MANONMANIAM SUNDARANAR UNIVERSITY

DEPARTMENT OF CHEMISTRY

STRUCTURE OF M.Sc. ORGANIC CHEMISTRY PROGRAM

For the academic year 2022-2023

1.VISION

To develop a Centre of Excellence for teaching as well a research at par with national and international standards. Reach a position of distinction by offering first-class education and serving the community in relevant areas of interest to the rural areas.

2. MISSION

- ✓ Provide an educational environment where students can realize their full potential in chemistry and attain quality education to face the challenges of the future.
- ✓ Provide a dynamic, challenging and ethical environment for pursuing high-quality teaching, learning, research and service.

3. Preamble

1. To impart training in Organic Chemistry at advanced level in a more holistic way and enthuse the students for the subject.
2. To train the students to make them confident and capable of accepting any challenge in Organic Chemistry.
3. To give a flavour of research in Organic Chemistry and train the students for research career.
4. To abreast the students about the current status and new developments in Organic Chemistry.
5. To make the students aware of the impact of Organic Chemistry on environment and imbibe the concept of sustainable developments.

4. Program Outcome

After completing the M.Sc. program the students will be able to

PO1 : Assimilate the impact of chemistry to solve problems in environmental (societal) context

PO2 : Understand the advanced concepts involved in chemistry

PO3 : Apply the principle/laws/ reactions in chemistry

PO4 : Acquire proficiency in laboratory skills

PO5 : Enrich with the knowledge and critical thinking to solve scientific problems

PO6 : Equip with standard and advanced procedures in analytical and spectral methods

PO7 : Expertise in laboratory techniques for industry-oriented jobs

PO8 : Skilled up fortheoretical and analysis in organic chemistry

PO9 : Execute innovative experiments, projects and techniques in medicinal fields

PO10 : Nurture constant leaning, moral values and professional ethics for our society

5. Program Specific Outcome

PS01 **:** MSU organic chemistry graduates will have the knowledge of fundamental concepts of Chemistry including physical, inorganic, analytical, nano science and in-depth in organic chemistry along with constant learning, human values and professional ethics.

PS02 **:** MSU Organic chemistry graduates will acquire additional knowledge and practical experience about the supramolecular & medicinal chemistry to work in Research institution and industries.

PS03 **:** MSU organic chemistry graduates will become proficient in drug designing, molecular modeling and operating advanced instrumentation techniques along with the standard methods and procedures.

6. Eligibility Norms

B.Sc. degree in Chemistry or any other equivalent Bachelor Degree is eligible for the admission in M.Sc. Chemistry program.

7. Internal Assessment

Distribution of marks between External and Internal Assessment is

- For Theory = 75: 25
- For Practical = 50 :50

Pass minimum of 50% for external and overall components.

Internal Marks for Theory shall be allotted in the following

The average of the best two from three compulsory tests.	15 Marks
Assignment	05 Marks
Seminar	05 Marks
TOTAL	**25 Marks**

Internal Marks for Practical shall be allotted in the following manner

Lab performance	25 Marks
Internal Test (Average of two test)	25 Marks
TOTAL	**50 Marks**

There is no internal passing minimum. There is a passing minimum of 50% for external and overall components.

8. Question Pattern

Scheme of Examination and question pattern

The question distribution as: Understand-35%, Apply-25%, Analyze-15%, Evaluate-15%, Create-10%

Time: 3 hours Max. marks:75

Part A	:	10 questions full of one or two sentence answer. Two questions from each unit of a paper. Each question carries one mark.	10 x1=10 marks
Part B	:	5 descriptive questions, of either a or b type (internal choice). One question is from each unit. Each question carries 5 marks	5 x 5 = 25 marks
Part C	:	5 descriptive type questions of either a or b type (internal choice). One question is from each unit. Each question carries 8 marks	5 x 8 = 40 marks

Course Weight:

In each of the courses, credits will be assigned on the basis of the lectures tutorials / lab work and other forms of learning in a 15 week schedule.

1. One credit for each lecture hr. per week
2. One credit for each tutorial hr. per week
3. One credit for every two hrs. of Lab or Practical Work per week

PROJECT

Project for IV semester shall be an individual project. Project evaluation will be done by Guide and another faculty member of the department. Viva voce Examination for the project students will be conducted jointly by the same examiners who evaluated the project report.

Course Structure for M.Sc Organic Chemistry Program

The credit and teaching hours of the program is distributed as under.

Sl. No.	Course Code	Papers	Credits	Hrs./ week
I Semester				
1	POCC11	Concepts of Organic Chemistry	4	4
2	POCC12	Inorganic Bonding & Reaction mechanism	4	4
3	POCC13	Quantum Mechanics	4	4
4	POCCPA	Thermodynamics (e- learning course)	4	4
5	POCEA-POCEH	Elective Paper –I	3	3
6	POCL11	Organic Chemistry Practical- I	2	4
7	POCL12	Organic Chemistry Practical– II	2	4
		Total	**23**	**27**
II Semester				
8	POCC21	Reaction and Mechanism of Organic Chemistry	4	4
9	POCC22	Organometallic Chemistry	4	4
10	POCC23	Analytical Chemistry	4	4
11	POCC24	Group Theory and Spectroscopy	4	4
12	MOOC	Supportive course paper I	3	3
13	POCL21	Physical Chemistry Practical – I	2	4
14	POCL22	Physical Chemistry Practical – II	2	4
15	POCVA21	Value added Course –Dyes and Pigments.	2(extra)	
		Total	**23**	**27**
III Semester				
16	POCC31	Organic Synthesis	4	4
17	POCC32	Electrochemistry	4	4
18	POCC33	Bio-inorganic chemistry	4	4
19	POCC34	Applications of organic Spectroscopy	4	4
20	MOOC	Supportive course Paper II	3	3
21	POCL31	Inorganic Chemistry Practical – I	2	4
22	POCL32	Inorganic Chemistry Practical– II	2	4
23	POCVA31/	Value added Course -Green energy and fuel/	2(extra)	

	POCVA32			
Total			**23**	**27**
IV Semester				
24	POC	Research Methodology	4	4
25	POCCPB	Supramolecular Chemistry	4	3
26	POCEA-POCEH	Elective Paper – III	3	3
		Elective Paper – III	3	3
27	POCL41	Advanced Organic practical	2	4
30	POC	Project	6	9
Total			**22**	**29**
Grand Total			**91**	**110**

Mapping -PO-PSO

Course Code	PO 1	PO 2	PO 3	PO 4	PO 5	PO 6	PO 7	PO 8	PO 9	PO1 0	PSO 1	PSO 2	PSO 3
POCC11	🟥	🟩	🟩		🟥						🟨		
POCC12	🟥	🟩	🟩		🟥			🟥			🟨		
POCC13	🟥	🟩	🟩		🟦		🟥		🟦		🟨		▨
POCCPA	🟥	🟩	🟩		🟩	🟥		🟥	🟥		🟨		
POCL11	🟥	🟩	🟩	🟩	🟦	🟩	🟩	🟦	🟦	🟩	🟨	🟪	▨
POCL12	🟥	🟩	🟩	🟩	🟦	🟩	🟩	🟦	🟦	🟩	🟨	🟪	▨
POCC21	🟥	🟩	🟩		🟥						🟨		
POCC22	🟥	🟩	🟩		🟩		🟦	🟥	🟦		🟨	🟪	
POCC23	🟩	🟩	🟩		🟦	🟦	🟦	🟦	🟦	🟥	🟨	🟪	▨
POCC24	🟥	🟩	🟩		🟥	🟩			🟦	🟥	🟨	🟪	▨
POCL21	🟥	🟩	🟩	🟩	🟦	🟩	🟩	🟦	🟦	🟩	🟨	🟪	▨
POCL22	🟥	🟩	🟩	🟩	🟦	🟩	🟩	🟦	🟦	🟩	🟨	🟪	▨
POCC31	🟥	🟩	🟩		🟦				🟥	🟥	🟨	🟪	
POCC32	🟥	🟩	🟩		🟩		🟦	🟥		🟥		🟪	▨
POCC33	🟥	🟥	🟥					🟩		🟦	🟨	🟪	
POCC34	🟥	🟦	🟥	🟦	🟩	🟩	🟩	🟩	🟩	🟩	🟨	🟪	▨
POCL31	🟥	🟩	🟩	🟩	🟦	🟩	🟩	🟦	🟦	🟩	🟨	🟪	▨
POCL32	🟥	🟩	🟩	🟩	🟦	🟩	🟩	🟦	🟦	🟩	🟨	🟪	▨
Research	🟩	🟩	🟩	🟦	🟩	🟩	🟩	🟩	🟩	🟩	🟨		
SUPRA	🟩	🟩	🟩		🟦		🟦	🟦	🟦	🟩	🟨	🟪	▨
POCL41	🟥	🟥	🟩	🟩	🟦	🟩	🟩	🟦	🟦	🟩	🟨	🟪	▨
POCEA	🟥	🟥	🟥		🟦	🟦	🟦	🟩	🟦	🟩	🟨	🟪	
POCEB	🟦	🟩	🟦	🟩	🟦			🟥	🟦	🟦	🟨	🟪	▨
POCEC	🟩	🟩	🟥		🟥	🟦	🟦	🟦	🟦	🟩		🟪	▨
POCED	🟥	🟥	🟦		🟦	🟩	🟦	🟩	🟩	🟩		🟪	▨
POCEE	🟥	🟥	🟦		🟦	🟩	🟦	🟩	🟩	🟩	🟨	🟪	▨
POCEF	🟩	🟥	🟦		🟦	🟥		🟦	🟦	🟩	🟨	🟪	
POCEG	🟩	🟥	🟦		🟦	🟥		🟦	🟦	🟩		🟪	▨
POCEH	🟩	🟥	🟦		🟦	🟥		🟦		🟥	🟨	🟪	
Project	🟩	🟥	🟦		🟦	🟥		🟦		🟥	🟨	🟪	

🟩 **Major Part**
🟦 **Significant**
🟥 **Small Extent**
🟨 **Scientific knowledge**
🟪 **Research and Job oriented**
▨ **Entrepreneurship / Innovation Technology**

SEMESTER - I

CONCEPTS OF ORGANIC CHEMISTRY

POCC11		
L (hrs)	**Credits**	**Course**
60	**4**	**Core**

Course Objectives:

1. To study the chemical bonding and structure of molecules
2. To study the mechanism of reactions
3. To understand the concept of Aromaticity and stability of molecules
4. To know about the Stereochemistry of molecules
5. To understand the concept of asymmetric synthesis of organic molecules

Course Prerequisites:

Student who have studied Organic Chemistry paper in B.Sc Chemistry.

Course Outcomes:

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

1. Remember the concept for interpreting reaction mechanisms.
2. Understand the concept of bond formation and breaking.
3. Analyse the stereochemistry and synthesis of various compounds and systems.
4. To design a new molecule using aromaticity and stereo chemistry
5. Solve the problems in aromaticity and stereo chemistry

Unit I Chemical Bonding and Structure: (12 hrs.)

Review of basic principles of structure and bonding, application of acid base concepts, Inductive effect – Mesomeric effect – Steric Inhibition of resonance – '$p\pi$-$d\pi$' bonding –hyperconjugation – cross conjugation – hydrogen bonding - acidity, basicity, factors affecting the strength of acids and bases - HSAB theory.Generation, structure, stability and reactivity of carbocations, carbanions, free radicals, carbenes and nitrenes.Effect of structure on reactivity.

Unit II Reaction Mechanism (12 hrs.)

Types of mechanisms, types of reactions, thermodynamic and kinetic requirements, Hammond postulate, Microscopic reversibility, Curtin-Hammett principle, transition states and intermediates, methods of determining mechanisms, isotopic effects.The Hammett equation and linear free energy relationship (sigma-rho) relationship, Taft equation.

Unit IIIAromaticity (12 hrs.)

Aromaticity and antiaromaticity, Hückel's rule, non-aromaticity, anti-aromaticity, homo-aromaticity n-annulenes, heteroannulene, Bonds weaker than covalent; addition compounds, inclusion compounds, crown ethers, cyclodextrins, catenanes and rotaxanes.

Unit IV Stereochemistry and conformation analysis (12 hrs.)

Conformational analysis of cycloalkanes, effect of conformation on reactivity. Elements of symmetry, chirality, molecules with more than one chiral center, projection formulae (i) Fischer (ii) Sawhorse (iii) Newman (iv) Flying Wedge; threo and erythro isomers, methods of resolution, optical purity, enantiotopic and diastereotopic atoms, groups and faces, stereospecific and stereoselective synthesis. Optical activity in the absence of chiral carbon-Biphenyl, allene and spiranes.

Unit VAsymmetric Synthesis (12 hrs.)

Chiral auxiliaries, methods of asymmetric induction – substrate, reagent and catalyst controlled reactions; determination of enantiometric and diastereomeric excess; enantio-discrimination. Resolution – optical and kinetic.Cram's rule, Prelog's rule-stereoselective and stereospecific synthesis.Cram's rule, Sharplessenantioselectiveepoxidation, hydroxylation, amino hydroxylation.

References

1. F. A. Carey and R. A. Sundberg, Advanced Organic Chemistry, Part A: Structure and Mechanisms, 5th Edition, Springer, New York,2007.
2. Stereochemistry of Carbon Compounds by E. J. Eliel, McGraw Hill, 2001
3. Organic Chemistry by S. H. Pine, McGraw Hill,1987
4. Stereochemistry of Organic Compounds by D. Nasipuri, Wiley1994.
5. Robert E. Gawley, Jeffrey Aube, Principles of Asymmetric Synthesis, pergamon, 2nd edition, 1996
6. V.K. Ahluwalia and R.K. Parashar, Organic Reaction Mechanisms, Narosa Publishing House, 2002.
7. Stereochemistry, D. G. Morris, RSC Tutorial Chemistry Text 1, 2001.
8. E. L. Eliel and S. H. Wilen, Stereochemistry of Organic Compounds, John Wiley & Sons, New York, 1994.
9. D. G. Morris, Stereochemistry, RSC Tutorial Chemistry Text 1, 2001

10. J. Kirby, Stereoelectronic effects, Oxford Chemistry Primers,2011.
11. Steric and Stereoelectronic Effects in Organic Chemistry, V. K. Yadav, Springer,2016.

COURSE OUTCOME MAPPING

	UNIT 1	UNIT 2	UNIT 3	UNIT 4	UNIT 5
CO1	**L2**	**L3**	**L1**		
CO2	**L3**	**L1**	**L1**		
CO3			**L1**	**L3**	**L3**
CO4		**L3**	**L3**	**L3**	**L2**
CO5			**L2**	**L3**	**L2**

L1: Addressed to small extent

L2: Addressed significantly

L3: Addressed Major Part

INORGANIC BONDING & REACTION MECHANISM

POCC12		
L (hrs)	**Credits**	**Course**
60	**4**	**Core**

Course Objectives:

1. To provide advanced concepts about bonding reactions and redox potentials of inorganic compounds
2. To introduce bonding concepts, magnetic spectra and optical behavior of coordination complexes
3. To disseminate knowledge on reaction mechanism of coordination complexes.

Course Prerequisites:

1. To know the significant of coordination chemistry
2. To have the knowledge of acids and bases

Course Outcomes:

At the end of the course Students are able to

1. Understand the structure and bonding of inorganic compounds.
2. Apply the concepts of acid and base theory, bonding in metal complexes
3. Examine the bonding by molecular orbital theory and VSPER
4. Analyse and present the concepts in transition metal complexes
5. Validate the knowledge and understand the electronic spectra

Unit I Bonding (12 hrs.)

Synthesis, Properties, structure and bonding of: Pseudo halogen, Interhalogen and Xenon compounds, Boranes, Carboranes, Metallocarboranes, Borazines, Phosphazenes, Sulfur-Nitrogen compounds, silicates.

Unit II Acid & Base (12 hrs.)

Redox Reactions: Latimer diagram, Electrochemical Series. Acids and Bases: Lewis acids and bases; HSAB concept. Transition Metal Chemistry: Nomenclature, Isomerism, Chelate effect, Macrocyclic ligands, thermodynamic stability, successive and overall stability constants, Irving-William series.

Unit III Structure & Bonding in coordination complexes (12 hrs.)

Bonding in Coordination Complexes: VSEPR theory, Crystal-Field theory, d-orbital Splitting in Octahedral, Tetrahedral, Square Planar geometries; Molecular Orbital Theory, p-bonding; Jahn-Teller effect, Spectrochemical series, nephelauxetic series. Electronic Spectra: d-d transitions, Orgel diagrams, charge-transfer spectra.

Unit IV Reaction Mechanism: **(12 hrs.)**

Substitution reaction in octahedral and square planar complexes; lability, trans-effect, Conjugate base mechanism, racemisation, Electron Transfer Reactions: inner sphere and outer sphere mechanism, application of electron transfer reaction in synthesis of coordination complexes.

Unit V Electronic Spectra **(12 hrs.)**

UV-Vis, charge transfer, colors, intensities and origin of transitions, interpretation, term symbols and splitting of terms in free atoms, selection rules for electronic transitions, calculation of Dq, B, C, Nephelauxetic ratio.

References

1. Inorganic Chemistry: Principles of Structure and Reactivity by J. E. Huheey, E. A. Keiter and R. L. Keiter, 4th ed. Pearson education, 2006.
2. Concepts and Models of Inorganic Chemistry by B. E. Douglas, D.H. Mc Daniel and J. J. Alexander, John Wiley, 1994, 3rded.
3. Physical Inorganic Chemistry: A Coordination Chemistry Approach by S.F.Kettle, Spektrum,1999, Oxford press.
4. Chemistry of the Elements by N. N. Greenwood and A. Earnshaw, Pergamon, Reprinted 2005.
5. Advanced Inorganic Chemistry by F. A. Cotton, G. W. Wilkinson, 5thedition, John-Wiley & Sons,1999.
6. Introduction to Magneto chemistry by A. Ernshaw, Academic press, 2013

COURSE OUTCOME MAPPING

	UNIT 1	UNIT 2	UNIT 3	UNIT 4	UNIT 5
CO1	**L3**		**L2**	**L1**	
CO2	**L2**	**L3**	**L1**		
CO3			**L3**	**L1**	**L1**
CO4	**L1**	**L1**	**L2**	**L2**	**L2**
CO5			**L3**	**L3**	**L3**

L1: Addressed to small extent

L2: Addressed significantly

L3: Addressed Major Part

QUANTUM MECHANICS

POCC13		
L (hrs)	**Credits**	**Course**
60	**4**	**Core**

Course Objectives:

1. To impart knowledge of advanced quantum mechanics for solving relevant physical problems
2. Use of mathematical concepts as a tool to understand atomic and molecular structure and properties as well as chemical reactivity

Course Prerequisites:

General Physical Chemistry, Fundamentals of Spectroscopy

Course Outcomes:

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

1. Define the postulates of quantum mechanics.
2. Apply the postulates of quantum mechanics to analyse Schrodinger equation
3. Solve time-independent and time-dependent Schrodinger equation for simple potentials
4. Use approximation method to solve many electrons system
5. Compile mathematical tools for quantum mechanical models

Unit – I: Quantum Mechanics – I (12 hrs.)

Postulates of quantum mechanics, Hermitian operators, Commutators and results of measurements in Quantum Mechanics. Eigen functions and eigen values of operators.

Unit – II: Quantum Mechanics – II (12 hrs.)

Solution of the Schrodinger equation for exactly solvable problems for bound states such as particle-in-a- box.

Unit – III: Quantum mechanics for H_2 atom and atomic orbital (12 hrs.)

Harmonic oscillator and rigid rotor, Solution of the Schrodinger equation for the hydrogen atom, radial and angular probability distributions, atomic orbitals and electron spin.

Unit–IV: Approximation methods (12 hrs.)

Perturbation theory and variation theorem Born-Oppenheimer approximation, VB and MO theory, H^{2+} , H_2 molecule problem, Hückel molecular orbital theory and its application to ethylene, butadiene and benzene.

Unit–V: Time dependent Mechanics (12 hrs.)

The time dependent Schrödinger equation. Co-ordinate and momentum space representation of operators and eigen states; Schrodinger and Heisenberg representations.

References:

1. Levine, N.I., Quantum Chemistry, Prentice Hall (2009) 6th ed.
2. Chandra, A.K., Introduction to Quantum Chemistry, Tata McGraw Hill (2004) 4th ed.
3. Atkins, P., Friedman, R., Molecular Quantum Mechanics, Oxford University Press, (2005) 4th ed.
4. Prasad, R.K., Quantum Chemistry, Wiley Easter (1992).
5. McQuarrie, D. A. Quantum Chemistry, Viva Books, India (2015).
6. McWeeny, R., Coulson's Valence, Oxford University Press, 3rd Ed., 1980.
7. Lowe J.P., Quantum Chemistry, Pubs: Academic Press, 1993.
8. Greimer, W. Quantum Mechanics : An Introduction, Springer, 3rd Ed.,1999.
9. McQuarrie, D. A. Quantum Chemistry, University Science books, 2nd Ed., 2008.
10. Bransden, B.H. and Joachain, C.J., Quantum Mechanics, Addison-Wesley. 2000.
11. Kreyszig, E., Advanced Engineering Mathematics, 5th edition, Wiley Eastern, 1989.
12. Arfken, G., Weber, H. J., Mathematical methods for Physicists, Prism Indian Edition,1995.
13. D. J. Griffiths, Introduction to Quantum Mechanics, Pearson Education, 2005.
14. Kuhn, H., Försterling, H.-D., Waldeck, D.H., Principles of Physical Chemistry, 2nd edition, Wiley,2009.
15. e-PG Pathshala – P-02- Physical Chemistry- I (Quantum Chemistry)
16. NPTEL link: **https://nptel.ac.in/courses/115101107**

COURSE OUTCOME MAPPING

	UNIT 1	UNIT 2	UNIT 3	UNIT 4	UNIT 5
CO1	**L3**	**L1**	**L1**		
CO2	**L2**	**L2**	**L2**	**L1**	**L1**
CO3		**L1**		**L1**	**L2**
CO4			**L1**	**L3**	**L2**
CO5	**L2**		**L2**	**L2**	**L3**

L1: Addressed to small extent

L2: Addressed significantly

L3: Addressed Major Part

THERMODYNAMICS (e- LEARNING)

POCCPA		
L (hrs)	**Credits**	**Course**
60	**4**	**Core**

Course Objectives

1. To study the fundamental concepts in thermodynamics, Chemical potential depend on temperature and pressure as well as how it co-exist in phase equilibria, chemical equilibrium and its relationship with thermodynamic quantities.
2. To understand basic concept of statistical thermodynamics with ensemble model and particle distribution of Boltzmann, Fermi-Dirac and Bose-Einstein model.
3. To apply the Canonical partition function for ideal gas of linear and nonlinear molecules
4. To examine the Canonical partition function for interacting particles.
5. To analyze the specific heat capacity of solid by Einstein and Debye model and evaluate electron distribution in metal and semiconductors by Fermi-Dirac and Bose-Einstein model.

Course Prerequisites

Students must study chemistry as major subject in B.Sc. Degree level.

Course Outcomes

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

1. Understand the importance of thermodynamic parameters.
2. Enumerate chemical potential for evaluating thermodynamic parameter.
3. Analyse ensembles and identify the molecular distribution.
4. Measure the intermolecular potential for real gas molecules.
5. Describe the concepts **S**tatistical thermodynamics.

Unit I Fundamental concepts of thermodynamics (12 hrs.)

Fundamental equations for open systems, Partial molar quantities and chemical potential, Chemical equilibrium, Phase behavior of one and two component systems, Ehrenfest classification of phase transitions.

Unit II Statistical Thermodynamics (12 hrs.)

Introduction, Concept of ensembles, partition functions and distributions, microcanonical, canonical and grand canonical ensembles, canonical and grand canonical partition functions, Boltzmann, Fermi-Dirac and Bose-Einstein distributions.

Unit III Thermodynamics of Ideal gases (12 hrs.)

Canonical partition function in terms of molecular partition function of non-interacting particles, Heat capacity (Cv, Cp) of an ideal gas of linear and nonlinear molecules, chemical equilibrium.

Unit IV Thermodynamics of Real gases (12 hrs.)

Canonical partition function for interacting particles, intermolecular potential (Lennard-Jones, Hard-sphere and Square-well) and virial coefficients. Temperature dependence of the second virial coefficient.

Unit V: Thermodynamics of solids & Metals (12 hrs.)

Solids: - Einstein and Debye models. T^3 dependence of heat capacity of solids at low temperatures (universal feature).

Metals: Fermi function, Fermi energy, free electron model and density of states, chemical potential of conduction electrons.

References

1. P. Atkins and J. Paula, Physical Chemistry, 10th Edition, Oxford University Press, Oxford,2014.
2. D. A. Mc Quarrie and J. D. Simon, Molecular Thermodynamics, University Science Books, California 2004.
3. R. S. Berry, S. A. Rice and J. Ross, Physical Chemistry, 2nd Edition, Oxford University Press, Oxford, 2007.
4. D. A. Mc Quarrie, Statistical Mechanics, University Science Books, California 2005
5. B. Widom, Statistical Mechanics - A Concise Introduction for Chemists, Cambridge, University Press, 2002.
6. Glasstone, Text Book of Physical Chemistry, 2nd Edition, Macmillan India Ltd, New Delhi , 1974.
7. e-PG Pathshala- P-06- Physical Chemistry.

COURSE OUTCOME MAPPING

	UNIT 1	UNIT 2	UNIT 3	UNIT 4	UNIT 5
CO1	**L3**	**L2**	**L2**		
CO2	**L2**	**L1**	**L1**		**L1**
CO3		**L3**	**L3**	**L1**	
CO4	**L1**			**L2**	**L3**
CO5		**L3**	**L3**	**L2**	**L3**

L1: Addressed to small extent

L2: Addressed significantly

L3: Addressed Major Part

ORGANIC CHEMISTRY PRACTICAL – I

POCL11		
P(hrs)	**Credit**	**Course**
60	2	Practical

Course objectives:

To know about the basic concept and to improve the practical knowledge of the students.

Course Prerequisites:

Students have done Organic Chemistry practicals inB.Sc Chemistry.

Course Outcomes:

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

1. List the properties of reagents/ solvents in laboratory.
2. Understand the method of preparations.
3. Apply the synthetic methods.
4. Determine the yield percentage of the reaction
6. Design a new methodology for synthesis of organic molecules.

Practicals

1. **Single stage preparations:**
    a. Diels – Alder Reaction, Bis – 2 – Naphthol, 1,2,3,4 – Tetrahydrocarbazole, Benzpinacol, Benzpinacolone, Aspirin, Phenol – formaldehyde resin, p – Nitroacetanilide, β – D – Glucopyranose, Fluorescein, p - Bromoacetanilide
2. **Two stage preparations:**
    a. Synthesis of Phthalamide, p – nitro aniline, p – Bromo aniline, m – nitrobenzoic acid

References

1. A. I. Vogel, a Text Book of Practical Organic Chemistry, 1989.
2. Ault, Techniques and Experiments for Organic Chemistry, 1998
3. N. K. Vishnoi, Advanced Practical Organic Chemistry, 1979.
4. Dey and M.V. Sitaraman, Laboratory Manual of Organic Chemistry, 2017.
5. Raj K. Bansal, Laboratory Manual in Organic Chemistry, 1994.

COURSE OUTCOME MAPPING

	EXPERIMENT 1	EXPERIMENT 2
CO1	L3	L3
CO2	L2	L2
CO3	L3	L3
CO4	L3	L3
CO5	L2	L1

L1: Addressed to small extent

L2: Addressed significantly

L3: Addressed Major Part

ORGANIC CHEMISTRY PRACTICAL – II

POCL11		
P(hrs)	**credit**	**Course**
60	2	Practical

Course objective:

To understand the basic concept and to enhance the technical skill of the students.

Course Prerequisites:

Students who have done Organic Chemistry practicals in B.Sc Chemistry.

Course Outcomes:

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

1. Classify the types of separation of organic binary mixtures
2. Identity the functional groups present in an organic compound.
3. Analyse the organic compounds
4. Determine the yield of organic derivatives.
5. Create a method for the qualitative and quantitative analysis of organic compounds

Practicals

1. Seperation and systematic analysis of Organic binary mixtures.
2. Estimation of phenol, aniline, methyl ethyl ketone, glucose.

References

1. A. I. Vogel, a Text Book of Practical Organic Chemistry, 1989.
2. Ault, Techniques and Experiments for Organic Chemistry, 1998
3. N. K. Vishnoi, Advanced Practical Organic Chemistry, 1979.
4. Dey and M.V. Sitaraman, Laboratory Manual of Organic Chemistry, 2017.
5. Raj K. Bansal, Laboratory Manual in Organic Chemistry, 1994.

COURSE OUTCOME MAPPING

	EXPERIMENT 1	EXPERIMENT 2
CO1	L3	
CO2	L2	L2
CO3	L3	L3
CO4	L2	L2
CO5	L1	L3

L1: Addressed to small extent

L2: Addressed significantly

L3: Addressed Major Part

SEMESTER – II

REACTION& MECHANISM IN ORGANIC CHEMISTRY

POCC21		
L (hrs)	**Credits**	**Course**
60	**4**	**Core**

Course objectives:

1. To study about the Aliphatic and aromatic nucleophilic substitution reactions
2. To study about the Aliphatic and aromatic electrophilic substitution reactions
3. To understand the concept of Free radical reactions
4. To know about the concept of substitution and addition reactions
5. To learn about the concept of elimination reactions

Course Prerequisites:

Students who have studied Organic Chemistry paper in B. Sc Chemistry.

Course Outcomes:

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

1. Remember the concept of substitution reactions.
2. Understand the types of elimination and addition reactions.
3. Analyse the types rearrangement in organic synthesis.
4. Create an idea to enhance the selectivity and reactivity of compounds.

Unit I Nucleophilic Substitution (12 hrs.)

AliphaticNucleophile Substitution: The S_N^2, S_N^1, mixed S_N^1 and S_N^2 and SET mechanisms. The neighbouring group mechanism.Classic al and nonclassicalcarbocations, phenonium ions, norbornyl system, common carbocation rearrangements.TheSN^i mechanism.Nucleophilic substitution at an allylic, aliphatic trigonal and a vinyl carbon. Reactivity effects of substrate structure, attaching nucleophile, leaving group and reaction medium.

Aromatic Nucleophile Substitution: The SNAr, SN^1, benzyne. Reactivity; effect of substrate structure, leaving group and attacking nucleophile.

Unit II Electrophilic Substitution (12 hrs.)

Aliphatic: Bimolecular mechanisms: SE^1, SE^2 and SE^i. The SE^1 mechanism, electrophilic substitution accompanied by double bond shifts. Effect of substrates, leaving group and the solvent polarity on the reactivity. Aromatic: The arenium ion mechanism, orientation and reactivity, energy profile diagrams. The ortho/para ratio, ipso attack, orientation in other ring systems. Quantitative treatment of reactivity in substrates and electrophiles.

Unit III Free Radical Reactions (12hrs.)

Types of free radical reactions, free radical substitution mechanism, mechanism at an aromatic substrate, neighbouring group assistance. Reactivity for aliphatic and aromatic substrates at a bridgehead.Reactivity in the attaching radicals.The effect of solvents on reactivity.

Unit IV Addition to Carbon-Carbon Multiple Bonds: (12 hrs.)

Mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals, regio- and chemo-selectivity, orientation and reactivity. Addition to cyclopropane ring.Hydroboration. Addition to Carbon-Hetero Multiple Bonds:Mechanism of metal hydride reduction of saturated and unsaturated carbonyl compounds, acids, esters and nitriles.

Unit V Elimination Reactions: (12 hrs.)

E^2, E^1 and E^1CB mechanisms and their spectrum. Orientation of the double bond. Reactivity effects of substrate structures, attaching base, the leaving group and the medium.

References:

1. Advanced Organic Chemistry by J. March, John Wiley & Sons,1992
2. Organic Chemistry by S. H. Pine, McGraw Hill, 1987.
3. Modern Synthetic Reactions by H. O. House, W.A. Benjamin, Inc.,1972
4. Understanding Organic Reaction Mechanism by A. Jacobs, Cambridge 1998.
5. Organic Chemistry by J. M. Horn back, Books Coley, 1998.
6. Organic Chemistry by P.Y. Bruice, Prentice Hall, 1998.
7. Organic Reaction and their Mechanism by P.S. Kalsi, New Age, 1996.

COURSE OUTCOME MAPPING

	UNIT 1	UNIT 2	UNIT 3	UNIT 4	UNIT 5
CO1	**L3**	**L3**	**L2**		
CO2			**L1**	**L3**	**L3**
CO3	**L2**	**L2**	**L2**	**L2**	**L2**
CO4	**L2**	**L2**	**L2**	**L2**	**L2**

L1: Addressed to small extent

L2: Addressed significantly

L3: Addressed Major Part

ORGANOMETALLIC CHEMISTRY

Course Objectives

POCC22		
L (hrs)	**Credits**	**Course**
60	**4**	**Core**

1. To study about the Classification of Organometallic compounds.
2. To understand the concept of alkene and alkyne system.
3. To study about the elimination and insertion reactions.
4. To know about the importance of Catalyst.
5. To learn about the fundamental process of transition metal complexes

Course Prerequisites:

A basic knowledge and understanding about inorganic chemistry and organometallic compounds studied in undergraduate level

Course Outcomes

On the successful completion of this course, student will able to

1. Know about the synthesis, structure and bonding of metal carbonyls, nitrosyls.
2. Understand the concept of alkene and alkyne complexes
3. To learn about the reaction mechanism of organometallic compounds
4. To know about the application of catalyst

Unit I Organometallic Compounds-1 (12 hrs.)

Definition, classifications and bonding in organometallic compounds. EAN rule and its correlation to stability of organometallic compounds - synthesis, structure and bonding of metal carbonyls, nitrosyls and dinitrogen complexes and halides; IR spectral characterization of carbonyls and nitrosyls

Unit II Organometallic Compounds-II (12 hrs.)

Pi acceptor complexes with alkene, alkyne, allyl and arene system: Bonding of alkenes to transition metal complexes - C-H activation of alkenes. Synthesis reactivity and bonding of alkyne allyl and arene complexes. Metallocenes; synthesis, properties, structure and bonding with particular reference to ferrocene and berryllocene.

Unit III Reaction Mechanisms of Organometallic Compounds (12Hrs)

Substitution reactions of carbonyls; oxidative addition and reductive elimination, migratory insertion and elimination reactions; nucleophilic and electrophilic attack of coordinated ligands; Reactivity- M-C bond cleavage reaction. Insertion of CO, alkene and alkynes.

Unit IV Organometallic Catalysis – I (12 hrs.)

Organometallic catalysts and the requirements; Terminology in catalysis - catalytic loop, Turnover, Turnover number (TON), Turnover frequency (TOF). Wilkinson's catalyst and hydrogenation reactions and its mechanism, Tolman's catalytic loop; hydroformylation (oxo) reaction, Wacker and Monsanto acetic acid processes. Cluster compound, and its classification.

Unit V Organometallic Catalysis – II (12 hrs.)

Water gas shift reactions-mechanism -and its application; Fischer Tropsch process and synthetic gasoline, The Heck Reaction, C-C coupling reaction, Suzuki process, The Stille Reaction, Oligomerizations, Lanthanoidocene Catalysts. Ziegler-Natta polymerization and its mechanism.

REFERENCES:

1. Inorganic Chemistry: Principles of Structure and Reactivity by J. E. Huheey, E. A. Keiter and R. L. Keiter, 4th Ed. Harper Collins 1993.
2. Concepts and Models of Inorganic Chemistry by B. E. Douglas, D.H. McDaniel, J. J. Alexander, John Wiley, 1993, 3rdEd.
3. Reaction Mechanism of Inorganic Chemistry and Organometallic system by R. R. Jordan Oxford Univ. Press, 2007. 2ndEd.
4. Advanced Inorganic Chemistry by F. A. Cotton and G. W. Wilkinson, John- Wiley & Sons, 1988, 5thEd.
5. Organometallics by Ch. Elschenbroich, VCH, 2006, 3rd Ed.
6. Organotransition Metal Chemistry: Fundamental Concepts and Applications by A. Yamamoto, John Wiley1986.
7. Organometallic Chemistry of the Transition Metals by R. H. Crabtree, John.John Wiley& Sons, April 11, 2014.
8. Basic Organometallic Chemistry, A.J Elias, January2013

COURSE OUTCOME MAPPING

	UNIT 1	UNIT 2	UNIT 3	UNIT 4	UNIT 5
CO1	L3		L1	L1	
CO2		L3	L1	L1	L1
CO3	L2	L2	L2	L2	L2
CO4	L1	L1		L3	L3

L1: Addressed to small extent

L2: Addressed significantly

L3: Addressed Major Part

ANALYTICAL CHEMISTRY

Course objectives:

POCC23		
L (hrs)	**Credits**	**Course**
60	**4**	**Core**

1. To learn about molecular spectroscopy.
2. To study the basic concept about the surface techniques.
3. To know about electroanalytical techniques, adsorption and emission spectroscopy.
4. To study about the advanced techniques in chromatography.

Course prerequisites:

A basic knowledge and understanding about Analytical techniques studied in B.Sc. level

Course outcomes

On the successful completion of this course, student will able to

1. Learn about analytical instrumentation techniques
2. Understand the working principle of analytical instrument.
3. Evaluate the analytical data from different analytical instruments
4. Identify the suitable analytical methods for selected application.

Unit I Molecular Spectroscopy (12 hrs.)

Working Principles, Instrumentation and Applications of Ultraviolet – Visible Spectroscopy (UV), Fluorescence Spectroscopy, Fourier Transformer Infra Red Spectroscopy (FTIR), X-Ray Diffraction Spectroscopy (XRD) and Raman Spectroscopy, Mossbauer Spectroscopy.

Unit II Surface Techniques I (12 hrs.)

Working Principles, Instrumentation and Applications of Scanning Electron Microscopy (SEM), Energy Dispersive X-Ray Spectroscopy (EDS), Transmission Electron Microscopy (TEM), Scanning Transmission Electron Microscope (STEM), X-ray Photoelectron spectroscopy (XPS), Electron Back Scatter Diffraction (EBSD), Auger Electron Spectroscopy (AES),Secondary Ion Mass Spectrometry (SIMS),and Brunauer Emmett Teller Spectroscopy (BET).

Unit III Surface Techniques II (12 hrs.)

Working Principle, Instrumentation and Application of Scanning Probe Microscopy - The Atomic Force Microscope (AFM) and The Scanning Tunneling Microscope (STM) and, Surface Plasmon Resonance (SPR),Magnetic Force Microscopy (MFM), Electrochemical Scanning Microscope (ECSM).

Unit IV Electroanalytical and Spectrometric techniques (12 hrs.)

1. An introduction to electroanalytical chemistry –Potentiometry, Voltammetry, Electrogravimetry, Chronoamperometry, Impedance Spectroscopy.
2. An introduction to spectrometric method – Working Principle, Instrumentation and Applications of Fluorimetry, Nephelometry, Turbidimetry, Dynamic Light Scattering, Atomic Absorption Spectroscopy and Atomic Emission Spectroscopy.

Unit V Advance Chromatographic Technique: (12 hrs.)

A general description of chromatography – Working Principles, Instrumentation and Applications of Gas Chromatography GC, Gas Chromatography Mass Spectroscopy GC/MS, High Pressurized Liquid Chromatography HPLC, Liquid Chromatography Mass Spectroscopy LC/MS, High-Resolution Mass Spectrometry (HRMS), Matrix-Assisted Laser Desorption Ionization Time-Of-Flight Mass Spectrometry (MALDI-TOF MS).

References:

1. D. A. Skoog, F. J. Holler and S. R. Crouch, Principles of Instrumental Analysis, 6th Edition,
2. Brooks/Cole Cengage Learning, Belmont, CA, 2007
3. H. H. Willard, L. L. Merrln, Jr., J. A. Dean, and F. A. Senle, Jr., Instrumental Methods of Analysis: Wadsworth, 7th Edition, Belmont.,1989
4. F. Rousseac and A. Roessac, Chemical Analysis: Modern Instrumentation Methods and Analysis,
5. 4th Edition, John Wiley & Sons, Ltd.,2000
6. B. Voigtlaender, Scanning Probe Microscopy: Atomic Force Microscopy and
7. Scanning Tunneling Microscopy: Springer - Verlag, Berlin 2015.

COURSE OUTCOME MAPPING

	UNIT 1	UNIT 2	UNIT 3	UNIT 4	UNIT 5
CO1	**L3**	**L3**	**L3**	**L3**	**L3**
CO2	**L2**	**L2**	**L3**	**L3**	**L2**
CO3	**L1**	**L1**	**L1**	**L1**	**L1**
CO4	**L3**	**L3**	**L3**	**L3**	**L3**

L1: Addressed to small extent

L2: Addressed significantly

L3: Addressed Major Part

GROUP THEORY AND SPECTROSCOPY

Course Objectives:

POCC24		
L (hrs)	**Credits**	**Course**
60	**4**	**Core**

The objective of the course is to help recognize symmetry in molecules and understand its role in Chemistry.

1. To give an exposure to the students the advanced concepts related with symmetry and point group specification of simple to complex molecular systems.
2. To know the fundamentals and applications of spectroscopy

Course pprerequisites:

General Physical Chemistry, Fundamentals of Spectroscopy in B.Sc. level

Course Outcomes:

The course will explore the students to understand the role of symmetry in

1. Learn the concepts of symmetry and group theory
2. Understand the fundamentals of spectroscopy
3. Classify the molecules based on molecular states and motions
4. Determine selection rules in spectroscopy
5. Evaluate the road map problems related to spectroscopy.

Unit I Molecular symmetry and point groups (12 hrs.)

Definition of group, symmetry, point groups, representation of group, orthogonality theorem, irreducible representation, character table, direct product representation.

Unit II Application of group theory (12 hrs.)

Application of group theory to normal mode analysis –symmetry selection rules for IR and Raman active fundamentals; symmetry of molecular orbitals and symmetry selection rule for electronic transitions in simple molecules (ethylene, formaldehyde and benzene); projection operators – SALC procedure – evaluation of energies and MO’s for ethylene, butadiene and cyclopropenyl systems – application of group theory to solve hybridization problems.

Unit III Molecular Spectroscopy- I (12 hrs.)

Classification of molecules, rigid rotor model, selection rules, intensity of spectral lines, effect of isotopic substitution. Stark effect. Infrared: Review of harmonic oscillator, selection rules, vibrational energy of diatomic molecules, zero point energy, force constant and bond strength; anharmonicity, Morse potential energy diagram, vibration-rotation spectroscopy, P, Q, R, branches.

Unit IV Molecular Spectroscopy- II (12 hrs.)

Electronic spectroscopy – Born- Oppenheimer approximation – vibrational coarse structure – Franck-Condon principle – dissociation energy – rotational fine structure of electronic – vibration transitions- Fortrat diagram – predissociation.

Classical and quantum theories of Raman effect, pure rotational, vibrational and vibrational- rotational Raman spectra, selection rules, mutual exclusion principle, Resonance Raman.

Unit V Spin resonance Spectroscopy (12 hrs.)

i. NMR Spectroscopy – spin and an applied field – nature of spinning particles – interaction of spin magnetic field – population of energy levels; chemical shift and coupling constant.
ii. NQR spectroscopy – principles- experimental set up- nuclear quadrupole coupling in atoms and molecules – applications.
iii. ESR spectroscopy – basis principles – hyperfine splitting – origin of hyperfine interaction – the g value – Mc Connel relationship – applications of ESR.

References

1. Chemical Applications of Group Theory by F.A. Cotton, Wiley Interscience, 1990, 3rdEd.
2. Fundamentals of Molecular Spectroscopy by C. N. Banwell and E.M. Mc Cash, Tata McGraw Hill, 1994.
3. Group Theory and Quantum Mechanics by M. Tinkham, McGraw Hill,1964.
4. Introduction to Molecular Spectroscopy by G. M. Barrow, McGrawHill,1962.
5. Modern Molecular Photochemistry by Nicholas J. Turro, University Science Books,1991.
6. P. W. Atkins, Molecular Quantum Mechanics, 2nd edition, Oxford University Press,1983.
7. P. F. Bernath, Spectra of Atoms and Molecules, 2nd Ed., Oxford University Press, 2005.
8. R.S. Drago, Physical Methods in Chemistry, W.B. Saunders, 1997.
9. NPETL link: https://nptel.ac.in/courses/104101099

COURSE OUTCOME MAPPING

	UNIT 1	UNIT 2	UNIT 3	UNIT 4	UNIT 5
CO1	**L3**	**L1**		**L1**	
CO2	**L1**		**L2**	**L2**	**L1**
CO3			**L2**	**L3**	**L3**
CO4	**L1**	**L1**	**L2**	**L2**	**L2**
CO5			**L2**	**L2**	**L3**

L1: Addressed to small extent

L2: Addressed significantly

L3: Addressed Major Part

PHYSICAL CHEMISTRY PRACTICAL – I

POCL21		
P(hrs)	**Credits**	**Course**
60	2	Practical

Course objectives

1. To understand the basic concept of conductivity of ions
2. To know about the chemical kinetics of acid hydrolysis

Course prerequisites

Basic knowledge in handling the equipment and the basic concept about kinetics, pH, conductance.

Course outcomes:

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

1. Understand the principle behind conductometric titration
2. Determine the rate constant of chemical reaction
3. interpret the experimental data's from conductometric and kinetics

Practical's

I. Conductometric Titration

1. Determination of cell constant and dissociation constant of a weak acid
2. Estimation of HCl and CH_3COOH in a mixture
3. Estimation of NH_4Cl and HCl in a mixture
4. Estimation of CH_3COOH and Sodium acetate in a buffer mixture

II. Kinetics

1. Acid hydrolysis of ester – comparison of strength of acids.

References:

1. W. J. Popiel, Laboratory Manual of Physical Chemistry, ELBS, London 1970
2. Findlay's Practical Physical Chemistry, B. P. Levitt, Longman, London, 1985
3. S. K. Sinha, Physical Chemistry A Laboratory Manual, Narosa Publishing Pvt, Ltd., 2014.

COURSE OUTCOME MAPPING

	EXPERIMENT 1	EXPERIMENT 2
CO1	L3	
CO2		L3
CO3	L2	L2

L1: Addressed to small extent

L2: Addressed significantly

L3: Addressed Major Part

PHYSICAL CHEMISTRY PRACTICAL – II

POCL22		
P(hrs)	**Credits**	**Course**
60	2	Practical

Course Objectives

1. To understand the concept of solubility product, dissociation constant and Potentiometry titrations
2. To study about the physical and chemical behavior of oxalic acid / acetic acid on charcoal

Course Prerequisites:

Source of practical knowledge about science skills

Course Outcomes:

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

1. Understand the principle behind potential metric titration
2. Study the adsorption isotherm
3. interpret the experimental data from potentiometric and adsorption isotherm

Practical's

I. Potentiometric Titration

1. Determination of solubility product of sparingly soluble silver salts.
2. Determination of dissociation constant of weak acids.
3. Potentiometric titrations:
    i. Redox titrations
        a. Fe^{2+}vs $Cr_2O_7^{2-}$
        b. Fe^{2+}vs Ce^{4+}
        c. I^-vs $KMnO_4$
    ii. Precipitation titration
        a. Mixture of Cl- and I-vs Ag+

II. Kinetics'

1. Adsorption isotherm of oxalic acid/acetic acid on charcoal

References:

1. W. J. Popiel, Laboratory Manual of Physical Chemistry, ELBS, London 1970
2. Findlay's Practical Physical Chemistry, B. P. Levitt, Longman, London, 1985
3. .S. K. Sinha, Physical Chemistry A Laboratory Manual, Narosa Publishing Pvt, Ltd. 2014

COURSE OUTCOME MAPPING

	EXPERIMENT 1	EXPERIMENT 2
CO1	L3	
CO2		L3
CO3	L2	L2

L1: Addressed to small extent

L2: Addressed significantly

L3: Addressed Major Part

SEMESTER-III

ORGANIC SYNTHESIS

POCC31		
L (hrs)	**Credits**	**Course**
60	**4**	**Core**

Course objectives:

1. To understand about the pericyclic reactions
2. To learn about the rearrangements in photochemistry
3. To study about the reagents and rearrangements in Organic synthesis

Course Pre-requisite:

1. Knowledge in basic organic chemistry

Course outcomes:

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

1. Understand and acquire knowledge about the different types of pericyclic reactions, photochemical reaction
2. Predict the feasibility of product based on stereochemistry of a starting molecule.
3. Analyse the types of reagents used for synthesis of organic compounds.
4. Explain the types of molecular rearrangement.
5. Design a new molecule by applying the learned concept

Unit I Pericyclic Reactions-I (12 hrs.)

Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene and allyl system. Classification of pericyclic reactions. Woodward-Hoffmann correlation diagrams. FMO and PMO approach. Electrocyclic reaction; conrotatory and disrotatory motions 4n, 4n+2 and allyl systems.

Unit II Pericyclic Reactions-II (12 hrs.)

Cycloaddition; antrafacial and suprafacial addition, 4n and 4n+2 systems, 2+2 addition of ketenes, 1,3 dipolar cycloadditions and cheleotropic reactions. Sigmatropic Rearrangements; suprafacial and antrafacial shifts of H, sigmatropic shifts involving carbon moieties, 3,3- and 5,5- sigmatropic rearrangements, Claisen, Cope and Aza-Cope rearrangements. Ene reaction.

Unit III Photochemistry (12 hrs.)

Quantum yields, intersystem crossing, photosensitization and energy transfer reactions. Photochemistry of olefins and carbonyl compounds, photo oxygenation and photofragmentation, Photochemistry of aromatic compounds: isomerisation, additions and substitutions. Singlet molecular oxygen reactions. Patterno-Buchi reaction, Di-pimethane rearrangement, Bartons reaction and Photo-Fries rearrangement.

Unit IV Reagents in Organic Synthesis (12 hrs.)

Use of the following reagents in organic synthesis and functional group transformations; complex metal hydrides, Gilman's reagent, lithium dimethylcuprate, lithium diisopropylamide (LDA), dicyclohexylcarbodiimide, 1,3-dithiane (reactivity Umpoloung), trimethylsilyl iodide, tri-n-butyltin hydride, Woodward and pervost hydroxylation, osmium tetroxide, DDQ, selenium dioxide, Phase transfer catalysts, crown ethers and Merrifield resin, Peterson's synthesis, Wilkinson's catalyst, Baker yeast.

Unit- V Rearrangements (12 hrs.)

General mechanistic considerations, nature of migration, migratory aptitude and detailed study of various arrangements reactions. :- Wagner-Meerwin Rearrangement, Pinacol-Pinacolone Rearrangement, Dienone-Phenol Rearrangement, Beckmann Rearrangement, Baeyer Villiger Oxidation, Stevens Rearrangement, Wittig Rearrangement, Sommelet Hauser Rearrangement, Benzil-Benzilic acid Rearrangement, Favorski Rearrangement, Claisen Rearrangement, Fries Rearrangement, Von-Richter Rearrangement.

References

1. Protective Groups in Organic Synthesis by T.W.Greene, Wiley-VCH, 1999.
2. Modern Heterocyclic Chemistry by L. A. Paquette, W.A. Benjamin, Inc.,1968.
3. Organic Chemistry by I. L. Finar, Vol II, ELBS,1968.
4. Heterocyclic Chemistry by T. R. Gilchrist, Longman,1989.
5. Selectivity in Organic Synthesis by Ward, Wiley-VCH,1999.
6. Robert E. Gawley, Jeffrey Aube, Principles of Asymmetric Synthesis, pergamon, 2nd
7. edition, 2012
8. V.K. Ahluwalia and R.K. Parashar, Organic Reaction Mechanisms, Narosa Publishing House, 4th edition, 2010
9. J. March and M. B. Smith, March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 6th Edition, Wiley, 2007.
10. Jagdamba Singh, Photochemistry and Pericyclic Reactions, May 2019

11. Fleming, Frontier Orbitals and Organic Chemical Reactions, Wiley, London, 1976.
12. S. Sankararaman, Pericyclic Reactions- A text Book, Wiley VCH, 2005

COURSE OUTCOME MAPPING

	UNIT 1	**UNIT 2**	**UNIT 3**	**UNIT 4**	**UNIT 5**
CO1	**L3**	**L3**	**L2**		
CO2	**L3**	**L3**	**L2**		
CO3			**L3**	**L2**	**L3**
CO4			**L3**	**L2**	**L3**
CO5	**L1**	**L1**	**L2**	**L3**	**L3**

L1: Addressed to small extent

L2: Addressed significantly

L3: Addressed Major Part

ELECTROCHEMISTRY

POCC32		
L (hrs)	**Credits**	**Course**
60	**4**	**Core**

Course objectives

1. To study about the Interaction of electromechanical interfaces.
2. To learn about the Electrochemical measurement and Galvanic cells.
3. To study about the Electrocatalysis, Photo electrochemistry and Water splitting.
4. To study about the Corrosion – types and its applications.

Course prerequisites:

The fundamental of electrochemistry studied in undergraduate level

Course outcomes

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

1. To impart the electrochemical interface
2. Understand the concept of electrochemical reaction
3. Learning in detail about the electrochemical measurement
4. To know about application of electrochemistry

Unit I Electrochemical Interface (12 hrs.)

Debye-Huckel-theory, Onsager theory, Debye-Huckel-Onsager theory, electrochemical interfaces – electrical double layer –Helmholtz and Gouy – Chapman – Stern models of the double layer, Lippmann equation..

Unit II Electrochemical Reaction & Equations (12 hrs.)

Galvanic cells: Reversible and Irreversible cells – EMF and its measurement, Electrochemical series, Nernst equation, Ohmic and diffusion overpotentials, Activation polarization, concentration polarization, Current-potential relationship - derivation of Butler-Volmer and Tafel equations.

Unit III Electrochemical measurements (12 hrs.)

Two electrode cell - Three electrode cell, Types of Electrodes - Reference, working and counter electrodes and its applications, Reversible and Irreversible systems: Quasi-reversible systems, Steady-State Polarization Measurements, Current and diffusion-controlled reactions, Impedance Measurements.

Unit IV Electrocatalysis & Photo Electrochemistry (12 hrs.)

- Electrocatalysis: Introduction, Interaction of reactant with electrode, Mechanism and application of hydrogen and oxygen evolution reactions (OER, ORR, HER), Electrocatalyst for fuel cells.
- Photo-Electrochemistry: Principle, Photo excitation charge–transfer process at Electrode/Electrolyte interface, photoelectrochemical cells and its applications of decontamination of water, water splitting, CO2 Photoreduction.

Unit V Corrosion & Electrochemical Sensors (12 hrs.)

- Corrosion: Different types of corrosion; Pourbaix diagram, mixed potential theory, corrosion rate measurements and prevention of corrosion.
- Electrochemical sensors: Introduction to electrochemical sensors and biosensors, electrochemical sensors in environmental analysis, glucose biosensor and immune sensors, ISFETs, CHEMFETS.

References

1. Carl H. Hamann, Andrew Hamnett and WolfVielstich, Wiley VCH, Electrochemistry,2007.
2. J. O'M. Bockris and A. K.N. Reddy, Kluwer Academic, Modern Electrochemistry 2000.
3. A. J. Bard and L. R. Faulkner, Electrochemical Methods, ,2000, 2nd edition.
4. E. Gileadi, Physical Electrochemistry, Fundamental, Techniques and Applications, Wiley-VCH, 2011.
5. J. Bard and L. R Faulkner Electrochemical Methods: Fundamentals and Applications, 2nd Edition, Wiley,2001.
6. P. H. Rieger, Electrochemistry, 2nd Edition, Springer1994.
7. J. Newman and K. E. Thomas-Alyea, Electrochemical Systems, 3rd Edition, Wiley Interscience,2004.
8. J. Wang, Analytical Electrochemistry, 3rd Edition, Wiley – VCH,2006.
9. P.T. Kissinger and W.R. Heineman, Laboratory Techniques in Electroanalytical Chemistry, 2nd Edition, Marcel Dekker Inc.,1996.

COURSE OUTCOME MAPPING

	UNIT 1	UNIT 2	UNIT 3	UNIT 4	UNIT 5
CO1	L3	Ll3	L1		
CO2	L3	L3	L3		
CO3	L1	L1	L2	L3	L3
CO4			L2	L3	L3

L1: Addressed to small extent

L2: Addressed significantly

L3: Addressed Major Part

BIO-INORGANIC CHEMISTRY

POCC33		
L (hrs)	**Credits**	**Course**
60	**4**	**Core**

Course objectives

1. To study about the Role of alkaline and alkaline earth metal & Electron transfer.
2. To learn about the Oxygen transport and activation and Enzymes
3. To study about the Various spectroscopic methods in Bioinorganic chemistry
4. To study about the uses of Coordination complexes and Metals in medicine

Course Prerequisites:

1. To know the significant of bioinorganic compounds
2. To have the knowledge of enzymes and metabolisms

Course Outcomes:

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

1. understand the concept of biomacro molecules.
2. get an idea on function of different bio inorganic molecules.
3. describe the significance of enzyme metabolism
4. validate of the therapeutic and toxic issues of metals in medicine.

Unit I Metals in Biology (12 hrs.)

Role of alkali and alkaline earth metal ions in biology; Na -K Pump, ionophores and crown ethers. Metal site structure, function. Metal ion transport and storage: Ferritin, Transferrin, Siderophores and metallothionein. Electron Transfer: Cytochromes, Iron-Sulfur Proteins and Copper Proteins.

Unit II Oxygen transport and activation (12 hrs.)

Oxygen transport and storage: Hemoglobin, myoglobin, hemerythrin, hemocyanin Oxygen activation: Cytochrome oxidase. Other metal containing enzymes: Catalase, peroxidase, superoxide dismutase, alcohol dehydrogenase, carbonic anhydrase, carboxypeptidase, vitamin B12 coenzyme, photosystem I and II, oxygen evolving center.

Unit III Enzymes and its role in Biochemistry (12 hrs.)

Nitrogen-cycle enzymes : Mo in N, and S-metabolism by Mo-pterin cofactors and Mo- Fe-cofactors. NOx reductases, sulfite oxidase, xanthine oxidase, nitrogenase, P and M-clusters in nitrogenase, transition-metal-dinitrogen complexes and insights into N2 binding, reduction to ammonia.

Unit IV Co-ordination complexes in biological systems. (12 hrs.)

Use of coordination complexes as models for various enzymes, metalloproteins. Role of hazardous materials such as nitric oxide, cyanide and methyl isocyanate etc. in biological systems.

Unit V Metals in Medicine (12 hrs.)

Metals in medicine - therapeutic applications of cis-platin, transition metal radio-isotopes (example: Tc, Co and Cu etc.) and MRI (Mn and Fe) agents. Toxicity of metals - Cd, Hg and Cr toxic effects with specific examples.

References:

1. S. J. Lippard and J. M. Berg, Principle of Bioinorganic Chemistry , University Science Books,1994.
2. Lawrence Que, Jr, Physical Methods in Bioinorganic Chemistry: Spectroscopy and Magnetism, University Science Books, 2000.
3. F. A. Cotton and G. W. Wilkinson, Advanced Inorganic Chemistry, 5John-Wiley & Sons, 1988
4. D. Banerjea, Coordination Chemistry, 2 Ed, Asian Books Pvt. Ltd., 2007.
5. J. E. Huheey, E. A. Keiter and R. L. Keiter, Inorganic Chemistry: Principal , Structure and Reactivity , 4 Ed. Harper Collins, 1993.

COURSE OUTCOME MAPPING

	UNIT 1	UNIT 2	UNIT 3	UNIT 4	UNIT 5
CO1	**L1**	**L3**	**L2**	**L1**	
CO2	**L2**	**L3**	**L2**	**L3**	**L2**
CO3		**L2**	**L3**	**L2**	
CO4	**L3**	**L2**	**L2**	**L2**	**L3**

L1: Addressed to small extent

L2: Addressed significantly

L3: Addressed Major Part

APPLICATIONS OF ORGANIC SPECTROSCOPY

POCC34		
L (hrs)	**Credits**	**Course**
60	**4**	**Core**

Course objectives

1. To study about the UV-Vis & FT-IR spectroscopic technique
2. To study about the vibration & ESR spectroscopy
3. To study about the basic concept of 1D NMR spectroscopy
4. To study about the 2 D NMR spectroscopy
5. To determine the molecular weight of the compounds

Course prerequisites:

A basic knowledge about organic chemistry studied in B.Sc. level.

Course Outcome:

1. To understand the importance of organic spectroscopy.
2. To acquire knowledge about electronic spectroscopy
3. To learn about magnetic and spin resonance spectroscopy
4. Elucidate and identify the organic molecules

Unit I UV-Vis & FT-IR Spectroscopy (12 hrs.)

i. UV-Vis Spectroscopy- Introduction, various electronic transition, Beer-Lamberts Law, Instrumentation & sample handling effect of solvents on electronic transitions, UV bands for saturated and unsaturated carbonyl compounds. Woodward-Fieser rules for conjugated dienes and carbonyl compounds.

ii. IR Spectroscopy- Introduction, instruments and sample handling – characteristic vibrational frequencies of alkanes, alkenes, alkynes, aromatic compounds, alcohols, ethers, phenols, and amines, Detailed study of vibrational frequencies of carbonyl compounds (aldehyde ketones, esters, acids, amides, anhydrides, lactones, lactams, and conjugated carbonyl compounds) Effect of hydrogen bonding and solvent effects on vibrational frequencies overtones, combination bands & Fermi resonance

Unit – II Vibrational & ESR spectroscopy (12 hrs.)

i. Vibrational: Symmetry and shapes of AB_2, AB_3, AB_4, AB_5 and AB_6, modes of bonding in ambidentate ligands, application of resonance Raman spectroscopy particularly for the study of active sites of metalloproteins.

ii. ESR spectroscopy for organic free radicals

Unit III Nuclear Magnetic Resonance -I (12 hrs.)

General introduction and definition, Inframentation and sample analysis technique- chemical shift, factors effecting nuclear relaxation, spin-spin interaction, shielding mechanism solvent effect, order of spectra, Nuclear over hauser effect (NOE) Resonance of other nuclei, FT-technique- spin relaxation, double resonance.

General consideration 13C NMR spectroscopy, proton coupled, Interpretation and application of organic compounds.

Unit III Nuclear Magnetic Resonance - II (12 hrs.)

Two dimensional NMR Spectroscopy: Introduction correlation spectroscopy (COSY), heteronuclear correlation spectroscopy (HETCOR), heteronuclear multiple- quantum coherence (HMQC), heteronuclear multiple-bond correlation spectroscopy (HMBC), Nuclear overhauser effect spectroscopy (NOESY), Magnetic resonance image (MRI), Functional Nuclear Magnetic Resonance image (FMRI).

.

Unit V Mass spectroscopy (12 hrs.)

i. Instrumentation, Mass spectral fragmentation of organic compounds, Mc Lafferty rearrangement, examples of mass spectral fragmentation of organic compounds with respect to their structure determination.
ii. ORD & CD: Definition, deduction of absolute configuration, octant rule for ketones.
iii. Combined spectroscopy problems: UV-Vis, FT-IR, NMR & Mass Spectral Data.

References

1. Physical Methods in Chemistry by R. S. Drago, Saunders,1992
2. Inorganic Electronic Spectroscopy by A. B. P. Lever, Elsevier, 1984, 2ndEd.
3. Spectrometric Identifications of Organic Compounds by R. M.Silverstein, John Wiley,1991.
4. Introduction to Spectroscopy by D.L. Pavia, G. M. Lampman, G. S.Kriz, Harcourt College Publisher, NY,2001.
5. Organic Spectroscopy by William Kemp, ELBS 3rd Ed. 1994.

COURSE OUTCOME MAPPING

	UNIT 1	UNIT 2	UNIT 3	UNIT 4	UNIT 5
CO1	**L2**	**L2**	**L2**	**L2**	**L2**
CO2	**L3**	**L3**			**L2**
CO3			**L3**	**L3**	**L2**
CO4	**L3**	**L3**	**L3**	**L3**	**L3**

L1: Addressed to small extent

L2: Addressed significantly

L3: Addressed Major Part

INORGANIC CHEMISTRY PRACTICAL- I

POCL31		
P(hrs)	**C**	**Course**
60	2	Practical

Course Objectives

1. To train identification of metal ions in a mixture with semi micro qualitative analysis technique
2. To train the estimation of metal ions in a mixture by complexometric titration method

Course prerequisites:

Already have the qualitative skills in Undergraduate level

Course Outcomes

On the successful completion of this course, student will able to

1. understand the qualitative and quantitative analysis
2. Identify and estimate the amount of cation

Practicals

1. Semi micro qualitative analysis of inorganic mixture containing two less-familiar cations. - W, Tl, Se, Te, Mo, Ce, Th, Zr, Ti, V, U and Li.
2. Complexometric titrations – Estimation of Cu, Zn and Mg by EDTA titration in the presence of either Pb or Ba; estimation after elimination of Pb or Ba.
3. Determination of Total hardness, Ca and Mg content of water by EDTA titration.

References:

1. V.V. Ramanujam, ‘Inorganic Semi micro Qualitative analysis, 3rd revised Edn, The National publishing Co., Chennai, 1988.
2. Vogel’s Text Book of Quantitative Chemical Analysis’, Eds. G.H. Jeffrey, J. Banett, J. Mendham and R.C. Denney, ELBS, 5thEdn. Reprint 1991.

COURSE OUTCOME MAPPING

	EXPERIMENT 1	**EXPERIMENT 2**	**EXPERIMENT 3**
CO1	**L3**	**L3**	**L3**
CO2	**L3**	**L3**	**L3**

L1: Addressed to small extent

L2: Addressed significantly

L3: Addressed Major Part

INORGANIC CHEMISTRY PRACTICAL – II

POCL32		
P(hrs)	**C**	**Course**
60	2	Practical

Course Objective

To Provide training in separation and estimation of metal ions by volumetric and gravimetric methods of analysis

Course Prerequisites:

Already have the quantitative skills in Undergraduate level

Course Outcomes

On the successful completion of this course, student will able to

1. Know the concept of volumetric and gravimetric methods.
2. Separate and Estimate the amount of element

Practicals

Separation and estimation of metal ions in a mixture by volumetric and gravimetric methods. Some typical recommended mixtures are:

Cu(II) & Ni(II); Fe(II) & Cu(II); Cu(II) & Zn(II); Ca(II) & Ba(II); Fe(II) & Ni(II);
Cu(II) &Ca(II)

References:

1. Vogel's Text Book of Quantitative Chemical Analysis', Eds. G.H. Jeffrey, J. Banett, J. Mendham and R.C. Denney, ELBS, 5thEdn. Reprint 1991.
2. A Collection of Interesting General Chemistry Experiments, Anil J. Elias,2008

COURSE OUTCOME MAPPING

	EXPERIMENT 1
CO1	**L3**
CO2	**L3**

L1: Addressed to small extent

L2: Addressed significantly

L3: Addressed Major Part

SEMESTER IV

RESEARCH METHODOLOGY

POC		
L (hrs)	**Credits**	**Course**
60	**4**	**Core**

Course objectives:

The objective of the paper is to train doctoral students in research methodology. It will facilitate the students in understanding the tools and techniques of conducting their thesis.

Course Prerequisites:

The students should have basic knowledge in all chemistry topics in Undergraduate level

Course outcomes:

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

1. Gain basic knowledge in research and methodology
2. Understand the data analysis and scientific writing
3. Acquire a complete practical training on research and methodologies

Unit I Research Basics (12hrs)

Research Basics: Definition, purpose -Significance of research in applied sciences; Process of research; Objectives and dimensions of research; Research Problem, Research questions, Research design. Qualitative and Quantitative; Systematic review of literature in applied sciences; Features of good study Preparations of Research proposal/Synopsis; Research Ethics (Issues relating to referencing and documentation, copyrights, plagiarism etc.), Impact Factor, H-Index, Citation Index, References/ bibliography. Structuring of a Thesis

Unit II Data analysis (12hrs)

Data: Types (primary and secondary data), collection methods; Data Analysis- quantitative and qualitative analysis; Basics of Regression Analysis- linear and multilinear analysis; introduction to PCA and PLS

Sampling: types, steps; sampling errors; sampling of attributes (including chi square test); sampling of small and large sample variables (including ANOVA); Hypothesis Testing: fundamentals of hypothesis testing in applied sciences. Statistical decision theory

Unit III Analytical methods (12 hrs)

Detail study on Laboratory Component such as UV-visible, fluorescence, FTIR, fluorometer, SEM, Electrochemical studies LC/LC-MS, HPLC, NMR, TGA

Unit IV Safety measures in Chemistry lab: (12 hrs)

i. Procedures for Common Categories of Hazardous Chemicals
ii. ***Emergency response :*** chemical spills, radiation spills, biohazard spills, leaking compressed gas cylinders, fires, medical emergency accident reporting
iii. ***General safety :*** General safety and operational rules, safety equipments, personal protective equipments, compressed gas safety, safety practices for disposal of broken glass wares, centrifuge safety, treated biomedical wastes and scientific ethics.

Unit V Scientific Writing and Seminar (12hrs)

Research survey pertaining to Chemical Sciences, primary sources of literature survey including journal and patents etc., secondary sources of literature survey including books, reference books and text books.

Selection of any four research papers from literature. Preparation of a report on a topic based on selected papers including title, objective, a brief presentation of results and discussion and outcome. The same report is to be presented in the form of a seminar.

References

1. C. R. Kothari, Research Methodology Methods and Techniques, 2nd. ed. New Delhi: New Age International Publishers, 2009.
2. R. Panneerselvam, Research Methodology, New Delhi: PHI, 2005.
3. P. Oliver, Writing Your Thesis, New Delhi: Vistaar Publications, 2004.
4. J. W. Creswell, Research Design: Qualitative, Quantitative, and Mixed Methods Approaches, 3nd. ed. Sage Publications, 2008.
5. Kumar, Research Methodology: A Step by Step Guide for Beginners, 2nd. ed. Indian: PE, 2005.
6. B. C. Nakra and K. K. Chaudhry, Instrumentation, Measurement and Analysis, 2nd. edision. New Delhi: TMH publishing Co. Ltd., 2005.
7. Gregory, Ethics in Research, Continuum, 2005.

COURSE OUTCOME MAPPING

	UNIT 1	UNIT 2	UNIT 3	UNIT 4	UNIT 5
CO1	**L2**	**L2**	**L2**	**L2**	**L2**
CO2	**L1**	**L3**	**L2**		**L1**
CO3	**L2**	**L1**	**L3**	**L3**	**L2**

L1: Addressed to small extent

L2: Addressed significantly

L3: Addressed Major Part

SUPRAMOLECULAR CHEMISTRY

POC		
L (hrs)	**Credits**	**Course**
60	**4**	**Core**

Course objectives:

1. To study about the Ions Interactions
2. To learn about the Host Guest Interactions
3. To know about the Crystal Engineering and Molecular devices
4. To study about the recent developments in Supramolecular chemistry

Course Pre-requisite:

The Students should have knowledge in macromolecules, types of bonding interaction between the molecules and metal, enzymatic catalyst reaction.

Course outcomes:

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

1. define the basic concepts and phenomena of supramolecular chemistry and recognizes the most typical supramolecular compounds.
2. understands the method of synthesis and connections-disconnections of macromolecules.
3. analyze the type of interactions and explains the role of interactions in supramolecules and macro molecules.
4. design simple potential supramolecular machines and biomimetic models.

Unit I Introduction of supramolecular chemistry (12 hrs.)

Definition of supramolecular chemistry. Nature of binding interactions in supramolecular structures: ion-ion, ion-dipole, dipole-dipole, H-bonding, cation-p, anion-p, p-p, and vander Waals interactions.

Unit II Synthesis and structure of Macromolecules & Molecular devices (12 hrs.)

Synthesis and structure of crown ethers, lariat ethers, podands, cryptands, spherands, calixarenes, cyclodextrins, cyclophanes, cryptophanes, carcerands and hemicarcerands., Host-Guest interactions, pre-organization and complimentarity, lock and key analogy.

Molecular devices: molecular electronic devices, molecular wires, molecular rectifiers, molecular switches, molecular logic.

Unit III Bonding reactions in supramolecular chemistry (12 hrs.)

Binding of cationic, anionic, ion pair and neutral guest molecules. Self-assembly molecules: design, synthesis and properties of the molecules, self assembling by H bonding, metal-ligand interactions and other weak interactions, metallomacrocycles, catenanes, rotaxanes, helicates and knots.

Unit IV Advanced supramolecular chemistry (12 hrs.)

Relevance of supramolecular chemistry to mimic biological systems: cyclodextrins as enzyme mimics, ion channel mimics, supramolecular catalysis etc. Examples of recent developments in supramolecular chemistry from current literature.

Unit IV Retrosynthesis (12 hrs.)

Strategy and planning-starting material-Linear and Convergent approach, protecting groups and activating groups. Regioselectivity, chemoselectivity. diastereoselectivity. Target molecules containing one functional group requiring a single disconnection- Synthons and synthetic equivalents. Latent polarity. Target molecules with two functional groups– 1,2-, 1,3-, 1,4-, 1,5-, and 1,6-dicarbonyl compounds, Umpolung reactions. Functional group interconversions. Retrosynthetic analysis of 2,4–dimethyl–2–hydroxypentanoic acid, trans-9-methyl–1–decalone, α-onocerin, β-bisabolene.

References

1. J.-M. Lehn; Supramolecular Chemistry-Concepts and Perspectives (WileyVCH, 1995)
2. P. D. Beer, P. A. Gale, D. K. Smith; Supramolecular Chemistry (Oxford University Press,1999)
3. J. W. Steed and J. L. Atwood; Supramolecular Chemistry (Wiley, 2000).
4. Desiraju, Raman Vittal, Crystal Engineering, University Press, 2019.
5. e-PG Pathshala- P-14- Organic Chemistry-IV (Supramolecular Chemistry).

COURSE OUTCOME MAPPING

	UNIT 1	UNIT 2	UNIT 3	UNIT 4	UNIT 5
CO1	**L2**	**L2**	**L2**		
CO2		**L2**	**L2**	**L1**	**L3**
CO3	**L3**	**L2**	**L2**	**L1**	**L1**
CO4	**L1**			**L3**	

L1: Addressed to small extent

L2: Addressed significantly

L3: Addressed Major Part

ELECTIVE

NUCLEAR CHEMISTRY

POCEA		
L(hrs)	**C**	**Course**
45	3	Elective

Course Objectives

1. To know about the Radioactivity.
2. To learn about the nuclear reactions and nuclear reactor.
3. To know about the Applications of Radioactivity.

Course Prerequisites:

A basic knowledge about nuclear chemistry studied in undergraduate level

Course Outcomes

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

1. To impart the knowledge of nuclear reaction
2. Understand the concept of nuclear radiation and its matter
3. Learning in detail about the radioactivity and its applications

Unit I Radioactivity and Its Measurement (9 hrs.)

Radioactivity -Discovery – types of decay – Properties of radioactive radiation- decay kinetics – half-life period, mean life, parent daughter decay – growth relationship – secular and transient equilibrium; Units of radioactivity; Theory of decay- alpha, beta and gamma decay; energies and properties.

Unit II Nuclear Reactions (9 hrs.)

Bohr Theory of nuclear reaction – Chemical reaction - nuclear fission, fusion, photonuclear reactions and thermonuclear reactions. Uses of radioisotopes - Artificial radioactivity. Detectors: ionization chamber, electron pulse counter, scintillation detectors.

Unit III Nuclear Reactor (9 hrs.)

The fission energy – enrichment of uranium - reproduction factor; Classification of reactors based on moderators, coolants, phase of fuel and generation. Breeder reactor India’s nuclear energy programmes – reprocessing of spent fuels.

Unit IV Radiation and Matter **(9 hrs.)**

Application of radioisotopes: probing by isotopes, reactions involved in the preparation of radioisotopes. The Szilard-Chalmers' reaction – Radiochemical principles in the use of Tracers.

Unit V Applications of Radioactivity **(9 hrs.)**

Applications of radioisotopes as tracers – chemical investigations, analytical applications, agricultural and industrial applications – Neutron activation analysis – Carbon and rock dating.

References

1. S. Glasstone, Source book on atomic energy, East West press, 3rdEdn,2014.
2. H.J. Arniker, Essentials of Nuclear Chemistry, New Age International, Reprint 2011.
3. M.G. Friedlander, J.M. Kennedy, E.S. Macian and J.M. Miller, Nuclear and Radiochemistry, 3rdEdn. John Wiley & Sons, 1981.
4. M.G. Arora and M. Singh, Nuclear Chemistry, Anmol Publications, 2002.

COURSE OUTCOME MAPPING

	UNIT 1	UNIT 2	UNIT 3	UNIT 4	UNIT 5
CO1	**L3**	**L3**	**L3**	**L1**	
CO2	**L1**	**L3**	**L2**	**L3**	**L1**
CO3	**L1**			**L3**	**L3**

L1: Addressed to small extent

L2: Addressed significantly

L3: Addressed Major Part

DRUG DESIGN AND MODELING

Course objectives:

POCEB		
L(hrs)	**C**	**Course**
45	3	Elective

This subject is designed to impart fundamental knowledge on the structure, chemistry and therapeutic value of drugs. The subject emphasis on modern techniques of rational drug design like quantitative structure activity relationship (QSAR), Prodrug concept, combinatorial chemistry and Computer aided drug design (CADD).

Course Pre-requisite:

The student should have

1. a sophisticated knowledge of biology and chemistry
2. Current knowledge in drugs available in market an its side effects

Course Outcomes:

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

1. Understand the basic principles and recognize the nature of information obtained in the different phases of Drug design and development to bring a drug to market
2. compares different sources of chemical entities for drug development
3. correlates the relationship between the chemical structure of a molecule and its biological activity
4. describe different types of the drug target interactions and how its activity is screened
5. understand how modern drugs were developed by using pharmacophore modelling and docking technique

Unit I Principles of Drug Discovery (9 hrs.)

Drug discovery without lead – Penicillin's and Librium drug. Lead discovery-random screening nonrandom screening (screening of natural products, medical folklore, screening synthetic banks, existing drugs from natural ligand or modulator, combinatorial synthesis, computer aided designing & serendipity – in brief). Drug metabolism studies – Phase I, Phase II metabolism.

Clinical observations : Phase-I, Phase-II, Phase-III and Phase-IV trials (introductory treatment).

Principles of drug design; agonist, antagonist drugs, structure pruning technique in drug design (eg. Morphine pharmacophore). Development of Cimetidine, Captopril from lead molecules- bioisosterism.

Unit II Structure – Activity Relationship Studies (9 hrs.)

i. Binding role of hydroxyl group, amino group, aromatic ring, double bond, ketones and amides.
ii. Variation of substituents –alkyl substituents, aromatic substituents, extension of structure, chain extension/contraction, ring expansion/contraction, ring variation, ring fusion. Isosteres
iii. Simplification of the structure, rigidification, conformational blockers, X-ray crystallographic studies. eg., a case study of Oxaminquine (schistosomiasis), Sulpha drugs (antibacterial), Benzodiazepines (Hypnotics) and Taxol analogues, (anticancer drugs).

Unit III Quantitative Structure –Activity Relationship Studies (9 hrs.)

i. Introduction -QSAR parameters – Substituent constants.
    a. Linear relationship between log p and biological activity
    b. Non-linear relationship between log p and biological activity.
    c. Electronic parameters, Steric parameters, effect of electronic and steric parameters on lipophilicity.
ii. Methods used in QSAR studies
    Linear free energy relationship (LFER). Application of Hammett equation, Hansch analysis, significance of slopes and intercepts in Hansch analysis. Craig's plot. Topliss Scheme

Unit IV Modelling Biomolecules (9 hrs.)

Introduction to modelling biomolecules, Protein structure prediction – Protein folding, secondary structure predication, sequence alignment, the inverse folding problem. Modelling by homology – the alignment, construction of the framework, selecting variable regions, side chain placement. Validation of protein models – Ramachandran plot. Molecular modelling in drug discovery, 3 D pharmacophores and detection methods, molecular docking, Denovo ligand design.

Unit V Combinatorial Synthesis (9 hrs.)

Introduction, Combinatorial approach, Combinatorial libraries, technologies. Solid phase synthesis, types of resins, Linkers, Reactants for solid phased synthesis, Methods of Parallel synthesis: Haughton's tea bag procedure, Automated parallel synthesis. Methods in Mixed combinatorial synthesis: general principles. Furkasmix and split combinatorial synthesis. Examples of Combinatorial Chemistry, Planning and designing of combinatorial synthesis, Spider like scaffolds, drug molecules, Automation in Combinatorial chemistry, High throughput screening.

References:

1. Donald J. Abraham (Author), David P. Rotella, Burger's Medicinal Chemistry, Drug Discovery and Development, 8 Volume Set (Burger's Medicinal Chemistry and Drug Discovery), Wiley; 7th Edition, 2010.
2. Manfred E. Wolff, Burger's medicinal chemistry and drug discovery: Therapeutic agents, Edition 5, Wiley, 1997.
3. Graham. L. Patrick, Introduction to Medicinal Chemistry, 5th Edition, Oxford University Press , USA, 2013.
4. Silverman ,Introduction to drug design, 2nd Edition, Elsevier Science & Technology books, 2008.
5. Corwin Hansch, Comprehensive Medicinal Chemistry, Pergamon Pr; 6 Volume Set edition, 1990.
6. David A. Williams, Foye's Principles of Medicinal Chemistry, Lippincott Williams & Wilkins; Seventh, North American Edition, 2012.
7. Thomas Nogrady (Author), Donald F. Weaver, Medicinal Chemistry: A Molecular and Biochemical Approach, Oxford University Press, USA; 3rd edition, 2005.
8. Hermann J. Roth, A. Kleemann, T. Beisswenger, M. D. Cooke, P. G. Sammes, Pharmaceutical Chemistry, Vol. 1: Drug Synthesis (Ellis Horwood Books in Biological Sciences, Series in Pharmaceutical Technology). Halstead Press / Ellis Horwood Ltd, 1988.
9. E J Ariens, Drug Design: v. 7 (Medicinal Chemical Monograph), Academic Press Inc., U.S., 1977.
10. Glenn L. Jenkins, Adelbert M. Knevel, Frank E. Digangi, Quantitative Pharmaceutical Chemistry 7th edition McGraw-Hill Inc.,US; 1977.

11. I.A. Khan and A. Khanum, Recent advances in Bioinformatics, 3rd Edition, John Wiley & Sons, 2008.
12. Hans-Dieter Höltje, Wolfgang Sippl, Didier Rognan, Gerd Folkers, Molecular Modeling, 3rd Edition, John Wiley & Sons, 2008.
13. Prof. Dr. K. C. Nicolaou, Dr. R. Hanko, Prof. Dr. W. Hartwig, Handbook of Combinatorial Chemistry: Drugs, Catalysts, Materials, Wiley-VCH Verlag GmbH, 2002
14. Andrew Leach ,Molecular modeling, 2nd Edition, Prentice Hall, 2001.

COURSE OUTCOME MAPPING

	UNIT I	**UNIT II**	**UNIT III**	**UNIT IV**	**UNIT V**
CO1	**L3**	**L1**		**L2**	
CO2		**L3**	**L2**		**L2**
CO3		**L3**	**L3**		**L1**
CO4	**L2**			**L3**	**L3**
CO5	**L1**			**L3**	**L1**

L1: Addressed to small extent

L2: Addressed significantly

L3: Addressed Major Part

TECHNOLOGY OF FINE CHEMICALS AND BULK DRUGS

Course objectives

POCEC		
L(hrs)	**C**	**Course**
45	3	Elective

This course facilitates an understanding of various unit processes involved in the manufacturing of pharmaceuticals, process development and optimization of bulk drugs and their synthesis and also study the industrial effluents ant its treatments.

Course prerequisites

Students should have a basic knowledge in basic chemistry, effluents and thermal methods.

Course outcomes

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

1. understand the basics in chemistry of drugs formulation
2. acquaint well with the preparative pathway of different class of medicinal compounds.
3. understand and learn methodologies of eco-friendly reaction.
4. Design new series of eco-friendly compound that can be used as catalyst in effluent industries and pharmaceutical industries

Unit I Unit Processes (9 hrs.)

Concept of unit processes in systematization of chemical reactions, explanation of one example each for unit processes: Alkylation, amination, (by ammonolysis, reduction), carbonylation, carboxylation, condensation, dehydration, diazotization, disproportionation, esterification, halogenation, hydration, hydroformylation, hydrogenation, hydrolysis, hydroxylation, nitration, oxidation and reduction.

Unit II Process Development and Optimization of Bulk drugs (9 hrs.)

a. Pilot- plant – Introduction – Appraisal for the need of pilot – plant – pilot plant (Vs) Small scale plant – Benefits of Pilot plant – Broad guidelines of process development.
b. Industrial manufacturing method and flow charts of Sulphamethoxazole, Ciprofloxacin, Chloramphenicol maleate, Furazolidone, Cephalosporin and Rifampicin.

Unit III Commercial Synthesis of Bulk drugs (9 hrs.)

Introduction to pharmaceutical manufacturing – raw materials, detailed manufacturing procedure, therapeutic function, common name, chemical name, structural formulae of the following drugs:

Acyclovir, alprazolam, propanolol, naproxen, ibuprofen, aspirin, levodopa and cimetidine. Licocaine, mephensin, ethambutal hydrochloride, 5-fluorouracil, norfloxacin, amoxycillin and levothroxin sodium.

Unit IV – Environment Health & Safety (9 hrs.)

Introduction to industrial effluents. Classification of effluents. Classification of basic methods of treating the effluents.

i. Purification of suspended and emulsified impurities by mechanical method. Purification of dissolved impurities
   a. from mineral matter by ion exchange, reverse osmosis, electrical and reagent methods.
   b. from organic matter by destructive methods, biological oxidation, ozonization, chlorination, extraction, adsorption and ion exchange.

ii. Purification of gases by desorption method.

iii. Purification by elimination and destruction-by thermal destruction, burying and pumping into depth of oceans.

Unit V catalysis and Green Chemistry (9 hrs.)

Introduction, basic principles of green chemistry. Designing a green synthesis: Green starting materials, green reagents, green solvents and reaction conditions, green catalysts. Use of the following in green synthesis with suitable examples. Green reagents: dimethylcarbonate, polymer supported reagents. Green catalysts: Acid catalysts, oxidation catalysts, basic catalysts, phase transfer catalysts and biocatalysts. Green solvents: water, ionic liquids, deep eutectic solvents, supercritical carbon dioxide. Solid state reactions: solid phase synthesis, solid supported synthesis. Microwave assisted synthesis: reactions in water, reactions in organic solvents, solvent free reactions. Ultrasound assisted reactions.

References:

1. B.K. Sharma, Industrial Chemistry, Goel Publishing House, Meerut, 14th Edn., 2004.
2. B.K. Sharma, Environmental chemistry. Goel Publishing House, Meerut, 11th Edn.,2007.

3. Philip Herkimer Groggins, Unit Processes in Organic Synthesis, 5th Edn., Tata McGraw-Hill, 1995.
4. Drydens, Unit processes in chemical engineering, McGraw-Hill Higher Education , 2004.
5. William Andrew, Pharmaceutical manufacturing encyclopedia Vol.I & II., 3rd Edn., William Andrew, 2007.
6. W.W.M. Wenland, Thermal Analysis, John Willey & Sons, New York, 2nd Edn., John Wiley & Sons, 1974.
7. S.B. Chandalia, Hand book of Process Development, Multitech Publishing Company, Mumbai. 1998.
8. Kumar G. Gadamasettia, Ambarish K. Singhb, Process Chemistry in Pharmaceutical industries, 3rd ., Edn., Taylor & Francis Group , 2013.
9. Randolph Norris Shreve, George T Autor Austin, Shreve's, Chemical Process Industries, 5th Edn, McGraw Hill Book Company.2000.
10. M.V. Krishnan – Safety Management in Industries, Jaico publishers, Mumbai, 2002.
11. S. Rao & S. Roy , Industrial Safe and Management, Khanna publications, New Delhi.
12. Rashmi Sanshi, M.M. Srivastra – Green Chemistry – Alpha Sciences, 2003.
13. R. Sanghi and M.M. Srivastava – Green Chemistry (Environment Friendly Alternatives), Alpha Science Internaional Ltd, Pangbourne England, 2003.
14. V.K. Ahluwalia – Green Chemistry (Environmentally Beingn Reactions), Ane Books India, New Delhi, 2006.

COURSE OUTCOME MAPPING

	UNIT I	**UNIT II**	**UNIT III**	**UNIT IV**	**UNIT V**
CO1	**L3**	**L3**	**L2**		
CO2	**L3**	**L3**	**L3**		
CO3		**L1**		**L2**	**L3**
CO4		**L1**	**L1**	**L3**	**L3**

L1: Addressed to small extent

L2: Addressed significantly

L3: Addressed Major Part

MEDICINAL CHEMISTRY

POCED		
L(hrs)	**C**	**Course**
45	3	Elective

Course objectives

1. To know about the Mechanism of drug action
2. To learn about the Synthesis of drugs
3. To know about the Enzymes and Nucleic acids

Course prerequisites

Students should have knowledge in DNA, RNA, Enzyme and basic concepts in chemistry

Course outcomes

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

1. learn the pharmacokinetic pathways of drug in body .
2. understand the drug discovery and delivery and therapeutic value of drugs
3. acquaint well with the synthesis of some important class of drugs
4. create an idea to develop a new chemical entity which can interact with macromolecules such as enzyme, DNA, protiens

Unit I Mechanism of drug action (9 hrs.)

Introduction to the history of pharmaceutical chemistry, general mechanisms of drug action on lipids, carbohydrates, proteins and nucleic acids, drug metabolism and inactivation, receptor structure and sites, drug discovery development, design and delivery systems, gene therapy and drug resistance.

Unit II Synthesis of Heterocyclic natural product and drugs (9 hrs.)

Chemistry heterocylics containing two hetroatoms: Pyrazines, pyradiazins, pyrimidines. ,1,2;1,3, and 1,4diaoxazines and thiazines: pyrazole pyrazolines and imidazoles, imidazolines. Synthesis of chloroquine, papavarine, amlodipine, bromouidine, ranitidine, Vit-B6, tryptophan, thiamine, histidine.

Unit III Synthesis of drugs (9 hrs.)

Classification of drugs based on structure and pharmacological basis with examples. Synthesis of important drugs such as α-methyl dopa, Chloramphenicol, griseo fulving, cephelosphorins and nystatin.

Unit IV Action of antibiotics (10hrs.)

General introduction to antibiotics, mechanism of action of lactam antibiotics and anon lactam antibiotics, antiviral agents, chemistry, stereochemistry, biosynthesis and degradation of penicillins – An account of semisynthetic pencillins – acid resistant, pencillinase resistant and broad spectrum semisynthetic pencillins.

Unit V Nucleic acids (8 hrs.)

DNA-protein interaction and DNA-drug interaction. Introduction to rational approach to drug design, physical and chemical factors associated with biological activities, mechanism of drug action.

References

1. A. Kar, Medicinal Chemistry, New Age International (P) Ltd, Delhi, 1997.
2. Principles of Biochemistry - L. Stryer (W.H. Freeman & Co.), 2002.
3. Principles of Biochemistry - A.L.Lehninger, D.W.Nelson & M.M.Cox (Macmillan), 1991.
4. Biochemistry - D.Voet & J.G.Voet (John Willey), 1995.
5. Harper's Illustrated Biochemistry - R.K.Murray et al. (McGraw Hill), January 8, 2005.
6. Lehninger's Principle of Biochemistry by David L. Nelson and Michael M. Cox. W. H. Freeman; 4th edition, 2004.
7. Text Book of Biochemistry with clinical correlation by Thomas .M. Devlin, John Wiley-Liss, Hobokhen NJ publishers, 2006.
8. A text book of pharmaceutical chemistry, Jayashree ghosh, S. Chand, 2003.
9. Medicinal chemistry, G.R.Chatwal, Himalaya Publishing House, New Delhi, 2002.
10. Pharmacology and Pharmatherapeutics – R.S. Satoskar and S.D. Bhandarkar, 1973.
11. Heterocyclic chemistry – J. A. Joule and K. Mills 4th edition Blackwell publishing, 2007.

COURSE OUTCOME MAPPING

	UNIT 1	UNIT 2	UNIT 3	UNIT 4	UNIT 5
CO1	L3			L1	L2
CO2		L1	L1	L2	L2
CO3		L3	L3	L2	
CO4	L1			L2	L2

L1: Addressed to small extent

L2: Addressed significantly

L3: Addressed Major Part

POLYMER CHEMISTRY

POCEE		
L(hrs)	**C**	**Course**
45	3	Elective

Course Objectives:

This course aims at acquainting the student's knowledge on the

1. basic concepts of polymers
2. to know about the kinetics and mechanism of polymerisation
3. to determine the molecular mass of polymers using various techniques
4. structural aspects of polymers
5. industrial and conducting polymers

Course prerequisites

Students studied general Physical Chemistry and Fundamentals of polymer chemistry in under-graduate level

Course Outcomes

On completion of this course, the students are expected to

1. Enumerate the concepts related to Polymer science
2. Describe the types of mechanisms involved in formation of polymers
3. Apply the processing techniques polymers
4. Understand the application of polymers.

Unit I Concept of macromolecules (9 hrs)

Principle of duality – molecular design – nomenclature and classification – raw material sources of polymers – classification of polymers - synthetic schemes – Molecular Weight determination.

Unit II Polymerization processes (9 hrs)

Free radical and addition polymerization; kinetics and mechanism, Chain transfer – molecular weight distribution and molecular weight control; Radical atom transfer and fragmentation – addition mechanism, Free radical living polymers, cationic and anionic polymerization- kinetics and mechanism.

Unit III Stereochemistry of Polymerisation (9 hrs)

Stereoregularity in polymers – isotactic, syndiotactic and atactic polymers; polar and non-polar polymers; stereospecific polymerization and the utility of Ziegler-Natta catalyst; Copolymerization – bulk solution, melt, suspension, emulsion and dispersion techniques; synthesis of graft and block copolymers.

Unit IV Organic polymers & Industrial polymers (9 hrs)

Semiconducting properties of organic polymers containing metal groups – semiconduction of biopolymers and its application to biochemical problems – superconductors. Industrial polymers – Synthesis, Structure and applications of industrially important polymers.

Unit V Conducting polymers (9 hrs)

Synthesis of conducting polymers - chemical structure and electronic behavior of polymers – doping of conducting polymers – p- & n- type doping – doping techniques.

References:

1. F. W. Billmeyer, Textbook of polymer Science, 3rdEdn, Wiley, New York, 1991.
2. V. R. Gowariker, N. V. Viswanathan, J. Sreedhar, Polmer Science, Wiley-Eastern, New Delhi, 1988.
3. A. Tager, Physical Chemistry of Polymers, Mir Publishers, Moscow, 1978.
4. R. J. Young, Principles of Polymer Science, 3rd Edn., Chapman and Hall, New York, 1991.
5. P. J. Flory, Polymer Science, Cornell University Press, Ithacka, 1953.
6. J. E. Katon, Organic Semiconducting Polymers, Marcel Dekker, New York, 1968.
7. B. Bahadur, N. V. Sastry, Principles of Polymer Science, Narosa, New Delhi, 2002.
8. e-PG Pathshala – P-06- Physical Chemistry –II (M-31-Polymers and their Classification)
9. NPTEL link: **https://nptel.ac.in/courses/113105028**

COURSE OUTCOME MAPPING

	UNIT 1	UNIT 2	UNIT 3	UNIT 4	UNIT 5
CO1	**L3**			**L3**	**L1**
CO2		**L3**	**L3**		**L2**
CO3	**L1**		**L3**		**L1**
CO4	**L1**		**L2**	**L3**	**L1**

L1: Addressed to small extent

L2: Addressed significantly

L3: Addressed Major Part

MATERIALS AND NANOCHEMISTRY

Course objectives:

POCEF		
L(hrs)	**C**	**Course**
45	3	Elective

1. To impart knowledge to the students on nanotechnology and nanomaterials.
2. To provide thorough knowledge on optical and photonic materials
3. To make the students conversant with the nanotubes, nanowires and nanorods.
4. To familiarize the students with preparation, properties of nano materials.
5. To create awareness about application of nanomaterials in various fields.

Course prerequisites:

The students should have basic Knowledge about nanoparticles and its nature

Course outcomes:

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

1. Learn the material preparation and properties
2. Create aware of the significance of nanomaterials, how to synthesize/make them.
3. Cchoose and identify the materials for various applications

Unit I Materials Chemistry and Synthesis **(9 hrs.)**

Solid state reaction: general principle, experimental methods, crystallization of solution, melts, glasses and gels; vapor phase transport method; synthesis of metastable phases by chimie dome; hydrothermal and high pressure methods. Solid electrolytes: β-alumina and silver compounds and their applications.

Unit II Materials for specialized applications **(9 hrs.)**

Optical and photonic materials – overview –refractive index – optical dispersion and birefringence; passive optical materials –materials and devices for passive optical applications –lenses, prisms, filters –optical wave guide, responsive optical materials-liquid crystalline materials –Photochromic, electrochromic and non-linear optical materials –light emitting materials.

Unit III Nanomaterials – Introduction and types **(9 hrs.)**

Introduction to Nanoscience: Introduction- definition of nanoscience, nanochemistry- classification of the nanomaterials – Zero dimensional nanostructures-one dimensional nanostructures- nanowires and nanorods - two dimensional nanostructures-films, nanotubes and biopolymers-three dimensional nanostructures-fullerenes and dendrimers- quantum dots and their properties.

Unit VI Nanomaterials – Preparation and Properties **(10 hrs.)**

Synthesis of nanomaterials : Introduction – precipitative methods – hydrothermal and solvothermal methods - chemical methods - reduction methods – colloidal and micellar approach – sol-gel method – chemical vapor deposition method.

Properties of nanomaterials – physical properties – finite size effects – optical, magnetic and electronic properties – chemical properties – semiconductor nanoclusters – applications of nanomaterials.

Unit V Specialized Nanomaterials **(8 hrs.)**

Nanomaterials and their occurrence in nature, nanogold and glass materials – monolayer protected metal nanoparticles – Brust method of preparation, characterization and their applications – core-shell nanoparticles – metal-metal oxide, bimetallic, semiconductor and polymer-coated core-shell nanoparticles, electrical and optical properties and applications in biology, catalysis, sensing and chemical reactivity.

References

1. H. R. Allcock, Introduction to Materials Chemistry, John Wiley & Sons, Inc. Publication, 2008.
2. A. R. West, Solid State Chemistry and its applications, Wiley 2004.
3. M. T. Weller, Inorganic Materials Chemistry, Oxford Chemistry Primes, 1996.
4. W. Jones, Organic molecular solids, CRC Press, 1997.
5. T. Pradeep, Nano: The Essentials, Tata Mc Graw-Hill, 2007.

COURSE OUTCOME MAPPING

	UNIT 1	UNIT 2	UNIT 3	UNIT 4	UNIT 5
CO1	**L3**	**L3**	**L2**	**L2**	**L2**
CO2	**L2**	**L2**	**L3**	**L3**	**L3**
CO3	**L2**	**L2**	**L2**	**L2**	**L2**

L1: Addressed to small extent

L2: Addressed significantly

L3: Addressed Major Part

PHOTOCHEMISTRY AND SURFACE CHEMISTRY

POCEG		
L(hrs)	**C**	**Course**
45	3	Elective

Course Objectives:

1. Imparting knowledge on the principles and theories on the fundamental aspects of photochemistry
2. Understanding the excited state dynamics of photophysical processes
3. Acquainting the knowledge on the basic concepts of surface kinetics

Course prerequisites:

Students studied general Physical Chemistry and Fundamentals of photochemistry in under-graduate level

Course Outcomes

1. Understand the fundamentals of photo and surface chemistry
2. Adapt the concepts on the applications of photochemistry
3. Apply the principal of adsorption isotherms for the application of surface chemistry

Unit I Photochemistry- I (9 hrs)

Properties of excited states, electronically excited states of metal complexes and charge transfer excitations - bimolecular deactivation and energy transfer processes; ligand field photochemistry – photosubstitution, photoisomerisation and photoredox reactions.

Unit II Photochemistry-II (9 hrs)

Synthesis, properties and charge transfer photochemistry of $[Ru(bpy)_3]^{2+}$- photochemical conversion and storage of solar energy - photochemistry at semiconductor electrodes –Honda cell and water photolysis.

Unit III Surface Chemistry-I (9 hrs)

Gibbs adsorption isotherm – surface films – spreading of one liquid on another – measurement of film pressure; solid-liquid interfaces – contact angle – wetting as a contact angle phenomenon – wetting as a capillary action phenomenon.

Unit IV Surface Chemistry-II (9 hrs)

Physisorption , chemisorptions –Langmuir, Freundlich and BET isotherms - surface area determination – heats of adsorption; heterogeneous catalysis – role of surfaces in catalysis – semiconductor catalysis – n-and p-type surfaces.

Unit V Mechanism of surface adsorption (9 hrs)

Reactions involving adsorbed species – Langmuir- Hinshelwood mechanism – Langmuir – Rideal mechanism. Detergents– factors in detergent action; foams and aerosols.

References:

1. J.K. Rohatgi – Mukherjee, Fundamentals of Photochemistry, Wiley Eastern Revised Edn, 1978.
2. J. Chem. Ed., October 1983 issue, American Chemical Society
3. A.W. Anderson and F.D. Fleischer, Concepts of Inorganic Photochemistry, John Wiley and Sons, New York, 1975.
4. A.W. Adamson, Physical Chemistry of Surfaces, 5th Edition, John Wiley and Sons, New York, 1990.
5. Glasstone, Text Book of Physical Chemistry, 2nd Edition, Macmillan India Ltd, New Delhi , 1974.
6. K.J. Laidler, Chemical Kinetics, 2nd Edition, Tata McGraw –Hill, New Delhi 1991.
7. J.C. Kuriacose, Catalysis, Macmillan India Ltd., New Delhi, 1991.
8. e-PG Pathshala- P-14- Organic Chemistry-IV (Surface Chemistry).

COURSE OUTCOME MAPPING

	UNIT 1	UNIT 2	UNIT 3	UNIT 4	UNIT 5
CO1	L3		L3	L3	L1
CO2	L1	L3			
CO3			L2	L3	L3

L1: Addressed to small extent

L2: Addressed significantly

L3: Addressed Major Part

CHEMISTRY OF NATURAL PRODUCTS

POCEH		
L(hrs)	**C**	**Course**
45	3	Elective

Course objectives:

This course facilitate

1. An understanding the field of chemistry of vitamins
2. An Understanding the biosynthesis of aromatic compounds particularly alkaloids
3. Identification of the terpenoids and their probable biosynthetic pathways;
4. enhancement of structure and stereochemistry of steroids
5. Identification of different types of antibiotics and its synthetic pathway

Course prerequisites:

The students should have basic Knowledge about chemistry of heterocyclic compounds.

Course outcomes:

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

1. Learn the different types of heterocyclic compounds and their chemistry
2. Understand isolation, purification and characterization of simple chemical constituents from alkaloids, terpenoids, steroids and vitamins.
3. Explain the importance of natural compounds as lead molecules for new drug discovery.
4. Learn advanced methods of structural elucidation of compounds of natural origin.

Unit – I Vitamins: **(9 hrs.)**

Definition and Classification – A detailed study of structural elucidation and synthesis of A,B, C, H

Unit- II Terpenoids **(9 hrs.)**

Classification – General Methods of determining structure – Chemistry of acyclic monoterpenes (Myrcene, Ocenene) Monocyclic monoterpenes (terpeniol, menthol) Bicyclic monoterpenes (α-pinene, camphor) sesquiterpenes (Squalene)- Abietic acid.

Unit-III Alkaloids **(9 hrs.)**

Definition and classification- General methods of structural elucidation – Structure, stereochemistry and synthesis of the papverine, morphine, reserpine, atropine and yohimbine – Biosynthesis of alkaloids.

Unit-IV Steroids **(9 hrs.)**

Classification and nomenclature – Structure and stereochemistry of cholesterol- Sex hormones - Ergosterol and its irradiation product- A General study of adrenocortical steroids- cardiac glycosides –diosgenin- Biosynthesis of steroids.

Unit-V :Antibiotics **(9 hrs.)**

Definition and Classification – A detailed study of structural elucidation and synthesis of penicillin (β- lactam) , Structure of streptomycin (aminoglycoside), tetracyclines and griseofulvin.

References

1. I.L. Finar, Organic Chemistry, Vol II , ELBS , 1975.
2. A.R. Kartitzkey and J.M. Lagowski, Principles of Heterocyclic Chemistry, Chapman & Hall, 1967.
3. R.M. Acheson., Chemistry of Heterocyclic compounds, Wiley Eastern, New Delhi, 1992.
4. R.K. Bansal, Heterocyclic Chemistry – Synthesis , reactions and mechanism, Wiley Eastern, New Delhi, 1990.
5. K.W. Bently, Alkaloids Vol. I, Interscience, 1957.
6. L.F. Fieser and M. Fieser, Steriods, Reinhold Pub. Co., New York.
7. G.A. Cordell, Introduction to Alkalodis, John Wiley & sons , New York.
8. K.B.G. Torsell, Natural Products Chemistry, John Wiley & Sons, New York.
9. Burger's Medicinal Chemistry and Drug Discovery Vol- I, 5th Edn. John Wiley & Sons, New York.
10. P.M. Ramwell, The Prostaglandins, Vol I , Plenum press, 1973.
11. Gurdeep Chatwal, Organic Chemistry of Natural Products, Vol. II, Himalaya Pub. House, Bombay 1985.
12. Manfred E. Wolff, Burger's Medicinal Chemistry, Part I to III, 4th Edn., John Wiley & Sons, New York, 1980.

COURSE OUTCOME MAPPING

	UNIT 1	UNIT 2	UNIT 3	UNIT 4	UNIT 5
CO1	L2	L2	L2	L2	L2
CO2	L3	L3	L3		
CO3	L1	L1	L3	L3	L3
CO4	L2	L2	L2	L2	L2

L1: Addressed to small extent

L2: Addressed significantly

L3: Addressed Major Part

ADVANCED ORGANIC PRACTICAL

POCL41		
P(hrs)	**C**	**Course**
60	2	Practical

Course Objectives

1. To study about the various types of separation methods for organic compounds
2. To study about the various distillation methods for organic compounds
3. To study about the various characterization methods for organic compounds

Course Prerequisites:

Student who have done Organic Chemistry practicals inB.Sc Chemistry.

Course Outcomes:

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

1. Remember the different methods for separation and characterization of organic compounds.
2. Apply the distillation and chromatographic methods for the separation of molecules.
3. Analyze and characterize the organic compounds.

Practicals

a) **Distillation Methods:**Fractional distillation, Azeotropic Distillation, Distillation under reduced pressure and Steam distillation.

b) **Separation of organic compounds:** Paper chromatography,TLC and Column chromatography.

c) **Characterization of organic compounds:** UV, FT-IR, Gas chromatography (GC), and LCMS.

References

1. R.M. Silverstein, G.C. Bassler, T.C. Morril, Spectrometric Identification of Organic Compounds, John Wiley & Sons, New York, 1991.
2. W. Kemp, Organic Spectroscopy, Macmillan Press Ltd. 1996.
3. Jag Mohan, Organic Spectroscopy, Principles and Applications, Narosa publishing House, New Delhi, 2001.
4. P.R.Young, Practical Spectroscopy, The Rapid Interpretation of Spectral Data Brooks/Cole, California, 2000.
5. R. Davis, M. Frearson, Mass Spectrometry, John Wiley & Sons, New York, 1991.

COURSE OUTCOME MAPPING

	EXPERIMENT 1	EXPERIMENT 2	EXPERIMENT 3
CO1	L2	L2	L2
CO2	L3	L3	
CO2	L1		L3

L1: Addressed to small extent

L2: Addressed significantly

L3: Addressed Major Part

Model question Paper

MANONMANIAM SUNDARANAR UNIVERSITY

DEPARTMENT OF CHEMISTRY

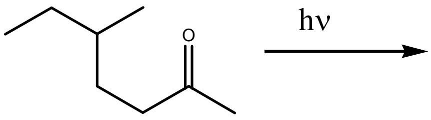
Organic synthesis

Time: Three hours Maximum: 75 marks

Part A - (10×1=10 marks)

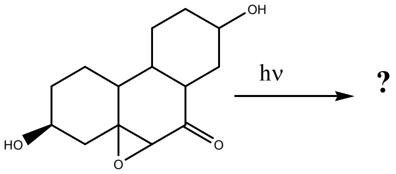
Answer **ALL** the questions

1.

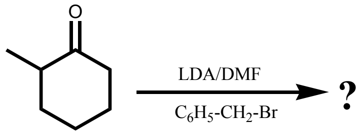


Find the product

2.



3. Write the selection rules for the cycloaddition using Hückel-Mobius rule
4. Define ene reaction.
5. How Oxitane is formed?
6. What is Intramolecular Hydrogen Abstraction in Carbonyl compounds?
7. Find the catalyst used in Beckmann rearrangement?
8. Define nucleophile and electrophile
9.



10. When lithium diphenylcuprate in ether crystallizes as a dimeric etherate, [{Li(OEt2)}(CuPh2)]2. Draw the structure

Part B - (5××5 = 25 marks)

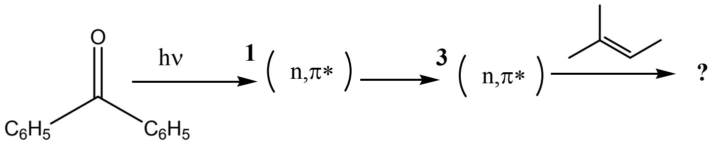
Answer **ALL** the questions choosing either (a) and (b)

11. a Write a note on conrotatory and disrotatory motion

(or)

b Explain the PMO theory for Electrocyclic reactions of 4nπ system.

12. a i



ii Draw the mechanism of conversion of barrelene to semibullvalene

(or)

b Write Brief note on Di-π-Methane Type Rearrangement.

13. a Draw the correlation diagram of [4 + 2] cycloaddition.

(or)

b With the help of FMO method, explain the stereochemistry of [3, 3] sigmatropic rearrangements under thermal and photochemical conditions

14. a Differentiate Woodward and Pervost hydroxylation.

(or)

b Write note on Selenium dioxide and osmium tetroxide as catalyst.

15. a Explain Baeyer villiger rearrangement with suitable examples.

(or)

b Write note on photofries Rearrangement

PART C - (5 x 8= 40 marks)

Answer **ALL** the questions choosing either (a) or (b).

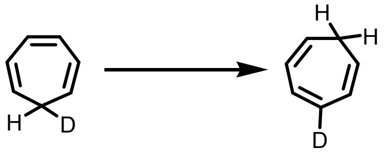
16. a What are Differentiate Woodward and pervost hydroxylation.electrocyclic reactions? With the help of correlation diagram, analyse the cis-3, 4-dimethylcyclobutene $\rightleftharpoons$ 2, 4-hexadiene system, giving stereochemistry under thermal and photochemical conditions.

(or)

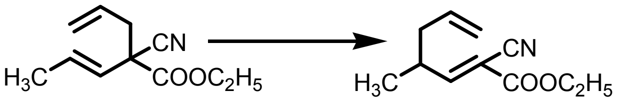
b Why cis-3, 4-dimethylcyclobutene on heating gives (2Z, 4E)-2, 4-hexadiene while on photochemical the product is (2E, 4E)-2, 4-hexadiene?

17. a Which of the following sigmatropic rearrangements would proceed readily and which slowly? Explain in detail.

1.



2.



(or)

b With the help of correlation diagram and PMO method, show that the Diels-Alder reaction is thermally allowed process.

18. a Discuss about Norrish type I and II.

(or)

b Explain the Photochemistry of olefins and carbonyl compounds.

19. a Explain Nucleophilic rearrangement with suitable examples.

(or)

b Explain electrophilic rearrangement with suitable examples.

20. a Explain how Phase transfer catalysts, crown ethers, Merrifield resin and Baker yeast can be used catalyst.

(or)

b Write note on complex metal hydrides.