Semester I

Teaching Plan

Department : Chemistry
Class : I M. Sc Chemistry
Title of the Course : **Core Course I:** Organic Reaction Mechanism – I
Semester : **I**
Course Code : CP231CC1

Course Code	L	T	P	Credits	Inst. Hours	Total Hours	Marks		
							CIA	External	Total
CP231CC1	**7**	**-**	**-**	**5**	**7**	**105**	**25**	**75**	**100**

Objectives

1. To understand the mechanism of various organic reactions.
2. To correlate and appreciate the differences involved in the various types of organic reaction mechanisms.
3. To design feasible synthetic routes for the preparation of organic compounds.

Course outcomes

CO	Upon completion of this course, the students will be able to:	PSO addressed	Cognitive level
CO-1	recall the basic principles of organic chemistry	PSO - 1	K2(U)
CO-2	understand the formation and detection of reaction intermediates of organic reactions.	PSO - 2	K2(U)
CO-3	predict the reaction mechanism of organic reactions and stereochemistry of organic compounds.	PSO - 3	K4(An)
CO-4	apply the principles of kinetic and non-kinetic methods to determine the mechanism of reactions.	PSO - 1	K3(Ap)
CO-5	design and synthesize new organic compounds by correlating the stereochemistry of organic compounds.	PSO - 2	K5(E)

Teaching plan

Total Contact hours: 105 (Including lectures, assignments and tests)

Unit	Module	Topic	Teaching Hours	Cognitive level	Pedagogy	Assessment/ Evaluation
I	**Methods of Determination of Reaction Mechanism**					
	1	Reaction intermediates, The transition state, Reaction coordinate diagrams, Thermodynamic and kinetic requirements of reactions:	5	K2(U)	Lecture with ppt	Oral test
	2	Hammond postulate. Methods of determining mechanism: non-kinetic methods - product analysis, determination of intermediates-isolation, detection, and trapping	7	K3(Ap)	Lecture with ppt	Short test
	3	Cross-over experiments, isotopic labelling, isotope effects and stereo chemical evidences. Kinetic methods - relation of rate and mechanism.	3	K4(An)	Lecture using chalk and talk	Slip test and MCQ
	4	Effect of structure on reactivity: Hammett and Taft equations. Linear free energy relationship, partial rate factor, substituent and reaction constants.	6	K3(Ap)	Lecture using chalk	Slip test and MCQ
II	**Aromatic and Aliphatic Electrophilic Substitution**					
	1	Aromaticity: Aromaticity in benzenoid, non-benzenoid, heterocyclic compounds and annulenes.	5	K2(U)	Lecture with ppt	Short summary
	2	Aromatic electrophilic substitution: Orientation and reactivity of di- and polysubstituted phenol, nitrobenzene and halobenzene.	4	K3(Ap)	Lecture using chalk and talk	Class test
	3	Reactions involving nitrogen electrophiles: nitration, nitrosation and diazonium coupling; Sulphur electrophiles: sulphonation;	5	K3(Ap)	Group discussion	Oral test

	4	Halogen electrophiles: chlorination and bromination; Carbon electrophiles: Friedel-Crafts alkylation, acylation and arylation reactions	4	K4(An)	Lecture using chalk and talk	Short test and quiz
	5	Aliphatic electrophilic substitution Mechanisms: SE2 and SEi, SE1-Mechanism and evidences.	3	K2(U)	Lecture with ppt	Oral test
III	**Aromatic and Aliphatic Nucleophilic Substitution**					
	1	Aromatic nucleophilic substitution: Mechanisms - S_NAr, S_N1 and Benzyne mechanisms - Evidences - Reactivity, Effect of structure, leaving group and attacking nucleophile.	5	K2(U)	Lecture using ppt	Concept explanations
	2	Reactions: Oxygen and Sulphur-nucleophiles, Bucherer and Rosenmund reactions, von Richter, Sommelet- Hauser and Smiles rearrangements.	5	K3(Ap)	Lecture using chalk and talk	Slip test
	3	S_N1, ion pair, S_N2 mechanisms and evidences. Aliphatic nucleophilic substitutions at an allylic carbon, aliphatic trigonal carbon and vinyl carbon.	5	K3(Ap)	Lecture using chalk and talk	Class test
	4	S_N1, S_N2, S_Ni, and S_E1 mechanism and evidences, Swain- Scott, Grunwald-Winstein relationship - Ambident nucleophiles	6	K4(An)	Lecture using chalk and talk	Slip test and quiz
IV	**Stereochemistry-I**					
	1	Introduction to molecular symmetry and chirality – axis, plane, center, alternating axis of symmetry. Optical isomerism due to asymmetric and dissymmetric molecules with C, N, S based chiral	4	K2(U)	Lecture using videos and ppt	Concept explanations and short summary

		centers				
	2	Optical purity, prochirality, enantiotopic and diastereotopic atoms, groups, faces, axial and planar chirality, chirality due to helical shape, methods of determining theconfiguration.	4	K3(Ap)	Lecture using chalk and talk	Class test
	3	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.	4	K3(Ap)	Lecture using chalk and talk	Short test
	4	Configurations of allenes, spiranes, biphenyls, cyclooctene, helicene, binaphthyls, ansa and cyclophanic compounds, exo-cyclic alkylidene-cycloalkanes. Topicity and prostereoisomerism, chiral shift reagents and chiral solvating reagents	5	K4(An)	Lecture using chalk and talk	Class test
	5	Criteria for optical purity: Resolution of racemic modifications, asymmetric transformations, asymmetric synthesis, destruction. Stereoselective and stereospecific synthesis.	4	K4(An)	Lecture using chalk and talk	Group discussion and class test
V	**Stereochemistry-II**					
	1	Conformation and reactivity of acyclic systems, intramolecular rearrangements, neighbouring group participation, chemical consequence of conformational equilibrium - Curtin-Hammett Principle	5	K3(Ap)	Lecture using chalk and talk	slip test
	2	Stability of five and six-membered rings: mono-, di- and polysubstituted cyclohexanes, conformation	5	K6(E)	Lecture using chalk and talk and Group	Short test

		and reactivity in cyclohexane systems.			discussion	
	3	Fused and bridged rings: bicyclic, poly cyclic systems, decalins and Brett's rule	5	K3(Ap)	Lecture using chalk and talk	Class test
	4	Optical rotation and optical rotatory dispersion, conformational asymmetry, ORD curves, octant rule, configuration and conformation, Cotton effect, axial haloketone rule and determination of configuration.	6	K4(An)	Lecture using ppt	Slip test and MCQ

Course Focusing on Employability/ Entrepreneurship/ Skill Development: Employability and Skill Development

Activities (Em/SD): Stereospecific and stereoselective synthesis

Demonstration of symmetry elements

Assignment:

Effect of structure, leaving group and attacking nucleophile, Assign R & S configuration of organic compounds- Reflective writing

Seminar Topic

Unit I

Determination of intermediates

Unit II

Reactions involving nitrogen electrophiles

Sample questions

PART A

1. Arrange the following carbocations in the order of increasing stability.

   (a) Benzyl > 3^o> 2^o> 1^o (b) Benzyl > 1^o> 2^o> 3^o

   (c) 3^o> 2^o> 1^o> Benzyl(d) 1^o> 2^o> 3^o > Benzyl

2. Benzyl radical is more stable than allyl radical. (True/ False)

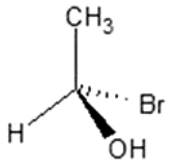
3. In SN1 reaction, the first step involves the formation of_____.

   (a) free radical (b) carbanion (c) carbocation (d) final product

4. Which of the following act as catalyst in the nitration of benzene

(a) Conc. H_2SO_4 (b) Dil. HCl (c) Conc. HNO_3 (d) HNO_2

5. Assign the R, S nomenclature of the following compound:

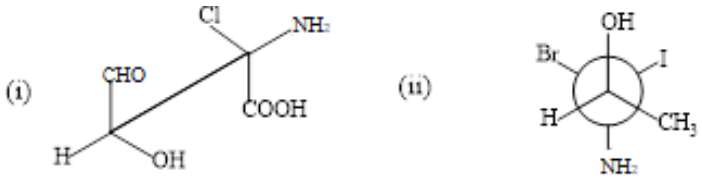


6. Predict the most stable conformation of cyclohexane.

(a) Chair (b) Boat (c) Half chair (d) Twist boat

PART B

1. Interpret any two applications of Hammett equation.
2. Explain Hammett and Taft equations.
3. Demonstrate aromatic nucleophilic substitution in aryl halides.
4. Convert the following sawhorse and Newman projections into equivalent Fischer projections:



(OR)

5. Evaluate the effect of conformation on the reactivity of S_N1 and S_N2 reactions of cyclic systems.
6. Validate the effect of conformation on the reactivity of base catalysed dehydrobromination of 1-bromo-1,2-diphenyl propane.

Part: C

1. Sketch and explain the energy profile diagrams of simple organic reactions.
2. Interpret the generation and stability of benzynes and carbocations.
3. Explain Sommelet- Hauser and Smiles rearrangements
4. Illustrate aliphatic nucleophilic substitutions in an allylic carbon
5. Illustrate the mechanism of S_N^{Ar} substitution with an example.
6. Elucidate planar chirality and helicity with suitable examples.
7. Illustrate Cram's rule with examples.
8. Verify Curtin-Hammet principle with an example.

Head of the Department **Course Instructor**

Dr. M. Anitha Malbi Dr. Y. Christabel Shaji

Teaching Plan

Department : Chemistry
Class : I M. Sc Chemistry
Title of the Course : **Core Course II:** Structure and Bonding in Inorganic compounds
Semester : **I**
Course Code : CP231CC2

Course Code	L	T	P	Credits	Inst. Hours	Total Hours	Marks		
							CIA	External	Total
CP231CC2	**7**	**-**	**-**	**5**	**7**	**105**	**25**	**75**	**100**

Objectives

- 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.

Course outcomes

CO	Upon completion of this course, the students will be able to:	PSO addressed	Cognitive level
CO-1	recall & predict the geometry of main group compounds and clusters.	PSO - 2	K3(Ap)
CO-2	explain about the packing of ions in crystals and apply the radius ratio rule to predict the coordination number of cations.	PSO - 2	K3(Ap)
CO-3	understand the various types of ionic crystal systems and analyze their structural features.	PSO - 3	K4(An)
CO-4	explain the crystal growth methods	PSO - 1	K2 (U)
CO-5	understand the principles of diffraction techniques and microscopic techniques and evaluate the structure of solids.	PSO - 2	K5(E)

Teaching plan

Total Contact hours: 105 (Including lectures, assignments and tests)

Unit	Module	Topic	Teaching Hours	Cognitive level	Pedagogy	Assessment/ Evaluation
I	**Structure of main group compounds and clusters**					
	1.	VB theory – Effect of lone pair and electronegativity of atoms (Bent's rule) on the geometry of the molecules	3	K3(Ap)	Introductory session, Lecture using Chalk and talk	Concept explanations, short summary
	2.	Applications of Paulings rule of electrovalence	2	K3(Ap)	Group Discussion and Lecture using Chalk and talk	Short summary
	3.	Structure of silicates - isomorphous replacements in silicates – ortho, meta and pyro silicates – one dimensional, two dimensional and three-dimensional silicates.	4	K4(An)	Lecture using videos and PPT	Simple definitions, MCQ
	4.	Structure of silicones	2	K2(U)	Review	True/False
	5.	Structural and bonding features of B-N, S-N and P-N compounds	3	K4(An)	Lecture using Chalk and talk, Group Discussion	Differentiate between bonding in B-N, S-N and P-N compounds
	6.	Poly acids – types, examples and structures	2	K2(U)	PPT	Simple definitions, short essay
	7.	Borane cluster: Structural features of closo, nido, arachano and klado; carboranes, hetero and metalloboranes	3	K4(An)	Group Discussion and Lecture using Chalk and talk	Evaluation through short test
	8.	Wade's rule to predict the structure	2	K3(Ap)	Group Discussion	Evaluation through quiz
II	**Solid state chemistry – I**					
	1.	Ionic crystals: Packing of ions in simple, hexagonal and cubic	4	K2(U)	Lecture using Chalk and talk	MCQ

		close packing				
	2.	Voids in crystal lattice, Radius ratio	2	K3(Ap)	Group Discussion	Evaluation through quiz
	3.	Crystal systems and Bravis lattices	3	K2(U)	PPT	Evaluation through short test
	4.	Symmetry operations in crystals	3	K3(Ap)	Demonstration, Review	Evaluation through short test
	5.	Glide planes and screw axis; point group and space group	4	K2(U)	Lecture using videos	Simple definitions
	6.	Solid state energetics: Lattice energy – Born-Lande equation - Kapustinski equation, Madelung constant.	5	K5(E)	Lecture using Chalk and talk	Problem-solving questions
III	**Solid state chemistry – II**					
	1.	Structural features of the crystal systems: Rock salt, zinc blende & wurtzite.	4	K2(U)	Lecture using PPT	Short summary
	2.	Fluorite and anti-fluorite, rutile and anatase	4	K2(U)	Lecture using Chalk and talk	Short essays
	3.	Cadmium iodide and nickel arsenide.	4	K2(U)	Lecture using PPT	Evaluation through short test
	4.	Spinels -normal and inverse types and perovskite structures	4	K4(An)	Group Discussion and Lecture using Chalk and talk	MCQ, simple definitions
	5.	Crystal Growth methods: From melt and solution (hydrothermal, sol-gel methods) – principles and examples.	5	K4(An)	Introductory session, Group Discussion and Lecture using Chalk and talk	Short essays
IV	**Techniques in solid state chemistry**					
	1.	X-ray diffraction technique: Bragg's law, Powder diffraction method – Principle and Instrumentation	4	K2(U)	Introductory session, and Lecture using Chalk and talk	Short essays
	2.	Interpretation of XRD data – JCPDS files	4	K3(Ap)	Demonstration	Review

	3.	Phase purity, Scherrer formula, lattice constants calculation	3	K5(E)	Lecture using Chalk and talk and Problem solving	Problem solving
	4.	Systematic absence of reflections; Electron diffraction technique – principle, instrumentation and application.	3	K3(Ap)	Lecture using PPT	True/False, MCQ
	5.	Electron microscopy – difference between optical and electron microscopy, theory, principle, instrumentation	4	K4(An)	Group Discussion and PPT	Evaluation through short test
	6.	Sampling methods and applications of SEM and TEM.	3	K3(Ap)	Demonstration	Short essays
V	**Band theory and defects in solids**					
	1.	Band theory – features and its application of conductors, insulators and semiconductors	4	K3(Ap)	Introductory session, Group Discussion	Simple definitions
	2.	Intrinsic and extrinsic semiconductors	3	K4(An)	Lecture using Chalk and Talk, Group Discussion	Evaluation through short test
	3.	Defects in crystals – point defects (Schottky, Frenkel, metal excess and metal deficient) and their effect on the electrical and optical property	6	K2(U)	Lecture using PPT	Sort essays, MCQ
	4.	laser and phosphors	4	K2(U)	Lecture using Chalk and Talk	True/False
	5.	Linear defects and its effects due to dislocations.	4	K2(U)	Lecture using videos	Review

Course Focussing on Employability/ Entrepreneurship/ Skill Development:
Employability

Activities (Em/ En/SD): Interpretation of XRD data of various samples– JCPDS files

Assignment: Classification of semiconductors.

1. Crystal defect and their effect on properties of semiconductors
2. Application of SEM and TEM

Seminar Topic:

Structure of silicates - isomorphous replacements in silicates – ortho, meta and pyro silicates – one dimensional, two dimensional and three-dimensional silicates.

Sample questions

Part A

1. The transition elements present in polyacids are _____.

2. An octahedral void is surrounded by _____ spheres.

   a) 4 b) 3 c) 6 d) 8

3. The general formula of perovskite structure is ABX 3. (True/False)

4. Define lattice energy.

5. The conduction band overlaps with the valence band in _____.

   a) conductors b) insulators c) semiconductors d) non metals

Part B

1. Classify the types of silicates.
2. Write a note on different types of voids.
3. Sketch the structure of rock salt
4. List out the difference between optical and electron microscopy
5. Mention the applications of band theory.

Part C

1. Predict the geometry of the molecules using Bent’s rule.
2. Calculate lattice energy of a crystal from the Born-Lande equation?
3. Compare the structure of zinc blende and wurtzite.
4. Explain the morphology of a sample using SEM and TEM.
5. Discuss the different types of defects in solids.

Head of the Department **Course Instructor**

Dr. M. Anitha Malbi Dr. M. Shirly Treasa

Teaching plan

Department : Chemistry
Class : I M. Sc Chemistry
Title of the Course : DS Elective I: b) Nano Materials and Nano Technology
Semester : **I**
Course Code : CP231DE2

Course Code	L	T	P	Credits	Inst. Hours	Total Hours	Marks		
							CIA	External	Total
CP231DE2	**4**	**1**	**-**	**3**	**5**	**75**	**25**	**75**	**100**

Objectives

- 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.

Course outcomes

CO	Upon completion of this course, the students will be able to:	PSO addressed	Cognitive level
CO - 1	Understand the methods of fabricating nanostructures.	PSO - 1	K2 (U)
CO - 2	relate the unique properties of nanomaterials to reduce dimensionality of the material.	PSO – 2,3	K4 (An)
CO - 3	describe the tools for properties of nanostructures.	PSO – 3, 4	K2 (U)
CO - 4	discuss the applications of nanomaterials.	PSO – 3, 5	K3 (Ap)
CO - 5	synthesize nano composites.	PSO - 3	K6 (C)

Teaching plan

Total Contact hours: 75 (Including lectures, assignments and tests)

Unit	Module	Topic	Teaching Hours	Cognitive level	Pedagogy	Assessment/ Evaluation
I	**Introduction of nanomaterials and nanotechnologies**					
	1	Introduction-role of size, classification-0D, 1D, 2D, 3D.	3	K2(U)	Lecture using chalk and talk, Group discussion	Recall definitions and concept explanations
	2	Synthesis-Bottom –Up, Top–Down, consolidation of nano powders.	4	K3(Ap)	Lecture using videos and ppt	MCQ and class test
	3	Features of nanostructures, Background of nanostructures.	2	K4(An)	Flipped classroom and lecture using chalk and talk	Group discussion and short test
	4	Techniques of synthesis of nanomaterials, Tools of the nanoscience.	3	K2(U)	Lecture using chalk and talk	Slip test and MCQ
	5	Applications of nanomaterials and technologies.	3	K3(Ap)	Lecture using chalk and talk and Group discussion	Short summary or overview
II	**Bonding and structure of the nanomaterials**					
	1	Predicting the Type of Bonding in a Substance crystal structure.	2	K4(An)	Lecture using chalk and talk	Short summary or overview
	2	Metallic nanoparticles, Surfaces of Materials, Nanoparticle Size and Properties.	4	K2(U)	Group discussion	Slip test and Quiz
	3	Synthesis- Physical and chemical methods - inert gas condensation, arc discharge, laser ablation, sol-gel, solvothermal and hydrothermal methods	5	K3(Ap)	Lecture using videos and ppt	Slip test and MCQ
	4	CVD-types, metallo organic, plasma enhanced, and low-pressure CVD.	2	K4(An)	Lecture using chalk and talk	Short test and quiz

	5	Microwave assisted and electrochemical synthesis.	2	K3(Ap)	Lecture using chalk and talk, videos	Short summary or overview
III	**Mechanical properties of nanomaterials**					
	1	Mechanical properties of materials, theories relevant to mechanical properties.	4	K2(U)	Lecture using chalk and talk	Concept explanations
	2	Techniques to study mechanical properties of nanomaterials, adhesion and friction, thermal properties of nanomaterials	5	K4(An)	Lecture using chalk and talk	Slip test and quiz
	3	Nanoparticles: gold and silver	3	K3(Ap)	Lecture using ppt	Short summary or overview
	4	Metal oxides: silica, iron oxide and alumina–synthesis and properties.	3	K3 (Ap)	Lecture using chalk and talk	Short test and MCQ
IV	**Electrical properties**					
	1	Electrical properties, Conductivity and Resistivity, Classification of Materials based on Conductivity, magnetic properties, electronic properties of materials.	4	K4(An)	Lecture using videos and ppt	Concept explanations and short summary
	2	Classification of magnetic phenomena. Semiconductor materials – classification-Ge, Si, GaAs, SiC, GaN, GaP, CdS, PbS.	4	K2(U)	Lecture using chalk and talk	Slip test and quiz
	3	Identification of materials as p and n –type semiconductor-Hall effect - quantum and anomalous, Hall voltage - interpretation of charge carrier density.	4	K4(An)	Lecture using chalk and talk	Short test and MCQ
	4	Applications of semiconductors: p-n junction as transistors and rectifiers, photovoltaic and photogalvanic cell.	3	K3(Ap)	Lecture using chalk and talk, mind mapping and group discussion	Class test
V	**Nanocomposites.**					

	1	Nano thin films, nanocomposites. Application of nanoparticles in different fields.	3	K2(U)	Group discussion and problem solving	Slip test
	2	Core-shell nanoparticles-types, synthesis, and properties.	4	K3(Ap)	Lecture using chalk and talk	Group discussion and slip test
	3	Nanocomposites-metal, ceramic and polymer matrix composites-applications.	4	K3(Ap)	Lecture using ppt	MCQ and short test
	4	Characterization– SEM, TEM and AFM - principle, instrumentation and applications.	4	K4(An)	Lecture using chalk and talk,Videos	Short summary

Course Focussing on Employability/ Entrepreneurship/ Skill Development: Employability and Skill Development

Activities (Em/ En/SD):

Preparation of nanoparticles, Checking the conductivity of nanomaterials, Characterizing the nanoparticle using SEM

Assignment:

Topic: Synthesis of nanomaterials by chemical methods, Applications of semiconductors -Reflective writing

Seminar Topic:

Unit- I

Synthesis-Bottom –Up, Top–Down, consolidation of nano powders.

Unit- II

Synthesis- Physical and chemical methods - inert gas condensation, arc discharge, laser ablation, sol-gel, solvothermal and CVD

Unit-III

Preparation of Gold and Silver nanoparticles, metal nanocomposites

Sample questions

Part A

1. Which one of the following is a two-dimensional nanoparticle?
   (a) Nanotubes (b) Nanorods
   (c) Nanosheets (d) Nano wires
2. One nanometer is equivalent to
   (a) 10^{-9}m (b) 10^{-9}cm (c) 10^{-9}dm (d) 10^{-9}pm
3. An example of Top-down approach is
   (a) Thermolysis (b) Sol-gel method
   (c) Sonochemical approach (d) Laser ablation method
4. Which one of the following is a polymer nanocomposite?
   (a) Epoxy nanocomposite (b) Bimetallic nanocomposite
   (c) Metal oxide nanomaterial (d) Trimetallic nanocomposite
5. In polymer nanocomposites, matrix phase is polymer and dispersed phase is_____.
   (a) Monomer (b) Compound
   (c) nanomaterial (d) Micromaterial
6. Quantum wire is a
   (a) 1-D structure (b) 3-D structure
   (c) 2-D structure (d) 0-D structure
7. Which of the following is an example of top-down approach of synthesis of the nano-material?
   (a) Physical vapour deposition (PVD) (b) Sputtering
   (c) Chemical vapour deposition (CVD) (d) Mechanical attrition

Part B

1. Classify the nanoparticles based on their structure.
2. Explain laser ablation process for producing nanomaterials with a neat diagram.
3. Discuss about the size dependent properties of nanomaterials.
4. With a neat sketch, explain Sol-gel synthesis for producing nanomaterials.
5. Discuss the properties and applications of metal matrix composites.
6. Analyse the p and n-type semiconductor in nanomaterials using Hall effect.

Part C

1. Validate the electrical properties of nanoparticles.
2. Write an informative note on the applications of nanomaterials.
3. Discuss the CVD and laser ablation techniques for the synthesis of nanoparticles.
4. Construct the diagram, working principle and procedure of Scanning Electron Microscopy.
5. Explain the preparation and properties of gold and silver nanoparticles.
6. Elaborate briefly the applications of semiconductor based on nanomaterials.

Head of the Department **Course Instructor**

Dr. M. Anitha Malbi Dr. M. Antilin Princela

Teaching plan

Department : Chemistry
Class : I M.Sc Chemistry
Title of the Course : **GElective II a:** Electrochemistry
Semester : **I**
Course Code : CP231GE1

Course Code	L	T	P	Credits	Inst. Hours	Total Hours	Marks		
							CIA	External	Total
CP231GE1	**4**	**1**	**-**	**3**	**5**	**75**	**25**	**75**	**100**

Objectives

- To understand the behavior of electrolytes in terms of conductance, ionic atmosphere, interactions.
- To get knowledge regarding the different types of over voltages and its applications in electro analytical techniques.

Course Outcomes (COs)

CO	Upon completion of this course, the students will be able to:	PSO Addressed	Cognitive level
CO - 1	understand the behaviour of electrolytes in solution and compare the structures of electrical double layer of different models	PSO - 1	K2(U)
CO - 2	predict the kinetics of electrode reactions applying Butler-Volmer and Tafel equations	PSO - 2,3	K3(Ap)
CO - 3	analyse different thermodynamic mechanism of corrosion	PSO - 2,4	K4(An)
CO - 4	evaluate the theories of electrolytes, electrical double layer, electrodics and activity coefficient of electrolytes	PSO - 2,3	K5(E)
CO - 5	construct fuel cells and storage devices	PSO – 4,5	K6(C)

Teaching plan
Total Contact hours: 75 (Including lectures, assignments and tests)

Unit	Module	Topic	Teaching Hours	Cognitive level	Pedagogy	Assessment/ Evaluation
I	**Ionics**					
	1	Arrhenius theory -limitations, van't Hoff factor and its relation to colligative properties. Deviation from ideal behavior	3	K2(U)	Lecture using Chalk and talk,PPT	Evaluation through short test,
	2	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	3	K3(Ap)	Flipped classroom and lecture using chalk and talk	Problem solving and class test
	3	Effect of solvent polarity on λ_{max}. Determination of activity coefficient ion solvent and ion-ion interactions.	3	K4(An)	Lecture using Chalk and talk,PPT, Group Discussion	Slip test and MCQ
	4	Derivation of Debye-Huckel limiting law at appreciable concentration of electrolytes modifications and applications.	3	K2(U)	Lecture using videos and ppt	Recall steps, Concept definitions
	5	Electrolytic conduction-Debye-Huckel Onsager treatment of strong electrolyte-qualitative and quantitative verification and limitations	3	K3(Ap)	Lecture using chalk and talk and Group discussion	Group discussion and short test
II	**Electrode-electrolyte interface**					
	1	Interfacial phenomena - Evidences for electrical double layer, polarizable and non-polarizable interfaces,	3	K2(U)	Lecture using videos and ppt	Short summary or overview
	2	Electrocapillary phenomena - Lippmann equation electro capillary curves.	2	K2(U)	Lecture using chalk and talk	Slip test and class test
	3	Electro-kinetic phenomena electro-osmosis, electrophoresis, streaming and sedimentation potentials	3	K3(Ap)	Group discussion and problem solving	Problem solving

	4	Colloidal and poly electrolytes.	2	K4(An)	Lecture using chalk and talk	Short test and quiz
	5	Structure of double layer: Helmholtz -Perrin, Guoy-Chapman and Stern models of electrical double layer	3	K3(Ap)	Lecture using chalk and talk	Short summary or overview
	6	Zeta potential and potential at zero charge. Applications and limitations.	2	K3(Ap)	Lecture using chalk and talk,PPT	Short test and quiz
III	**Electrodics of Elementary Electrode Reactions**					
	1	Behavior of electrodes: Standard electrodes and electrodes at equilibrium. Anodic and Cathodic currents, condition for the discharge of ions.	3	K2(U)	Lecture using chalk and talk,Videos	Evaluation through short test,
	2	Nernst equation, polarizable and non-polarizable electrodes. Model of three electrode system, over potential.	3	K4(An)	Lecture using chalk and talk	Slip test
	3	Rate of electro chemical reactions: Rates of simple elementary reactions.	2	K3(Ap)	Lecture using chalk and talk	Short summary or overview
	4	Butler-Volmer equation-significance of exchange current density, net current density and symmetry factor.	3	K5(E)	Lecture using chalk and talk	Slip test and quiz
	5	Low and high field approximations. symmetry factor and transfer coefficient Tafel equations and Tafel plots.	4	K3(Ap)	Lecture using ppt	Group discussion
IV	**Electrodics of Multistep Multi Electron System**					
	1	Rates of multi-step electrode reactions. Rate determining step, electrode polarization and depolarization	3	K2(U)	Lecture using videos and ppt	Concept explanations and short summary
	2	Transfer coefficients, its significance and determination, Stoichiometric number	2	K4(An)	Lecture using chalk and talk	Slip test and quiz
	3	Reduction of I^{3-}, Fe^{2+}, and dissolution of Fe to Fe^{2+}..	2	K2(U)	Lecture using chalk and talk	Short test

	4	Overvoltage - Chemical and electro chemical, Phase, activation and concentration over potentials	4	K4(An)	Lecture using chalk and talk,	Group discussion and class test
	5	Evolution of oxygen and hydrogen at different pH, Pourbaix and Evan's diagrams	4	K4(An)	Mind mapping and group discussion	Concept explanation and short test
V	**Concentration Polarization, Batteries and Fuel cells:**					
	1	Modes of Transport of electro active species - Diffusion, migration and hydrodynamic modes.	3	K3(Ap)	Group discussion and Lecture using chalk and talk	Slip test
	2	Role of supporting electrolytes. Polarography-principle and applications.	3	K3(Ap)	Lecture with chalk and talk, PPT	Discussion and slip test
	3	Cyclic voltammetry- anodic and cathodic stripping voltammetry and differential pulse voltammetry.	3	K3(Ap)	Lecture with chalk and talk,PPT	Concept explanation and short test
	4	Sodium and lithium-ion batteries and redox flow batteries	3	K5(E)	Group discussion and Lecture using chalk and talk	Concept explanations and short summary
	5	Energy production systems: FuelCells: classification, alkaline fuel cells, phosphoric acid fuel cells, high temperature fuel cells.	3	K6(C)	Lecture with chalk and talk,videos	Discussion and slip test

Course Focusing on Employability/ Entrepreneurship/ Skill Development: Employability and Skill Development

Activities (Em/SD): Demonstration of Pourbaix and Evan's diagrams, Construction of Fuel Cells

Assignment:

Topic: Structure of double layer: Helmholtz -Perrin, Guoy- Chapman and Stern models of electrical double layer

Type: Poster presentation on different models of electrical double layer**.**

Seminar Topic

Unit I

Arrhenius theory -limitations, van't Hoff factor and its relation to colligative properties.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

Unit II

Electro-kinetic phenomena electro-osmosis,electrophoresis, streaming and sedimentation potentials Zeta potential and potential at zero charge. Applications and limitations

Unit V

Sodium and lithium-ion batteries and redox flow batteries. Energy production systems:
Fuel Cells: classification, alkaline fuel cells, phosphoric acid fuel cells, high temperature fuel cells.

Sample questions

Part A

1. What is the value of the Van't Hoff factor (i) for solutes that dissociate in water?
   a) > 1
   b) < 1
   c) = 0
   d) Not defined
2. The Van't Hoff Factor for a solution of glucose in water is equal to 1.
   a) True
   b) False
3. A polarizable electrode is an electrode in an electrochemical cell that is characterized by _____at the electrode-electrolyte boundary.
4. Selective discharge of ions depends on:
   A. the nature of the electrode
   B. the relative concentration of ions
   C. the relative position of ions in the electrochemical (activity) series
   D. all of the above
5. Exchange current density is the current per unit area of either oxidation or reduction process at_____.
6. Voltammetry is based on the measurement of _____ as function of applied potential conductance pH current concentration.
7. Supporting electrolyte is used in Polarography to suppress_____ Diffusion current Migration current convention current limiting current.

Part B

1. Enlist the limitations of Arrhenius theory.

2. Correlate the terms Ionic activity, mean ionic activity and mean ionic activity coefficient.
3. Differentiate polarizable and non-polarizable interfaces.
4. Comment on the significance of exchange current density, net current density and symmetry factor.
5. Discuss the types of overvoltage.
6. Write a note on the role of supporting electrolytes.
7. What are the types of fuel cells?

Part C

1. Derive Debye-Huckel limiting law at appreciable concentration of electrolytes.
2. Discuss Debye-Huckel Onsager treatment of strong electrolyte-qualitative and quantitative verification and limitations.
3. Analyse the various models proposed for the structure of electrical double layer.
4. Derive the Butler-Volmer equation.
5. Sketch and explain the Pourbaix diagram and its significance.
6. Discuss the principle and application of polarography.
7. Explain the principle of cyclic voltammetry and its types.

Head of the Department **Course Instructor**

Dr. M. Anitha Malbi Dr. S. Lizy Roselet

Teaching plan
Semester-III

Department : Chemistry
Class : II M.Sc Chemistry
Title of the Course : **Core VII:** Organic Spectroscopy
Semester : **III**
Course Code : **PG2031**

Course Code	L	T	P	Credits	Inst. Hours	Total Hours	Marks		
							CIA	External	Total
PG2031	**6**	**-**	**-**	**5**	**6**	**90**	**40**	**60**	**100**

Objectives

- To understand the principle and applications of UV, IR, NMR and Mass spectroscopic techniques.
- To elucidate the structure of simple organic compounds using spectral data.

Course Outcomes (COs)

CO	Upon completion of this course, the students will be able to:	PSO Addressed	Cognitive level
CO - 1	understand the principle and applications of various spectroscopic techniques	PSO - 1	K2(U)
CO - 2	apply the spectroscopic concepts to determine the structure of organic compounds	PSO - 2,3	K3(Ap)
CO - 3	analyze the functional groups, molecular formula, structure and spectral data of compounds	PSO - 2,3	K4(An)
CO - 4	evaluate the purity, structure and molecular mass of compounds using various spectroscopic methods	PSO - 2,3	K5(E)
CO - 5	create and characterize novel organic compounds	PSO - 3,4	K6(C)

Teaching plan

Total Contact hours: 90 (Including lectures, assignments and tests)

Unit	Module	Topic	Teaching Hours	Cognitive level	Pedagogy	Assessment/ Evaluation
I	**UV-Visible and IR spectroscopy**					
	1	UV-Visible spectroscopy - principle - types of electronic excitations - chromophore - auxochrome - bathochromic - hypsochromic - hypochromic and hyperchromic shifts.	3	K2(U)	Flipped classroom and lecture using chalk and talk	Slip test and concept explanations
	2	Woodward-Fieser rules to calculate λ_{max} values of conjugated dienes - α,β-unsaturated carbonyl compounds and aromatic compounds. Fieser-Khun rule.	6	K3(Ap)	Group discussion and problem solving	Problem solving and class test
	3	Effect of solvent polarity on λ_{max}.	1	K4(An)	Flipped classroom and lecture using chalk and talk	Short test
	4	IR spectroscopy: principle - Hooke's law - types of molecular vibrations.	2	K2(U)	Lecture using videos and ppt	Slip test and MCQ
	5	Factors influencing the vibrational frequency. Identification of functional groups in organic compounds.	3	K3(Ap)	Lecture using chalk and talk and Group discussion	Group discussion and short test
	6	Finger print region. Fermi resonance - overtones and combination bands.	3	K2(U)	Lecture using chalk and talk	Concept explanations and slip test
II	**^{1}H NMR Spectroscopy**					
	1	^{1}H NMR Spectroscopy: principle - instrumentation - shielding and deshielding.	3	K2(U)	Lecture using videos and ppt	Short summary or overview
	2	Chemical shift - factors affecting chemical shift - electronegativity - hybridization - hydrogen bonding - anisotropic effect - double bond - triple bond -	4	K2(U)	Lecture using chalk and talk	Slip test and class test

		aromatic compounds - carbonyl compounds and annulenes.				
	3	Spin-spin splitting pattern of simple organic compounds	3	K3(Ap)	Group discussion and problem solving	Problem solving
	4	Types of coupling - germinal - vicinal - long range and through space coupling. Karplus equation. Coupling constant - AB, AB_2 and A_2B_3.	4	K4(An)	Lecture using chalk and talk	Short test and quiz
	5	Simplification of complex spectra - chemical exchange, double resonance and NMR shift reagents. Temperature dependent NMR.	4	K3(Ap)	Lecture using chalk and talk	Short summary or overview
III	**^{13}C, ^{19}F and ^{31}P NMR Spectroscopy**					
	1	^{13}C NMR spectroscopy: principle - comparison of ^{13}C NMR and ^{1}H NMR. Chemical shift - factors affecting chemical shift.	3	K2(U)	Lecture using ppt	Concept explanations
	2	Homonuclear and heteronuclear coupling. Broad band decoupling and OFF - resonance decoupling.	3	K4(An)	Lecture using chalk and talk	Slip test
	3	Distortionless Enhancement by Polarization Transfer (DEPT) spectrum - DEPT-45 - DEPT-90 and DEPT-135.	3	K3(Ap)	Lecture using chalk and talk	Short summary or overview
	4	2D Correlation spectroscopy (COSY) - HOMCORR - ^{1}H-^{1}H and ^{13}C-^{13}C connectivity. HETCORR - ^{1}H-^{13}C connectivity and MRI.	3	K5(E)	Lecture using chalk and talk	Slip test and quiz
	5	^{19}F NMR spectroscopy: precessional frequency and heteronuclear coupling. Identification of organofluoro compounds CF_3CO_2Et and CF_3CH_2OH.	3	K3(Ap)	Lecture using ppt	Group discussion

	6	^{31}P NMR spectroscopy: chemical shift - heteronuclear coupling and P-P bond in NMR. Identification of organophosphorous compounds $(Me)_3P$ - $(EtO)_3P=O$ and Ph_3P.	3	K3(Ap)	Lecture using ppt	Group discussion
IV	**Mass Spectrometry**					
	1	Principle - production of ions - Electronic Ionization (EI), Chemical Ionization (CI) and Fast Atom Bombardment (FAB).	4	K2(U)	Lecture using videos and ppt	Concept explanations and short summary
	2	Molecular ion peak - base peak - meta stable peak and isotopic peaks.	2	K4(An)	Lecture using chalk and talk	Slip test and quiz
	3	Nitrogen rule. McLafferty rearrangement and Retro Diels Alder reaction.	2	K2(U)	Lecture using chalk and talk	Short test
	4	General modes of fragmentation. Fragmentation pattern of simple organic compounds - alkenes - alkyl and aryl halides - alkylbenzene - benzene - aliphatic alcohols - phenols - aliphatic and aromatic acids - ketones - aldehydes - furan - pyrrole and pyridine.	10	K4(An)	Lecture using chalk and talk, mind mapping and group discussion	Group discussion and class test
V	**Structural Elucidation using Analytical and Spectral Data**					
	1	Determination of molecular formula of organic compounds using elemental (CHN) analysis data.	4	K3(Ap)	Group discussion and problem solving	Solving problems and slip test
	2	Structural determination of simple organic compounds using UV - IR - NMR and Mass spectral data.	14	K6(C)	Group discussion, problem solving and Peer tutoring	Solving problems, group discussion and slip test

Course Focusing on Employability/ Entrepreneurship/ Skill Development: Employability and Skill Development

Activities (Em/SD): Demonstration of UV-Visible spectroscopy

Demonstration of IR spectroscopy

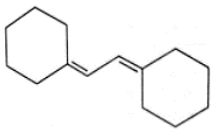
Assignment:

Calculation of absorption spectrum of organic compounds - Reflective writing

Sample questions

Part A

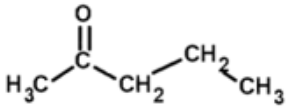
1. Identify the λ_{max} value of the following compound:



(a) 237 nm (b) 245 nm (c) 247 nm (d) 240 nm

2. Calculate the vibrational degrees of freedom in the following molecules:
   (i) CO_2 (ii) NH_3

3. Assertion (A) : Coupling constant is a measure of the effectiveness of spin-spin coupling. Reason (R) : Geminal protons are separated by three bonds.
   (a) Both A and R are true but R is not the correct explanation of A
   (b) Both A and R are true and R is the correct explanation of A
   (c) A is true but R is false
   (d) R is true but A is false
4. Predict the ^{1}H NMR splitting pattern of ethylbromide.
5. How many ^{13}C peaks will appear in noise decoupled spectrum of naphthalene?
6. DEPT 135 gives negative value for CH_2group. Say true or false.
7. Which among the following is the base peak of toluene?
   (a) m/z = 58 (b) m/z = 92 (c) m/z = 65 (d) m/z = 91
8. Identify the peak corresponding to McLafferty rearrangement in the following compound:



   (a) m/z = 28 (b) m/z = 31 (c) m/z = 43 (d) m/z = 58
9. Calculate the DBE of the compound $C_{10}H_7Br$.
   (a) 1 (b) 5 (c) 7 (d) 3
10. 0.30g of an unknown organic compound X gave 0.733g of carbon dioxide and 0.30g of water in a combustion analysis. Determine the empirical formula of X.

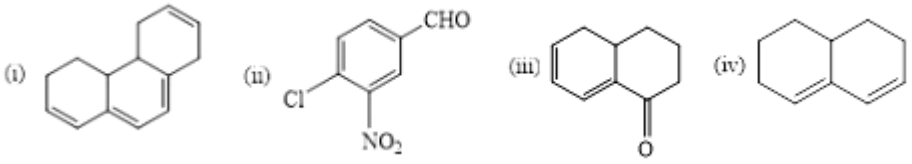
Part B

1. Analyze the effect of solvent polarity in UV-Visible spectroscopy.
2. Differentiate inter and intramolecular hydrogen bonding using IR spectroscopy.
3. Describe the types of coupling in ^{1}H NMR spectroscopy.
4. Explain chemical exchange with an example.
5. Differentiate ^{13}C NMR and ^{1}H NMR spectroscopy.
6. Sketch and explain the ^{19}F NMR spectrum of CF_3CH_2OH.
7. Validate nitrogen rule with examples.

8. Elucidate McLafferty rearrangement with an example.
9. A pale-yellow compound of molecular formula $C_6H_5NO_3$ is slightly acidic in nature and gave the following data: UV: 280 nm, λ_{max} 6600; IR: 3460, 3035 (m), 1608 (m), 1585 (m), 1510 (m), 1360 (s), 1320 (s) and 740 cm^{-1}. The band at 3460 cm^{-1} does not shift even on diluting the sample. NMR: 7.9 δ (singlet) ^1H and an unsymmetrical pattern at 7.25-7.39 δ (4 H). Deduce the structure of the compound.
10. An unknown organic compound Z of molecular weight 58.124 g/mol gave 8.8 g of carbon dioxide and 4.5 g of water in a combustion analysis for C and H. Determine the empirical and molecular formula of Z.

Part C

1. Determine the λ_{max} for the following compounds.



2. Analyse the use of IR spectroscopy for identifying the functional groups in organic compounds.
3. Discuss the factors which affect the chemical shift in ^1H NMR spectroscopy.
4. Explain NMR shift reagents and double resonance with examples.
5. Generalize DEPT technique with an example.
6. Illustrate ^1H-^1H COSY and ^1H-^{13}C COSY with examples.
7. Interpret the fragmentation patterns of aliphatic and aromatic acids, aldehydes and ketones.
8. Compare electronic ionization, chemical ionization and FAB methods for the production of ions in mass spectrometry.
9. Assign the structure of the compound on the basis of the spectral data. Molecular formula: $C_4H_6O_2$; UV: λ_{max}290 nm; IR: 1708 cm^{-1}; ^1H NMR: δ 2.29 (6H, s); Mass (m/z): 86 (M+)43 (100 %). Deduce the structure and predict the fragmentation pattern of the compound.
10. Assign the structure of the compound on the basis of the spectral data: Molecular Formula: $C_4H_8O_2$. UV, λ_{max}: 271 nm. IR (cm^{-1}): 1718, 3430 cm^{-1}. ^1H NMR (δ ppm): 4.22 (1H, q); 3.73 (1H, s); 2.18 (3H, s); 1.36 (3H, d). MS (m/z); 88 (M^+), 45 (100 %), 43 (80 %).

Head of the Department: Dr. M. Anitha Malbi **Course Instructor:** Dr. Sheeba Daniel

Teaching plan

Department **:** Chemistry
Class **:** II M. Sc Chemistry
Title of the Course **:** Core VIII: Thermodynamics and Group Theory
Semester **: III**
Course Code **: PG2032**

Course Code	L	T	P	Credits	Inst. Hours	Total Hours	Marks		
							CIA	External	Total
PG2032	6	-	-	5	6	90	40	60	100

Objectives

- To learn the various concepts of thermodynamics and statistical thermodynamics.
- To apply the concepts of group theory to molecules.

Course outcomes

CO	Upon completion of this course, the students will be able to:	PSO addressed	Cognitive level
CO-1	understand the concepts and applications of thermodynamics and group theory	PSO - 1	K2(U)
CO-2	apply thermodynamics and group theory to determine thermodynamic parameters, vibrations and hybrid orbitals	PSO - 2	K3(Ap)
CO-3	analyze the thermodynamic functions, point groups and normal mode of vibration of molecules	PSO - 2	K4(An)
CO-4	evaluate the thermodynamic parameters and delocalization energy in molecules	PSO - 2	K5(E)

Teaching plan

Total Contact hours: 90 (Including lectures, assignments and tests)

Unit	Module	Topic	Teaching Hours	Cognitive Level	Pedagogy	Assessment/ Evaluation
I	**Thermodynamics and Non-Ideal Systems**					
	1	Concepts of partial molar properties - partial molar free energy and partial molar volume. Gibbs-Duhem equation.	4	K2(U)	Lecture using Chalk and Talk	Evaluation through short test

	2	Chemical potential - variation of chemical potential with temperature and pressure - Van't Hoff isotherm and solution.	4	K3(Ap)	Group Discussion	MCQ, Recall steps
	3	Fugacity - determination of fugacity of gases by graphical method - variation of fugacity with temperature and pressure .	4	K5(E)	Peer Tutoring	Short essays
	4	Lewis Randal rule and Duhem-Margules equation	3	K2(U)	Lecture using Chalk and Talk	Longer essay
	5	Determination of activity and activity coefficient of non-electrolyte by e.m.f method - excess functions.	3	K5(E)	Lecture using videos	MCQ, True/False
II	**Irreversible Thermodynamics**					
	1	Nernst heat theorem - Third law of thermodynamics - applications of third law.	4	K3(Ap)	Group discussion	Recall steps, Evaluation through short test
	2	entropy change - calculation of absolute entropies - apparent exceptions to third law.	3	K5(E)	Group discussion and problem solving	Problem-solving questions
	3	Non-equilibrium thermodynamics - basic concepts - forces and fluxes - entropy of irreversible processes.	3	K1(R)	Introductory session	Recall, MCQ

	4	Clausius inequality - phenomenological equations - Onsager reciprocity relations and coupled reactions.	4	K2(U)	Lecture using Chalk and Talk	Longer Essay
	5	Principle of microscopic reversibility - the Onsager reciprocal relations - verification. Entropy production.	4	K2(U)	Peer tutoring and group discussion	Short essay, Short summary
III	**Statistical Thermodynamics**					
	1	Statistical thermodynamics - concept of distributions - types of particles (bosons, fermions, mesons) - types of ensembles.	4	K1(R)	Introductory session	MCQ, True/False
	2	Thermodynamic probability - most probable distribution law - classical statistics - Maxwell-Boltzmann (MB) statistics	3	K3(Ap)	Lecture using Chalk and Talk and Group Discussion	Short essay
	3	Quantum statistics - Bose-Einstein (BE) and Fermi-Dirac (FD) statistics - derivation of distribution function - MB, BE and FD statistics - comparison.	5	K4(An)	Peer group tutoring and group discussion	Differentiate between various ideas
	4	Partition functions - translational - rotational - vibrational and electronic partition function	3	K2(U)	Lecture using Chalk and Talk	Short summary
	5	calculation of thermodynamic parameters and equilibrium constants in terms of partition function. Debye and Einstein heat capacity of solids.	3	K5(E)	Group discussion and problem solving	Longer essay, problem solving

IV	**Group Theory I**					
	1	Molecular symmetry elements - symmetry operations - molecular symmetry and point groups.	4	K1(R)	Lecture using videos	MCQ, True/False
	2	Group multiplication tables - abelian - non-abelian - cyclic and sub groups - conjugacy relation and classes.	3	K2 (U)	Lecture and group discussion	Recall steps, simple definition
	3	Representation of symmetry operations by matrices - representation for C_{2v} - C_{3v} and C_{2h} point groups.	4	K3(Ap)	Lecture and demonstration	Recall steps, Evaluation through class test
	4	Reducible and irreducible representations. The great orthogonality theorem and its consequences.	3	K3(Ap)	Lecture and PPT	Short essay
	5	Construction of the character tables C_{2v}, C_{3v} and C_{2h}.	4	K6(C)	Group Discussion	Suggest idea with examples
V	**Group Theory – II**					
	1	Standard reduction formula - symmetry of normal modes of vibration in H_2O - NH_3 and CO_2. Application of group theory to normal mode analysis of H_2O and NH_3.	4	K4(An)	Lecture and group discussion	Recall, MCQ, Erue/False
	2	Symmetry properties of integrals and symmetry based selection rule for vibrational spectra. Identification of IR and Raman active fundamentals - symmetry of molecular orbitals	4	K4(An)	Lecture and group discussion	Recall steps, Evaluation through class test

	3	symmetry based selection rule for electronic transition - prediction of electronic transitions in ethylene and formaldehyde.	4	K2(U)	Lecture & PPT	Short essay
	4	Determinationof π-electron energy in ethylene.HMO theory - HMO calculations	3	K3(Ap)	Lecture and Group Discussion	Suggest idea with examples
	5	delocalization energy in trans-1,3-butadiene and benzene. Application of Determination of hybridization in CH_4 and BF_3.	3	K4(An)	Lecture and videos	Recall steps, Evaluation through class test

Course Focussing on Employability/ Entrepreneurship/ Skill Development : Employability
Activities (Em/ En/SD): Seminar and model making – Point group
Course Focussing on Cross Cutting Issues(Professional Ethics/ Human Values/Environment Sustainability/ Gender Equity): (Mention)
Activities related to Cross Cutting Issues : Nil
Assignment : (Mention Topic and Type)
1.Determination of absolute entropies of solids and liquids
2. Entropy change for reversible and irreversible process.
3. Symmetry properties of integrals and symmetry based selection rule for vibrational spectra
Seminar Topic: (if applicable)
Unit I : Partial molar free energy and partial molar volume. Gibbs-Duhem equation. Chemical potential - variation of chemical potential with temperature and pressure - Van't Hoff isotherm and solution. Determination of activity and activity coefficient of non-electrolyte by e.m.f method.
Unit II: Nernst heat theorem - Third law of thermodynamics - applications of third law.

Sample questions

Part A

1. Partial molar free energy is _____
   (a) fugacity (b) Gibb's free energy (c) chemical potential (d) entropy
2. Entropy is state function. (True / False)
3. Define ensemble.
4. The character of identity operation is
   (a) 1 (b) 0 (c) 3 (d) 2
5. The number of normal modes of vibration of a nonlinear molecule is
   (a) 3N-5 (b) 3N- 6 (c)3N (d) 3N-1

Part B

1. Discuss the significance of partial molar properties.

2. Prove $\Delta G = \Delta H$ using Nernst heat theorem.
3. Classify the types of ensembles.
4. Enumerate the characteristics of a group.
5. Apply group theory to obtain the normal mode analysis of vibration of NH_3.

Part C

1. Derive Gibb,sDuhem equation using partial molar properties.
2. Verify the Onsager reciprocity relations.
3. Compare MB, BE and FD.
4. Using the Great Orthogonality theorem construct the character table for C_{3v} point group.
5. Calculate the delocalisation energy in trans-1,3-butadiene with HMO considerations

Head of the Department
Dr.M.Anitha Malbi

Course Instructor
Dr.M.Shirly Treasa

Teaching plan

Department **:** Chemistry
Class **:** II M.Sc Chemistry
Title of the Course **: Elective III (a) -** Advanced Topics in Chemistry
Semester **: III**
Course Code **: PG2033**

Course Code	L	T	P	Credits	Inst. Hours	Total Hours	Marks		
							CIA	External	Total
PG2033	4	-	-	4	4	60	40	60	100

Objectives

- To acquire knowledge about nanoparticles and green chemistry.
- To gain idea about supramolecular chemistry.
- To study the applications of medicinal and biophysical chemistry.

Course Outcomes (COs)

CO	Upon completion of this course, the students will be able to:	PSO Addressed	Cognitive level
CO - 1	understand the principles and application of advanced areas in chemistry	PSO-1	K2(U)
CO - 2	apply the principle of nanochemistry and green chemistry to design and synthesise novel compounds	PSO-2,3	K3(Ap)
CO - 3	analyze the properties of nanoparticles, supramolecular interactions, therapeutic action of drugs and reactions in biomolecules	PSO-2,3	K4(An)
CO - 4	evaluate atom economy in green synthesis, structure and therapeutic action of various drugs and role of singlet oxygen in biology	PSO-2,4	K5(E)
CO - 5	create novel nanoparticles and compounds using green chemistry techniques	PSO-3,4	K6(C)

Teaching plan

Total Contact hours: 60 (Including lectures, assignments and tests)

Unit	Module	Topic	Teaching Hours	Cognitive level	Pedagogy	Assessment/ Evaluation
I	**Nanochemistry**					
	1	General principles of nanotechnology. Nanoparticles - definition - size relationship - nanoparticles of metals - semiconductors and oxides.	3	K2(U)	Lecture using Chalk and talk, PPT	Evaluation through short test,
	2	Synthesis of nanosized compounds - reduction methods and solgel methods. Optical and electrical properties of nanoparticles.	3	K3(Ap)	Flipped classroom and lecture using chalk and talk	Problem solving and class test
	3	Nanosystems - introduction - synthesis and purification of fullerenes. Carbonnanotubes - types - preparation - Arc and chemical vapour deposition methods.	2	K4(An)	Lecture using Chalk and talk,PPT, Group Discussion	Slip test and MCQ
	4	Nanoshells - gold and silver nanoshells and its applications. Nanosensors - introduction - nanoscale organization - characterization and optical properties.	2	K2(U)	Lecture using videos and ppt	Recall steps, Concept definitions
	5	Nanomedicines - introduction - approach to developing nanomedicines - protocol for nanodrug administration - diagnostic and therapeutic applications.	2	K3(Ap)	Lecture using chalk and talk and Group discussion	Group discussion and short test
II	**Green Chemistry**					
	1	Green chemistry and sustainable development - principles and applications of green chemistry. Atom economy - atom economy vs. yield. Prevention of waste/byproducts.	3	K2(U)	Lecture using videos and ppt	Short summary or overview

	2	Prevention or minimization of hazardous products. Designing safer chemicals through Sommelet-Hauser - Cope - Wolff - Witting and Bamberger reactions.	2	K2(U)	Lecture using chalk and talk	Slip test and class test
	3	Energy requirement for synthesis. CFC alternatives - green chemistry in organic synthesis. Selection of appropriate solvent and starting material.	3	K3(Ap)	Group discussion and problem solving	Problem solving
	4	Use of protecting groups and catalyst. Methods of greening organic reactions - solvent free reactions and reactions at ambient temperature.	2	K4(An)	Lecture using chalk and talk	Short test and quiz
	5	Microwave assisted reactions. Sonication assisted reactions - Reformatsky - Ullmann coupling - Wurtz and Bouveault reaction. Reactions in ionic solvents and super critical fluids. Tandem reactions.	2	K3(Ap)	Lecture using chalk and talk	Short summary or overview
III	**Supramolecular Chemistry**					
	1	Supramolecular interactions - discussion of host-guest systems - cation and anion binding host.	3	K2(U)	Lecture using chalk and talk,Videos	Evaluation through short test,
	2	Crown ethers - synthesis - properties and applications. Lariat ethers.	3	K4(An)	Lecture using chalk and talk	Slip test
	3	Podants - properties and 3-dimensional podants. Cryptands - synthesis - properties and applications.	2	K3(Ap)	Lecture using chalk and talk	Short summary or overview
	4	Spherands - synthesis - structure and uses. Supramolecular chemistry of fullerenes and cyclodextrins.	2	K5(E)	Lecture using chalk and talk	Slip test and quiz

	5	Molecular devices - non-linear optical switches and electrophotoswitching, Liquid crystal display. Supramolecular photochemistry.	2	K3(Ap)	Lecture using ppt	Group discussion
IV	**Medicinal Chemistry**					
	1	Modern drugs for diseases. Anticancer drugs - classification - synthesis and assay of cyclophoshamide - chlorambucil - cisplatin - vinblastine and vincristine.	3	K2(U)	Lecture using videos and ppt	Concept explanations and short summary
	2	Antimalarial drugs - classification - synthesis and assay of chloroquine and primaquine.	2	K4(An)	Lecture using chalk and talk	Slip test and quiz
	3	Diuretics - classification - synthesis and assay of Frusemide and benzthiazide.	2	K2(U)	Lecture using chalk and talk	Short test
	4	Anti-inflammatory drug - synthesis and therapeutic action of phenylbutazone and ibuprofen.	2	K4(An)	Lecture using chalk and talk,	Group discussion and class test
	5	Antipyretics and non-narcotic analgesics - synthesis and therapeutic action of paracetamol and aspirin	3	K4(An)	Mind mapping and group discussion	Concept explanation and short test
V	**Biophysical Chemistry**					
	1	Thermodynamics in biology and limitations of equilibrium thermodynamics. Irreversible thermodynamics - postulates and methodologies.	3	K3(Ap)	Group discussion and Lecture using chalk and talk	Slip test
	2	Irreversible thermodynamics and biological systems. Biochemical standard state - ATP. Currency of energy.	3	K3(Ap)	Lecture with chalk and talk,PPT	Discussion and slip test
	3	Oxidative phosphorylation. Role of singlet oxygen in biology.	2	K3(Ap)	Lecture with chalk and talk,PPT	Concept explanation and short test

	4	Reactions in biomolecules - membrate potential and ion pumps. Photoacoustic effect and its application in biology.	2	K5(E)	Group discussion and Lecture using chalk and talk	Concept explanations and short summary
	5	Biophysical applications of Moss-bauer effect. NMR imaging - applications of spin labeling in membrane research.	2	K6(C)	Lecture with chalk and talk,videos	Discussion and slip test

Course Focusing on Employability/ Entrepreneurship/ Skill Development: Employability and Skill Development

Activities (Em/SD): Demonstration of Nanoparticle synthesis

Assignment:

Topic: Nanoshells - gold and silver nanoshells and its applications.

Seminar Topic

Unit II

Green chemistry and sustainable development - principles and applications of green chemistry. Atom economy - atom economy vs. yield. Prevention of waste/byproducts. Prevention or minimization of hazardous products. Designing safer chemicals through Sommelet-Hauser - Cope - Wolff - Witting and Bamberger reactions.

Unit IV

Modern drugs for diseases. Anticancer drugs - classification - synthesis and assay of cyclophoshamide - chlorambucil - cisplatin - vinblastine and vincristine. Antimalarial drugs - classification - synthesis and assay of chloroquine and primaquine.

Unit V

Biophysical applications of Moss-bauer effect. NMR imaging - applications of spin labeling in membrane research.

Sample questions

Part A

1. A nanometer is
   (a) 10^{-9}m (b)10^{-9}cm (c)10^{-9}mm (d)10^{-9}pm
2. The tensile strength of carbon nanotube is 30 times greater than that of steel. (True/False)
3. An example for green solvent is
   (a) benzene (b) toluene (c) supercritical CO_2
4. If a reaction has 100% atom economy,the reaction has_____yield.
   (a) 100% (b)76% (c) 80% (d) 99%

5. Interactions between host and guest in supramolecular chemistry are covalent.(True/False)
6. Solubility of the crown ether depends upon the nature of the _____.
7. Primaquine phosphate is _____.
   (a)Antipyretic analgesics (b) Anti-malarial drug
   (c)Anti-inflammatory drug (d) Diuretics
8. List out any two examples for anti-inflammatory drugs.
9. The hydrolysis of ATP is carried out at pH_____.
   (a)7 (b)8 (c)9 (d)5
10. In Mossbauer Effect, a nucleus emits or absorbs gamma rays without loss of energy. (True/False)

Part: B

11. Explain the preparation of carbon nanotubes using Arc method.
12. Analyze the advantages and disadvantages of nanomedicine.
13. Deduce the mechanism in Witting and Wolff reactions for the design of safer chemicals
14. Suggest the CFC alternatives used in green chemistry.
15. Differentiate cryptands and spherands.
16. Compare lariat ethers and podants
17. Discuss the types of diuretics with examples.
18. Explain the synthesis and assay of cyclophosphamide
19. Explain the role of singlet oxygen in biology.
20. Explain the application of photo acoustic effect.

Part: C

21. Discuss optical and electrical properties of nanoparticles.
22. Describe the synthesis and applications of gold nanoshells.
23. Defend the statement green chemistry with its twelve principles.
24. Justify the reactions in ionic solvents and super critical fluids as green reactions.
25. Discuss the working principle of LCD with its advantages.
26. Elaborate the different types of supramolecular interactions.
27. Discuss the classification of anticancer drugs.
28. Explain the synthesis and therapeutic action of phenylbutazone and benzthiazide.
29. Explain the role of ion pump in the biological system.
30. Discuss in detail about NMR imaging.

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