structures. , Application dosage of different pesticides. , Analysis of specific pesticides.

Analysis of Ores and Alloys**10Hrs**

Analysis of ores :Composition and analysis of Dolomite, Bauxite, Ilmenite, Zinc blend, hematite, pyrolusite and calcite for their major constituents using one of the standard methods of analysis. **Analysis of alloys :** Composition, Properties, uses and analysis of : Brass, Bronze Solder, Stainless Steel, Monel-metal, gun-metal, Silver coin for their major constituents using one of the standard methods of analysis

References Books

1. Chemical analysis of food -Pearson.
2. Introductions to food science and technology, series by G.F.Stewart and M.A.Amerine
3. Food analysis -Nielson.
4. Food additives - S.N.Mahindry (APH) publication
5. Analytical chemistry of foods (C.S.James) Blackie Academic and professional
6. Food Analysis principles and techniques D.W.Gruenwedel, J.R.Whitaker, MercelDekker
7. Food analysis Theory and practice Y.pomeranz and C.E.Meloan,Chapman and Hill
8. Food Analysis ,2ndEdn. S.S Nelsen, Aspen publishers
9. Food analysis - A. G. Woodman, McGraw Hill
10. Chemical analysis of food By Pearson.
11. Introductions to food science and technology, series by G.F.Stewart and M.A.Amerine Academic process.
12. Applied chemistry .AText book for Engineers and technologists by H.D.Gesser.
13. A Text book of Quantitative Inorganic Analysis; A. I. Vogel

Course Name: Inorganic Chemistry -III

Course Code: ICHTE-656

Course type : DSE-15

2 Hrs/ Week

Total contact hours :30 Hrs Theory Credit: 2

Marks :50

Course outcomes:*On completion of this course, the students will be able:*

1. To understand various types of interaction between same and different molecules in solution phase and their examples and structure .
2. To understand the hydrogen bonding interaction organic compounds
3. To know the concept of polar and nonpolar solvent and factors responsible for polarity of solvent .
4. To understand the role of polar and nonpolar solvent in chemical reaction.
5. To describe the Synthesis, structure , nature of bonding and properties of Borazines, phosphazenes, Sulfur- nitrogen, Xenon compounds
6. To understand the structural aspect of oxy acid of phosphorous, sulphur, nitrogen and halogens
7. To understand the theoretical concept of different types of hybridizations
8. To draw the MOT diagram of any molecules .

Unit-I : Unit-IV: Chemical forces and its importance

10Hrs

Types of chemical forces, covalent bonding, ionic bonding, dipole-dipole interaction, induced dipole interactions, dipole-induced dipole interactions, with suitable examples, interpretation of hydrogen bonding interactions in common organic compounds , solubility of ionic substances, ion solvent interactions with examples, Polarity of solvent, factors affecting the polarity of solvents, importance of polar and non polar solvent in chemical reactions.

Unit-II :Chemistry of main group elements

10Hrs

Synthesis, structure and properties of Borazines, Phosphazenes and their polymers, Heterocyclic inorganic systems, Sulfur- nitrogen chain and ring compounds, Xenon compounds, interhalogens compounds, Structural aspect of oxy acid of phosphorous, Sulfur, nitrogen and halogens.

Unit-III : Valence bond model

10Hrs

Theoretical concept of hybridization, construction of wave functions for sp , sp^2 , sp^3 , dsp^2 and d^2sp^3 hybridizations. Identification of nature of bonds in molecules/ complex. Applications. Construction of molecular orbital energy level diagram of H_2O , NH_3 , BF_3 , octahedral and tetrahedral molecules

References Books

1. Inorganic Chemistry - J E Huhey
2. Concept and models of Inorganic chemistry – Bodil E Douglas and Darl H McDaniel, Oxford & IBH Pub. Co.
3. Inorganic chemistry- Gary L Miessler, Donald A Tarr 3rdEdn
4. Inorganic chemistry – Puri and Shrma
5. Inorganic chemistry – J D Lee
6. Inorganic chemistry- Attken
7. Quantum chemistry and spectroscopy- Engel
8. Physical chemistry - A molecular approach – Donald A Mc Quarrie , John D Simon

Course Name: Technology for Converting Agriculture waste Biomass into Energy Course Code: ICHTE-658

Course type : DSE-16

2 Hrs/ Week

Total contact hours : 30 Hrs Theory Credit: 2

Marks : 50

Course outcomes:

On completion of this course, the students will be able:

1. To understand the how to convert agriculture waste into useful materials
2. Describe the fundamentals of biomass, types , sources and their value added products
3. To understand the process of conversion of agriculture waste biomass
4. To know the process of conversion of agriculture waste biomass into activated carbon and their various application
5. To understand the production chemicals form agriculture waste
6. To know the production process of biodiesel

Unit-I : Sources of Biomass &Physical conversion of biomass 10Hrs

Biomass, classification of biomass, characteristics of biomass, composition of biomass, Properties of Biomass, Classification of Conversion Technologies. Waste agricultural biomass, Types and composition, moisture content, energy content.; Sizing separation, drying ,dewatering, densification technologies .torrefaction,. thermo chemical conversion of biomass, combustion, stages of combustion.

Unit-II : Activated carbon from agriculture waste 10Hrs

Sources of agriculture waste, Preparation of activated carbon, process, types of charcoal Kiln, factors influencing charcoal yield, surface area, BET Analysis, pore size, characterization and application of activated carbons, Gas-Phase applications, liquid-Phase applications, Treatment of textile effluents, textile dyes, classification of textile colorants.

Unit-III :Production of chemicals form agriculture waste biomass 10Hrs

Ethanol production process : Ethanol production by fermentation, sugar fermentation, starch fermentation, enzymatic hydrolysis, acid hydrolysis, factors that influence the ethanol fermentation.**Biodiesel from agriculture waste**:Production process, transesterification reaction, types of esterification, catalysts for biodiesel Production, catalytic transesterification, acid catalyzed transesterification.

References Books

1. Technologies for converting waste agricultural biomass to energy- UNEP
2. Biodiesel Production Technology – J. Van Gerpen

Course Name: Research project-2

Course Code: ICHRP-699

Course type : Research project

12 Hrs/ Week

Total contact hours :180 Hrs

Theory Credit: 6

Marks :150

Course outcomes:

On completion of this course, the students will be able:

- 1 To able to design research oriented project on particular context
- 2 To know how to search literature on selected research oriented project work
- 3 To know the recent advances in current research
- 4 To able to conduct experiment scientifically with safety
- 5 To characterize the prepared material by using microscopic, spectroscopic, diffraction, adsorption and thermal techniques.
- 6 To develop the skill to write dissertation , communication skill in presentation
- 7 To know the research paper publishing agencies, Impact factor of Journals, Citations etc.
- 8 To develop handling of computer based software such as MS word, Power point presentation, EXCEL, Chem office, XRD analysis Software's etc.
- 9 To demonstrate dissertation writing, communication and presentation skill
- 10 To interpret observed data scientifically
- 11 To know the Project writing framework (Introduction, Experimental, Results, Discussion, Conclusion & References)

Tentative topic

1. Transition/ non-transition metal complexes
2. Application of heterogeneous catalysts – Zeolite, MOF, Mixed metal oxides, Hydrotalcite, Metal / metal oxide supported catalyst,
3. Application of metal salts catalyzed reactions
4. Green catalyst for organic functional group transformations.
5. Agriculture waste biomass transformation into value added product
6. Application of computational software in chemistry
7. Application of Inorganic nano materials for biological & catalytic applications
8. Design & development of sensor for metal ions.
9. Conducting polymers
10. Synthesis & application of ionic liquids
11. Isolation of value added product from Agricultural plants / fruit waste / pulp
12. Isolation of magnetic material from fly ash and its use as catalyst
13. Design & development of micro reactor for chemical reactions
14. Synthesis of organic photosensitizer molecules

**DR. BABASAHEB AMBEDKAR MARATHWADA UNIVERSITY,
CHHATRAPATI SAMBHAJINAGAR**



NAAC Re-accredited 'A' Grade

Department of Chemistry

FACULTY OF SCIENCE & TECHNOLOGY

Two Years P.G. Programme in Chemistry

(M. Sc. Organic Chemistry Semester III& IV)

As Per National Education Policy-2020

Course structure and Curriculum

(OBE with Choice Based Credit System)

Subject : Chemistry
Specialization : Organic Chemistry

Effective From :2024-25

Sankarwar
31/05/2024

PREFACE

National Education policy 2020 has been intensely debated policies come into existence. In January, 2020 UGC has given the guideline for Learning outcome based curriculum framework (LOCF) work towards more holistic experience for the students. while focussing not just on knowledge delivery in higher education but also on the application of knowledge through field and laboratory work and emphasis on application of knowledge to real life experiences, LOCF is student-centric education in the context of development of personal, social, professional and acquired knowledge requirements in their career and life building, which focuses on measuring student performance through outcomes. It includes the knowledge, skills and attitudes enhancement in the students.

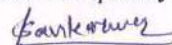
The aspects of LOCF is all-round development of the students, skill acquisition outside chosen subjects and research were undetermined but NEP has changed all of these in one stroke. The prominent features of the NEP framework are:

- Student centric education
- Flexibility in postgraduate programmes
- Multiple entry and exit points
- Skill based & outcome base education
- Credit based evaluation system
- Academic bank credits

It also focuses on evaluation of outcomes of the program by considering the knowledge, skill and behaviour of a students after completion of two year program. The educational triangle of Teaching-Learning and Evaluation process is the unique features of the OBE approach. The curriculum practices such as Competency based curriculum, Tailor-made curriculum development, spades, curriculum principles, Blooms Taxonomy and further use of assessment methodologies like, Norm-reference testing and Criterion reference testing, etc is being practiced since decades. It is also interesting to know that, globally, different countries and universities adopts the curriculum development models/approaches such as, CDIO (Conceive-Design-Implement-Operate), Evidence based education systems approach, etc as the scientific and systematic approaches in curriculum design.

Maharashtra state government and the authorities of Dr. Babasaheb Ambedkar Marathwada University, Chhatrapati Sambhajanagar has decided to implement National Education Policy-2020 from the academic year 2023-24 for postgraduate program with outcome based education

As per guideline of OBE the department has prepared curriculum for Master of science in chemistry with specialization Inorganic chemistry, Organic Chemistry, Physical Chemistry and self-supported Analytical Chemistry. The OBE syllabus will help to improve the quality and employability of the Post-graduates of the university department.



Professor & Head
Department of Chemistry
Dr. Babasaheb Ambedkar
Marathwada University,
Chhatrapati Sambhajanagar

Professor & Head
Department of Chemistry,
Dr. Babasaheb Ambedkar Marathwada University,
Chhatrapati Sambhajanagar - 431004.

1. **Vision of Department :**

A respectable teaching- learning and research organization nationally and internationally in the area of chemical sciences by providing competitive trained chemists which will assist the chemical world, industries and stake holders.

2. **Mission Department :**

- To bring sustainable progress of society by nurturing chemistry with responsibilities
- To create and maintain programs of excellence in the areas of research, education and public outreach
- Department will produce students who are knowledge in chemistry and can think critically.
- To develop the researcher and scientist in chemical science through post-graduate education and research programme.
- To develop the competent manpower with technology based experimentation methodologies and value based practices for business and industries.
- To undertake projects to solve field base problems.
- To provide student centric learning facilities for the development of overall personality of learner.

3. **Eligibility Criteria :**

4. **Assessment and Evaluation :**

5. **Duration of Course Programme : Two years**

6. **Credit Allotted for two year master programme in chemistry :88 Credit**

Semester - I : 22

Semester -II : 22

Semester -III : 22

Semester -IV : 22

7. **Program Educational Objectives:**

The program educational objectives (PEO's) are the statement that describes the career and professional achievement after the program of studies (post-graduation). The PEO's are driven from the Mission statement (What is the purpose of organization). The PEO's can be minimum three and maximum five.

PEO1:To have advanced knowledge of chemistry domain.

PEO2:To provide the professional services to industry, Research organization and institutes.

PEO3:To provide the professional consultancy and research support for therelevant organization in the domain of super specialization.

PEO4: To opt for higher education, disciplinary & multi-disciplinary research and to be a life-long learner.

PEO5: To provide, value based and ethical leadership in the professional and social

life.

8. Program Outcomes:

The program outcomes (PO's) are the statement of competencies/ abilities. POs are the statement that describes the knowledge and the abilities the post-graduate will have by the end of program studies.

- (i) In-depth and detailed functional knowledge of the fundamental theoretical concepts and experimental methods of chemistry.
- (ii) Apply/implement interface between on the one hand, the history of chemistry and natural science and, on the other hand, issues pertaining to the areas of modern technology, health, and environment.
- (iii) Skills in planning and conducting advanced chemical experiments and applying structural-chemical characterization techniques.
- (iv) Skill in examining specific phenomena theoretically and/or experimentally.
- (v) Generation of new scientific insights or to the innovation of new applications of chemical research.

9. Course Program outcome

Course Program Outcomes are developed through the curriculum (curricular/co-curricular-extra-curricular activities). The program outcomes are attained through the course implementation. As an educator, one must know, **"To which POs his/her course is contributing?"** So that one can design the learning experiences, select teaching method and design the tool for assessment.

M.Sc. Organic Chemistry Semester-III Course Structure

Sr. No.	Course Code	Course Name	Teaching (Hr/W)	Credits Assigned	Continuous Internal Assessment	End Semester Exam	Total Marks
Course type : DSC-Major Mandatory:							
1.	OCHTC-600	Structural Elucidation by Spectral Methods	4	4	40	60	100
2.	OCHTC-601	Reagents in Organic Synthesis	4	4	40	60	100
3.	OCHTC-602	Pericyclic Reactions and Free radicals	2	2	20	30	50
4.	OCHLC-603	Organic Chemistry Laboratory Course	4	2	20	30	50
5.	OCHLC-604	Organic Chemistry Laboratory Course	4	2	20	30	50
Course Type : DSE (Choose any two from pool of the course):							
6.	OCHTE-605	Organic Photochemistry and Green Chemistry	2	2	20	30	50
7.	OCHTE-606	Synthetic Organic Chemistry	2	2	20	30	50
8.	OCHTE-607	Bioorganic and Enzyme Chemistry	2	2	20	30	50
9.	OCHTE-608	Emerging Topics in Organic Chemistry	2	2	20	30	50
Course Type : Research Project:							
10.	OCHRP-649	Research Project -I	8	4	40	60	100
Total			32	22	220	330	550

Course code Nomenclature :

DSC-Discipline Specific Core ,**DSE**- Discipline Specific Elective, **T**-Theory,

L- Laboratory course, **OCHTC**- Organic Chemistry Theory Core ,**OCHLC**- Organic Chemistry Laboratory Core , **OCHTE**- Organic Chemistry Theory Elective , **OCHRP**- Organic Chemistry Research Project

[Signature]
31/05/2024

Professor & Head
Department of Chemistry,
Dr. Babasaheb Ambedkar Marathwada University,
Chhatrapati Sambhajnagar - 431004.

Course Name: Structural Elucidation by Spectral Methods

Course Code: OCHTC-600

Course type: DSC-15

Total contact hours: 60 h (04 h/Week)

Credits: 04

Marks: 100

Course Outcomes:

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

1. Review elementary concepts of nuclear magnetic resonance spectroscopy and delve into spin-spin couplings, factors affecting coupling constants, and spin systems like AB, AX, and ABX.
2. Explore techniques such as INEPT, INADEQUATE, and the Nuclear Overhauser effect.
3. Grasp elementary concepts of ^{13}C NMR spectroscopy, including chemical shifts for various carbon types and the impact of substituents on these shifts.
4. Understand the fundamentals of mass spectrometry, including ion production methods, ion analysis, factors affecting fragmentation, and the interpretation of mass spectra.
5. Explore fragmentation patterns for various functional groups and phenomena like the molecular ion peak and McLafferty rearrangement.
6. Grasp the principles of Mössbauer spectroscopy, understanding factors influencing line position and shape, including the isomer effect and quadrupole splitting.
7. Integrate UV, IR, ^1H NMR, ^{13}C NMR and Mass data to solve complex and deduce the structure.

UNIT-I: Nuclear Magnetic Resonance Spectroscopy (^1H NMR)

[12 h]

Elementary ideas (Recapitulation); Spin-spin couplings, Different types of couplings, factors affecting on coupling constants, Karplus equation, Spin systems (AB, AX, ABX, AMX), Rate processes, spin decoupling, shift reagents, Nuclear Overhauser effect (NOE), INEPT and INADEQUATE.

UNIT-II: ^{13}C Nuclear Magnetic Resonance Spectroscopy

[12h]

Elementary ideas, instrumental problems, chemical shifts (aliphatic, olefinic, alkyne, aromatic, heteroaromatic and carbonyl carbons); Effect of substituents on chemical shifts.

UNIT-III: Mass Spectroscopy

[12h]

Introduction, ion production (EI, CI, FD and FAB), ion analysis, ion abundance, factors affecting on fragmentation, fragmentation of different functional groups, molecular ion peak, isotopic peaks, metastable peak, Nitrogen rule, McLafferty rearrangement, Retro-Diels-Alder reaction.

UNIT-IV

[12h]

Problems based on joint applications of UV, IR, ^1H NMR, ^{13}C NMR and Mass spectroscopy.

UNIT-V

[12h]

Mossbauer spectroscopy: Principle, factors affecting the line position and shape, isomer effect and Quadrupole splitting iron salt like compounds, complexes, carbonyl compounds (temperature dependence of isomer shift and Quadrupole splitting in simple compound and coordination, polynuclear complexes), Numericals. **Electron Spin Resonance Spectroscopy:** Introduction, principle of ESR spectroscopy, presentation of spectrum, hyperfine splitting in various structures, hyperfine splitting diagram of representative examples; factors affecting the magnitude of 'g' values, Zero field splitting, Kramer's degeneracy, Anisotropy in the hyperfine coupling constant, electron delocalization, instrumentation and applications.

Reference Books:

1. Introduction to Spectroscopy: D. L. Pavia, G. M. Lampman, G. S. Kriz
2. Spectrometric Identification of Organic Compounds: R. M. Silverstein & F. X. Webster
3. ^{13}C NMR Spectroscopy: G. C. Levy, R. L. Lichter, G. L. Nelson
4. Spectroscopic Methods in Organic Chemistry: D. H. Williams & I. Fleming
5. Spectroscopy of Organic Compounds: V. M. Parikh
6. Mass Spectrometry: K. G. Das & James
7. Coordination Chemistry by Experimental Methods: K. Barger
8. Coordination Chemistry vol. I: E. Martell
9. Physical Methods for Chemistry: R. S. Drago
10. Structural Methods in Inorganic Chemistry: E. A. V. Ebsworth & D. W. H. Rankin
11. Organic Structure Analysis: Philips Crews

Course Name: Reagents in Organic Synthesis

Course Code: OCHTC-601

Course type: DSC-16

Total contact hours: 60 h (04 h/Week)

Credits: 04

Marks: 100

Course Outcomes:

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

1. Explore metal and non-metal based oxidising agents for functional group transformations.
2. Understand the selectivity in the reagents for carrying oxidations
3. Learn the utility of the reagents
4. Explore the suitable methods to carry out oxidation and dihydroxylation
5. Explore the synthetic utility of various hydride transfer reagents for reduction of functional groups
6. Understand the preparation and applications of organic reagents for different types of reactions
7. Utilize the various organometallic reagents for carbon-carbon bond formations
8. Achieve the preparation of ylides and their synthetic utility]

UNIT-I Oxidation**[18 h]**

(a) Oxidation of alcohol to aldehyde, ketone or acid: Jones reagent, Collins reagent, Fetizon's reagent, PCC, PDC, PFC, Activated MnO_2 , Chromyl chloride (Etard reaction), TEMPO, CAN, NMO,

(b) DMSO activated oxidation of alcohols to carbonyls: Kornblum oxidation, Moffatt-Pfitzner oxidation, Parikh-Doering oxidation, Albert-Goldman oxidation, Swern oxidation and Corey-Kim oxidation

(c) Oxidative cleavage of Carbon-Carbon double bonds: KMnO_4 , Ozonolysis.

(d) Oxidations using SeO_2 , PhSeBr and related applications of the reagents.

(e) Selective cleavages at functional groups: Cleavage of glycols, IO_4^- , $\text{Pb}(\text{OAc})_4$.

(f) Dihydroxylation of alkenes: (i) OsO_4 ; Mitsunobu dihydroxylation, Upjohn dihydroxylation and Johnson-Leimux reaction (ii) Ruthenium tetroxide

UNIT-II Reductions**[12 h]**

(a) Catalytic Hydrogenation under homogeneous and heterogeneous conditions; Reduction of alkenes, alkynes, nitriles, oximes and nitro compounds; (b) Reduction of carbonyls, acids, amides, esters, lactones, lactams, cyanides, imines by boron and aluminium based reagents such as LiAlH_4 , LiBH_4 , $\text{Li}(\text{OEt})_3\text{AlH}$, NaBH_4 , $\text{Ca}(\text{BH}_4)_2$, $\text{Zn}(\text{BH}_4)_2$, DIBAL-H, $\text{BH}_3\cdot\text{THF}$ complex, Catechol borane, Disiamylborane, Thexylborane, IP_2BH , IPcBH_2 (c) Reduction of carbonyls to hydrocarbons: Clemenson reduction, Wolf-Kishner reduction (d) Birch reduction and related reactions

UNIT-III Organic Reagents

[12 h]

Preparation and synthetic applications of: DCC, EDC, DDQ, 1,3 Dithiane, LDA, DMDO, Iodoxybenzoic acid, Dess-Martin Periodinane, Diazomethane, Lawesson's reagent.

UNIT-IV

[06 h]

Ylides and Enamines

Ylides: Preparation and their synthetic applications along with their stereochemical aspects of

(i) Phosphorous ylides: Wittig, Wittig-Horner, Horner-Wadsworth-Emmons reactions

(ii) Sulphur ylides: Corey-Chaykovskyepoxidation, cyclopropanation and aziridination reactions

Enamines: Generation & application in organic synthesis with mechanistic pathways, stork enamine reaction.

UNIT-V Formation of Carbon-Carbon bonds via organometallic reagents

[12 h]

Synthesis and applications of organo Lithium, Magnesium, Titanium, Cerium, Copper, Chromium, Zinc, Boron, Silicon, Cadmium, Palladium, Tin

Reference Books:

1. Organic Chemistry: Clayden, Greeves, Warren and Wothers
2. Stereochemistry of Organic Compounds (Principle and application): D. Nasipuri
3. Stereochemistry of Organic compounds: Ernest L. Eliel / Samuel H. Wilen
4. Organic Synthesis: W. Carruthers
5. Organic Reagents: Fieser&Fieser
6. Organic Synthesis: M. B. Smith
7. Advanced Organic Chemistry; Part A and B: F. A. Carey & R. J. Sundberg
8. Modern Organic Synthesis: An Introduction: G. S. Zweifel& M. H. Nantz
9. A Guidebook To Mechanism In Organic Chemistry: Peter Sykes
10. Organic Synthesis Concepts, Methods, Starting Materials: J. Fuhrhop, G. Penzlin
11. Organic Chemistry: An Intermediate Text: Robert V. Hoffmann
12. Advanced Organic Chemistry: Jerry March
13. Organic Synthesis: R. O. C. Norman and Coxan
14. Name Reactions: Jie Jack Li

Course Name: Pericyclic Reactions and Free Radicals

Course Code: OCHTC-602

Course type: DSC-17

Total contact hours: 30 h (02 h/Week)

Credits: 02

Marks: 50

Course Outcomes:

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

1. Understand the photochemical and thermal reactions
2. Classify the various types of pericyclic reactions
3. Apply the orbital correlation and frontier molecular orbital methods for pericyclic reactions
4. Predict the stereochemical outcome of pericyclic reactions
5. Understand various free radical reactions

UNIT-I: Pericyclic Reactions-I

[10 h]

Features and classification of pericyclic reactions, Phases, nodes and symmetry properties of molecular orbital in ethylene, 1,3-butadiene, 1,3,5-hexatriene. Allylation, allyl radical, pentadienylation and pentadienyl radical. Thermal and photochemical reactions.

Electrocyclic reactions: Woodward-Hoffmann selection rules for electrocyclic reactions. Explanation for the mechanism of electrocyclic reactions by: (i) Symmetry properties of HOMO of open chain partner; (ii) Conservation of orbital symmetry and orbital symmetry correlation diagram and (iii) Huckel-Mobius aromatic and antiaromatic transition state method.

UNIT-II: Pericyclic Reactions-II

[10 h]

Cycloaddition reactions: Diels-Alder reaction. Woodward-Hoffmann selection rules for cycloaddition reactions. Explanation for the mechanism of cycloaddition reactions by 1) Conservation of orbital symmetry and orbital symmetry correlation diagrams 2) Fukui Frontier Molecular Orbital (FMO) theory and (3) Huckel-Mobius aromatic and antiaromatic transition state method. Endo-exo selectivity in Diels-Alder reaction and its explanation by FMO theory. Examples of cycloaddition reactions.

Sigmatropic reactions: Selection rules for [i,j] shifts. Cope, degenerate Cope and Claisen rearrangements. Explanation of sigmatropic reactions by (i) symmetry properties of HOMO (ii) Huckel-Mobius aromatic and antiaromatic transition state method. Introduction to chelotropic reactions and the explanation of mechanism by FMO theory.

UNIT-III:Free radical reactions

[10 h]

Introduction, generation, stability, reactivity, characteristics, structural and stereo chemical properties of free radicals, Persistent free radicals.

Reaction of free radicals: Addition, substitutions, fragmentations, Oxidations and reductions, Detection of free radicals, Homolysis and free radical displacement. Radical chain reactions, Addition and rearrangements, radical cyclization, reactivity of aliphatic and aromatic substrates at bridgehead, Coupling of alkynes and arylation of aromatic compound by diazonium salt, Sandmeyer reaction, Hunsdieker reaction, Allylic halogenations, McMurry reaction, Acyloin condensation, Birch reduction, Bouveault-Blank reduction.

Reference Books:

1. Advanced Organic Chemistry Part A & Part B: F. A. Carey & R. J. Sundberg
2. Advanced Organic Chemistry: Jerry March
3. Organic Chemistry: Clayden, Greeves, Warren &wother.
4. Organic Chemistry: Stanley H. Pine
5. Organic Synthesis: W. Carruthers
6. Organic Synthesis: Norman and Coxon

Course Name: Organic Chemistry Laboratory Course

Course Code: OCHLC-603

Course type: DSC-18

Total contact hours: 60 h (04 h/Week)

Credits: 02

Marks: 50

Course Outcomes:

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

1. Understand the multistep organic synthesis
 2. Explore the theoretical knowledge to predict the mechanism of reactions
 3. Explore the purification techniques
 4. Allow carry out various reactions
 5. Determine the overall yield of the reaction
-

Contents:

Preparations involving at least two stage based on name reactions, condensations, cyclo-condensations, reagents and rearrangements (as covered under the theory). Separation purification of the product is desired.

1. Preparation of sulphanilamide from acetanilide
2. Preparation of benzilic acid from benzoin
3. Preparation of acetanilide from acetophenone via Beckmann rearrangement
4. Preparation of Benzanilide from Benzophenone via Beckmann rearrangement
5. Preparation of para-nitroaniline from aniline
6. Preparation of para-bromoaniline from aniline
7. Preparation of epoxyketone from chalcone
8. Anthanilic acid to 2-Iodoxybenzoic acid

Reference Book:

1. Practical Organic Chemistry: Vogel
-

Course Name: Organic Chemistry Laboratory Course

Course Code: OCHLC-604

Course type: DSC-19

Total contact hours: 60 h (04 h/Week)

Credits: 02

Marks: 50

Course Outcomes:

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

1. Understand the the use of green chemistry principles
 2. Explore the use of microwave and ultrasound irradiation technique for the synthesis
 3. Explore the purification techniques
 4. Carry out various reactions
 5. Utilize the knowledge of spectroscopic techniques for structure ilucidation
-

Part-A: Preparations involving one stage based upon the green synthetic protocols (as covered in theory syllabus). (Minimum 10 experiments)

Experiments will be based on use of Microwave and Ultrasound, Mild catalysts, Mechanochemistry, Water as solvent and solvent-free reactions.

1. Knoevenagel condensation
2. Hantzsch condensation
3. Biginelli condensation
4. Pechmann condensation
5. Preparation of 1, 1-bis-2-naphthol
6. Various Multicomponent reactions

Part-B Structure elucidation of organic compounds and drugs by spectral analyses

Use of UV, IR, ^1H NMR, ^{13}C NMR and Mass. A minimum of 40 representative examples should be discussed.

Reference Books:

1. Spectrometric Identification of Organic Compounds: R. M. Silverstein and others (8th Ed. Wiley)
 2. Monograph on Green Chemistry Laboratory Experiments: Green Chemistry Task Force Committee, DST
-

Course Name: Organic Photochemistry and Green Chemistry

Course Code: OCHTE-605

Course type: DSE-9

Total contact hours: 30 h (02 h/Week)

Credits: 02

Marks: 50

Course Outcomes:

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

1. Understand the photochemical and thermal reactions
2. Classify the various types of photochemical reactions
3. Predict the stereochemical outcome of photochemical reactions
4. Understand the concept of green chemistry
5. Utilize the knowledge of Microwave and Ultrasound assisted reactions for bioactive molecules

UNIT-I: Photochemistry-I

[10 h]

Photochemistry of (π , π^*) transitions: Excited state of alkenes, cis-trans isomerisation, photochemistry state, electrocycloaddition and Sigmatropic rearrangements, di π -methane rearrangement.

Intermolecular reactions: photocycloadditions, photodimerisation. Photoaddition reactions. Excited states of aromatic compounds, photodimerisation of benzene, photosubstitution reactions of aromatic compounds and Photo-Fries rearrangement.

UNIT-II: Photochemistry-II

[10 h]

Photochemistry of (n , π^*) transitions: Excited state of carbonyl compounds, Norrish-I and Norrish-II

Addition to C-C multiple bonds: Paterno-Buchi reaction, photochemistry of alkyl peroxides, hypohalites and nitriles. Barton reaction. Photochemistry of azo compounds, diazo compounds, azides and diazonium salts. Singlet oxygen-photo oxygenation reactions. Ene reaction, formation of dioxetanes and endoperoxides. Chemiluminescent reactions. Oxidative coupling.

UNIT-III: Green Chemistry

[10 h]

Green chemistry, relevance and goals, Anastas' twelve principles of green chemistry-Tools of green chemistry: alternative starting materials, reagents, catalysts, solvents and processes with suitable examples.

Microwave and Ultrasound assisted organic synthesis

Activation and specific effects of microwave and ultrasound irradiations, Neat reactions, solid supports reactions, Functional group transformations, condensations reactions, oxidations, reductions reactions, multi-component reactions.

Use of Ionic liquids

General synthesis and properties of ionic liquids, applications in various organic transformations, multicomponent reactions.

Reference Books:

1. Green Chemistry-Designing Chemistry for the Environment. Paul T. Anastas & Tracy C. Williamson.
2. Green Chemistry-Frontiers in benign chemical synthesis and processes. Paul T. Anastas & Tracy C. Williamson
3. Advanced Organic Chemistry Part A & Part B: F. A. Carey & R. J. Sundberg
4. Advanced Organic Chemistry: Jerry March
5. Organic Chemistry: Clayden, Greeves, Warren & Wothers.
6. Organic Chemistry: Stanley H. Pine
7. Organic Synthesis: W. Carruthers
8. Organic Synthesis: Norman and Coxon

Course Name: Synthetic Organic Chemistry

Course Code: OCHTE-606

Course type: DSE-10

Total contact hours: 30 h (02 h/Week)

Credits: 02

Marks: 50

Course Outcomes:

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

1. Understand the types of reactions and rearrangements
2. Predict the applications of named reactions and rearrangements in organic synthesis particularly natural products and drugs.
3. Allow to utilize the concept of carbon-carbon single and multiple bonds
4. Understand the concept of Multicomponent reactions and their utility

UNIT-I: Name Reactions-I

[10 h]

Arndt-Eistert, Hunsdiecker reaction, Baeyer-Villiger, Dakin, Gabriel synthesis, Michael, Darzen, Prins, Henry, Reimer-Tiemann, Hoffmann-Löffler-Freytag, Dieckmann cyclization, Chichibabin, Vilsmeier, Ene, Ullmann reaction, Mannich, Strecker amino acid synthesis. Bamford-Stephen, Baylis-Hillmann, Corey-Fuchs Reaction, Julia olefination, Mukaiyamaaldol, Mitsunobu, Peterson olefination, Corey-Winter olefination,

UNIT-II: Name Reactions-II

[10 h]

Woodward and Prevost dihydroxylation, Shapiro, Ritter, Stille, Heck, Sonogashira, Suzuki, Duff, Chugaev, Petasis, McMurry reaction and Coupling. Ring closing metathesis (Grubb's metathesis), Aldol-Tishchenko (Evans-Tishchenko reaction), Ugi, Passerini, Biginelli, Hantzsch condensation.

UNIT-III: Name Rearrangements

[10 h]

Pummerer, Payne, Eschenmoser fragmentation, Brook, Wagner-Meerwein, Wolf, Semipinacol, Epoxide rearrangement with Lewis acid, Dienone-Phenol rearrangement, Tiffeneau-Demjanov, Favorskii, von Richter, Wittig, Neber, Smiles, Fries, Curtius, Lossen, Schmidt, Steven, Hofmann, Iodolactonisation.

Reference Books

1. Organic Synthesis: M. B. Smith
2. Advanced Organic Chemistry; Part A and B: F. A. Carey & R. J. Sundberg
3. Modern Organic Synthesis: An Introduction: G. S. Zweifel & M. H. Nantz
4. A Guidebook To Mechanism In Organic Chemistry: Peter Sykes
5. Organic Synthesis Concepts, Methods, Starting Materials: J. Fuhrhop, G. Penzlin

6. Organic Chemistry: An Intermediate Text: Robert V. Hoffmann
7. Advanced Organic Chemistry: Jerry March
8. Organic Synthesis: R. O. C. Norman and Coxan
9. Name Reactions: Jie Jack Li
10. Name Reactions and Reagents in Organic Synthesis: B. P. Mundy, M. G. Eller, F. G. Favaloro

Course Name: Bioorganic and Enzyme Chemistry

Course Code: OCHTE-607

Course type: DSE-11

Total contact hours: 30 h (02 h/Week)

Credits: 02

Marks: 50

Course Outcomes:

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

1. Understand the concept of bioorganic chemistry
2. Know about the types of enzymes, structures.
3. Understand the applicability of various enzymes

UNIT-I: Introduction to Bioorganic chemistry [10 h]

Basic concepts, Proximity effects in organic chemistry, Molecular adaptation, Molecular recognition.

UNIT-II: Enzyme Chemistry [10 h]

Introduction, Nomenclature, Classification and Extraction of enzymes, Introduction to catalysis and enzymes; Multifunctional catalysis, Intramolecular Catalysis, Mechanism of enzyme action, Factors responsible for enzyme specificity, Enzyme activity and kinetics (Michaelis-Menten and Lineweaver-Burk plots), Enzyme Inhibitions (Reversible and irreversible), Structure, Mechanism of action and applications of α -Chymotrypsin, Ribonuclease, lysozyme and Carbopeptidase-A. Enzymes in synthetic organic chemistry. [Additions, eliminations, substitutions, condensations, cyclocondensations, oxidations, reductions and rearrangement reactions are to be covered]

UNIT-III: Co-Enzyme Chemistry [10 h]

Chemical structures of co-enzymes and cofactors, Oxidoreduction (NAD^+ , NADP^+), Pyridoxal phosphate (PLP), Thiamine pyrophosphate (TPP), Biotin (CO_2 carrier), Haemoglobin (O_2 -carrier), Flavin (FMN, FAD, FADH_2), Oxene Reactions, Lipoic acid, Mechanisms of reactions catalyzed by co-factors.

Reference Books

1. Bioorganic chemistry (A chemical approach to enzyme action): Hermann Dugas
2. Biotransformation in Organic chemistry: K. Faber
3. Enzyme structure and Mechanism: Alan Fersht.
4. Enzyme catalysis in organic synthesis vol.1: Karlheinz Drauz and Herbert Waldmann.
5. Bioorganic, Bioinorganic and supramolecular chemistry: P. S. Kalsi and J. P. Kalsi.

Course Name: Emerging Topics in Organic Chemistry

Course Code: OCHTE-608

Course type: DSE-12

Total contact hours: 30 h (02 h/Week)

Credits: 02

Marks: 50

Course Outcomes:

At the end of the course, the student will be able to:

1. Understand the concepts of multicomponent reactions and their mechanisms.
2. Understand the tandem reactions in organic synthesis.
3. Apply the principles of click chemistry in drug discovery, biology and materials chemistry.
4. Discuss the flow chemistry, micro reactors, separation techniques and process chemistry in organic synthesis.

UNIT-I Advanced Multicomponent Reactions**[10 h]**

Recent Developments in the multicomponent reactions (MCRs): General Approaches of MCRs, Synthesis of different heterocyclic compounds using 3, 4 and 5 component reactions, MCRs using homogeneous and heterogeneous catalysts.

UNIT-II Click and Flow Chemistry**[10**

h] Importance of Click chemistry, Applications of click chemistry in drug discovery, biology and materials chemistry.

Recent advances in Flow chemistry and Micro reactors,

UNIT-III Tandem Reactions**[10**

h] Tandem (cascade/domino) reactions in Organic Synthesis, Metal Carbenes in Organic Synthesis, N-heterocyclic carbenes in organic synthesis, Hypervalent iodine reagents in organic synthesis.

Reference Books:

1. Multicomponent Reactions: Concepts and Applications for Design and Synthesis, Raquel P. Herrera, Eugenia Marqués-López, John Wiley & Sons. 2015, 1st Edition.
2. Click Reactions in Organic Synthesis, Srinivasan Chandrasekaran, John Wiley & Sons, 2016, 1st Edition.
3. Domino Reactions in Organic Synthesis, Lutz F. Tietze, Gordon Brasche, Kersten Gericke, John Wiley & Sons, 2006
4. Microreactors in Organic Synthesis and Catalysis, Ed. by Thomas Wirth Title, John Wiley & Sons, 2008

Course Name: Research Project-I

Course Code: OCHRP-649

Course type: Project

Total contact hours: 120 h (08 h/Week)

Credits: 04

Marks: 100

Course Outcomes:

At the end of the course, the student will be able to:

1. Know how to carry out literature survey by using various search engines and database
2. Handle various chemicals, solvents, instruments and others
3. Perform reactions, monitoring by TLC
4. Purification techniques
5. Understand the structure of organic compounds by using spectral techniques

Research project will be assigned to the students on the basis of theory components, such as Multicomponent reactions, use of ionic liquids/surfactants in organic synthesis, Microwave/ Ultrasound assisted synthesis of bioactive molecules etc.

Literature Survey, Studies of Reactions, Synthesis, Mechanism, Standardization of Reaction Conditions, New Synthetic Methods etc

Note: Student should attend the National/International Conference in this semester and present their project work (if possible)

M.Sc. Organic Chemistry Semester-IV Course Structure

Sr. No.	Course Code	Course Name	Teaching (Hr/W)	Credits Assigned	Continuous Internal Assessment	End Semester Exam	Total Marks
Course Type: DSC-Major Mandatory:							
1.	OCHTC-650	Organic synthesis: Retrosynthetic approach	4	4	40	60	100
2.	OCHTC-651	Chemistry of Natural Products and Asymmetric Synthesis	4	4	40	60	100
3.	OCHTC-652	Heterocyclic Chemistry	2	2	20	30	50
4.	OCHLC-653	Organic Chemistry Laboratory Course	4	2	20	30	50
Course Type : DSE (Choose any two from pool of the course):							
5.	OCHTE-654	Introduction to Medicinal Chemistry	2	2	20	30	50
6.	OCHTE-655	Drug Synthesis	2	2	20	30	50
7.	OCHTE-656	Polymer Chemistry	2	2	20	30	50
8.	OCHTE-657	Advanced Spectroscopy	2	2	20	30	50
Course type : Research Project:							
9.	OCHRP-699	Research Project -2	12	6	60	90	150
Total			32	22	220	330	550

Course code Nomenclature :

DSC-Discipline Specific Core **DSE**- Discipline Specific Elective, **T**-Theory, **L**- Laboratory course, **OCHTC**- Organic Chemistry Theory Core , **OCHLC**- Organic Chemistry Laboratory Core, **OCHTE**- Organic Chemistry Theory Elective , **OCHRP**- Organic Chemistry Research Project,

Course Name: Organic synthesis: Retrosynthetic approach

Course Code: OCHTC-650

Course type: DSC-20

Total contact hours: 60 h (04 h/Week)

Credits: 04

Marks: 100

Course Outcomes:

At the end of the course, the student will be able to:

1. Understand the basic concepts of retrosynthetic analysis
2. Describe disconnection approaches applied on synthetic strategies and mechanism prediction.
3. Understand the use of protecting groups
4. Allow to disconnect the molecules by using different strategies
5. Explore the various reactions for designing the synthesis of target molecules
6. Allow to construct the various rings
7. Utilize the knowledge of retrosynthetic analysis and synthesis for natural products, drugs and complex molecules

UNIT-I Disconnection Approach

[12 h]

An introduction to synthons, synthetic equivalents, disconnection approach, functional group interconversions, importance of order of events in organic synthesis, one and two group C-X disconnections, selective organic transformations: chemoselectivity, regioselectivity, stereoselectivity, enantioselectivity, Reversal of polarity, cyclization reactions, amine synthesis.

UNIT-II Protecting Groups

[12 h]

Protection and deprotection of hydroxyl, carbonyls in aldehydes and ketones, amines, carboxylic acids, alkenes and alkynes.

UNIT-III C-C Disconnections

[12 h]

(i) One group C-C Disconnections:

Alcohols (including stereoselectivity), carbonyls (including regioselectivity), Alkene synthesis, use of acetylenes and aliphatic nitro compounds in organic synthesis.

(ii) Two group C-C Disconnections:

Diels-Alder reactions, 1,3difunctionalized compounds and α , β -unsaturated compounds, control in carbonyl condensations, 1,5 difunctionalized compounds, Michael addition and Robinson annelation.

UNIT-IV Ring Synthesis

[12 h]

Introduction to ring synthesis, saturated heterocycles, synthesis of 3, 4, 5 and 6 membered rings, rearrangements and photochemistry in synthesis, aromatic heterocycles.

UNIT-V Complex molecules

[12h]

Synthetic routes based on retrosynthetic analysis for following molecules: Longifoline, Reserpine, Juvabione, Aphidicoline, Taxol.

Reference Books:

1. Organic Synthesis: The Disconnection Approach: Stuart Warren
2. Designing Organic Synthesis: Stuart Warren
3. Organic Synthesis: Strategy and Control: Paul Wyatt and Stuart Warren
4. The Logic of Chemical Synthesis: E. J. Corey and Xue-Min Chelg
5. Classics in Total Synthesis I, II and III: K. C. Nicolaou and others
6. Organic Synthesis Concepts, Methods, Starting Materials: J. Fuhrhop, G. Penzlin
7. Some Modern Methods of Organic Synthesis: W. Carruthers
8. Organic Synthesis: M. B. Smith
9. Principles of Organic Synthesis: R. Norman and J. M. Coxan.
10. Advanced Organic Chemistry: Jerry March
11. Organic Chemistry: Clayden, Greeves, Warren and Wothers

Semester-IV

Course Name: Chemistry of Natural Products and Asymmetric Synthesis

Course Code: OCHTC-651

Course type: DSC-21

Total contact hours: 60 h (04 h/Week)

Credits: 04

Marks: 100

Course Outcomes:

At the end of the course, the student will be able to:

1. Understand the concept of structure elucidation of natural compounds
2. Build the synthetic schemes of natural products and bioactive molecules
3. Analyze the stereochemistry of drug molecules
4. Apply the knowledge of biosynthesis in total synthesis of organic molecules.
5. Design new synthetic methodologies
6. Understand the concepts involved in asymmetric synthesis

UNIT-I:Terpenoids& Carotenoids

[12 h]

Classification, Nomenclature, occurrence, isolation, general methods of structure determination, isoprene rule, Structure determination, stereochemistry, and synthesis of the following representative molecules: Citral, Geraniol, α -Terpineol, Menthol, Farnesol, Zingiberene, Phytol, Abietic acid and β - Carotene.

UNIT-II:Alkaloids

[12 h]

Occurrence, isolation, general methods of structure elucidation, degradation, classification based on nitrogen heterocyclic ring, role of alkaloids in plants. Structure, stereochemistry and synthesis of the following: Ephedrine, (+)-coniine, nicotine, atropine, Quinine and Morphine.

UNIT-III:Steroids

[12 h]

Occurrence, nomenclature, basic skeleton, Diel's hydrocarbon and stereochemistry. Isolation, structure determination and synthesis of Bile acids, Androsterone, Testosterone, Estrone, Progesterone.

UNIT-IV:Asymmetric Synthesis-I

[12 h]

Chiral pool, Chiral auxiliary, Enantio- & Diastereoselective synthesis, Chiral reagent and chiral catalyst including CBS reagent, NADH, Asymmetric hydrogenation including BINAP,

UNIT-V:Asymmetric Synthesis-II

[12 h]

Hydroboration- Ipc_2BH , IpcBH_2 , Asymmetric epoxidation- (+) DET & (-) DET, Sharpless, Jacobson, Asymmetric dihydroxylation- $(\text{DHQD})_2\text{PHAL}$ & $(\text{DHQ})_2\text{PHAL}$, Felkin-Anh model, Zimmermann-Traxler transition state model, Prolinecatalyzed asymmetric reactions

Reference Books

1. The Organic Chemistry of Drug Design and Drug Action: R. B. Silverman, Academic press.
2. Natural Products: Chemistry and Biological Significance: J. Mann, R. S. Davidson, J. B. Hobbs, D. V. Banthrope and J. B. Harborne, Longman, Essex.
3. Organic Chemistry: Vol. II, I. L. Finar, ELBS.
4. New Trends in Natural Product Chemistry: Atta-ur-Rahman and M. I. Choudhary, Harwood Academic publishers.
5. Stereochemistry of Organic Compounds (Principle and application): D. Nasipuri
6. Stereochemistry of Organic compounds: Ernest L. Eliel / Samuel H. Wilen
7. Advanced Organic Chemistry; Part A and B: F. A. Carey & R. J. Sundberg
8. Organic Chemistry: Clayden, Greeves, Warren and Wothers
9. Organic Synthesis: M. B. Smith

Course Name: Heterocyclic Chemistry

Course Code: OCHTC-652

Course type: DSC-22

Total contact hours: 30 h (02 h/Week)

Credits: 02

Marks: 50

Course Outcomes:

At the end of the course, the student will be able to:

1. Classify heterocyclic compounds and their nomenclature
2. Understand the physical and chemical properties of simple and fused heterocyclic compounds
3. Apply the knowledge of heterocyclic chemistry to synthesize the natural products and drug molecules
4. Distinguish aromatic and homoaromatic compounds using spectral data

UNIT-I**[10 h]**

Nomenclatures of all types of heterocycles, Classification of heterocycles: as aromatics based upon various membered ring systems.

UNIT-II**[10 h]**

General synthetic routes based on name reactions, reactivities, utilities and wherever possible spectral analyses of the following class of heterocycles.

Four membered: Azetidines, including β - lactams.

Five membered: Thiazoles, Oxazoles, Pyrazoles and Imidazoles.

Six membered: Pyridines, Pyrimidines.

UNIT-III**[10 h]**

Fused heterocycles: Flavones, Chromones, Coumarines, Indoles, Quinolines, Benzodiazepines, and Phenothiazines.

Reference Books:

1. Heterocyclic Chemistry: vol. I, II, III: R. R. Gupta, M. Kumar and M. Gupta
2. Heterocyclic Chemistry: Joules and Mills
3. Modern heterocyclic Chemistry: L. A. Paquette (Benjamin)
4. Organic Chemistry: Jonathan Clayden

Course Name: Organic Chemistry Laboratory Course

Course Code: OCHLC-653

Course type: DSC-23

Total contact hours: 60 h (04 h/Week)

Credits: 02

Marks: 50

Course Outcomes:

At the end of the course, the student will be able to:

1. Understand the principles involved in separation and purification techniques
 2. Analyze the functional groups in organic molecules
 3. Understand the principles involved in separation of ternary mixtures
 4. Obtain practical experience in the separation and identification of individual compounds in the ternary mixtures
 5. Develop the knowledge and skills in the synthetic organic chemistry useful for industrial applications
-

Qualitative analysis of ternary mixtures.

In a mixture at least one liquid one water soluble compound be given. (minimum 08 mixtures)

- (i) Separation of Ternary Mixture
- (ii) Identification of Two Components
- (iii) Element Detections
- (iv) Functional Groups
- (v) Physical Constant
- (vi) Derivatives

Course Name: Introduction to Medicinal Chemistry

Course Code: OCHTE-654

Course type: DSE-13

Total contact hours: 30 h (02 h/Week)

Credits: 02

Marks: 50

Course Outcomes:

At the end of the course, the student will be able to:

1. Understand basic concepts of drug discovery.
2. Apply the concepts in lead discovery.
3. Identify the importance of Lipinski rule and bioisosterism.
4. Understand the concept of Pharmacokinetics and Pharmacodynamics

UNIT-I: Basic consideration of drug activity

[10 h]

Definition and Introduction of following terms-Drug, Prodrug, Hard and Soft drugs, agonists, antagonists, affinity, efficacy, potency, isosterism, bioisosterism, pharmacophores, lead molecule, lethal dose (LD₅₀) and effective dose (ED₅₀) (i) Factors affecting bioactivity, (ii) Theories of drug activity, (iii) Structure activity relationship (SAR), QSAR (2D and 3D method) and Hantzsch equation (iv) Drug receptor mechanism.

UNIT-II Pharmacokinetics

[10 h]

- (i) Drug absorption, Distribution and deposition of drugs.
- (ii) Excretion and elimination of drugs, Bioavailability.

UNIT-III Pharmacodynamics

[10 h]

(i) Mechanism of drug action: Enzyme stimulation and enzyme inhibition, antimetabolites, membrane active drugs, chelation; (ii) Drug metabolism and inactivation: Factors affecting drug metabolism, pathways of drug metabolism [Metabolicreaction (Phase I) and conjugation reaction (Phase II)].

Reference Books:

1. FOYE'S Principles of Medicinal Chemistry VIth Edition: Thomas L. Lemke, David A. Williams, Victoria F. Roche and S. William Zito.
2. Introduction of Medicinal Chemistry:A. Gringuage, Wiley-VCH.
3. Synthesis of Essential Drugs:R. S. Vardanyan and V. J. Hruby.
4. Volumes of Burger's Medicinal Chemistry: M. E. Wolf, JohnWiley.
5. Medicinal Chemistry: David J. Triggle.
6. Essentials of Medicinal Chemistry IInd: AndrejusKorolkovas, WileyVCH.

Course Name: Drug Synthesis

Course Code: OCHTE-655

Course type: DSE-14

Total contact hours: 30 h (02 h/Week)

Credits: 02

Marks: 50

Course Outcomes:

At the end of the course, the student will be able to:

1. Understand classification of drugs.
2. Explore the knowledge of pharmacokinetics and dynamics of the drugs
3. Understand the mode of action of drugs.
4. Explore the knowledge of synthetic organic chemistry to drug synthesis

UNIT-I Classification of Drugs

[06 hrs]

The detail contents of the each class of the drugs.

UNIT-II Drug Synthesis-I

[12 hrs]

Synthesis and Utilities of the following drug molecules (at least one convenient synthetic route with possible mechanism) from following classes:

I. Anti inflammatory Drugs: (a) Naproxen (b) Ibuprofen (c) Oxaprozin (d) Diclofenac Sodium (e) Rofecoxib (f) Celecoxib.

II. Anti-hypertensive Drugs: (a) Verapamil (b) Captopril (c) d-sotalol (d) Atenolol (e) Diltiazem (f) Semotiadilfumarate.

III. Drugs acting on CNS: (a) CNS Stimulant :Dextro-amphetamine

(b) Respiratory Stimulant :Doxapram

(c) CNS anti-depressant : (i) Chlorpromazine (Antipsychotic) (ii) Diazepam (Anxiolytic)

(iii) Phenobarbitol (Antiepileptic)

UNIT-III Drug Synthesis-II

[12 hrs]

I Anesthetic Drugs:

(a) General : Ketamine (b) Local : (i) Lidocaine (ii) Procaine

II. Antibiotics: (a) Chloramphenicol (b) Ampicillin (c) Amoxycillin (d) Cefepime (e) Cefpirome (f) Antimycobacterial: Ethambutol (g) Antiviral: Acyclovir (h) Antimicrobial: Sulfamethoxazole

III. Antidiabetics :(a) Troglitazone (b) Chlorpropamide (c) Tolbutamide

IV. Antineoplastic Drugs: (a) Antagonist: Fluorouracil (b) Alkylating agents: i) Chlorambucil (ii) Cis-Platin

Reference Books:

1. FOYE'S Principles of Medicinal Chemistry VIth Edition: Thomas L. Lemke, David A. Williams, Victoria F. Roche and S. William Zito.
1. Introduction of Medicinal Chemistry:A. Gringuage, Wiley-VCH.
2. Synthesis of Essential Drugs:R. S. Vardanyan and V. J. Hruby.
3. Volumes of Burger's Medicinal Chemistry: M. E. Wolf, JohnWiley.
4. Medicinal Chemistry: David J. Triggle.
5. Essentials of Medicinal Chemistry IInd: AndrejusKorolkovas,

Course Name: Polymer Chemistry

Course Code: OCHTE-656

Course type: DSE-15

Total contact hours: 30 h (02 h/Week)

Credits: 02

Marks: 50

Course Outcomes:

At the end of the course, the student will be able to:

1. Understand the basic concepts in Polymer chemistry.
2. Learn the determination of molecular weight and properties of polymers.
3. Know about the polymer processing and polymerization techniques.
4. Explore synthesis and applications of commercial polymers and conducting polymers.

UNIT-I Basic Concepts

[10 h]

Hours) Monomers, repeat units, degree of polymerization, Linear, branched and network polymers, Addition polymerization, Condensation polymerization, Mechanism of free radical, cationic and anionic polymerization and co-ordination polymerization. Ziegler- Natta catalyst. Kinetics of free radical, cationic, anionic and co-polymerisation. Determination of Reactivity ratio, Reactivity ratio and co-polymerisation behavior.

UNIT-II Molecular Weight, Physical Properties, Polymer Processing & Techniques

[10 h]

Concept of Average molecular weight, number- average, weight- average molecular weight and viscosity- average molecular weights. Determination of molecular weight - viscosity, light scattering, osmotic and ultracentrifugation methods.

Polymers processing- Plastics, elastomers and fibres. Compounding, Processing techniques- calendaring, die casting, injection molding, thermofoaming and fibre spinning. Polymerization techniques- Bulk polymerization, solution polymerization, suspension polymerization, emulsion polymerization and melt polycondensation.

UNIT-III Commercial Polymers

[10 h]

Synthesis and applications of polyethylene, polyvinyl chloride, polyamide, polyester, phenol resins, epoxy resins, silicone polymers, polybenoxazoles, polyimidazole, polyurethane, polymethylmethacrylate, poly(tetrafluoro ethylene) and polyacrylonitrile.

Reference Books:

1. Organic Polymer Chemistry: K. J. Saunders
2. Textbook of Polymer Science: F.W. Billmeyer, Wiley Student Edition, 3rd Edition.
3. Polymer Science: V.R. Gowariker, N. V. Viswanathan, J. Sreedhar

Course Name: Advanced Spectroscopy

Course Code: OCHTE-657

Course type: DSE-16

Total contact hours: 30 h (02 h/Week)

Credits: 02

Marks: 50

Course Outcomes:

At the end of the course, the student will be able to:

1. Analyze the concepts of ^{19}F spectroscopy in determining the structures of molecules.
2. Apply the principles of 2D NMR spectroscopy in resolving the structures of organic molecules.
3. Discuss the principle of ^{31}P and mass spectrometry and their applications.
4. Solve the structures of organic compounds using spectral data.

UNIT-I 2D-NMR spectroscopy**[10 h]**

Principles of 2D NMR, Classification of 2D-experiments. Correlation spectroscopy (COSY) HOMOCOSY (^1H - ^1H COSY), TOCSY (Total Correlation Spectroscopy), Hetero COSY (^1H , ^{13}C COSY, HMQC), long range ^1H , ^{13}C COSY (HMBC), Homonuclear and Heteronuclear 2D-J-resolved spectroscopy, ROESY, NOESY and 2DINADEQUATE experiments and their applications.

UNIT-II ^{19}F NMR spectroscopy:**[10 h]**

Introduction, ^{19}F chemical shifts, spin-spin coupling, coupling constants. Homonuclear couplings, Applications of ^{19}F NMR involving coupling with ^{19}F , ^1H and ^{31}P : 1, 2 dichloro-1, 1 difluoro ethane, BrF_5 , SF_4 , PF_5 , ClF_3 , IF_5 , $\text{CF}_3\text{CH}_2\text{OH}$.

UNIT-III ^{31}P NMR spectroscopy:**[10 h]**

^{31}P chemical shifts, coupling constants. Applications of ^{31}P NMR involving coupling with ^{31}P , ^{19}F , ^1H and ^{13}C : Simple molecules ^{31}P , P_4S_3 , H_3PO_4 , H_3PO_3 , H_3PO_2 and HPF_2 .

Reference Books:

1. Introduction to Spectroscopy, Donald Pavia, G. M. Lampman, George S. Kriz, Thomson/Brooks/Cole, 2001, 3rd Edition.
2. Organic Spectroscopy, William Kemp, Palgrave Publishers, 2007, 3rd Edition.
3. Spectrometric Identification of Organic Compounds, Robert M. Silverstein, Francis X. Webster, David J. Kiemle, David L. Bryce, Wiley, 2014, 8th Edition.

Semester-IV

Course Name: Research Project-II

Course Code: OCHRP-699

Course type: Project

Total contact hours: 120 h (12 h/Week)

Credits: 06

Marks: 150

Course Outcomes:

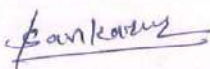
At the end of the course, the student will be able to:

1. Know how to carry out literature survey by using various search engines and database
2. Handle various chemicals, solvents, instruments and others
3. Perform reactions, monitoring by TLC
4. Purification techniques
5. Understand the structure of organic compounds by using spectral techniques

Research project will be assigned to the students on the basis of theory components, such as Multicomponent reactions, use of ionic liquids/surfactants in organic synthesis, Microwave/ Ultrasound assisted synthesis of bioactive molecules etc.

Literature Survey, Studies of Reactions, Synthesis, Mechanism, Standardization of Reaction Conditions, New Synthetic Methods etc

Note: Student should participate in National/International Conference and Present the project work.



Professor & Head
Department of Chemistry,
Dr. Babasaheb Ambedkar Marathwada University,
Chhatrapati Sambhajnagar - 431004.

**DR. BABASAHEB AMBEDKAR MARATHWADA UNIVERSITY,
CHHATRAPATI SAMBHAJINAGAR**



NAAC Re-accredited 'A' Grade

Department of Chemistry

FACULTY OF SCIENCE & TECHNOLOGY

Two Years P.G. Programme in Chemistry

(M. Sc. Physical Chemistry Semester III & IV)

As Per National Education Policy-2020

Course structure and Curriculum

(OBE with Choice Based Credit System)

Subject : Chemistry
Specilization : Physical Chemistry

Effective From :2024-25

Sankarwar

Professor & Head
Department of Chemistry,
Dr. Babasaheb Ambedkar Marathwada University,
Chhatrapati Sambhajinagar - 431004.

PREFACE

National Education policy 2020 has been intensely debated policies come into existence. In January, 2020 UGC has given the guideline for Learning outcome based curriculum framework (LOCF) work towards more holistic experience for the students. while focussing not just on knowledge delivery in higher education but also on the application of knowledge through field and laboratory work and emphasis on application of knowledge to real life experiences, LOCF is student-centric education in the context of development of personal, social, professional and acquired knowledge requirements in their career and life building, which focuses on measuring student performance through outcomes. It includes the knowledge, skills and attitudes enhancement in the students.

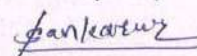
The aspects of LOCF is all-round development of the students, skill acquisition outside chosen subjects and research were undetermined but NEP has changed all of these in one stroke. The prominent features of the NEP framework are:

- Student centric education
- Flexibility in postgraduate programmes
- Multiple entry and exit points
- Skill based & outcome base education
- Credit based evaluation system
- Academic bank credits

It also focuses on evaluation of outcomes of the program by considering the knowledge, skill and behaviour of a students after completion of two year program. The educational triangle of Teaching-Learning and Evaluation process is the unique features of the OBE approach. The curriculum practices such as Competency based curriculum, Tailor-made curriculum development, spades, curriculum principles, Blooms Taxonomy and further use of assessment methodologies like, Norm-reference testing and Criterion reference testing, etc is being practiced since decades. It is also interesting to know that, globally, different countries and universities adopts the curriculum development models/approaches such as, CDIO (Conceive-Design-Implement-Operate), Evidence based education systems approach, etc as the scientific and systematic approaches in curriculum design.

Maharashtra state government and the authorities of Dr. Babasaheb Ambedkar Marathwada University, Chhatrapati Sambhajnagar has decided to implement National Education policies -2020 from the academic year 2023-24 for postgraduate program with outcome based education

As per guideline of OBE the department has prepared curriculum for Master of science in chemistry with specialization Inorganic chemistry, Organic Chemistry, Physical Chemistry and self-supported Analytical Chemistry. The OBE syllabus will help to improve the quality and employability of the Post-graduates of the university department.



Professor & Head
Department of Chemistry
Dr. Babasaheb Ambedkar
Marathwada University,
Chhatrapati Sambhajnagar

Professor & Head
Department of Chemistry,
Dr. Babasaheb Ambedkar Marathwada University,
Chhatrapati Sambhajnagar - 431004.

1. **Vision of Department :**
A respectable teaching- learning and research organization nationally and internationally in the area of chemical sciences by providing competitive trained chemists which will assist the chemical world, industries and stake holders.
2. **Mission Department :**
 - To bring sustainable progress of society by nurturing chemistry with responsibilities
 - To create and maintain programs of excellence in the areas of research , education and public outreach
 - Department will produce students who are knowledge in chemistry and can think critically.
 - To develop the researcher and scientist in chemical science through post-graduate education and research programme.
 - To develop the competent manpower with technology based experimentation methodologies and value based practices for business and industries.
 - To undertake projects to solve field base problems.
 - To provide student centric learning facilities for the development of overall personality of learner.
3. **Eligibility Criteria :**
4. **Assessment and Evaluation :**
5. **Duration of Course Programme : Two years**
6. **Credit Allotted for two year master programme in chemistry :88 Credit**
Semester - I : 22
Semester -II : 22
Semester -III : 22
Semester -IV : 22
7. **Program Educational Objectives:**
The program educational objectives (PEO's) are the statement that describes the career and professional achievement after the program of studies (post-graduation). The PEO's are driven form the Mission statement (What is the purpose of organization). The PEO's can be minimum three and maximum five.
 - PEO1:**To have advanced knowledge of chemistry domain.
 - PEO2:**To provide the professional services to industry, Research organization and institutes.
 - PEO3:**To provide the professional consultancy and research support for therelevant organization in the domain of super specialization.
 - PEO4:** To opt for higher education, disciplinary & multi-disciplinary research and to be a life-long learner.
 - PEO5:** To provide, value based and ethical leadership in the professional and social

life.

8. **Program Outcomes:**

The program outcomes (PO's) are the statement of competencies/ abilities. POs are the statement that describes the knowledge and the abilities the post-graduate will have by the end of program studies.

i). In-depth and detailed functional knowledge of the fundamental theoretical concepts and experimental methods of chemistry.

ii). Apply/implement interface between on the one hand, the history of chemistry and natural science and, on the other hand, issues pertaining to the areas of modern technology, health, and environment.

iii). Skills in planning and conducting advanced chemical experiments and applying structural-chemical characterization techniques.

iv). Skill in examining specific phenomena theoretically and/or experimentally.

v). Generation of new scientific insights or to the innovation of new applications of chemical research.

9. **Course Program outcome**

Course Program Outcomes are developed through the curriculum (curricular/co-curricular-extra-curricular activities). The program outcomes are attained through the course implementation. As an educator, one must know, **"To which POs his/her course is contributing?"** So that one can design the learning experiences, select teaching method and design the tool for assessment.

Professor & Head
Department of Chemistry
Dr. Babasaheb Ambedkar Marathwada University,
Chhatrapati Sambhaji Nagar - 431004

M.Sc. Physical Chemistry Semester-III Course Structure

Sr. No.	Course Code	Course Name	Teaching (Hr/W)	Credits Assigned	Conti.I nter.As smen.	End. Sem. Exam	Total Marks
Course type : DSC-Major Mandatory:							
1.	PCHTC-600	Structural Elucidation by Spectral Methods	4	4	40	60	100
2.	PCHTC-601	Thermodynamics	4	4	40	60	100
3.	PCHTC-602	Electrochemistry -I	2	2	20	30	50
4.	PCHLC-603	Physical Chemistry Laboratory Course	4	2	20	30	50
5.	PCHLC-604	Physical Chemistry Laboratory Course	4	2	20	30	50
Course Type : DSE (Choose any two from pool of the course):							
6.	PCHTE -605	Solid State Chemistry	2	2	20	30	50
7.	PCHTE -606	Electrochemistry II	2	2	20	30	50
8.	PCHTE -607	Nuclear Chemistry	2	2	20	30	50
9.	PCHTE -608	Chemical Mathematics and Computer Programming	2	2	20	30	50
Course Type :Research Project:							
10.	PCHRP-649	Research Project -I	8	4	40	60	100
Total			32	22	220	330	550

Course code Nomenclature :

DSC-Discipline Specific Core , **DSE**- Discipline Specific Elective, **T**-Theory, **L**- Laboratory course, **PCHT**- Physical Chemistry Theory Core , **PCHLC**- Physical Chemistry Laboratory Core , **PCHTE**- Physical Chemistry Theory Elective **PCHRP**- Physical Chemistry Research Project

Sankar
Professor & Head
 Department of Chemistry,
 Dr. Babasaheb Ambedkar Marathwada University,
 Chhatrapati Sambhajinagar - 431004.

Course Name: Structural Elucidation by Spectral Methods

Semester : III

Course type : DSC-15

Course Code: PCHTC-600

Total contact hours : 60 Hrs **Theory Credit: 4**

4 Hrs/ Week

Marks : 100

Course outcomes:

On completion of this course, the students will be able:

1. Students will review elementary concepts of nuclear magnetic resonance spectroscopy and delve into spin-spin couplings, factors affecting coupling constants, and spin systems like AB, AX, and ABX.
2. They'll also explore techniques such as INEPT, INADEQUATE, and the Nuclear Overhauser effect.
3. Students will grasp elementary concepts of ^{13}C -nuclear magnetic resonance spectroscopy, including chemical shifts for various carbon types and the impact of substituents on these shifts.
4. They'll also address instrumental challenges associated with ^{13}C -NMR spectroscopy.
5. Students will understand the fundamentals of mass spectrometry, including ion production methods, ion analysis, factors affecting fragmentation, and the interpretation of mass spectra.
6. They'll explore fragmentation patterns for various functional groups and phenomena like the molecular ion peak and McLafferty rearrangement.
7. Students will grasp the principles of Mössbauer spectroscopy, understanding factors influencing line position and shape, including the isomer effect and quadrupole splitting.
8. They'll also delve into Electron Spin Resonance spectroscopy, analyzing hyperfine splitting, zero field splitting, and instrumentation in varied applications.
9. Students will integrate UV, IR, ^1H NMR, ^{13}C NMR, and Mass Spectroscopy data to solve complex problems in structural elucidation and compound identification.

Unit-I : Nuclear Magnetic Resonance Spectroscopy (^1H NMR)

12Hrs

Elementary ideas (Recapitulation); Spin-spin couplings, Different types of couplings, factors affecting on coupling constants, Karplus equation, Spin systems (AB, AX, ABX, AMX), Rate processes, spin decoupling, shift reagents, Nuclear Overhauser effect (NOE), INEPT and INADEQUATE.

Unit-II : ^{13}C -Nuclear Magnetic Resonance Spectroscopy

12Hrs

Elementary ideas, instrumental problems, chemical shifts (aliphatic, olefinic, alkyne, aromatic, heteroaromatic and carbonyl carbons); Effect of substituents

on chemical shifts.

Unit-III : Mass Spectroscopy

12Hrs

Introduction, ion production (EI, CI, FD and FAB), ion analysis, ion abundance, factors affecting on fragmentation, fragmentation of different functional groups, molecular ion peak, isotopic peaks, metastable peak, Nitrogen rule, McLafferty rearrangement, Retro-Diels-Alder reaction.

Unit-IV :

12Hrs

Problems based on joint applications of UV, IR, ^1H NMR, ^{13}C NMR and Mass spectroscopy.

Unit- V :Mossbauer Spectroscopy

12Hrs

Principle, factors affecting the line position and shape, isomer effect and Quadrupole splitting iron salt like compounds, complexes, carbonyl compounds (temperature dependence of isomer shift and Quadrupole splitting in simple compound and coordination, polynuclear complexes), Numericals. **Electron Spin Resonance Spectroscopy:** Introduction, principle of ESR spectroscopy, presentation of spectrum, hyperfine splitting in various structures, hyperfine splitting diagram of representative examples, factors affecting the magnitude of 'g' values, Zero field splitting, Kramer's degeneracy, Anisotropy in the hyperfine coupling constant, electron delocalization, instrumentation and applications.

References Books

1. Introduction to Spectroscopy: D. L. Pavia, G. M. Lampman, G. S. Kriz
2. Spectrometric Identification of Organic Compounds: R. M. Silverstein & F. X. Webster
3. ^{13}C NMR Spectroscopy: G. C. Levy, R. L. Lichter, G. L. Nelson
4. Spectroscopic Methods in Organic Chemistry: D. H. Williams & I. Fleming
5. Organic Structure Analysis: Philips Crews
6. Structural Methods in Inorganic Chemistry: E. A. V. Ebsworth & D. W. H. Rankin
7. Physical Methods for Chemistry: R. S. Drago
8. Coordination Chemistry vol. I: E. Martell
9. Coordination Chemistry by Experimental Methods: K. Barger
10. Mass Spectrometry: K. G. Das & James
11. Absorption Spectroscopy of Organic Compounds: V. M. Parikh

Semester : III

Course Name: Thermodynamics

Course Code: PCHTC-601

Course type : DSC-16

4 Hrs/ Week

Total contact hours : 60 Hrs Theory Credit: 4

Marks : 100

Course outcomes:

On completion of this course, the students will be able:

1. **Understanding Fundamental Principles:** Understand microstates vs. macrostates and how macroscopic properties emerge. Learn statistical ensembles (microcanonical, canonical, grand canonical) and their uses.
2. **Probability and Statistics:** Apply probability theory to particle distributions and energy levels. Calculate statistical averages to predict macroscopic properties.
3. **Classical and Quantum Statistics:** Apply Boltzmann statistics to classical systems. Understand and apply Fermi-Dirac and Bose-Einstein statistics to quantum systems of fermions and bosons.
4. **Thermodynamic Quantities and Relations:** Use partition functions to link microscopic properties to macroscopic quantities. Utilize thermodynamic potentials (internal energy, Helmholtz free energy, Gibbs free energy, and enthalpy).
5. **Applications to Physical Systems:** Analyse ideal gases using classical and quantum mechanics. Calculate heat capacity of solids with Einstein and Debye models. Describe phase transitions and critical phenomena, including order parameters and critical exponents, using statistical mechanics.
6. **Experimental and Practical Applications:** Apply statistical thermodynamics to real systems (gases, solids, liquids, plasmas). Interpret experimental data to validate theoretical models with empirical observations.

Unit-I : Introduction

12Hrs

Ensembles-canonical, grand canonical and micro canonical Combinatorial problems, Thermodynamics probability and most probable distribution, Stirlings approximation, distribution laws, the law of equipartition of energies. Quantum statistics- Max Well-Boltzmann, Bose-Einstein and Fermi-Dirac, limit and applicability of various distribution laws.

Unit-II : Molecular Partition function

12Hrs

Partition function, Expression for translational, rotational, vibrational and electronic partition functions, Third law of thermodynamics and partition function, Numerical problems.

Unit-III : Application to chemical systems

12Hrs

Partition function and Thermodynamic functions, Sackur-Tetrode equation (derivation), determination of equation of state of an ideal gas. Internal rotation, residual entropies, heat capacity of solids: Einstein model, Debye modification (model), characteristic temperature, statistical mechanics of solutions ideal and nonideal.

Unit-IV : Applications to quantum systems

12Hrs

Nuclear spin statistics, ortho and para nuclear states, ortho and para hydrogen. Fermi energy, Fermi energy of electron gas in metals, Planck's distribution law and radiation, Bose-Einstein degenerate gas (He gas).

Unit-V : Irreversible Thermodynamics

12Hrs

Postulates, entropy production in heat, entropy production in matter flow, entropy production in chemical reactions, Onsager's theory, microscopic reversibility and Onsager's reciprocity, stationary states and entropy production, Prigogine's principle of minimum entropy, application to thermoelectric effects-Seebeck and Peltier effect.

References Books

1. Statistical Thermodynamics, Donald A. Mc Quirrie, Harper & Row, New York 1973.
2. Statistical Thermodynamics, M.C. Gupta, Wiley Eastern Ltd. New Delhi.
3. Elements of Statistical Thermodynamics, L. K. Nash Addison Wesley, Menlo Park, 1972.
4. Physical chemistry, P. W. Atkins, ELBS
5. Non Equilibrium Thermodynamics, Prigogine Kalyani Publication.
6. Thermodynamics and Non Equilibrium Thermodynamics, Gurudeep & Raj.

Course Name: Electrochemistry

Course Code: PCHTC-602

Course type : DSC-17

2 Hrs/ Week

Total contact hours : 30 Hrs Theory Credit: 2

Marks: 50

Course outcomes:

On completion of this course, the students will be able:

1. Fundamentals: Understand oxidation, reduction, and redox reactions.
2. Describe galvanic and electrolytic cells. Use electrode potentials and Nernst equation.
3. Understand bio-electrochemistry and electrocatalysis principles.
4. Explain biological redox reactions, enzyme electrochemistry, electrode design, and nanomaterials.
5. Study biosensors, biofuel cells, catalytic mechanisms, and applications in medicine and environment. Practice safety and ethics.
6. Students will define polarization and overvoltage in electrochemical systems, differentiate between types like hydrogen and metal overvoltages, and analyze their influencing factors.
7. They'll also describe experimental methods, understand Tafel theory, and solve numerical problems related to electrode kinetics.

Unit-I : Oxidation - Reduction Systems:**10Hrs**

Oxidation potentials, reversible ox-red systems, determination of standard ox-red potentials, variation of ox-red potential, ox-red equilibria, ox-red systems in analytical chemistry, ox-red indicators, two stage ox-red , semiquinone formation constant. Numericals.

Unit-II :Bio- electrochemistry and Electrocatalysis:**10Hrs**

Donnan membrane equilibrium, membrane potential, theories of membrane potential, introduction to electrocatalysis, relative power of electrocatalysts, mechanism of electrocatalysis, bioelectro catalysis, immobilization, application of enzymes on electrodes.

Unit-III : Polarization and Overpotentials:**10Hrs**

Polarization, concentration polarization, decomposition potentials, over voltage, hydrogen, oxygen and metal overvoltages, types of overvoltages, factors affecting overvoltages, experimental determination of decomposition potential and overvoltage, Tafels theory and Tafel equation, simultaneous deposition of metals .Numericals.

References Books

1. Modern Electrochemistry, Vol 1,2A and 2B, John O" M Bokris
2. An Introduction to Electrochemistry, Samuel Glasstone.
3. Theoretical Electrochemistry, L.Antropov.
4. Advanced Physical Chemistry, Gurtu and Gurtu.
5. Principles of Physical Chemistry, Puri,Sharma and Pathania.
6. Text Book of Physical Chemistry, S. Glasstone
7. Physical Chemistry, Robert J. Silbey.
8. Physical Chemistry, G.K.Vemulapalli.
9. Physical Chemistry, Maron and Pruton.
10. Physical Chemistry, P.W. Atkins

Semester : III

Course Name: Physical Chemistry Laboratory Course

Course Code: PCHLC-603

Course type : DSC-18

4 Hrs/ Week

Total contact hours :60 Hrs Lab. Work Credit: 2

Marks : 50

Course outcomes:

On completion of this course, the students will be able:

1. Students will gain proficiency in spectrophotometer operation, experimental design, and data analysis, utilizing these abilities for quantitative analysis and interdisciplinary chemistry applications.
2. They'll develop a comprehensive understanding of spectroscopic techniques and their relevance in various scientific disciplines beyond chemistry.
3. Students will learn to determine the percentage of two optically active substances in a mixture.
4. Investigate complex ion formation between Fe(II) and thiocyanate ion.
5. Explore the effect of chloride ion substitution on the rate constant of cane sugar inversion using different catalysts
6. Students will determine refractive indices of salt solutions, analyzing to find salt concentrations in unknown solutions.
7. They'll also investigate refractive index variations in carbon tetrachloride-ethyl acetate mixtures, determining compositions and molar refractions of unknown mixtures, enhancing skills in quantitative analysis and experimental design.
8. Students will determine the critical solution temperature of phenol-water with various additives, constructing phase diagrams for ethanol-benzene-water systems.
9. They'll also find equilibrium constants for tri-iodide formation and complex formulae of cupric ion-ammonia complexes using distribution methods, enhancing skills in thermodynamics and analytical chemistry.

List of experiments

Spectroscopy:

1. To determine the indicator constant pK_{in} of an indicator by using half height method (Bromo cresol purple)
2. To determine the concentration of Fe(II) and Cu(II) by spectrophotometric titration with EDTA.
3. To investigate the reaction kinetics between $K_2S_2O_8$ and KI by spectrophotometrically.

4. To determine simultaneously the dichromate and permanganate ions in the given solution.

Polarimetry:

5. Determine the percentage of two optically active substances in a mixture.
6. To investigate the complex ion formation between Fe(II) and thiocyanate ion.
7. Investigate the effect of substitution of chloride ions on rate constant of inversion of cane sugar by using mono, di and trichloro acetic acid as catalyst.

Refractometry:

8. Determine the refractive indices of series of solution of a salt and determine the concentration of the salt in the given unknown solution.
9. Study the variation of refractive indices with composition of mixture of carbon tetrachloride and ethyl acetate and determine the composition and molar refraction of the given unknown mixture.

Phase equilibria

10. Determine the critical solution temperature of phenol and water in presence of
1) 1% NaCl 2) 0.5% naphthalene 3) succinic acid. Construct the phase diagram of three-component system containing ethanol benzene and water.
11. Determine the equilibrium constant of the tri-iodide formation in aqueous solution by distribution method.
12. Determine the formula of the complex formed between cupric ion and ammonia by distribution method.

References Books

1. Systematic experimental physical chemistry – S.W. Rajbhoj and T. K. Chondhekar
2. Experiments in chemistry – D.V. Jahagirdar

Course Name: Physical Chemistry Laboratory Course

Course Code: PCHLC-604

Course type : DSC-19

4 Hrs/ Week

Total contact hours :60 Hrs Lab. Work Credit: 2

Marks : 50

Course outcomes:

On completion of this course, the students will be able:

1. Students will titrate ferrous ammonium sulfate with ceric sulfate to find formal redox potentials of $\text{Fe}^{2+}/\text{Fe}^{3+}$ and $\text{Ce}^{3+}/\text{Ce}^{4+}$ systems.
2. They will titrate phosphoric acid potentiometrically against NaOH to calculate pK_1 , pK_2 , and pK_3 .
3. Students will determine standard free energy changes (ΔG°), equilibrium constants for reactions, and activity coefficients of silver ions using a concentration cell without transference.
4. Students will determine the proton-ligand and metal-ligand stability constants of organic acids and their complexes via pH measurements.
5. They will calculate the Hammett constant of substituted benzoic acids, the dissociation constant of acetic acid, and the hydrolysis constant of aniline hydrochloride through pH analysis of various mixtures.
6. Study surfactant effects on water's surface tension and determine the alcohol molecule's limiting cross-sectional area using a stalagmometer.
7. Analyze surface tension using parachor measurements.
8. Students will determine the partial molar volumes of ethanol and water in a mixture through density measurements.
9. They will measure the heat of neutralization for strong acids and the heat of ionization for weak acids using calorimetry. Additionally, they will determine the integral heat of solution for KNO_3 .

List of experiments**Potentiometer:**

1. Titrate ferrous ammonium sulphate with ceric sulphate and find out formal redox potential of $\text{Fe}^{2+}/\text{Fe}^{3+}$ and $\text{Ce}^{3+}/\text{Ce}^{4+}$ system.
2. Titrate potentiometrically phosphoric acid solution against NaOH and calculate pK_1 , pK_2 and pK_3 of the acid.
3. To determine the standard free energy changes ΔG° and equilibrium constant for reaction



4. Determine the activity coefficient of silver ions using a concentration cell without transference.

pH metry:

5. To determine the proton-ligand stability constant of an organic acid and the metal-ligand stability constant of its complex by pH measurements.
6. Determine the Hammett constant of a given substituted benzoic acid by pH measurements.
7. Determine the pH values of various mixtures of sodium acetate and acetic acid in aqueous solution and hence find out the dissociation constant of the acid.
8. To determine the hydrolysis constant of aniline hydrochloride by pH measurements.

Surface Tension:

9. Study the effect of surfactant (n-propyl alcohol) at various concentrations on the surface tension of water and hence determine the limiting cross sectional area of alcohol molecule by stalagmometer.
10. To study the effect of surfactant on surface tension of water by parachor of a solid by stalagmometer.

Thermodynamics:

11. Determine the partial molar volume of ethanol and water in a given composition by density measurements.
12. To determine heat of neutralization of strong acid and heat of ionization of weak acid calorimetrically.
13. To determine the integral heat of solution of KNO_3 .

References Books

1. Systematic Experimental Physical Chemistry – S.W. Rajbhoj and T. K. Chondhekar
2. Experiments In Chemistry – D.V. Jahagirdar

Course Name: Solid State Chemistry

Course Code: PCHTE-605

Course type : DSE-9

2 Hrs/ Week

Total contact hours : 30Hrs Theory Credit: 2

Marks : 50

Course outcomes:

On completion of this course, the students will be able:

1. Students will understand general principles and classifications of solid-state reactions, Wagner reaction mechanism, nucleation laws, and nuclei growth.
2. They'll explore improving solids' reactivity, co-precipitation, kinetics, and factors affecting solid-state reactivity.
3. They'll learn principles and methods for growing single crystals, including slow evaporation, cooling, solvent and reactant diffusion, sublimation, and seed crystals.
4. Students will understand perfect and imperfect crystals, point defects, stoichiometric (Schottky and Frenkel) and nonstoichiometric defects, including thermodynamics of formation, color centers, metal excess and deficiency defects.
5. They will also study line imperfections, edge and screw dislocations, Burger's circuits, and surface imperfections like grain boundaries and stacking faults.
6. Students will learn free electron theory, band theory, and metal band structures.
7. They'll understand insulators, semiconductors, x-ray generation, interaction, scattering, diffraction, Bragg's law, Miller indices, instrumentation, and methods like Bragg's, single crystal, and Debye-Scherrer.
8. They'll explore unit cell identification, structure determination, structure factor, phase problem, lattice plane indexing, NaCl and KCl structures, Avogadro's number, and x-ray diffraction applications.

Unit-I : Solid State Reactions and Imperfections in solids**10Hrs**

General Principles, Classification, Wagner reaction mechanism, Laws governing nucleation, Growth of nuclei, improving reactivity of solids, co precipitation as a precursor to solid state reactions, Kinetics of solid state reactions, factors affecting the reactivity of solid state reactions.

Perfect and imperfect crystal, Point defects, Stiochiometric defects, Schottky and Frenkel defects. Thermodynamics of their formation, colour centers. Nonstoichiometric defects. Metal excess and metal deficiency defects. Line imperfections, edge dislocation and screw dislocation, Burger's circuits. Surface imperfection, grain boundaries and stacking faults.

Unit-II : Semiconductors and their devices

10Hrs

Intrinsic and extrinsic semiconductors, semiconductors materials and their fabrication, semiconductors devices p-n junctions, properties of p-n junctions, semiconductors diode as rectifier, Filters circuits, Zener diode as a voltage stabilizer, transistors transistor as an amplifier Super conductivity: conventional super conductors, organic super conductors (organic metals), fullerece, high temperature super conductors, organic charge transfer complexes Applications.

Unit-III : Theories of solid state and properties of solids

10Hrs

Free electron theory, Conduction by free electrons, Band theory, refinement to simple band theory, band structure of metals. Insulator and semiconductors. Generation of x-rays, interaction of X-rays with matter, scattering and diffraction, Bragg's law, Miller indices, General instrumentation, Bragg's method, single crystal method, Debye-Scherrer method, Identification of unit cells from systematic absences, x-ray, Phase problem. Indexing of lattice planes in a cubic system, structure of NaCl and KCl, applications of x-ray diffraction.

References Books

1. Solid State chemistry and its Applications-A. R. West (John Wiley and sons)
2. Principles of Solid State –H.V. Keer (Wiley Eastern Limited)
3. Material science and Engineering-V.Raghavan (prentice Hall of India)
4. Principles of Electronics- V.K.Metha (S.Chand and co.)
5. Industrial chemistry –B.K. Sharma (Goel publishing House)
6. Engineering chemistry –P.C. Jain and M. Jain (Shanpat Rai and Sons)
7. X-ray Structure Determination A Practical Guide, 2nd edition George H. Stout and Lyle H. Jensen, John Wiliey& Sons, New York, 1989.
8. Crystals and Crystal Growing, Alan Holden and Phylis Singer, Anchor Books Doubleday, New York, 1960
9. The growth of crystals from liquids J.C. Brice, North Hollond/American Elesvier(1973)
10. Chemistry of imperfect crystal-F.A. Krogen

Course Name: Electrochemistry

Course Code: PCHTE-606

Course type : DSE-10

2 Hrs/ Week

Total contact hours : 30 Hrs Theory Credit: 2

Marks : 50

Course outcomes:

On completion of this course, the students will be able:

1. Students will grasp metal electrogrowth, ion surface diffusion, and factors influencing cathodic deposition.
2. They'll understand electrochemical dissolution, passivity theories, anodic dissolution, and electroplating mechanisms, including applications and numerical problem-solving in electrodeposition processes.
3. Students will understand storage cell varieties like batteries, evaluating cell performance through charging and discharging.
4. They'll explore classical and modern batteries, including zinc-air, nickel-metal oxide, and lithium batteries, examining their characteristics and applications.
5. Students will explore the history and efficiency of fuel cells, including hydrogen-oxygen, phosphoric acid, direct methanol, and biochemical fuel cells.
6. They'll also learn about solar cells, understanding their principles, operation, and advantages.
7. Students will study electrochemical gas sensors, exploring their application in detecting CO₂, N₂, and nitrate reduction.
8. They'll also delve into agricultural electrochemistry, examining its relevance and potential contributions to sustainable farming practices.

Unit-I :Electrodeposition**10Hrs**

Introduction, the electrogrowth of metals on electrodes , the reaction pathway for electro deposition, surface diffusion of ions, cathodic deposition of metals from solutions, factors affecting cathodic deposition of metals, electrochemical dissolution and passivity of metals, anodic dissolution of metals, film and adsorption theories of passivity.

Electroplating of metals, mechanism, throwing power of an electroplating bath, factors affecting throwing power, typical electrodeposition processes, and applications of electroplating of metals. Numericals.

Unit-II :Conversion and storage of electrochemical energy**10Hrs**

Introduction of storage cells, fuel cells, solar cells Types of storage cells

(batteries), measure of cell performance, charging and discharging, introduction of classical batteries, modern batteries –zinc-air, nickel-metal oxide and lithium batteries.

Brief history of fuel cells, efficiency of fuel cells, hydrogen-oxygen fuel cell, phosphoric acid fuel cell, direct methanol and biochemical fuel cells;

Solar cells introduction, principle and working of solar cells, advantages.

Unit-III : Environmental Electrochemistry

10Hrs

Electrochemical gas sensors, Electrochemical CO₂, N₂, Nitrate reduction, Agricultural electrochemistry, Electrochemical studies on pesticides and insecticides.

References Books

1. Modern Electrochemistry, Vol 1,2A and 2B, John O" M Bokris
2. An Introduction to Electrochemistry, Samuel Glasstone.
3. Principles of Physical Chemistry, Puri, Sharma and Pathania.
4. Theoretical Electrochemistry, L. Antropov.
5. Physical Chemistry, P.W. Atkins
6. Physical Chemistry, Maron and Pruton.
7. Physical Chemistry, G.K. Vemulapalli.
8. Physical Chemistry, Robert J. Silbey.

Course Name: Nuclear and Radiochemistry

Course Code: PCHTE-607

Course type : DSE-11

2 Hrs/ Week

Total contact hours : 30Hrs Theory Credit: 2

Marks : 50

Course outcomes:

On completion of this course, the students will be able:

1. Students will explore the shell model, periodicity in nuclear properties, and forces of nuclear potential, including energy levels in potential wells and nuclear configuration.
2. They'll also study the liquid drop model, Fermi gas model, radioactive elements, decay kinetics, detection methods, and decay theories.
3. Students will understand nuclear reaction definitions, energetics, and threshold energies, along with reaction characteristics, conservation laws, and cross sections.
4. They'll explore compound nucleus theory, optical and direct interaction models, and specific reactions like photonuclear, evaporation, spallation, and thermonuclear reactions.
5. Students will grasp radiation-matter interactions, including primary effects, linear energy transfer (LET), Bremsstrahlung, and Cherenkov radiation.
6. They'll explore electron, neutron, heavy charged particle, and gamma ray interactions with matter, along with isotopic preparations, radiochemical principles, and applications as tracers in various fields.

Unit-I : Nuclear Models and Radioactivity

10Hrs

The shell model and its salient features, periodicity in nuclear properties- magic numbers, forces of nuclear potential, energy level in nuclear potential well, the sequence of filling the orbital including models, nuclear configuration. The liquid drop model, and its details and The Fermi gas model.

Historical, background, natural radioactive elements, general characteristics of α , β , γ rays, detection and measurement of radioactivity, the theory of radioactive disintegration, decay kinetics, units of radioactivity, parent daughter growth relationship- secular and transient equilibrium, theory of α decay, β decay – energetics of β decay problems of β decay, fermis theory of β decay, nuclear de-excitation – emission, numerical

Unit-II :Nuclear Reactions

10Hrs

Definition and Bethes notation, nuclear reaction energetic, nuclear reaction and threshold energy, characteristics of nuclear reactions, types of nuclear reactions, conservation in nuclear reactions, nuclear reactions cross section, cross section and reaction rate, the compound nucleus theory, general properties of compound nucleus, optical model, direct interaction model, specific nuclear reactions- photonuclear reactions, stripping and pickup reactions evaporation, spallation, fragmentation, direct nuclear reactions, thermonuclear reactions.

Unit-III : Radiation chemistry and its applications

10Hrs

Introduction of radiation with matter, primary effects due to charged particle/radiation, Linear energy transfer(LET), Bethes equation for LET, Bremsstrahlung, the cerenkov radians, interactions of electron with matter, interaction of neutrons with matter, interaction of heavy charged particles with matter, interaction of rays with matter, units for measuring radiation absorption, absorption in water.

Typical reactions involved in the preparations of isotopes: the scillard-chalmers reactions, radiochemical principles in the use of tracers, typical application of radioisotopes as tracers- chemical investigation, physio-chemical research, analytical applications, agricultural applications, industrial applications, use of nuclear radiations, radioisotope as a source of electricity.

References Books

1. Source of Atomic energy by s. Glasstance, D. Van Nostrand co. INC.
2. Essentials of nuclear chemistry by H.J. Arnikar 4th Edn, New Age International(p) Ltd.
3. Introduction to Nuclear By chemistry B. G. Harvey,
4. Nuclear chemistry by M. G. Arora & M. Singh Anmol publication, New Delhi
5. Elements of nuclear chemistry by A. K. Srivastav, P. C. Jain, S. Chand & Co.
6. A text book of Nuclear chemistry by C.V. ShekarDeminant publication & distribution, New Delhi.
7. Radiochemistry & nuclear chemistry, 3rd edn G. chappin, Butterwerth Heinemann.

Course Name: Chemical Mathematics and Computer Programming **Course Code: PCHTE-608**

Course type : DSE-12

2 Hrs/ Week

Total contact hours : 30Hrs Theory Credit: 2

Marks : 50

Course outcomes:

On completion of this course, the students will be able:

1. Students will understand functions, differential and integral calculus, including limits, derivatives, and their physical significance.
2. They'll explore differentiation rules, maxima, minima, and applications in chemistry, along with exact and inexact differentials, Taylor/Maclaurin series, curve sketching, partial differentiation, integration rules, and exponential/Gaussian function integrals.
3. Students will comprehend vectors, dot/cross products, and matrix algebra, including addition, multiplication, inverses, adjoints, and transposes.
4. They'll explore determinants, unit/diagonal matrices, and their applications in mathematical operations and problem-solving.
5. Students will grasp hardware/software concepts, binary/decimal numbers, constants/variables, and basic programming constructs like assignment, flow charts, IF statements, loops, input/output formatting, subroutines, algorithms, and an introduction to programming languages.

Unit-I : Chemical Mathematics

10Hrs

Functions, differential and integral calculus, limits, derivative, physical significance, basic rules of differentiation, maxima and minima, applications in chemistry, exact and inexact differential, Taylor and McLaurin series, curve sketching, partial differentiation, rules of integration, definite and indefinite integrals, integral involving exponential and Gaussian functions

Unit-II : Matrices And Determinants

10Hrs

Vectors, matrices and determinants Vectors, dot, cross and triple products, introduction to matrix algebra, addition and multiplication of matrices, inverse, adjoint and transpose of matrices, unit and diagonal matrices

Unit-III : Elements of Computer Programming

10Hrs

Hardware and software, binary and decimal numbers, constants and variables, assignment statement, flow chart and their use, IF and GO TO statements, Do loops. Input, output and format statements, Subroutines,

function subprograms, Algorithms, Introduction to programming languages

References Books

1. The Chemical Maths Book, E. Steiner, Oxford University Press (1996).
2. Mathematical Preparation for Physical Chemistry, F. Daniels, McGraw Hill.
3. Computer programs for chemistry D. F. Detar W. A. Benjamin Inc, New York Vol. 1-3 (1968-69).
4. Computer and Chemistry: introduction to programming and numerical methods T. R. Dickson, Freeman (1968).
5. Computer Programming in Fortran-90 V. Rajaraman, Prentice Hall, New Delhi (1990).
6. Computers and Common Sense R. Hunt and Shelley, Prentice Hall, New Delhi (1998).
7. Maths for Chemists, Volumes 1 and 2, Martin C. R. Cockett and Graham Doggett, Royal Society of Chemistry , Cambridge (2003).

Semester : III

Course Name: Research project-1

Course Code: PCHRC-649

Course type : Research project

8 Hrs/ Week

Total contact hours : 120Hrs

Theory Credit: 4

Marks : 100

Course outcomes:

On completion of this course, the students will be able:

- 1.
- 2.
- 3.
- 4.
- 5.
- 6.
- 7.
- 8.
- 9.

Professor & Head
Department of Chemistry
Dr. B. R. Ambedkar National University
Chhatrapati Sambhaji Maharaj - 431004

M. Sc. Physical Chemistry Semester-IV Course Structure

Sr. No.	Course Code	Course Name	Teaching (Hr/W)	Credits Assigned	Conti.I nter. Assmen.	End. Sem Exam	Total Marks
Course Type :DSC-Major Mandatory:							
1.	PCHTC-650	Chemical Dynamics and Catalysis	4	4	40	60	100
2.	PCHTC-651	Polymer Chemistry	4	4	40	60	100
3.	PCHTC-652	Nanochemistry-I	2	2	20	30	50
4.	PCHLC-653	Physical Chemistry Laboratory Course	4	2	20	30	50
Course Type : DSE (Choose any two from pool of the course):							
5.	PCHTE -654	Nanochemistry-II	2	2	20	30	50
6.	PCHTE -655	Surface and Magnetochemistry	2	2	20	30	50
7.	PCHTE -656	Advanced Quantum Chemistry	2	2	20	30	50
8.	PCHTE -657	Biophysical Chemistry	2	2	20	30	50
Course type :Research Project:							
9.	PCHRP -699	Research Project -2	12	6	40	60	150
Total			32	22	220	330	550

Course code Nomenclature :

DSC-Discipline Specific Core DSE- Discipline Specific Elective, T-Theory, L- Laboratory course, PCHTC- Physical Chemistry Theory Core , PCHLC- Physical Chemistry Laboratory Core , PCHTE- Physical Chemistry Theory Elective, PCHRP- Physical Chemistry Research Project


Professor & Head
Department of Chemistry,
Dr. Babasaheb Ambedkar Marathwada University,
Chhatrapati Sambhajinagar - 431004.

Course Name: Chemical Dynamics and Catalysis

Course Code: PCHTC-650

Course type : DSC-20

4 Hrs/ Week

Total contact hours : 60 Hrs Theory Credit: 4

Marks : 100

Course outcomes:

On completion of this course, the students will be able:

1. Students will comprehend various types of reactions such as opposing, parallel, competitive, consecutive, and chain reactions, including hydrogen-oxygen reactions and polymerization kinetics.
2. They will also explore how temperature influences reaction rates.
3. Students will explore diffusion-controlled reactions, substitution and correlation effects, including the Hammett equation and Taft effects, alongside electron and proton transfer reactions.
4. They'll examine ion-dipole and dipole-dipole interactions and pressure's influence on reaction rates, supplemented with numerical problem-solving.
5. Students will explore the law of photochemical equivalence, various photocatalytic reactions such as photooxidation, photoreduction, degradation, and chemiluminescence, alongside photosynthesis, with additional practice in numerical problem-solving.
6. Students will grasp the introduction and mechanism of catalysis, including acid-base and micellar catalysis, enzyme kinetics, autocatalysis, and oscillatory reactions, supplemented with numerical problem-solving.
7. Students will explore unimolecular and bimolecular surface reactions, considering temperature effects, transition state theory, and heterogeneous catalysis.
8. They'll also examine catalyst preparation, characterization, and applications.

Unit-I :Kinetics of Complex Reactions**12Hrs**

Opposing or reversible reactions, parallel and competitive reactions, consecutive reactions, chain reactions, branched chain reactions and explosions, hydrogen-oxygen reactions, kinetics of polymerization-step wise and free radical polymerization Effect of temperature on rates of simple and complex reactions. Numericals

Unit-II :Reactions in Solution**12Hrs**

Diffusion controlled reactions, substitution and correlation effect, Hammett equation, Taft effects, compensation effect. Electron transfer reactions, proton transfer reactions. Ion dipole and dipole-dipole interactions.

Influence of pressure on rate in solution. Numericals

Unit-III : Photochemical Reactions

12Hrs

Introduction, low of photochemical equivalence, photocatalytic reactions, types of photocatalytic reactions, photooxidation, photoreduction, photosensitization, photocatalytic degradation. Chemiluminescence, photosynthesis. Numericals

Unit-IV : Homogeneous Catalysis

12Hrs

Introduction, mechanism of catalysis, Acid-base catalysis, effect of pH on rate constant. Micellar catalysis, enzyme catalysis, factors governing rate of enzyme reactions, kinetics of enzyme catalysed reactions. Autocatalysis and oscillatory reaction, Lotka-Volterra mechanism, the brusselator, the eragonator, bistability, chemical chaos. Numericals

Unit- V : Surface Reactions and Heterogeneous Catalysis

12Hrs

Unimolecular surface reactions, bimolecular surface reactions, effect of temperature on heterogeneous reactions, transition state theory and the rates of surface reactions, theory of heterogeneous catalysis, structure of solid surfaces, absolute rates of desorption's, electronic theories of chemisorption and heterogeneous catalysis. Preparation and characterization of catalysts, applications.

References Books

1. Chemical kinetics- E.S.Laidler Pearson Education
2. Kinetics and Mechanism Of Chemical Transformations. Rajaram Macmillan India Ltd J.C.Curiacose.
3. Physical chemistry- Atkin and D.Paula, Oxford University press
4. Physical chemistry- Berry, Rice, Ross Oxford University press
5. Physical chemistry-principles And Appllication in Biological Sciences - Tinoco, Sauer Pearson Education.
6. Physical chemistry-W.J.Moore.
7. Chemical kinetics and Reaction Mechanism -F-Wilkinson-VanNostralReinhdd
8. Chemical kinetics and Reaction dynamics -Bul Houston

Semester : IV

Course Name: Polymer Chemistry

Course Code: PCHTC-651

Course type : DSC-21

4 Hrs/ Week

Total contact hours : 60 Hrs Theory Credit: 4

Marks : 100

Course outcomes:

On completion of this course, the students will be able:

1. Students will comprehend the chemical bonds and properties of water in biological systems, thermodynamic principles, amino acid properties, nucleic acid structures, protein structure-function relationships, and nucleotide composition.
2. They'll also grasp electrophoresis principles, types, and applications in genetic analysis, DNA sequencing, and foot-printing.
3. Students will understand the formation and classification of synthetic high polymers, including chain and step polymerization reactions.
4. They'll also learn about methods for determining molar masses, such as viscosity, osmometry, ultracentrifugation, light scattering, and diffusion.
5. Students will comprehend various polymerization mechanisms including free radical, ionic, and coordination polymerization, along with the role of Ziegler-Natta catalysts.
6. They'll also explore step polymerization processes like polycondensation, polyaddition, and ring opening, as well as electrochemical and group transfer polymerization techniques.
7. Students will understand the mechanisms of free radical, anionic, and cationic polymerization, as well as copolymerization processes and their applications in polymer synthesis.
8. Students will grasp the theories of electronic conduction in conducting polymers, including band theory and hopping conduction, as well as doping mechanisms and stimuli-sensitive properties.
9. They'll explore applications such as photovoltaic devices, sensors, LEDs, solar cells, and batteries.

Unit-I : Fundamentals of Biological Macromolecules **12Hrs**

Chemical bonds in biological systems; Properties of water; Thermodynamic principles in biological systems; Properties and classification of amino acids; Structures of nucleic acids, Protein structure and function, Properties of nucleosides and nucleotides, Composition of nucleic acids, Electrophoresis, Factors affecting on Electrophoretic Mobility; Types of Electrophoresis; Free electrophoresis and Gel electrophoresis; Electrophoresis in genetic analysis; DNA Sequencing and DNA foot Printing.

Unit-II : Macromolecules **12Hrs**

Introduction, Formation of synthetic high polymers classification, Polymerization reactions: Chain and Step. Average molecular weight, Number average weight, Methods of determination of molar masses of polymers; Viscosity, Osmometry, Molar mass of charged macromolecules, Donnan membrane equilibrium, Ultracentrifugation, light scattering, Diffusion.

Unit-III : Chemistry of Polymerization **12Hrs**

Chain polymerization: free radical polymerization, ionic polymerization, coordination polymerization, Ziegler-Natta catalysts. Step Polymerization: polycondensation, polyaddition, ring opening, electro chemical polymerization, group, Transfer polymerization, Polymerization techniques.

Unit-IV : Kinetics of Polymerization **12Hrs**

Free radical chain polymerization, Anionic polymerization, Cationic polymerization, Copolymerization, Free radical copolymerization, Ionic copolymerization, Copolycondensation.

Unit-V : Electronically Conducting Polymers **12Hrs**

Introduction, Theories of electronic conduction; Band theory of conduction, Hopping conduction, Super conduction, Mechanism of conduction, Doping mechanism, p-type, n-type, auto doping, Stimuli sensitive (smart) polymers, pH and temperature sensitive smart polymers, Applications: Photovoltaic devices, Sensors, LED and Solar cells, Electro chemical devices, Batteries etc.

References Books

1. Cantor, C. R. and Schimmel Biophysical Chemistry Vols. 1-3, W. H. Freeman (1980).
2. Polymer Science and Technology. By Premamoy Ghosh.

3. Lehninger, A.L., Nelson, D. L. and M. M. Lehninger, Principles of Biochemistry 4th Ed., W. H. Freeman (2004).
4. U. Satyanarayana; Biochemistry.
5. Upadhyay; Biophysical Chemistry.
6. L. Stryer, Biochemistry, 5th Edition, (2002) Freeman and Co. New York.
7. D. Voet, J. G. Voet, Biochemistry 3rd Edition (2004), Wiley International Publication.
8. D. L. Nelson and M. M. Cox, Lehninger Principles of Biochemistry 3rd Edition (2002) McMillan North Publication.

Course Name: Nanochemistry-I

Course Code: PCHTC-652

Course type : DSC-22

2 Hrs/ Week

Total contact hours : 30Hrs Theory Credit: 2

Marks : 50

Course outcomes:

On completion of this course, the students will be able:

1. Students will learn nanoparticle synthesis via physical methods like high energy ball milling, melt mixing, and physical vapor deposition.
2. They'll explore advanced techniques like ionized cluster beam deposition, laser methods, sputter deposition, electric arc deposition, and chemical vapor deposition (CVD).
3. Students will study colloids, their interactions with mediums, and charge effects, learning synthesis and growth of nanoparticles by various methods.
4. They'll explore the Langmuir-Blodgett method, sol-gel method, and electrochemical techniques.
5. Students will learn about various microscopes including SEM, TEM, SPM, STM, and AFM, alongside X-ray diffraction, UV-visible, and IR spectroscopy.
6. They will understand their applications and operational principles.

Unit-I : General introduction & synthesis of nanomaterials by physical methods 10Hrs

Objective of study, synthesis of nanoparticles by physical method, mechanical methods- high energy ball milling, melt mixing, method based on evaporation, physical vapour deposition with consolidation. Ionized cluster beam deposition. Laser vaporization, Laser pyrolysis, sputter deposition, electric arc deposition, Chemical Vapour Deposition (CVD).

Unit-II : Synthesis of Nanomaterials by Chemical Methods**10Hrs**

Introduction, colloids and colloids in solution, interaction of colloids and medium, colloids in vacuum, colloids in medium, effect of charge on colloids, steric repulsion, synthesis of colloids, growth of nanoparticles, synthesis of metal and semiconductor nanoparticles by colloidal route, Langmuir-Blodgett (L-B) method, sol gel method, electrochemical method.

Unit-III : Analysis Technique**10Hrs**

Introduction, microscopes, electron microscopes, SEM, TEM, Scanning probe microscope (SPM), Scanning Tunnelling microscope, Atomic force microscope, X-ray diffraction, UV-visible and IR spectroscopy.

References Books

1. Nanotechnology: Principles and practices- Sulabha K. Kulkarni (capital Pub. Co.)
2. NANO- The next revolution –Mohan SurendraRajan(Natioinal book Trust, India)
3. Fundamental of Nanotechnology – Gabor L. Hornyak, John J. Moore, Harry F. Tibbals, Joydeep Dutta.
4. Recent advances in the liquid phase synthesis of Inorganic Nanoparticles- B. LCushing,
5. V. L. Kolesmichenko&C.J.O".Connor Chemical Review 104, 3893-3946.(2004)
6. Hand book of Thin film technology- H. R. Khan.
7. Thin film phenomenon- K. N. Chopra. Mcgrawa Hill publication
8. Material Science deposition & structure –Milton.

Semester : IV

Course Name: Physical Chemistry Laboratory Course

Course Code:PCHLC-653

Course type : DSC-23

4 Hrs/ Week

Total contact hours :60 Hrs Lab. Work Credit: 2

Marks : 50

Course outcomes:

On completion of this course, the students will be able:

1. Students will determine the pK_{in} of an indicator using the half-height method and analyze Fe(II) and Cu(II) concentrations via spectrophotometric titration.
2. They will also investigate reaction kinetics between $K_2S_2O_8$ and KI and simultaneously determine dichromate and permanganate ions in a solution.
3. Students will determine the percentage of optically active substances in a mixture and investigate chloride ion substitution effects on cane sugar inversion rate.
4. They will also study Fe(II) and thiocyanate ion complex formation.
5. Students will investigate ionic strength effects on the $K_2S_2O_8$ and KI reaction rate and determine reaction order using substitution, fractional change, and differential methods.
6. They will also study the kinetics of bromic acid-hydrochloric acid and acetone iodination reactions.
7. Students will determine the critical solution temperature of phenol and water with additives and construct a phase diagram for ethanol, benzene, and water.
8. They will also determine the equilibrium constant of tri-iodide formation and the formula of the cupric ion-ammonia complex using distribution methods.

List of Experiments:

Spectroscopy:

- 1) To determine the indicator constant pK_{in} of an indicator by using half height method (Bromo cresol purple) (DVJ-200)
- 2) To determine the concentration of Fe(II) and Cu(II) by spectrophotometric titration with EDTA.
- 3) To determine simultaneously the dichromate and permanganate ions in the given solution.
- 4) To investigate the reaction kinetics between $K_2S_2O_8$ and KI by spectrophotometrically (TKC-223)

Polarimetry:

- 5) Determine the percentage of two optically active substances in a mixture.(TKC-

194).

- 6) Investigate the effect of substitution of chloride ions on rate constant of inversion of cane sugar by using mono, di and trichloro acetic acid as catalyst.
- 7) To investigate the complex ion formation between Fe(II) and thiocyanate ion.

Chemical Dynamics

- 8) Investigate the influence of ionic strength on the rate constant of the reaction between $K_2S_2O_8$ and KI.(TKC-335)
- 9) Determine the order of a reaction by I) substitution method, (II) fractional change method and (III) differential method.
- 10) Investigate the reaction between bromic acid and hydrochloric acid.(TKC-335)

- 11) Investigate the kinetics of iodination of acetone.

Phase equilibria

- 12) Determine the critical solution temperature of phenol and water in presence of
1) 1% NaCl 2) 0.5% naphthalene 3) succinic acid
- 13) Construct the phase diagram of three-component system containing ethanol benzene and water.
- 14) Determine the equilibrium constant of the tri-iodide formation in aqueous solution by distribution method.
- 15) Determine the formula of the complex formed between cupric ion and ammonia by distribution method.

References Books

1. Systematic experimental physical chemistry – S.W. Rajbhoj and T. K. Chondhekar
2. Experiments in chemistry – D.V. Jahagirdar

Course Name: Nanochemistry –II

Course Code: PCHTE-654

Course type : DSE-13

2 Hrs/ Week

Total contact hours : 30Hrs Theory Credit: 2

Marks : 50

Course outcomes:

On completion of this course, the students will be able:

- 1) Students will explore the mechanical, electrical, optical, magnetic, electrochemical, and photochemical properties of nanomaterials.
- 2) They will analyse how these properties differ from bulk materials.
- 3) Students will study special nanomaterials such as carbon nanotubes, porous silicon, aerogels, and zeolites.
- 4) Applications include electronics, energy, automobiles, sports, textiles, cosmetics, biotechnology, medical, space, defence, and environment.
- 5) Students will learn about thin films, including deposition by chemical and electrochemical reactions, chemical vapor deposition of inorganic thin films, and chemical etching.

Unit-I : Properties of Nanomaterials**10Hrs**

Properties of nanomaterials – Mechanical, Electrical, Optical, Magnetic, Electrochemical and Photochemical properties

Unit-II : Some Special Nanomaterials and Application of Nanomaterials**10Hrs**

Some special nanomaterials – Carbon nanotubes, porous silicon, Aerogels, Zeolites.

Application – Electronic, energy automobiles, sport and toys, textile, cosmetics, domestic appliances, biotechnology, medical, space, defence & environment.

Unit-III : Thin films**10Hrs**

Introduction, deposition by chemical reactions, deposition by electrochemical reaction, chemical vapor deposition of inorganic Thin films, chemical etching.

References Books

1. Nanotechnology: Principles and practices- Sulabha K. Kulkarni (capital Pub. Co.)
2. NANO- The next revolution –Mohan SurendraRajan(Natioinal book Trust, India)
3. Fundamental of Nanotechnology – Gabor L. Hornyak, John J. Moore,

- Harry F. Tibbals, Joydeep Dutta.
4. Recent advances in the liquid phase synthesis of Inorganic Nanoparticles- B. LCushing,
 5. V. L. Kolesmichenko & C.J.O". Connor Chemical Review 104, 3893-3946.(2004)
 6. Hand book of Thin film technology- H. R. Khan.
 7. Thin film phenomenon- K. N. Chopra. Mcgrawa Hill publication
 8. Material Science deposition & structure –Milton.

Course Name: Surface and Magnetochemistry

Course Code: PCHTE-656

Course type : DSE-14

2 Hrs/ Week

Total contact hours : 30Hrs Theory Credit: 2

Marks : 50

Course outcomes:

On completion of this course, the students will be able:

- 1) Students will understand surface chemistry concepts such as adsorption and Langmuir's unimolecular theory, including the statistical derivation of Langmuir's adsorption isotherm and the BET theory.
- 2) Students will comprehend colloids, their properties, and specific characteristics such as electrical properties, including the origin and behaviour of charges, and electrokinetic properties like electrophoresis.
- 3) They'll explore applications and perform numerical exercises to determine colloidal particle size.
- 4) Students will grasp the definition of magnetic properties, types of magnetic behavior, and sources of paramagnetism, including Pascal's constants and their applications.
- 5) They'll also learn to determine magnetic susceptibility through numerical exercises.

Unit-I : Surface Chemistry**10Hrs**

Adsorption, adsorption isotherms, Langmuir's unimolecular theory of adsorption statistical derivation of Langmuir's adsorption isotherm, BET theory of multilayer adsorption and its determination

Unit-II : Colloidal state of Matter**10Hrs**

Introduction to colloids, classification, properties, specific properties like, electrical properties, charge on colloidal particles, origin of charge, electrical double layer, electrokinetic properties, electrophoresis, electroosmosis, streaming potential, sedimentation potential, determination of size of colloidal particles, applications of colloids, Numericals.

Unit-III : Introduction to Magnetochemistry**10Hrs**

Definition of magnetic properties, types of magnetic behaviour, sources of paramagnetism, Pascal's constants and its applications, Determination of magnetic susceptibility. Numericals.

References Books

1. K.J.Laidler, J.H.Meiser and B.C. Sanctuary, Physical Chemistry, Houghton

- Mifflin Company, New York, 2003.
2. R.I.Dutta and Syamal, Elements of magnetochemistry
 3. A.W. Adamson, Physical Chemistry of Surfaces, 4 th edition, Interscience, New York, 1982.
 4. A.R.West, Solid State Chemistry and its Applications, John Wiley and Sons, 2003(reprint 2009)
 5. S.Glasstone, Text book of Physical Chemistry.
 6. A.Earn Shaw, Introduction to Magnetochemistry, Academic Press.
 7. Gurdeep and Raj, Advanced Physical Chemistry.
 8. H.V.Keer, Principles of Solid State.

Course Name: Advanced Quantum Chemistry	Semester : IV
Course type : DSE-15	Course Code: PCHTE-656
Total contact hours : 30Hrs	2 Hrs/ Week
Theory Credit: 2	Marks : 50

Course outcomes:

On completion of this course, the students will be able:

- 1) Students will understand energy and wave-function corrections for degenerate states, applied to scenarios like the Stark effect, hydrogen atom, anharmonic oscillators, and particle in a box.
- 2) They'll also explore time-dependent perturbation theory applications.
- 3) Students will comprehend the Hartree-Fock theory including Slater determinants, antisymmetry postulates, and computational aspects such as basis sets and UHF methods.
- 4) They will also learn about Slater-Condon rules, Hartree-Fock equations, and related theorems like Koopman and Brillouin.
- 5) Students will review the Huckel and extended Huckel methods, along with semi-empirical theories like CNDO/INDO, MINDO, AM1, and PM3.
- 6) They'll compare these methods and explore their computational aspects and applications in predicting molecular properties.

Unit-I : Perturbation Theory **10Hrs**

Energy and wave-function corrections to wave-function degenerate states, applications including stark effect, hydrogen atom, anharmonic, - quartic oscillators, particle in a box- ground and excited states, time dependent perturbation theory

Unit-II : HartreeFock Theory **10Hrs**

Slater determinants, Postulate of antisymmetry, Slater- Condon rules for matrix elements, Hartree-Fock equations, Koopman and Brillouin theorems, Roothaan formulation, basis sets, computational aspects, UHF method, PopleNesbet equations

Unit-III : Semi-empirical Theories **10Hrs**

Recapitulation of Huckel method, extended Huckel method, ZDO approximation, CNDO/INDO methods, Molecular Properties, Computational aspects, MINDO, AM1, PM3 methods, comparison of these methods

References Books

1. Modern Quantum Chemistry, A. Szabo and N.L. Ostlund, Dover, New York (1996)
2. Approximate Molecular Orbital Theory, J. A. Pople and D. L. Beveridge, McGraw Hill, New York (1971)
3. Molecular Modeling, A. Leach, Longman, London (1996)
4. Density Functional Theory of Atoms and Molecules, R. G. Parr and W. Yang, Oxford University Press, Oxford (1989)

Semester : IV

Course Name: Biophysical Chemistry

Course Code: PCHTE-658

Course type : DSE-16

2 Hrs/ Week

Total contact hours : 30Hrs Theory Credit: 2

Marks : 50

Course outcomes:

On completion of this course, the students will be able:

- 1) Students will study biomolecules such as carbohydrates, lipids, proteins, nucleic acids, enzymes, and vitamins, along with their roles in cells.
- 2) They'll also learn about free energy changes in biochemical reactions, including exergonic, endergonic, and ATP hydrolysis reactions, and biological oxidation reactions.
- 3) Students will grasp the basic principles of centrifugation and become familiar with various types of centrifuges, including desktop, high-speed, and ultracentrifuges, and analytical centrifuges.
- 4) They'll also learn about rotors and the principles behind differential and density gradient centrifugation.
- 5) Students will understand the factors influencing electrophoretic mobility and different types of electrophoresis, including free, zone, and gel electrophoresis.
- 6) They'll explore applications like genetic analysis, DNA sequencing, and DNA footprinting using electrophoresis techniques.

Unit-I : Biomolecules and Bioenergetics

10Hrs

Biomolecules and the cells, carbohydrates, lipids, proteins and amino acids, nucleic acids and nucleotides, enzymes and vitamins, Free energy change in biochemical reactions, exergonic, endergonic, hydrolysis, ATP Biological oxidation reaction.

Unit-II : Centrifugation

10Hrs

Basic principle of centrifugation, Instrumentation, desktop centrifuges, high speed centrifuge, the ultracentrifuge, analytical centrifuges, rotors, differential, density gradient, analytical centrifugation.

Unit-III : Electrophoresis

10Hrs

Factors affecting electrophoretic mobility, types of electrophoresis, free electrophoresis, zone electrophoresis and gel electrophoresis, electrophoresis in genetic analysis, DNA sequencing and DNA footprinting.

References Books

1. U. Satyanarayana; Biochemistry.
2. Upadhyay; Biophysical Chemistry.
3. L. Stryer, Biochemistry, 5th Edition, (2002) Freeman and Co. New York.
4. Lehninger, A.L., Nelson, D. L. and M. M. Lehninger, Principles of Biochemistry 4th Ed., W. H. Freeman (2004).
5. Biophysical Chemistry.- M. Satake
6. Biostatistical Analysis- A. M. Mungikar

