K.M.G. COLLEGE OF ARTS AND SCIENCE

(AUTONOMOUS)

Approved by the Government of Tamil Nadu
Permanently Affiliated to Thiruvalluvar University, Vellore
Recognized under Section 2(f) and 12(B) of the UGC Act 1956
Accredited by NAAC (2nd Cycle) with (CGPA of 3.24/4) 'A' Grade

P.G. AND RESEARCH DEPARTMENT OF CHEMISTRY

M.Sc., CHEMISTRY

SYLLABUS

(CHOICE BASED CREDIT SYSTEM)

Under

LEARNING OUTCOMES-BASED CURRICULUM

FRAMEWORK (LOCF)

(Effective for the Batch of Students Admitted from 2024-2025)

PREFACE

"Life is simply a matter of Chemistry - James Watson"

The outcome-based curriculum for post graduate courses in chemistry is focused on the advanced level of learning fields such as inorganic, physical, organic and analytical chemistry. Chemistry is beyond the science of mere observation and understanding of nature. The curriculum is designed to include scientific research methodology and project as components of research along with the necessary provision for employability and entrepreneurship. The periodical restructuring of the syllabi is carried out to fulfill the requirements of graduate attributes, qualification descriptors, program learning outcomes and course-level learning outcomes. The purpose of the outcome-based education is meant to provide an exposure to the fundamental and advanced concepts in different branches of chemistry and its applications keeping in mind the growing needs for higher education, employability, entrepreneurship and social responsibility.

The outcome-based education enriches the curriculum to achieve self-learning module, minor projects and industrial internship to enable students to get equipped for higher studies and employment.

The program also includes training to students for seminar presentation preparation of internship reports, hands-on training in lab courses, skills to handle instruments, synthesis and analysis of compounds, developing leadership qualities, organization and participation in the inter-collegiate academic competitions. The papers studied under different categories such as subject elective, cross-disciplinary, value-added course, life skill training etc. provide additional strength to augment students' interest in related fields.

The outcome-based curriculum is intended to enrich the learning pedagogy to global standards. ICT enabled teaching learning methodology seminar invited lectures endowment lectures provide ample opportunities to students for interactions with industrialists, entrepreneurs, academics, researchers, alumni, etc. to update with recent trends in different fields of chemistry. The exposure to the academic/industrial internship and MOUs with industries can open an avenue for a start-up and its progress would be followed regularly. The OBE based evaluation methods will reflect the true cognitive levels of the students as the curriculum is designed with course outcomes and cognitive level correlations as per BLOOM's Taxonomy.

PREAMBLE

Taxonomy forms three learning domains: the cognitive (knowledge), affective (attitude), and psychomotor (skill). This classification enables to estimate the learning capabilities of students.

Briefly, it is aimed to restructure the curriculum as student-oriented, skill-based, and institution- industry-interaction curriculum with the various courses under

"Outcome Based Education with Problem Based Courses, Project Based Courses, and Industry Aligned Programmes" having revised Bloom's Taxonomy for evaluating students' skills.

1. Cognitive Domain
   (Lower levels: K1: Remembering; K2: Understanding; K3: Applying;Higher levels: K4: Analysing ; K5: Evaluating; K6: Creating)
2. Affective Domain
3. Psychomotor Domain

ABOUT THE COLLEGE

The College was founded in the new millennium 2000 by the vision of late Shri.K.M.Govindarajan fondly known as Iyah, with a mission to offer higher education in the fields of Arts and Science to the needy and the poor middle class students of this area and make them fully employable and economically self-reliant. With a humble beginning of launching an elementary school named Thiruvalluvar Elementary School in the year 1952, Iyah groomed it into a Higher Secondary School and later into a college. Education was his soul and breath. The college has grown into a full-fledged educational hub offering 12 under graduate programmes, 8 post graduate programmes, 5 M.Phil. research programmes and 4 Ph.D. programmes. The college has been accredited with 'A' grade by NAAC in 2nd cycle and recognized under section 2(f) & 12(B) of the UGC act 1956. The College is permanently affiliated to Thiruvalluvar University. The College is also acquired the status of Autonomous from the academic year 2024-2025. The College is an associate member of ICT Academy and registered member of NPTEL and Spoken Tutorials of IIT Bombay. The college is also a member of INFLIBNET and NDL.

VISION OF THE COLLEGE

Empower young men and women by educating them in the pursuit of excellence, character building and responsible citizen.

MISSION OF THE COLLEGE

Offer higher education in the fields of Arts, Science & Management to the needy and make them fully self-dependent.

QUALITY POLICY OF THE COLLEGE

KMG Students achieve the best learning results and personal growth with modern education that equip them for working life and a changing society to become deserving citizens.

ABOUT THE DEPARTMENT

The knowledge of basic science is essential for the sustainable development of the society. To get the basic knowledge in chemical science to young students the Department of Chemistry initiated in the academic year 2007-2008. The objective of our department is to motivate students to excel in chemistry at the global level, which is necessary for chemists getting placement as well as becoming an entrepreneur in future. The department was uplifted as the post graduate department in the year 2010-2011. The department has been recognized as a research department since 2014-15 to offer M.Phil., Followed that the Thiruvallur University accorded recognition to the Department as a centre for Doctoral research in Chemistry from 2019-2020. The focus of the department is the holistic development of the students and involves them in curricular and co-curricular activities. The Chemistry Department pledges itself to serve in the broadest, innovative and most liberal manner towards the advancement of chemistry in all of its branches through academics, research and service missions upholding the values and entrepreneurial skills. The job potential to the chemist is very high now and opportunities to provoke research in chemistry are ample. Needless to say that for a developing country likes ours, “CHEMISTRY IS OUR LIFE AND FUTURE”.

VISION OF THE DEPARTMENT

The Department is determined to educate and graduate rural students. The department is committed to produce the quality chemist with highest caliber who would engage in research, technological design and development to lend-a-hand in the national economic development.

MISSION OF THE DEPARTMENT

- To develop a basic knowledge in Chemistry with practical experience.
- To kindle the interest of students towards the development of technical skills to start their own business through mini projects and in-plant training.
- To enhance the students with the capacity of application oriented skills, which is a gateway to professional chemists.

PROGRAM EDUCATIONAL OBJECTIVES (PEOs)

PEO1 - Professional Skill Development: To provide professional training and skill development to students in physical sciences, related disciplines and nurture them to become responsible persons in the society.

PEO2 - Core Competency Development: To augment their core-competencies and knowledge levels in science, humanities and inter-disciplinary areas by imparting education of high standards and advanced technological tools with specialized research orientation.

PEO3 - Innovative Curriculum of Global Relevance: To upgrade the curriculum periodically based on scientific advancements, innovations and societal relevance, so as to cater to the shifting global demands as cited by University Grants Commission, CSIR, etc.

PEO4 - Environmental Sensitivity and Sustainability: To infuse environmental sensitivity in students through academic activities and hence equip them with technical skills and scientific knowledge required to protect and safeguard the environment for a sustainable future by respecting ecological balance of the globe.

PEO5 - Ethical Principles and Holistic Development: To promote ethical values and special focus on the holistic development of students to become proficient, skilled, competent and socially responsible people.

PEO6 - Accessibility and Academic Excellence: To provide an accessible learning environment of excellence and equal opportunity to students, enabling them to develop their creativity, critical thinking, leadership, employability skills and making them competent for job market.

PROGRAM OUTCOMES (POs)

On successful completion of the programme, the students will be able to:

POs	Graduate Attributes	Statements
PO1	**Disciplinary Knowledge**	Capable of demonstrating detailed knowledge and expertise in all the disciplines of the subject.
PO2	**Communication Skills**	Ability to develop communication, managerial and interpersonal skills.
PO3	**Decision Making Skill**	Foster analytical and critical thinking abilities for data-based decision-making.
PO4	**Analytical Reasoning**	Ability to evaluate the reliability and relevance of evidence, identify flaws, analyze and synthesize data from different sources.
PO5	**Problem Solving Skill**	Apply knowledge of Scientific and Management theories and Human Resource practices to solve business problems through research in Global context.
PO6	**Employability and Entrepreneurial Skill**	Equip the skills in current trends and future expectations for placements and be efficient entrepreneurs by accelerating qualities to facilitate startups in the competitive environment.
PO7	**Individual and Team Leadership Skill**	Capability to lead themselves and the team to achieve organizational goals and contribute significantly to society.
PO8	**Multicultural competence**	Possess knowledge of the values and beliefs of multiple cultures and a global perspective.
PO 9	**Moral and ethical awareness/reasoning**	Ability to embrace moral/ethical values in conducting one's life.
PO10	**Lifelong Learning**	Identify the need for skills necessary to be successful in future at personal development and demands of work place.

PROGRAM SPECIFIC OUTCOMES (PSOs)

On successful completion of the M.Sc., Chemistry, the students will be able to:

PSOs	Statements
PSO1	To create effective entrepreneurs by enhancing their critical thinking, problem solving, decision making and leadership skill that will facilitate startups and high potential organizations.
PSO2	Design and implement practices in research that comply with employment laws, leading the organization towards growth and development.
PSO3	To contribute to the development of the society by collaborating with stakeholders for mutual benefit.

Correlation Rubrics:

High	Moderate	Low	No Correlation
3	2	1	-

Mapping of PSOs with POs:

	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10
PSO1	3	3	3	3	3	3	2	1	-	2
PSO2	3	3	2	3	3	2	2	-	2	3
PSO3	3	3	1	2	-	2	2	2	3	-

K.M.G. COLLEGE OF ARTS AND SCIENCE

(AUTONOMOUS)

Subject and Credit System- M.Sc., Chemistry

(Effective for the Batch of Students Admitted from 2024-2025)

Semester–I	Credit	Hours	Semester-II	Credit	Hours	Semester-III	Credit	Hours	Semester–IV	Credit	Hours
1.1. Core-I	5	7	2.1. Core-IV	5	6	3.1. Core-VII	5	6	4.1. Core-XI	5	6
1.2 Core-II	5	7	2.2 Core-V	5	6	3.2 Core-VIII	5	6	4.2 Core-XII	5	6
1.3 Core – III	4	6	2.3 Core – VI	4	5	3.3 Core – IX	5	6	4.3 Project with viva voce	7	10
1.4 Discipline Centric Elective -I	3	5	2.4 Discipline Centric Elective – III	3	4	3.4 Core – X	4	6	4.4Elective - VI (Industry / Entrepreneurship) 20% Theory 80% Practical	3	4
1.5 Generic Elective-II:	3	5	2.5 Generic Elective -IV:	3	4	3.5 Discipline Centric Elective - V	3	3	4.5 Skill Enhancement course / Professional Competency Skill	2	4
			2.6 NME I	2	3	3.6 NME II	2	3	4.6 Extension Activity	1	
			2.7 Human Rights	2	2	3.7 Internship/ Industrial Activity	2	-			
			2.8 MOOC	2	-						
	20	**30**		**26**	**30**		**26**	**30**		**23**	**30**
Total Credit Points -95											

Semester	Part	Category	Course Code	Course Title	Ins.Hrs/	Credit	Maximum Marks

					Week		Internal	External	Total
SEMESTER - I	Part - I	Core-I	APCCH11	Organic Reaction Mechanism-I	7	5	25	75	100
		Core-II	APCCH12	Structure and Bonding in Inorganic Compounds	7	5	25	75	100
		Core-III	APCPCH13	Organic Chemistry Practical	6	4	25	75	100
		Elective – I (Choose any One)	APECH14A	Pharmaceutical Chemistry	5	3	25	75	100
			APECH14B	Electrochemistry					
		Elective – II (Choose any One)	APECH15A	Nanomaterials and Nanotechnology	5	3	25	75	100
			APECH15B	Molecular Spectroscopy					
	Semester Total				**30**	**20**			
SEMESTER - II	Part - I	Core-IV	APCCH21	Organic Reaction Mechanism-II	6	5	25	75	100
		Core-V	APCCH22	Physical Chemistry – I	6	5	25	75	100
		Core-VI	APCPCH23	Inorganic Chemistry Practical	6	4	25	75	100
		Elective-III (Choose any One)	APECH24A	Medicinal Chemistry	4	3	25	75	100
			APECH24B	Green Chemistry					
		Elective-IV (Choose any One)	APECH25A	Bio-inorganic Chemistry	4	3	25	75	100
			APECH25B	Material Science					
		SEC - I	APSCH26	Skill Enhancement Course (One from Group G)	2	2	25	75	100
	Part - II	Compulsory	APHR20	Human Rights	2	2	25	75	100
		Compulsory	APMOOC20	MOOC course	-	2	-	100	100
	Semester Total				**30**	**26**			

Semester	Part	Category	Course Code	Course Title	Ins.Hrs/ Week	Credit	Maximum Marks		
							Internal	External	Total
SEMESTER - III	Part - I	Core-VII	APCCH31	Organic Synthesis and Photochemistry	6	5	25	75	100
		Core-VIII	APCCH32	Coordination Chemistry – I	6	5	25	75	100
		Core-IX	APCPCH33	Physical Chemistry Practical	6	5	25	75	100
		Core-X	APCPCH34	Analytical Instrumentation Technique Practical	6	4	25	75	100
		Elective-V (Choose any One)	APECH35A	Pharmacognosy and Phytochemistry	4	3	25	75	100
			APECH35B	Biomolecules and Heterocyclic compounds					
		SEC - II	APSCH36	Skill Enhancement Course - Professional Communication	2	2	25	75	100
		Compulsory	APICH37	Internship / Industrial Activity (Carried out in Summer Vacation at the end of I year – 30 hours)	-	2	100	-	100
				Semester Total	**30**	**26**			
SEMESTER - IV	Part - I	Core-XI	APCCH41	Coordination Chemistry –II	6	5	25	75	100
		Core-XII	APCCH42	Physical Chemistry – II	6	5	25	75	100
		Core-XIII	APPCH43	Core Project with viva voce	10	7	25	75	100
		Elective VI (Choose any One)	APECH44A	Chemistry of Natural Products	4	3	25	75	100
			APECH44B	Polymer Chemistry					
		SEC - III	APSCH45A	Professional Competency Skill Enhancement Course Training for Competitive Examinations • Chemistry for NET / UGC - CSIR/ SET / TRB Competitive Examinations (2 hours) • General Studies for UPSC / TNPSC / Other Competitive Examinations (2 hours)	4	2	25	75	100
			APSCH45B	Chemistry for Advanced Research Studies (4 hours)					
	Part - II	Compulsory	APEA40	Extension Activity	-	1	100	-	100
				Semester Total	**30**	**23**			

Consolidated Semester wise and Component wise Credit distribution

Parts	Semester-I	Semester-II	Semester-III	Semester-IV	Total Credits
Part-I	20	22	26	22	90
Part-II	-	04	-	01	05
Total	20	26	26	23	**95**

*****Part I and Part II components will be separately taken into account for CGPA calculation and classification for the post graduate programme and has to be completed during the duration of the programme as per the norms, to be eligible for obtaining the PG degree.

Elective Courses

Courses are grouped (Group A to Group F) so as to include topics from Pure Chemistry (PC), Applied Chemistry (AC) and Industrial Components (IC) like pharmaceutical industries, Polymer labs courses for flexibility of choice by the stakeholders / institutions.

Semester I: Elective I and Elective II

Elective I to be chosen from Group A and **Elective II** to be chosen from Group B

Group A: (PC/AC/IC)

1. Pharmaceutical Chemistry
2. Electrochemistry

Group B:(PC/AC/IC)

1. Nanomaterials and Nanotechnology
2. Molecular Spectroscopy

Semester II: Elective III & Elective IV

Elective III to be chosen from **Group C** and **Elective IV** to be chosen from **Group D**

Group C:**(PC/AC/IC)**

1. Medicinal Chemistry
2. Green Chemistry

Group D :(PC/AC/IC)

1. Bioinorganic Chemistry
2. Material Science

Semester III: Elective V

Elective V to be chosen from Group E.

Group E: (PC/AC/IC)

1. Pharmacognosy and Phytochemistry
2. Biomolecules and Heterocyclic compounds

Semester IV: Elective VI

Elective VI to be chosen from Group F.

Group F:(PC/AC/IC)

1. Chemistry of Natural products
2. Polymer Chemistry

Skill Enhancement Courses

Skill Enhancement Courses are chosen to keep in pace with the latest developments in the academic / industrial front and provides flexibility of choice by the stakeholders / institutions.

Group G (Skill Enhancement Courses) SEC:(Practical based paper)

- Computational Chemistry
- 3D printing in Chemistry
- Preparation of Consumer products
- Chemistry in everyday life
- Cosmetic Chemistry
- Origin lab
- Industrial Chemistry
- Research Tools and Techniques

Instructions for Course Transaction

Courses	**Lecture Hrs**	**Tutorial hrs**	**Lab Practice**	**Total hrs**
Core	75	15	--	90
Electives	75	15	--	90
ED	75	15	--	90
Lab Practice Courses	-	15	75	90
Project	20	--	70	90

Written Examination: Theory Paper (Bloom's Taxonomy based)

Question paper Model

Intended Learning Skills	**Maximum 75 Marks** **Passing Minimum: 50%Duration:** **Three Hours**
	Part –A (10x 2 = 20 Marks) Answer ALL questions **Each Question carries 2mark**
Memory Recall / Example/ Counter Example / Knowledge aboutthe Concepts/ Understanding	Two questions from each UNIT
	Question 1 to Question 10
	Part – B (5 x 5 = 25 Marks)Answer ALL questions **Each questions carries 5 Marks**
Descriptions/ Application(problems)	**Either-or Type** Both parts of each question from the same UNIT
	Question 11(a) or 11(b) To **Question 15(a) or 15(b)**
	Part-C (3x 10 = 30 Marks) Answer any THREE questions Each question carries 10 Marks
Analysis /Synthesis / Evaluation	There shall be FIVE questions covering all the five units
	Question 16 to Question 20

COURSE DESCRIPTORS

Title of the Course	ORGANIC REACTION MECHANISM - I	**Hours/Week**	07
Course Code	APCCH11	**Credits**	05
Category	Core-1	**Year & Semester**	I & I
Prerequisites	Basic concepts of organic Chemistry	**Regulation**	2024

Objectives of the course:

- To explain the concepts of advanced organic chemistry with mechanistic approach.
- To discuss about the methods of determining the reaction mechanism and stereochemistry.
- To explain the evidences in favour of the mechanism of organic reactions and rearrangements.
- Detaille discussed stereochemical aspects of organic reaction mechanisms.
- To describes the important aspects involved in the preparation of various functional organic compounds..

UNITS	Contents	COs	Cognitive Levels
UNIT-I	**UNIT - I** Methods of Determination of Reaction Mechanism: Reaction intermediates. The transition state, Reaction coordinate diagrams. Methods of determining mechanism: non-kinetic methods – product analysis, determination of intermediates-isolation, detection, and trapping. Cross-over experiments, isotopic labelling, isotope effects and stereo chemical evidences. Kinetic methods - relation of rate and mechanism. Effect of structure on reactivity: Hammett and Taft equations. Linear free energy relationship, partial rate factor, substituent and reaction constant	CO1 CO2	K1 K2
UNIT-II	**UNIT – II: Aromatic and Aliphatic Electrophilic Substitution:** Aromaticity: Aromaticity in benzenoid, non-benzenoid, heterocycliccompounds and annulenes. Aromatic electrophilic substitution: Orientation and reactivity of di- and polysubstituted phenol, nitrobenzene andhalobenzene. Reactions involving nitrogen electrophiles: nitration, nitrosation and diazonium coupling; Sulphur electrophiles: sulphonation; Halogen electrophiles: chlorination and bromination; Carbon electrophiles: Friedel-Crafts alkylation, acylation and arylation reactions. Aliphaticelectrophilic substitution Mechanisms: SE_2 and SE_i, SE_1- Mechanism and evidences.	CO1 CO2 CO3	K1 K2 K4

UNIT-III	**UNIT - III** Aromatic and Aliphatic Nucleophilic Substitution: Aromatic nucleophilic substitution: Mechanisms - SNAr, SN1 and Benzyne mechanisms - Evidences - Reactivity, Effect of structure, leaving group and attacking nucleophile. Reactions: Oxygen and Sulphur-nucleophiles, Bucherer and Rosenmund reactions, von Richter, Sommelet- Hauser and Smiles rearrangements. SN1, ion pair, SN2 mechanisms and evidences. Aliphatic nucleophilic substitutions at an allylic carbon, aliphatic trigonal carbon and vinyl carbon.SN1, SN2, SNi, and SE1 mechanism and evidences.	CO3 CO4	K1 K2 K3 K5
UNIT-IV	**UNIT – IV: Stereochemistry-I:** Introduction to molecular symmetry and chirality – axis, plane, centre, alternating axis of symmetry. Optical purity, prochirality, enantiotopic and diastereotopic atoms, groups, faces, axial and planar chirality, chirality due to helical shape, methods of determining the configuration. Racemic modifications: Racemization by thermal, anion, cation, reversible formation, epimerization, mutarotation. D, L system, Cram's and Prelog's rules: R, S notations, proR, proS, side phase and re phase Cahn-Ingold- Prelog rules, absolute and relative configurations. Configurations of allenes, spiranes, biphenyls.	CO4 CO5	K4 K5 K6
UNIT-V	**UNIT-V: Stereochemistry-II** Conformation and reactivity of acyclic systems, intramolecular rearrangements, neighbouring group participation, chemical consequence of conformational equilibrium. Stability of five and six-membered rings: mono-, di- and polysubstituted cyclohexanes, conformation and reactivity in cyclohexane systems. Fused and bridged rings: bicyclic, poly cyclic systems, decalins and Brett's rule. Optical rotation and optical rotatory dispersion, conformational asymmetry, ORD curves, octant rule, configuration and conformation.	CO5	K3 K4 K5 K6

Recommended Text Books

1. *J. March and M. Smith, Advanced Organic Chemistry, 5th edition, John-Wiley and Sons.2001.*
2. *E. S. Gould, Mechanism and Structure in Organic Chemistry, Holt, Rinehart and Winston Inc., 1959.*
3. *P.S.Kalsi, Stereochemistry of carbon compounds, 8th edition, New Age International Publishers, 2015.*
4. *P. Y. Bruice, Organic Chemistry, 7th edn, Prentice Hall, 2013.*
5. *J.Clayden, N. Greeves, S. Warren, Organic Compounds, 2nd edition, Oxford University Press, 2014.*

Reference Books

1. Maron, S. H. and Prutton C. P. Principles of Physical Chemistry,4thed.; The Macmillan Company: Newyork,1972.

2. Lee, J. D. Concise Inorganic Chemistry, 4th ed.; ELBS William Heinemann: London,1991.

3. Gurudeep Raj, Advanced Inorganic Chemistry, 26thed.; Goel Publishing House: Meerut, 2001.

4. Atkins, P.W. & Paula, J. Physical Chemistry, 10th ed.; Oxford University Press:New York, 2014.

5. Huheey, J. E. Inorganic Chemistry: Principles of Structure and Reactivity, 4th ed .; Addison, Wesley Publishing Company: India,1993.

Website and e-learning source

1) https://sites.google.com/site/chemistryebookscollection02/home/organic- chemistry/organic
2) https://www.organic-chemistry.org/

Course Learning Outcomes (for Mapping with POs and PSOs)

On completion of the course the students should be able to

COs	CO Description	Cognitive Level
CO1	Comprehend the concepts of stereochemistry and write the configurational nomenclature	K1,K2
CO2	Examine the mechanisms of nucleophilic substitution reactions and describe nucleophilic substitution on aromatic rings.	K3
CO3	Compose multiple ways for addition-elimination reactions and predict the stereochemistry of elimination mechanisms.	K4
CO4	Assess the concept of aromaticity and classify the reactions on aromatic rings.	K5
CO5	Evaluate the orientation of aliphatic and aromatic substitution reactions	K6

	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10	PSO1	PSO2	PSO3
CO1	3	3	-	2	-	-	-	-	-	2	2	1	2
CO2	3	2	2	3	2	-	-	-	-	1	2	1	1
CO3	3	2	-	2	2	-	-	-	-	-	1	2	1
CO4	3	2	-	-	-	-	-	-	-	-	2	2	2
CO5	3	2	-	2	2	-	-	-	-	-	3	2	1

COURSE DESCRIPTORS

Title of the Course	Structure and Bonding in Inorganic Compounds	**Hours/Week**	07
Course Code	APCCH12	**Credits**	05
Category	Core-2	**Year & Semester**	I & I
Prerequisites	Basic concepts of Inorganic Chemistry	**Regulation**	2024

Objectives of the course:

This course aims at providing knowledge on

- To determine the structural properties of main group compounds and clusters.
- To gain fundamental knowledge on the structural aspects of ionic crystals.
- To familiarize various diffraction and microscopic techniques.
- To study the effect of point defects and line defects in ionic crystals.
- To evaluate the structural aspects of solids.

UNITS	Contents	COs	Cognitive Levels
UNIT-I	Structure of main group compounds and clusters: VB theory – Effect of lone pair and electronegativity of atoms (Bent's rule) on the geometry of the molecules. Structural and bonding features of B-N, S-N and P-N compounds; Poly acids – types, examples and structures; Borane cluster: Structural features of closo, nido, arachano; carboranes, hetero and metalloboranes; Wade's rule to predict the structure of Borane cluster; main group clusters	CO1 CO2	K1 K2 K3
UNIT-II	**Solid state chemistry – I:** Ionic crystals: Packing of ions in simple, hexagonal and cubic close packing, voids in crystal lattice, Radius ratio, Crystal systems and Bravais lattices, Symmetry operations in crystals, glide planes and screw axis; point group and space group; Solid state energetics: Lattice energy – Born-Lande equation - Kapustinski equation, Madelung constant.	CO1 CO2	K1 K2 K3

UNIT-III	**Solid State Chemistry – II:** Structural features of the crystal systems: Rock salt, zinc blende & wurtzite, fluorite and anti-fluorite, rutile and anatase, cadmium iodide and nickel arsenide; Spinels -normal and inverse types and perovskite structures. Crystal Growth methods: From melt and solution (hydrothermal, sol-gel methods) – principles and examples.	CO1 CO2 CO3	K1 K4
UNIT-IV	**Techniques in Solid State Chemistry:** X-ray diffraction technique: Bragg's law, Powder diffraction method – Principle and Instrumentation; Interpretation of XRD data, Phase purity, lattice constants calculation; Systematic absence of reflections; Electron diffraction technique – principle, instrumentation and application. Electron microscopy – difference between optical and electron microscopy, theory, principle, instrumentation, sampling methods and applications of SEM and TEM.	CO2 CO3 CO4 CO5	K1 K2 K3 K4 K5
UNIT-V	**Band theory and defects in solids** Band theory – features and its application of conductors, insulators and semiconductors, Intrinsic and extrinsic semiconductors; Defects in crystals – point defects (Schottky, Frenkel, metal excess and metal deficient) and their effect on the electrical and optical property, laser and phosphors; Linear defects and its effects due to dislocations.	CO3 CO5	K1 K2 K4 K5

Recommended Text Books

1. *A R West, Solid state Chemistry and its applications, 2ndEdition (Students Edition), John Wiley & Sons Ltd., 2014.*
2. *A K Bhagi and G R Chatwal, A textbook of inorganic polymers, Himalaya Publishing House, 2001.*
3. *L Smart, E Moore, Solid State Chemistry – An Introduction, 4th Edition, CRC Press, 2012.*
4. *K. F. Purcell and J. C. Kotz, Inorganic Chemistry; W.B. Saunders company: Philadelphia, 1977.*
5. *J. E. Huheey, E. A. Keiter and R. L. Keiter, Inorganic Chemistry; 4th ed.; Harper and Row: NewYork, 1983.*

Reference Books

1. *D. E. Douglas, D.H. McDaniel and J. J. Alexander, Concepts and Models in Inorganic Chemistry, 3rd Ed, 1994.*
2. *R J D Tilley, Understanding Solids - The Science of Materials, 2nd edition, Wiley Publication, 2013.*
3. *C N R Rao and J Gopalakrishnan, New Directions in Solid State Chemistry, 2nd Edition, Cambridge University Press, 199.*
4. *T. Moeller, Inorganic Chemistry, A Modern Introduction; John Wiley: New York, 1982.*
5. *D. F. Shriver, P. W. Atkins and C.H. Langford; Inorganic Chemistry; 3rd ed.; Oxford University Press: London, 2001.*

Website and e-learning source

https://ocw.mit.edu/courses/3-091-introduction-to-solid-state-chemistry-fall-2018/video_galleries/lecture-videos/

Course Learning Outcomes (for Mapping with POs and PSOs)

On completion of the course the students should be able to

COs	CO Description	Cognitive Level
CO1	Predict the geometry of main group compounds and clusters.	K1,K2,K3
CO2	Explain about the packing of ions in crystals and apply the radius ratio rule to predictthe coordination number of cations.	K1,K2,K3
CO3	Understand the various types of ionic crystal systems and analyze their structuralfeatures.	K1,K4
CO4	Elucidate the crystal growth methods and principles of diffraction and microscopic techniques	K3,K4,K5
CO5	To recognize the important of Defects in crystals	K1,K2,K3

	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10	PSO1	PSO2	PSO3
CO1	3	3	-	3	2	-	-	-	-	-	2	2	2
CO2	3	3	-	-	-	-	-	-	-	-	2	1	2
CO3	3	3	-	2	1	-	-	-	-	-	1	1	1
CO4	3	3	2	3	2	1	-	-	-	2	3	2	1
CO5	3	3	-	2	-	-	-	-	-	1	1	2	1

COURSE DESCRIPTORS

Title of the Course	**Organic Chemistry Practical**	**Hours/Week**	06
Course Code	APCPCH13	**Credits**	04
Category	**Core Practical**	**Year & Semester**	I & I
Prerequisites	**Basic concepts of Organic Chemistry**	**Regulation**	2024

Objectives of the course:

The course aims at giving an overall view of the

- To understand the concept of separation, qualitative analysis and preparation of organic compounds.
- To develop analytical skill in the handling of chemical reagents for separation of binary and ternaryorganic mixtures.
- To analyze the separated organic components systematically and derivatize them suitably.
- To construct suitable experimental setup for the organic preparations involving two stages.
- To experiment different purification and drying techniques for the compound processing.

UNITS	Contents	COs	Cognitive Levels
UNIT-I	**Separation and analysis:** Two component mixtures. Ternary component (Demo)	CO1 CO2 CO3	K1,K2 K3,K4
UNIT-II	**Estimations:** **a)** Estimation of Phenol (bromination) **b)** Estimation of Aniline (bromination) **c)** Estimation of Ethyl methyl ketone (iodimetry) **d)** Estimation of Glucose (redox) **e)** Estimation of Ascorbic acid (iodimetry).	CO2	K1,K2 K3,K4 K5

UNIT-III	**Two stage preparations:** a) p-Bromoacetanilide from aniline b) p-Nitroaniline from acetanilide c) 1,3,5-Tribromobenzene from aniline d) Acetyl salicyclic acid from methyl salicylate e) Benzilic acid from benzoin f) m-Nitroaniline from nitrobenzene g) m-Nitrobenzoic acid from methyl benzoate	CO2 CO4 CO5	K1,K2 K3, K4

Recommended Text Books

1. *Ganapragasm, N. S., & Ramamurthy, C. (2015). Organic Chemistry Lab Manual, (2nd Ed.). Vishwanathan S Printers and Publishers (P) Ltd.*
2. *Furniss, B. S., Hannaford, A. J., Smith, P. W. G., & Tatchell, A. R. Vogel's Textbook of Practical Organic Chemistry, (5th Ed.). Pearson publication.*

Reference Books

1. *Venkateswaran, V., Veeraswamy, R., & Kulandaivelu, A. R. (1997). Basic principles of practical chemistry, (2nd ed.). Sultan Chand & Sons.*
2. *Organic Chemistry Lab Manual for Micro Qualitative Analysis. Department of Chemistry, KMG College of Arts And Science (AUTONOMOUS), Gudiyatham,635803 (Private circulation).*

Website and e-learning source

1. *https://youtu.be/EyWGc-vizic*
2. *https://youtu.be/mQ035ZrdD4Y*
3. *https://youtu.be/N96JaRnE7n0*

Course Learning Outcomes (for Mapping with POs and PSOs)

On completion of the course the students should be able to

COs	CO Description	Cognitive Level
CO1	To recall the basic principles of organic separation, qualitative analysis and preparation.	K1,K2,K3,K4
CO2	To explain the method of separation and analysis of separated organic mixtures and convert them as derivatives by suitable preparation method.	K1,K2
CO3	To determine the characteristics of separation of organic compounds by various chemical reactions.	K1,K2,K3,K4,K5
CO4	To develop strategies to separate, analyze and prepare organic compounds.	K3,K4,K5
CO5	To formulate a method of separation, analysis of organic mixtures and design suitable procedure for organic preparations.	K3,K4,K5

	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10	PSO1	PSO2	PSO3
CO1	3	2	-	3	-	-	-	-	-	2	3	3	1
CO2	3	3	-	3	-	-	-	-	-	1	3	2	-
CO3	3	2	2	3	-	-	-	-	-	-	3	3	-
CO4	3	3	3	3	3	-	2	-	2	2	3	3	2
CO5	3	3	2	3	2	-	-	-	-	2	3	3	-

COURSE DESCRIPTORS

Title of the Course	PHARMACEUTICAL CHEMISTRY	Hours/Week	05
Course Code	APECH14A	Credits	03
Category	ELECTIVE - I	Year & Semester	I & I
Prerequisites	Basic knowledge on drugs and doses	Regulation	2024

Objectives of the course:

This course aims at providing knowledge on

- To understand the advanced concepts of pharmaceutical chemistry.
- To recall the principle and biological functions of various drugs.
- To train the students to know the importance as well the consequences of various drugs.
- To have knowledge on the various analysis and techniques.
- To familiarize on the drug dosage and its structural activities.

UNITS	Contents	COs	Cognitive Levels
UNIT-I	Physical properties in Pharmaceuticals: Physical properties of drug molecule: physical properties. Refractive index- Definition, explanation, formula, importance, determination, specific & molar refraction. Dielectric constant & Induced Polarization- Dielectric constant explanation & determination. Rheology of pharmaceutical systems: Introduction, Definition, Applications, concept of viscosity, Newton's law of flow, Kinematic, Relative, Specific, Reduced & Intrinsic viscosity.	CO1 CO2	K1 K2 K3
UNIT-II	**Isotopic Dilution analysis:** Principle and applications, Neutron activation analysis: Principle, advantages and limitations, Scintillation counters: Body scanning. Introduction to radiopharmaceuticals. Properties of various types of radiopharmaceuticals, Radio-pharmaceuticals As diagnostics, as therapeutics, for research and sterilization. Physico Chemical Properties and drug action. Physico chemical properties of drugs (a) Partition coefficient, (b) solubility (c) surface activity, (d) degree of ionization.	CO1 CO2	K1 K2

UNIT-III	**Drug dosage and product development:** Introduction to drug dosage Forms & Drug Delivery system – Definition of Common terms. Drug Regulation and control, pharmacopoeias formularies, sources of drug, drug nomenclature, routes of administration of drugs products, need for a dosage form, classification of dosage forms. Drug dosage and product development. Introduction to drug dosage Forms & Drug Delivery system – Definition of Common terms. Drug Regulation and control, pharmacopoeias formularies, sources of drug, drug nomenclature, routes of administration of drugs products, need for a dosage form, classification of dosage forms.	CO1 CO2 CO3 CO5	K1 K3 K4
UNIT-IV	**Development of new drugs:** Introduction, procedure followed in drug design, the research for lead compounds, molecular modification of lead compounds. Structure-Activity Relationship (SAR) Factors effecting bioactivity, resonance, inductive effect, isoterism, bioisosterism, spatial considerations, biological properties of simple functional groups, theories of drug activity, occupancy theory, rate theory, induced-fit theory.	CO2 CO3 CO5	K3 K4 K5
UNIT-V	**Computers in Pharmaceutical Chemistry:** Need of computers for chemistry. Computers for Analytical Chemists Introduction to computers: Organization of computers, CPU, Computer memory, I/O devices, information storage, software components. Application of computers in chemistry: Quantitative structure activity relationship (QSAR): Development of QSAR, drug receptor interactions, the additivity of group contributions, physico-chemical parameters, lipophilicity parameters, electronic parameter, ionization constants, steric parameters, chelation parameters, redox potential, indicator-variables	CO3 CO4 CO5	K1 K2 K4

Recommended Text Books

1. *Physical Chemistry- Bahl and Tuli.*
2. *Text Book of Physical Pharmaceutics, IInd edition, Vallabh Prakashan-.C.V.S. Subramanyam.*
3. *Medicinal Chemistry (Organic Pharmaceutical Chemistry), G.R Chatwal, Himalaya Publishing house.*
4. *Instrumental method of Analysis: Hubert H, Willard,7th edition.*
5. *Textbook of Pharmaceutical Chemistry by,Jayshree Ghosh, S. Chand & company Ltd.Pharmaceutical Chemistry by Dr. S. Lakshmi, Sultanchand & Sons.*

Reference Books

1. *Computers in chemistry, K.V. Raman, Tata Mc.Graw-Hill, 1993.*
2. *Computers for Chemists, S.K Pundir, Anshu bansal, A pragate prakashan., 2 nd edition, New age international (P) limited, New Delhi.*
3. *Physical Pharmacy and Pharmaceutical Sciences by Martins, Patrick J. Sinko, Lippincott. William and Wilkins.*
4. *Cooper and Gunn's Tutorial Pharmacy ,6th edition by S.J. Carter, CBS Publisher Ltd.*
5. *Ansels pharmaceutical Dosage forms and Drug Delivery System by Allen Popvich and Ansel, Indian edition-B.I. Publication Pvt. Ltd.*

Website and e-learning source

https://www.ncbi.nlm.nih.gov/books/NBK482447/

https://training.seer.cancer.gov/treatment/chemotherapy/types.html

Course Learning Outcomes (for Mapping with POs and PSOs)

On completion of the course the students should be able to

COs	CO Description	Cognitive Level
CO1	To identify the suitable drugs for various diseases.	K1,K2
CO2	To apply the principles of various drug action and drug design.	K2,K3,K4
CO3	To acquire the knowledge on product development based on SAR.	K1,K2,K3
CO4	To apply the knowledge on applications of computers in Chemistry.	K3,K4,K5
CO5	To synthesize new drugs after understanding the concepts SAR.	K1,K5,K6

	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10	PSO1	PSO2	PSO3
CO1	3	2	2	3	-	-	-	-	-	-	3	3	3
CO2	3	3	2	2	-	-	-	-	-	-	3	2	2
CO3	3	3	2	3	2	-	-	-	-	-	3	2	2
CO4	3	3	-	-	-	3	-	-	-	3	3	3	2
CO5	3	3	2	3	2	2	-	-	-	2	2	2	2

COURSE DESCRIPTORS

Title of the Course	ELECTROCHEMISTRY	Hours/Week	05
Course Code	APECH14B	Credits	03
Category	ELECTIVE - I	Year & Semester	I & I
Prerequisites	Basic knowledge of Electrochemistry	Regulation	2024

Objectives of the course:

This course aims at providing knowledge on

- To understand the behavior of electrolytes in terms of conductance, ionic atmosphere, interactions.
- To familiarize the structure of the electrical double layer of different models.
- To compare electrodes between current density and over potential.
- To discuss the mechanism of electrochemical reactions.
- To highlight the different types of over voltages and its applications in electroanalytical techniques.

UNITS	Contents	COs	Cognitive Levels
UNIT-I	**Ionics**: Arrhenius theory -limitations, van't Hoff factor and its relation to colligative properties. Deviation from ideal behavior. Ionic activity, mean ionic activity and mean ionic activity coefficient-concept of ionic strength, Debye Huckel theory of strong electrolytes, activity coefficient of strong electrolytes Determination of activity coefficient ion solvent and ion-ion interactions. Born equation. Debye-Huckel Bjerrum model. Derivation of Debye-Huckel limiting law at appreciable concentration of electrolytes modifications and applications. Electrolytic conduction -Debye- Huckel Onsager treatment of strong electrolyte-qualitative and quantitative verification and limitations.	CO1	K1 K2
UNIT-II	**Electrode-electrolyte interface:** Interfacial phenomena - Evidences for electrical double layer, polarizable and non-polarizable interfaces, Electrocapillary phenomena - Lippmann equation electro capillary curves. Electro-kinetic phenomena electro-osmosis, electrophoresis, streaming and sedimentation potentials. Structure of double layer: Helmholtz - Perrin, Guoy Chapman and Stern models of electrical double layer. Zeta potential and potential at zero charge. Applications and limitations.	CO1 CO4	K1 K2 K3

UNIT-III	**Electrodics of Elementary Electrode Reactions:** Behavior of electrodes: Standard electrodes and electrodes at equilibrium. Anodic and Cathodic currents, condition for the discharge of ions. Nernst equation, polarizable and non-polarizable electrodes. Model of three electrode system, over potential. Rate of electro chemical reactions: Rates of simple elementary reactions. Butler-Volmer equation-significance of exchange current density, net current density and symmetry factor. Low and high field approximations. Symmetry factor and transfer coefficient Tafel equations and Tafel plots.	CO1 CO2	K1 K2 K3 K4
UNIT-IV	**Electrodics of Multistep Multi Electron System:** Rates of multi-step electrode reactions, Butler - Volmer equation for a multi-step reaction. Rate determining step, electrode polarization and depolarization. Transfer coefficients, its significance and determination, Stoichiometric number. Electro-chemical reaction mechanisms-rate expressions, order, and surface coverage. Reduction of I^{3-}, Fe^{2+}, and dissolution of Fe to Fe^{2+}. Overvoltage - Chemical and electro chemical, Phase, activation and concentration over potentials. Evolution of oxygen and hydrogen at different pH. Pourbiax and Evan's diagrams.	CO2 CO3 CO4	K1 K2 K3 K4
UNIT-V	**Concentration Polarization, Batteries and Fuel cells:** Modes of Transport of electro active species - Diffusion, migration and hydrodynamic modes. Role of supporting electrolytes. Polarography principle and applications. Principle of square wave polarography. Cyclic voltammetry- anodic and cathodic stripping voltammetry and differential pulse voltammetry. Sodium and lithium-ion batteries and redox flow batteries. Mechanism of charge storage: conversion and alloying. Capacitors-mechanism of energy storage, charging at constant current and constant voltage. Energy production systems: Fuel Cells: classification, alkaline fuel cells, phosphoric acid fuel cells, high temperature fuel cells.	CO4 CO5	K1 K2 K3 K4

Recommended Text Books

1. *D. R. Crow, Principles and applications of electrochemistry, 4thedition, Chapman & Hall/CRC, 2014.*
2. *J. Rajaram and J.C. Kuriakose, Kinetics and Mechanism of chemical transformations Macmillan India Ltd., New Delhi, 2011.*
3. *S. Glasstone, Electro chemistry, Affiliated East-West Press, Pvt., Ltd., New Delhi, 2008.*
4. *B. Viswanathan, S. Sundaram, R. Venkataraman, K. Rengarajan and P.S. Raghavan, Electrochemistry-Principles and applications, S. Viswanathan Printers, Chennai,2007.*
5. *Joseph Wang, Analytical Electrochemistry, 2nd edition, Wiley, 2004.*

Reference Books

1. *J.O.M. Bockris and A.K.N. Reddy, Modern Electro chemistry, vol.1 and 2B, Springer, Plenum Press, New York, 2008.*
2. *J.O.M. Bockris, A.K.N. Reddy and M.G. Aldeco Morden Electro chemistry, vol. 2A, Springer, Plenum Press, New York, 2008.*
3. *Philip H. Rieger, Electrochemistry, 2nd edition, Springer, New York, 2010.*
4. *L.I. Antropov, Theoretical electrochemistry, Mir Publishers, 1977.*
5. *K.L. Kapoor, A Text book of Physical chemistry, volume-3, Macmillan, 2001.*

Website and e-learning source

. https://www.pdfdrive.com/modern-electrochemistry-e34333229.

Course Learning Outcomes (for Mapping with POs and PSOs)

On completion of the course the students should be able to

COs	CO Description	Cognitive Level
CO1	Understand the behaviour of electrolytes in solution and compare the structures of electrical double layer of different models.	K2,K3
CO2	Predict the kinetics of electrode reactions by applying Butler-Volmer and Tafel equations.	K1,K3,K4
CO3	Analyze the mechanism of corrosion using Pourbiax and Evan's diagrams.	K2,K3,K4
CO4	Discuss the necessity electrical double layer and activity coefficient of electrolytes.	K1,K2
CO5	Describe electrochemical reaction mechanism in storage devices.	K3,K4

	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10	PSO1	PSO2	PSO3
CO1	3	3	-	3	-	-	-	-	-	-	3	2	2
CO2	3	3	3	3	3	-	-	-	-	-	3	3	2
CO3	3	3	-	2	-	-	-	-	-	-	3	2	1
CO4	3	3	-	-	-	-	-	-	-	-	3	2	2
CO5	3	3	2	-	-	-	-	-	-	-	3	1	2

COURSE DESCRIPTORS

Title of the Course	**NANO MATERIALS AND NANO TECHNOLOGY**	**Hours/Week**	05
Course Code	APECH15A	**Credits**	03
Category	ELECTIVE - II	**Year & Semester**	I & I
Prerequisites	**Basic knowledge of crystallography and material science**	**Regulation**	2024

Objectives of the course:

This course aims at providing knowledge on

- To understand the concept of nano materials and nano technology.
- To understand the various types of nano materials and their properties.
- To understand the applications of synthetically important nano materials.
- To correlate the characteristics of various nano materials synthesized by new technologies.
- To design synthetic routes for synthetically used new nano materials.

UNITS	Contents	COs	Cognitive Levels
UNIT-I	Introduction of nanomaterials and nanotechnologies, Introduction-role of size, classification-0D, 1D, 2D, 3D. Synthesis Bottom – Up, Top–Down, consolidation of Nano powders. Features of nanostructures, Background of nanostructures. Techniques of synthesis of nanomaterials, Tools of the nanoscience. Applications of nanomaterials and technologies.	CO1 CO4 CO5	K1 K2
UNIT-II	Bonding and structure of the nanomaterials, Predicting the Type of Bonding in a Substance crystal structure. Metallic nanoparticles, Surfaces of Materials, Nanoparticle Size and Properties. Synthesis Physical and chemical methods - inert gas condensation, arc discharge, laser ablation, sol-gel, solvo-thermal and hydrothermal- CVD-types, metalloorganic, plasma enhanced, and low-pressure CVD. Microwave assisted and electrochemical synthesis.	CO1 CO2	K1 K2
UNIT-III	Mechanical properties of materials, theories relevant to mechanical properties. Techniques to study mechanical properties of nanomaterials, adhesion and friction, thermal properties of nanomaterials Nanoparticles: gold and silver, metal oxides: silica, iron oxide and alumina - synthesis and properties	CO1 CO3	K1 K2 K3

UNIT-IV	Classification of Materials based on Conductivity, magnetic properties, electronic properties. Semiconductor materials – classification-Ge, Si, GaAs, SiC, GaN, GaP, CdS, PbS. Identification of materials as p and n – type semiconductor-Hall effect - quantum and anomalous, Hall voltage - interpretation of charge carrier density. Applications of semiconductors: p-n junction as transistors and rectifiers, photovoltaic and photogalvanic cell**.**	CO1 CO2 CO5	K1 K2 K3 K4
UNIT-V	Nano thin films, nanocomposites. Application of nanoparticles in different fields. Core-shell nanoparticles - types, synthesis, and properties. Nanocomposites - metal-, ceramic- and polymer-matrix composites applications. Characterization – SEM, TEM and AFM - principle, instrumentation and applications.	CO4 CO5	K2 K3 K4

Recommended Text Books

1. *S.Mohan and V. Arjunan, Principles of Materials Science, MJP Publishers, 2016.*
2. *Arumugam, Materials Science, Anuradha Publications,2007.*
3. *Giacavazzo et. al., Fundamentals of Crystallography, International Union of Crystallography. Oxford Science Publications, 2010*
4. *Woolfson, An Introduction to Crystallography, Cambridge University Press, 2012.*
5. *James F. Shackelford and Madanapalli K. Muralidhara, Introduction to Materials Science for Engineers. 6th ed., PEARSON Press, 2007.*

Reference Books

1. *S.Mohan and V. Arjunan, Principles of Materials Science, MJP Publishers, 2016.*
2. *Arumugam, Materials Science, Anuradha Publications,2007.*
3. *Giacavazzo et. al., Fundamentals of Crystallography, International Union of Crystallography. Oxford Science Publications, 2010*
4. *Woolfson, An Introduction to Crystallography, Cambridge University Press, 2012.*
5. *James F. Shackelford and Madanapalli K. Muralidhara, Introduction to Materials Science for Engineers. 6th ed., PEARSON Press, 2007.*

Website and e-learning source

1. http://xrayweb.chem.ou.edu/notes/symmetry.html.
2. http://www.uptti.ac.in/classroom-content/data/unit%20cell.pdf.

Course Learning Outcomes (for Mapping with POs and PSOs)

On completion of the course the students should be able to

COs	CO Description	Cognitive Level
CO1	Describe and consolidate the various types of nanomaterials.	K1,K2
CO2	Explain the fabricating methods of nanostructures	K1,K2
CO3	Narrate the unique properties of nanomaterials to reduce dimensionality of the material.	K2,K3
CO4	Discuss the tools to characterize the nanoparticles.	K2,K3
CO5	Analyze the advanced applications of nanomaterials.	K3,K4

	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10	PSO1	PSO2	PSO3
CO1	3	3	-	-	-	-	-	-	-	-	3	1	2
CO2	3	3	-	2	-	-	-	-	-	-	3	1	1
CO3	3	3	-	-	-	-	-	-	-	-	3	2	1
CO4	3	3	-	2	-	-	-	-	-	-	3	2	2
CO5	3	3	-	3	-	-	-	-	-	-	3	3	2

COURSE DESCRIPTORS

Title of the Course	MOLECULAR SPECTROSCOPY	Hours/Week	05
Course Code	APECH15B	Credits	03
Category	ELECTIVE - II	Year & Semester	I & I
Prerequisites	Basic Knowledge of Spectroscopy	Regulation	2024

Objectives of the course:

This course aims at providing knowledge on

- To understand the influence of rotation and vibrations on the spectra of the polyatomic molecules.
- To study the principle of Raman spectroscopy, ESR spectroscopy, EPR spectroscopy and fragmentation patterns in Mass spectroscopy.
- To highlight the significance of Franck-Condon principle to interpret the selection rule, intensity and types of electronic transitions.
- To interpret the first and second order NMR spectra in terms of splitting and coupling patterns using correlation techniques such as COSY, HETCOR, NOESY.
- To carry out the structural elucidation of molecules using different spectral techniques.

UNITS	Contents	COs	Cognitive Levels
UNIT-I	**Rotational and Raman Spectroscopy:** Rotational spectra of diatomic and polyatomic molecules. Intensities of rotational spectral lines, effect of isotopic substitution. Non-rigid rotators. Classical theory of the Raman effect, polarizability as a tensor, polarizability ellipsoids, quantum theory of the Raman effect, Pure rotational Raman spectra of linear and asymmetric top molecules, Stokes and anti-Stokes lines. Vibrational Raman spectra, Raman activity of vibrations, rule of mutual exclusion, rotational fine structure-O and S branches, Polarization of Raman scattered photons.	CO1	K1 K2

UNIT-II	**Vibrational Spectroscopy:** Vibrations of molecules, harmonic and anharmonic oscillators-vibrational energy expression, energy level diagram, vibrational wave functions and their symmetry, selection rules, expression for the energies of spectral lines, computationof intensities, hot bands, effect of isotopic substitution. Diatomic vibrating rotor, vibrational-rotational spectra of diatomic molecules, P, R branches, breakdown of the Born-Oppenheimer approximation. Vibrations of polyatomic molecules – symmetry properties, overtone and combination frequencies. Influence of rotation on vibrational spectra of polyatomic molecule, P, Q, R branches, parallel and perpendicular vibrations of linear and symmetric top molecules.	CO2	K2 K3
UNIT-III	**Electronic spectroscopy:** Electronic Spectroscopy: Electronic spectroscopy of diatomic molecules, Frank-Condon principle, dissociation and pre dissociation spectra. $\pi \rightarrow \pi^*$, $n \rightarrow \pi^*$ transitions and their selection rules. Photoelectron Spectroscopy: Basic principles, photoelectron spectra of simple molecules, X-ray photoelectron spectroscopy (XPS). Lasers: Laser action, population inversion, properties of laser radiation, examples of simple laser systems.	CO3	K3 K4 K5
UNIT-IV	**NMR and ESR spectroscopy:** Chemical shift, Mechanism of shielding and de-shielding. Spin systems: Simplification of complex spectra. Spin-spin interactions: Homonuclear coupling interactions - AX, AX2, AB types. Vicinal, germinal and long-range coupling-spin decoupling. Nuclear Overhauser effect (NOE), Factors influencing coupling constants and Relative intensities. 13CNMR and structural correlations, Satellites. ESR spectroscopy Characteristic features of ESR spectra, line shapes and line widths; The g value and the hyperfine coupling parameter (A). Interpretation of ESR spectra and structure elucidation of organic radicals using ESR spectroscopy; Spin orbit coupling and significance of g tensors, zero/non-zero field splitting, Kramer's degeneracy.	CO4	K3 K4 K5

UNIT-V	**Mass Spectrometry, EPR and Mossbauer Spectroscopy:** Ionization techniques- Electron ionization (EI), chemical ionization (CI), isotope abundance, molecular ion, fragmentation processes of organic molecules, deduction of structure through mass spectral fragmentation, high resolution. Effect of isotopes on the appearance of mass spectrum. EPR spectra of anisotropic systems - anisotropy in g value, causes of anisotropy, anisotropy in hyperfine coupling, hyperfine splitting caused by quadrupole nuclei. Principle of Mossbauer spectroscopy: Doppler shift, Isomer shift, Applications: Mossbauer spectra of high and low-spin Fe and Sn compounds.	CO5	K3 K4

Recommended Text Books

1. *C. N. Banwell and E. M. McCash, Fundamentals of Molecular Spectroscopy, 4th Ed., Tata McGraw Hill, New Delhi, 2000.*
2. *R. M. Silverstein and F. X. Webster, Spectroscopic Identification of Organic Compounds, 6th Ed., John Wiley & Sons, New York, 2003.*
3. *W. Kemp, Applications of Spectroscopy, English Language Book Society, 1987.*
4. *D. H. Williams and I. Fleming, Spectroscopic Methods in Organic Chemistry, 4th Ed., Tata McGraw-Hill Publishing Company, New Delhi, 1988.*
5. *R. S. Drago, Physical Methods in Chemistry; Saunders: Philadelphia, 1992.*

Reference Books

1. *P.W. Atkins and J. de Paula, Physical Chemistry, 7th Ed., Oxford University Press, Oxford, 2002.*
2. *I. N. Levine, Molecular Spectroscopy, John Wiley & Sons, New York, 1974.*
3. *A. Rahman, Nuclear Magnetic Resonance-Basic Principles, Springer-Verlag, New York,1986.*
4. *K. Nakamoto, Infrared and Raman Spectra of Inorganic and coordination Compounds, PartB: 5th ed., John Wiley& Sons Inc., New York, 1997.*
5. *J. A. Weil, J. R. Bolton and J. E. Wertz, Electron Paramagnetic Resonance; Wiley Interscience, 1994.*

Website and e-learning source

https://onlinecourses.nptel.ac.in/noc20_cy08/preview

https://www.digimat.in/nptel/courses/video/104106122/L14.html

Course Learning Outcomes (for Mapping with POs and PSOs)

On completion of the course the students should be able to

COs	CO Description	Cognitive Level
CO1	Explain the importance of rotational and Raman spectroscopy.	K1,K2
CO2	Apply the vibrational spectroscopic techniques to diatomic and polyatomic molecules.	K2,K3
CO3	Evaluate different electronic spectrum of simple molecules using electronicspectroscopy.	K3,K4,K5
CO4	Predict the spectrum of 2D NMR – COSY, NOESY and ESR spectroscopic techniques.	K3,K4,K5
CO5	Describe the Mass Spectrometry, EPR and Mossbauer Spectroscopy techniques.	K3,K4

	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10	PSO1	PSO2	PSO3
CO1	3	3	-	-	-	-	-	-	-	-	3	3	2
CO2	3	3	-	2	-	-	-	-	-	-	3	3	1
CO3	3	3	2	3	2	-	-	-	-	-	3	3	2
CO4	3	3	2	3	1	-	-	-	-	-	3	3	2
CO5	3	3	3	2	-	-	-	-	-	-	3	3	2