Semester I
Structure and Bonding (Core I)
Subject Code: PG2011

No. of hours per week	Credit	Total no. of hours	Marks
6	5	90	100

Objectives:

- To provide knowledge about the concepts in structure and bonding of simple molecules
- To understand the structure and diffraction methods of solids
- To attain knowledge about the structure of boron, inorganic chains and cluster compounds

Course Outcomes (COs)

CO No.	*Upon completion of this course, the students will be able to:*	PSO Addressed	Cognitive Level
CO-1	understand the structure and bonding in inorganic compounds	PSO-1	U
CO-2	apply the concepts of chemical bonding to predict the structure of compounds	PSO-2	A
CO-3	analyze the types of bonding, crystal lattices and crystal defects	PSO-2	Y
CO-4	evaluate bond energy, lattice energy and properties of inorganic compounds	PSO-2	E

Unit I Chemical Bonding (18 Hours)

VB approach to bonding - Heitler-London - Pauling and Slater refinements. Concept of hybridization and structure of molecules. VSEPR theory - shapes of molecules. MO approach to covalent bonding - symmetry and overlap of atomic orbitals - symmetry of molecular orbitals - sigma and pi bonding - energy levels in homo and hetero nuclear diatomic systems - bond length - bond order and bond energy - application to small molecules such as $BeCl_2$ - BCl_3 - CCl_4 and SF_4. Ionic character in a covalent bond and concept of multicentre bonding. Pseudo halogens - structure and bonding in ClF_3 - BrF_3 - BrF_5 - IF_5 - IF_7 etc. Oxides and oxyacids of halogens. Bonding in noble gas compounds - $XeCl_2$ - XeF_4 - $XeOF_4$ and XeF_6.

Unit II Chemistry of Solid State I (18 Hours)

Weak chemical forces - van der Waals forces and hydrogen bonding. Close packing of atoms and ions - HCP and BCC - types of packing voids - radius ratio - derivation - its influence on structures. Lattice energy - Born-Lande equation - Kapustinski equation and Madelung constant. Representative structures of AB and AB_2 types of compounds - rock salt - cesium chloride - wurtzite - zinc blende - rutile - fluorite - antifluorite - cadmium iodide and

nickel arsenide. Structure of graphite and diamond. Spinels - normal and inverse types and perovskite structures.

Unit III Chemistry of Solid State II (18 Hours)

Defects in crystal - line - plane defects - stoichiometry and non-stoichiometry defects. Band theory of solids. Electrical properties of solids - conductor - insulator - semiconductor - intrinsic and extrinsic semiconductors. Optical properties - lasers and phosphors. Elementary study of liquid crystals. Difference between point group and space group - screw axis - glide plane - symmetry elements - relationship between molecular symmetry and crystallographic symmetry. Concept of reciprocal lattice. X-ray diffraction by single crystal - rotating crystal and powder diffraction. Neutron diffraction - elementary treatment and comparison with X- ray diffraction. Electron diffraction- basic principle. Crystal growth methods from melt and solution. Hydrothermal and gel methods.

Unit IV Boron Compounds and Clusters (18 Hours)

Chemistry of boron - preparation - properties and structure of boranes - higher boranes - borazines - boron nitrides - hydroborate ions - STYX numbers - Wade's rules.

Carboranes - types - preparation - properties and structure of nido - closo - arachno. Metallocarboranes - general study. Metal clusters - chemistry of low molecularity metal clusters. Structure of Re_2Cl_8 and multiple metal-metal bonds.

Unit V Inorganic Chain and Cluster Compounds (18 Hours)

Types of inorganic polymers - comparison with organic polymers - silanes - higher silanes - multiple bonded systems - silicon nitrides and siloxanes. P-N compounds - cyclophosphazenes and cyclophosphazanes. S-N compounds - S_4N_4 and $(SN)_x$.

Isopoly and heteropoly acids - structure and bonding of 6- and 12- isopoly and heteropoly anions. Structure of silicates - applications of Paulings rule of electrovalence - isomorphous replacements in silicates - ortho - meta and pyro silicates - one dimensional - two dimensional and three dimensional silicates.

Text Books:

1. Cotton, F.A. & Wilkinson, G. (1999). Advance Inorganic Chemistry. (6^{th}ed.). New York: Wiley Interscience.
2. Puri B.R., Sharma, L.R. & Kalia, K.C. (2012). Principles of Inorganic Chemistry. (4^{th} ed.). India: Milestone publishers.

3. Kittle, C. (2012). Introduction to Solid State Physics. (8th ed.). New York: Wiley Eastern Ltd.
4. Puri, R.K. & Babber, V.K. (2001). Solid State Physics. (1st ed.). India: S. Chand and Company Ltd.
5. Lee, J.D. (2008). Concise Inorganic Chemistry. (5th ed.). New York: Wiley Interscience.
6. Huheey, J.E., Keiter, E.A., Keiter, R.L. & Medhi, O.K. (2011). Inorganic Chemistry: Principles of Structure and Reactivity. (4th ed.). India: Pearson Education.

Reference Books:

1. Purcell, K.F. & Kotz, J.C. (2012). Inorganic Chemistry. (2nd ed.). India: Cengage Learning India Pvt. Ltd.
2. Azaroff, L.V. (1989). Introduction to Solids.India: Tata McGraw Hill Publishing Ltd.
3. Dougles, D.E., McDaniel, D.H.& Alexander, J.J. (1994). Concepts and Models of Inorganic Chemistry. (3rd ed.). New York: John Wiley and Sons Ltd.
4. Malik, W.U., Tuli, G.D. & Madan, R.D. (2012). Selected topics Inorganic Chemistry. (5th ed.). New Delhi: S. Chand Company Ltd.
5. Miessler, G.L. (2004). Inorganic Chemistry, (3rd ed.). India: Pearson Education.

Module

Credit: 5 ***Total Hours: 90 (Incl. Seminar & Test)**

Unit	Section	Topics	Lecture Hours	Learning Outcome	Pedagogy	Assessment/ Evaluation
I	**Chemical Bonding**					
	1	VB approach to bonding - Heitler-London - Pauling and Slater refinements. Concept of hybridization and structure of molecules.	3	Understand the concept of hybridization and structure of molecules	Lecture with ppt	Evaluation through online quiz Formative assessment I
	2	VSEPR theory - shapes of molecules. MO approach to covalent bonding - symmetry and overlap of atomic orbitals - symmetry of molecular orbitals - sigma and pi bonding - energy levels in homo and hetero nuclear diatomic systems	4	Apply the concepts to predict the structure and shapes of molecules	Lecture and Group discussion	
	3	Bond length - bond order and bond energy - application to small molecules such as $BeCl_2$ - BCl_3 - CCl_4 and SF_4	3	Evaluate bond order and bond energy of small molecules	Lecture and Seminar	
	4	Ionic character in a covalent bond and concept of multicentre bonding. Pseudo halogens - structure and bonding in ClF_3 - BrF_3 - BrF_5 - IF_5 - IF_7 etc.	4	Analyse the types of bonding in pseudohalogens	Lecture	
	5	Oxides and oxyacids of halogens. Bonding in nobl gas compounds - $XeCl_2$ XeF_4 - $XeOF_4$ and XeF_6	4	Analyse the bonding in noble gas compounds	Lecture with ppt	
II	**Chemistry of Solid State I**					
	1	Weak chemical forces - van der Waals forces and hydrogen bonding	3	Understand the weak chemical forces	Lecture	Evaluation through class test, online quiz and group discussion Formative assessment I
	2	Close packing of atoms and ions - HCP and BCC - types of packing voids - radius ratio - derivation - its influence on structures	3	Analyse the types of packing of atoms and ions	Lecture with ppt	

	3	Lattice energy - Born-Lande equation - Kapustinski equation and Madelung constant	3	Understands lattice energy, Born-Lande equation and Kapustinski equation	Lecture and group discussion	
	4	Representative structures of AB and AB_2 types of compounds - rock salt - cesium chloride - wurtzite - zinc blende - rutile - fluorite - antifluorite - cadmium iodide and nickel arsenide	5	Analyse the types of bonding in AB and AB_2 types of compounds	Lecture	
	5	Structure of graphite an diamond. Spinels - norma and inverse types an perovskite structures.	4	Analyse the structure of graphite and diamond, normal and inverse types of spinels	Lecture with ppt	
III	**Chemistry of Solid State II**					
	1	Defects in crystal - line - plane defects - stoichiometry and non-stoichiometry defects	3	Analyse the types of defects in crystal	Lecture with ppt	Evaluation through class test, online quiz and group discussion Formative assessment II
	2	Band theory of solids. Electrical properties of solids - conductor - insulator - semiconductor - intrinsic and extrinsic semiconductors. Optical properties - lasers and phosphors. Elementary study of liquid crystals	4	Evaluate the optical and electrical properties solids	Lecture	
	3	Difference between point group and space group - screw axis - glide plane - symmetry elements - relationship between molecular symmetry and crystallographic symmetry. Concept of reciprocal lattice	4	Understand the differences between point group and space group, molecular symmetry and concepts of reciprocal lattice	Lecture with models	

	4	X-ray diffraction by single crystal - rotating crystal and powder diffraction. Neutron diffraction - elementary treatment and comparison with X-ray diffraction	4	Compare X-ray diffraction and neutron diffraction	Lecture	
	5	Electron diffraction- basic principle. Crystal growth methods frommelt and solution. Hydrothermal and gel methods	3	Understand electron diffraction and apply crystal growth methods.	Lecture	
IV	**Boron Compounds and Clusters**					
	1	Chemistry of boron - preparation - properties and structure of boranes - higher boranes	4	Understand the structure and properties of boranes	Lecture	Evaluation through class test and group discussion Formative assessment II
	2	Borazines - boronnitrides - hydroborate ions - STYX numbers - Wade's rules	4	Understand the structure of borazines, STYX numbers and wade rule	Lecture and group discussion	
	3	Carboranes - types - preparation - properties and structure of nido – closo and arachno	3	Analyse the structure of carboranes	Lecture	
	4	Metallocarboranes - general study. Metal clusters - chemistry of low molecularity metal clusters	4	Understand the chemistry of low molecularity metal clusters	Lecture	
	5	Structure of Re_2Cl_8 and multiple metal-metal bonds	3	Analyse the metal-metal bonds in Re_2Cl_8	Lecture	
V	**Inorganic Chain and Cluster Compounds**					
	1	Types of inorganic polymers - comparison with organic polymers silanes - higher silanes - multiple bonded systems - silicon nitrides and siloxanes	5	Understand the types of inorganic polymer and organic polymer	Lecture	Evaluation through class test, group discussion and quiz Formative assessment II
	2	P-N compounds - cyclophosphazenes. S-N compounds - S_4N_4 and $(SN)_x$	4	Understand the structure of P-N and S-N compounds	Lecture	

	3	Isopoly and heteropoly acids - structure and bonding of 6- and 12-isopoly and heteropoly anions	3	Analyse the structure and bonding in polyacids	Lecture	
	4	Structure of silicates - applications of Paulings rule of electrovalence - isomorphous replacements in silicates - ortho - meta and pyro silicates	3	Apply Pauling's rule of electrovalence to structure of silicates	Lecture and Group Discussion	
	5	One dimensional - two dimensional and three dimensional silicates	3	Understand one dimensional and two dimensional silicates	Lecture	

Course Instructor: Dr. S. Lizy Roselet HOD: Dr. G. Leema Rose

Semester I
Reaction Mechanism and Stereochemistry (Core II)
Subject Code: PG2012

No. of hours per week	Credit	Total no. of hours	Marks
6	5	90	100

Objectives:

- To understand the fundamental mechanisms involved in electrophilic and nucleophilic reactions
- To familiarize the basic aspects of stereochemistry and conformation

Course Outcomes (COs)

CO No.	*Upon completion of this course, the students will be able to:*	PSO Addressed	Cognitive Level
CO-1	understand the basic concepts of reaction mechanisms, stereochemistry and conformation in organic compounds	PSO-1	U
CO-2	apply the reaction mechanism, stereochemistry and conformation for the synthesis of organic compounds	PSO-2	A
CO-3	analyse the types of reaction mechanisms involved in synthetic organic transformation.	PSO-2	Y
CO-4	create novel organic compounds	PSO-3,4	C

Unit I Reaction Mechanism and Reactive Intermediates (18 Hours)

Reaction mechanism - energy diagram of simple organic reactions - transition state and intermediate. Kinetic and non-kinetic methods of determining organic reaction mechanisms. Isolation - trapping of intermediates and isotopic labeling studies. Primary kinetic isotopic effect. Correlation analysis - linear free energy relationships - Hammett equation - significances of σ and ρ - applications of Hammett equation. Taft equation and applications. Reactive intermediates - generation - stability and reactivity - carbocations - carbanions - free radicals - carbenes - benzynes and nitrenes.

Unit II Aliphatic Nucleophilic Substitution (18 Hours)

Mechanism of aliphatic nucleophlic substitution reaction - S_N1 - S_N2 and S_Ni mechanisms. Solvent and leaving group effects on aliphatic nucleophlic substitution reactions. Neighbouring group participation (NGP). Substitution at carbonyl - vinylic and bridgehead system. Substitution with ambident nucleophiles- "O" Vs "C"alkylation. Role of LDA - crown ethers and phase transfer catalysts (PTC) in nucleophilic substitution

reactions. Mechanism of ester hydrolysis (only BAc^2 - AAc^2 and AAl^1). Alkylation of active methylene compounds. Asymmetric alkylation - Evans - Enders and Meyers procedures. Preparation and synthetic utility of enamines - Finkelstein reaction and Wurtz coupling.

Unit III Aromatic Electrophilic and Nucleophilic Substitutions (18 Hours)

Aromatic electrophilic substitution - mechanism of nitration - sulfonation - Friedel-Crafts alkylation and acylation reactions. Synthesis of di- and tri-substituted benzenes from benzene or mono-substituted benzenes. Haworth reaction for naphthalene - Scholl reaction - Vilsmeier-Haack formylation - Gattermann reaction - Reimer-Tiemann and Bischler-Napieralski reactions.

Aromatic nucleophilic substitution in aryl halides by Meisenheimer complexmechanism and benzyne mechanism. Reactions of aryldiazonium salts. Zeigler alkylation - Vicarious Nucleophlic Substitution (VNS) - Chichibabin and Schiemann reactions.

Unit IV Stereochemistry (18 Hours)

Chirality - symmetry elements - asymmetric and dissymmetric chiral molecules. Relative and absolute nomenclature. Newman - Sawhorse - Fischer projections - their conversions. Axial chirality - planar chirality - helicity - allenes - spiranes - biphenyls - ansa compounds and trans-cycloalkenes. Stereochemistry of compounds containing nitrogen - sulphur and phosphorus. Topicity - homotopic - enantiotopic and diastereotopic ligands - groups and faces. Stereospecific and stereoselective synthesis. Asymmetric synthesis. Cram's rule - open chain - cyclic and dipolar model. Prelog's rule.

Unit V Conformational Analysis (18 Hours)

Conformation - definition - differences between configuration and conformation. Conformation of simple acyclic systems. Effect of conformation on reactivity of acyclic system - cis- and trans- eliminations. Conformation of cyclic systems upto six membered rings. Conformation of mono and di-substituted - three - four - five and six membered ring systems. Effect of conformation on reactivity of cyclic systems - S_N1 and S_N2 reactions. Quantitative correlation between conformation and reactivity - Winstein-Eliel equation and Curtin-Hammet principle. Conformations of decalin - perhydrophenanthrene and perhydroanthracene.

Text books:

1. March, J. (2006). Advanced Organic Chemistry. (4^{th} ed.). New York: John Wiley and Sons.
2. Sykes, P. (2003). A Guidebook to Mechanism in Organic Chemistry. (6^{th} ed.). India: Pearson.

3. Norman, R.O.C. & Coxon, J.M. (1993). Principles of Organic Synthesis, (3rd ed.). New York: CRC press, Taylor and Francis Group.
4. Ahluwalia, V.K. & Parshar, R.K. (2010). Organic Reaction Mechanism. (4th ed.). India: Narosa publishing House, 2010.
5. Nasipuri, D. (2011). Stereochemistry of Organic Compounds - Principles and Applications. (3rd ed.). India: New Age International, Ltd.
6. Kalsi, P.S. (2015). Stereo chemistry Conformation and Mechanism. (8th ed.). India: New Age International, Ltd.

Reference books:

1. Morrison, R.T. & Boyd, R.N. (1997). Organic Chemistry. (6th ed.). New Jersey: Prentice Hall.
2. Carey, F. & Sundberg, R.J. (2007). Advanced Organic Chemistry-Part A and B. (5thed.). USA: Springer.
3. Smith, M.B. & March, J. (2001). Advanced Organic Chemistry. (5thed.). New York: John Wiley and Sons.
4. Bansal, R.K. (2005). Reaction Mechanism in Organic Chemistry. (3rd ed.). Tata McGraw Hill.
5. Clayden, J. Greeves, N& Warren, S. (2012). Organic Chemistry. (2nd ed.). Oxford University Press.
6. Eliel, E.L. & Wilen, S.H. (2003). Stereochemistry of organic compounds. (1st ed.). New York: Wiley.

Teaching Module

Credit: 5 ***Total Hours: 90 (Incl. Seminar & Test)**

Unit	Section	Topics	Lecture Hours	Learning Outcome	Pedagogy	Assessment/ Evaluation
I	**Reaction Mechanism and Reactive Intermediates**					
	1	Reaction mechanism - energy diagram ofsimple organic reactions - transition state and intermediate	4	Understand the basic concepts of reaction mechanisms in organic compounds	Lecture with ppt	Evaluation through online quiz Formative assessment I
	2	Kinetic and non-kinetic methods of determining organic reaction mechanisms. Isolation - trapping of intermediates and isotopic labelling studies	4	Compare Kinetic and non-kinetic methods of determining organic reaction mechanisms	Lecture and Group discussion	
	3	Primary kinetic isotopic effect. Correlation analysis - linear free energy relationships - Hammett equation - significances of σ and ρ - applications of Hammett equation	4	Interpret the reaction mechanisms using linear free energy relationship.	Lecture and Seminar	
	4	Taft equation and applications	2	Understand the principle and applications of Taft equation	Lecture	
	5	Reactive intermediates - generation - stabilityand reactivity- carbocation- carbanions - free radicals - carbenes - benzynes and nitrenes	4	Understand and analyze the generation, stability and reactivity of reaction intermediates	Lecture with ppt	
II	**Aliphatic Nucleophilic Substitution**					
	1	Mechanism of aliphatic nucleophlic substitution reaction - S_N^1 - S_N^2 and S_N^i mechanisms. Solvent and leaving group effects on aliphatic nucleophlic substitution reactions	4	Identify S_N^1, S_N^2 and S_N^i mechanisms in organic reactions	Lecture with models	Evaluation through class test, online quiz and group discussion Formative

	2	Neighbouring group participation (NGP). Substitution at carbonyl - vinylic and bridgehead system. Substitution with ambident nucleophiles- "O" Vs "C"alkylation	5	Understand the concept of neighbouring group participation and substitution reactions	Lecture	assessment I
	3	Role of LDA - crown ethers and phase transfer catalysts (PTC) in nucleophilic substitution reactions	4	Understand the role of LDA - crown ethers and phase transfer catalysts (PTC) in organic reactions	Lecture and group discussion	
	4	Mechanism of ester hydrolysis (only BAc^2 - AAc^2 and AAl^1). Alkylation of active methylene compounds. Asymmetric alkylation - Evans - Enders and Meyers procedures. Preparation and synthetic utility of enamines - Finkelstein reaction and Wurtz coupling	5	Understand the reaction and mechanism of aliphatic nucleophlic substitution reactions	Lecture	
III	**Aromatic Electrophilic and Nucleophilic Substitutions**					
	1	Aromatic electrophilic substitution - mechanism of nitration - sulfonation - Friedel-Crafts alkylation and acylation reactions	4	Understand the mechanism of aromatic electrophilic substitution	Lecture with models	Evaluation through class test, online quiz and group discussion Formative assessment II
	2	Synthesis of di- and tri-substituted benzenesfrom benzene or mono-substituted benzenes. Haworth reaction for naphthalene - Scholl reaction - Vilsmeier-Haack formylation	6	Synthesize benzene derivatives using aromatic electrophilic substitution reactions	Lecture	
	3	Gattermann reaction - Reimer-Tiemann and Bischler-Napieralski reactions. Aromatic nucleophilic substitution in aryl halides by Meisenheimer complex mechanism and benzyne mechanism	5	Understand the mechanism of aromatic electrophilic and nucleophilic substitution reactions	Lecture and group discussion	

	4	Reactions of aryldiazonium salts. Zeigler alkylation - Vicarious Nucleophlic Substitution (VNS) - Chichibabin and Schiemann reactions	3	Understand the mechanism of aromatic nucleophilic substitution reactions)	Lecture	
IV	**Stereochemistry**					
	1	Chirality - symmetry elements - asymmetric and dissymmetric chiral molecules	3	Understand the concept of chirality	Lecture	Evaluation through class test and group discussion Formative assessment II
	2	Relative and absolute nomenclature. Newman - Sawhorse - Fischer projections - their conversions	4	Convert Newman, Sawhorse and Fischer projections	Lecture and group discussion	
	3	Axial chirality - planar chirality - helicity - allenes - spiranes - biphenyls - ansa compounds and trans-cycloalkenes	4	Differentiate axial and planar chirality	Lecture	
	4	Stereochemistry of compounds containing nitrogen - sulphur and phosphorus. Topicity - homotopic - enantiotopic and diastereotopic ligands - groups and faces	4	Understand the concept of topicity	Lecture	
	5	Stereospecific and stereoselective synthesis Asymmetric synthesis. Cram's rule - openchain - cyclic and dipolar model. Prelog's rule	3	Illustrate asymmetric synthesis using Cram's rule and prelog'srule	Lecture	
V	**Conformational Analysis**					
	1	Conformation - definition - differences between configuration and conformation. Conformation of simple acyclic systems. Effect of conformation on reactivity of acyclic system - cis- and trans-eliminations	5	Understand the conformation of simple acyclic systems	Lecture with videos	Evaluation through class test, group discussion and quiz Formative assessment I

	2	Conformation of cyclic systems upto six membered rings. Conformation of mono and di-substituted - three - four - five and six membered ring systems	5	Understand the conformation of cyclic systems	Lecture	
	3	Effect of conformation on reactivity of cyclic systems - S_N1 and S_N2 reactions	2	Evaluate the effect of conformation in cyclic system	Lecture	Evaluation through class test, group discussion and quiz Formative assessment II
	4	Quantitative correlation between conformation and reactivity - Winstein-Eliel equation and Curtin-Hammet principle	3	Correlate Winstein-Eliel equation and Curtin-Hammet principle	Lecture and Group Discussion	
	5	Conformations of decalin - perhydrophenanthrene and perhydroanthracene	3	Understand the conformation of bi- and tri-cyclic systems		

Course Instructor: Dr. Sheeba Daniel HOD: Dr. G. Leema Rose

Semester I
Chemical Kinetics and Electrochemistry (Core III)
Subject Code: PG2013

No. of hours per week	Credit	Total no. of hours	Marks
6	5	90	100

Objectives:

- To understand the mechanism of kinetics and catalysis of chemical reactions
- To attain knowledge about the concepts of photochemistry and electrochemistry

Course Outcomes (COs)

CO No.	*Upon completion of this course, the students will be able to:*	PSO Addressed	Cognitive Level
CO-1	understand the concepts of chemical kinetics, catalysis, photochemistry and electrochemistry	PSO-1	U
CO-2	apply the mechanism of kinetics and catalysis to chemical reactions	PSO-2,3	A
CO-3	analyze the principles and applications of kinetics, catalysis, photochemistry and electrochemistry	PSO-2,3	Y
CO-4	evaluate the kinetics and mechanism of chemical reactions	PSO-4	E

Unit I Chemical kinetics **(18 Hours)**

Arrhenius equation - Simple collision theory - ARRT theory - statistical and thermodynamic treatments. Ionic reactions - primary and secondary salt effects. Derivation and significance of volume of activation.

Kinetic isotopic effect - Kinetics of unimolecular reaction - Lindemann-Hinshelwood and Rice-Ramsperger-Kassel Marcus. Fast reactions - general features - flow techniques - relaxation theory and relaxation techniques (T-jump and p jump) - crossed molecular beam technique.

Unit II Catalysis **(18 Hours)**

Homogenous Catalysis - General catalytic mechanism - equilibrium treatment and steady state treatment - general acid-base catalysis and determination of catalytic co- efficient. Discussion of protolytic and prototropic mechanisms of acid catalysis. Bronsted relationships as linear free energy relationships. Acidity functions and correlation of mechanisms.

Heterogeneous Catalysis - physisorption and chemisorption - Langmuir adsorption isotherm - mechanism of surface reactions. Langmuir - Hinshelwood and Eley-Rideal mechanism. Absolute rate of surface reactions.

Unit III Photochemistry (18 Hours)

Introduction to photochemistry - laws of photochemistry - quantum yield calculation. Physical properties of electronically excited molecules - excited state dipole moment - acidity constant and redoxpotential. Photophysical processes in electronically excited molecules - Jablonski diagram - intersystem crossing - internal conversion - fluorescence - phosphorescence - delayed fluorescence and other deactivation processes.

Stern-Volmer equation and its application. Photosensitation and chemiluminescence. Chemical lasers - photoexplosion and dissociation laser - experimental techniques. Chemical actinometry and flash photolysis.

Unit IV Electrochemistry - I (18 Hours)

Deviation from ideal behavior - ion-solvent and ion-ion interactions. Debye-Hückel-Bjerrum model - ion association and triple ion formations. Expression for the mean activity coefficient. Debye-Hückel limiting law and its applications - diverse ion effect. Van't Hoff factor and its relation to colligative properties. Debye-Hückel theory of strong electrolytes. Debye-Huckel length and potential around a central ion - interpretation. Transport of ions in solution - electrolytic conduction - Debye - Huckel-Onsager treatment of strong electrolytes - ionic atmosphere and anomalous conductance of non-aqueous electrolytes.

Unit V Electrochemistry – II (18 Hours)

Electrical double layer - electrocapillary phenomena - surfactants and Lipmann's equation. Electrokinetic phenomena - zeta potential and its applications. Structure of electrical double layer - Helmholtz-Perrin - Guoy-Chapmann and Stern models. Butler-Volmer equation for one electron transfer reaction - equilibrium and exchange current densities - symmetry factor and transfer coefficient. Cyclic voltammetry and stripping voltammetry - principle and instrumentation. Corrosion and passivation of metals - Pourbaix diagram - Evans diagram. Batteries and fuel cells. Ion selective electrodes.

Text books

1. Laidler, K.J. (1987). Chemical Kinetics. (3rd ed.). New York: Harper and Row.
2. Atkins, P. & Atkins, J.P. (2002). Physical Chemistry. (7th ed.). USA: Oxford university press
3. Puri, B.R., Sharma, L.R. & Pathania, M.S.(2016). Principles of Physical Chemistry. (47th ed.). India: Vishal Publications.
4. G. W. Castellan, (2004).Physical Chemistry. (4th ed.). India: Narosa publishing House.

5. Turro, N.J. (1978). Modern Molecular Photochemistry. (1st ed.). California: Benjamin/Cummings, Menlo Park.
6. Glastone, S.A. (1969). Text Book of Physical Chemistry. (2nd ed.). London: Macmillan and Co Ltd.
7. Hamann, C.H., Hamnett, A. & Vielstich, W. (2001). Electrochemistry. (4th ed.). New York: John Wiley and Sons.
8. Perez, N. (2016). Electrochemistry and Corrosion Science. New York: Springer.

Reference Books

1. Agarwal, G.L. (1990). Basic Chemical Kinetics. (1st ed.). India: Tata McGraw Hill.
2. Silbey, R.J., Alberty, R.A. & Bawendi, M.G. (2015). Physical Chemistry.(4th ed.).India: Wiley.
3. Barrow, G.M. (2018). Physical Chemistry. (6th ed.). Ney York: Tata McGraw Hill.
4. Rohatgi-Mukhergee, K.K. (1997). Fundamentals of Photochemistry. (3rd ed.). India: New Age International Ltd.
5. Holze, R. (2009). Experimental Electrochemistry. New York: John Wiley and Sons.
6. Rieger, P.H. (2010). Electrochemistry. (2nded.). New York: Chapmann and Hall.

Teaching Module

Credit: 5 ***Total Hours: 90 (Incl. Seminar & Test)**

Unit	Section	Topics	Lecture Hours	Learning Outcome	Pedagogy	Assessment/ Evaluation
I	**Chemical kinetics**					
	1	Arrhenius equation-Simple collision theory-ARRT theory-statistical and thermodynamic treatments	4	Gain knowledge about chemical kinetics	Lecture	Evaluation through class test and quiz Formative assessment I
	2	Ionic reactions - primary and secondary salt effects	3	Explain the principle of ionic reactions	Lecture	
	3	Derivation and significance of volume of activation	4	Know about the significance of volume of activation	Lecture and Seminar	
	4	Kinetic isotopic effect-Kinetics of unimolecular reaction-Lindemann-Hinshelwood and Rice-Ramsperger-Kassel Marcus	3	Understand the mechanism of unimolecular reaction	Lecture	
	5	Fast reactions- general features - flow techniques - relaxation theory and relaxation techniques (T-jump and p jump) - crossed molecular beam technique	4	Know about the general features of fast reactions	Lecture	
II	**Catalysis**					
	1	Homogenous Catalysis-General catalytic mechanism - equilibrium treatment and steady state treatment - general acid-base catalysis	4	Infer the catalytic mechanism of equilibrium	Lecture	Evaluation through class test, group discussion and online quiz Formative assessment I
	2	Determination of catalytic co-efficient. Discussion of protolytic and prototropic mechanisms of acid catalysis	4	Compare protolytic and prototropic mechanisms	Lecture and group discussion	

	3	Bronsted relationships as linear free energy relationships. Acidity functions and correlation of mechanisms	4	Correlate Bronsted and linear free energy relationships	Lecture	
	4	Heterogeneous Catalysis –physisorption and chemisorption - Langmuir adsorption isotherm - mechanism of surface reactions	3	Differentiate homogeneous and heterogeneous catalysis	Lecture	
	5	Langmuir - Hinshelwood and Eley-Rideal mechanism. Absolute rate of surface reactions	3	Identify Langmuir - Hinshelwood and EleyRideal mechanism	Lecture	
III	**Photochemistry**					
	1	Introduction to photochemistry - laws of photochemistry, quantum yield calculation. Physical properties of electronically excited molecules.	5	Deduce photochemical relations	Lecture	Evaluation through class test and group discussion Formative assessment I
	2	Excited state dipolemoment, acidity constant and redox potential. Photophysical processes - electronically excited molecules	3	Understand excited state dipolemoment, acidity constant and redox potential	Lecture and seminar	
	3	Jablonski diagram, intersystem crossing, internal conversion, fluorescence, phosphorescence and other deactivation processes	2	Explain Jablonski diagram	Lecture and group discussion	
	4	Delayed fluorescence. Stern-Volmer equation and its application. Photosensitation and chemiluminescence. Chemical lasers	3	Derive Stern-Volmer equation	Lecture and seminar	
	5	Photoexplosion and dissociation laser - experimental techniques. Chemical actinometry and flash photolysis	5	Understand laser methods	Lecture	

IV	**Electrochemistry – I**					
	1	Deviation from ideal behavior - ion-solvent and ion-ion interactions. Debye-Hückel-Bjerrum model - ion association and triple ion formations. Expression for the mean activity coefficient	4	Understand the basic concepts of electrochemistry	Lecture	Evaluation through class test, group discussion and online quiz Formative assessment II
	2	Debye-Hückel limiting law and its applications - diverse ion effect. Van't Hoff factor and its relation to colligative properties	3	Derive Debye Huckel equation	Lecture and group discussion	
	3	Debye-Hückel theory of strong electrolytes. Debye-Huckel length and potential around a central ion - interpretation. Transport of ions in solution	4	Explain the principles and applications of Huckel theory	Lecture	
	4	Electrolytic conduction-. Debye - Huckel-Onsager treatment of strong electrolytes- ionic atmosphere	4	Apply Debye - Huckel-Onsager treatment to strong electrolytes	Lecture	
	5	Anomalous conductance of non-aqueous electrolytes	3	Gain knowledge about the non aqueous electrolytes	Lecture	
V	**Electrochemistry – II**					
	1	Electrical double layer - electrocapillary phenomena -surfactants and Lipmann's equation. Electrokinetic phenomena - zeta potential and its applications	4	Derive Lippmann equation	Lecture	Evaluation through class test, group discussion and quiz Formative assessment II
	2	Structure of electrical double layer - Helmholtz-Perrin - Guoy-Chapmann and Stern models. Butler-Volmer equation for one electron transfer reaction equilibrium	4	Derive Butler-Volmer equation		

	3	Exchange current densities- symmetry factor and transfer coefficient.Cyclic voltammetry and stripping voltammetry - principle and instrumentation	4	Know about the Transfer coefficients	Lecture	
	4	Corrosion and passivation of metals - Pourbaix diagram - Evans diagram.	3	Employ the methods of preventing corrosion	Lecture with videos	
	5	Batteries and fuel cells. Ion selective electrodes	3	Employ the methods of the Construction of fuel cells	Lecture	

Course Instructor: Dr. M. Shirly Treasa HOD: Dr. G. Leema Rose

Semester I
Analytical Chemistry (Elective I)

Subject Code: PG2014

No. of hours per week	Credit	Total no. of hours	Marks
4	3	60	100

Objectives

- To attain the ability to identify the errors.
- To understand various analytical techniques.

Course Outcomes (COs)

CO No.	*Upon completion of this course, the students will be able to:*	PSO Addressed	Cognitive Level
CO-1	understand the principle and instrumentation of various analytical techniques	PSO-1	U
CO-2	apply the principle of analytical techniques to predict the purity, stability and concentrations of compounds	PSO-2,4	A
CO-3	analyse chemical compound using various analytical techniques	PSO-2,3	Y
CO-4	evaluate the quality and quantity of chemical compounds	PSO-3	E

Unit I Error Analysis **(12 Hours)**

Significant figures - rounding off the values - accuracy and precision. Errors - classification of errors. Expression and calculation of errors in different forms. Precision and accuracy with respect to random errors. Minimization of errors - calibration of apparatus - analysis of standard samples - running a blank determination and independent analysis. Confidence limits. Tests of significance - F-test - t-test - chi square test and annova. Correlation and regression analysis.

Unit II Chromatography **(12 Hours)**

General principle - classification of chromatographic methods - nature of partition forces and chromatographic behaviour of solutes. Plate and rate theories. Normal and reversed phase liquid chromatography. Column chromatography - principle - experimental technique and applications. Gas chromatography - gas-solid and gas-liquid chromatography. Thin layer chromatography - ion exchange chromatography and high performance liquid chromatography.

Unit III Colorimetric and Spectrophotometric Analytical Techniques (12 Hours)

Colorimetry - fundamental laws - instrumentation and applications. Spectrophotometry - instrumentation and applications. Principle - instrumentation - applications of fluorimetry - phsophorimetry - flame photometry - nephelometry and turbidimetry. Turbidimetric titrations and applications.

Unit IV Thermoanalytical Techniques (12 Hours)

Thermogravimetric analysis (TGA) - principle - instrumentation - factors affecting thermogram - decomposition of calcium oxalate monohydrate and copper sulphate pentahydrate. Differential thermal analysis (DTA) - principle - instrumentation and thermal behaviour of copper sulphate pentahydrate by DTA. Differential scanning calorimetry (DSC) - principle - instrumentation - phase transition studies by DSC. Thermometric titrations - principle - working and applications.

Unit V Electroanalytical Techniques (12 Hours)

Electrogravimetric analysis - theory - instrumentation and applications. Coulometric analysis - coulometric titrations and applications. Potentiostatic coulometry. Polarography - principle - current-voltage relationship - dropping mercury electrode (DME) - experimental assembly - polarogram - half-wave potential - Ilkovic equation - applications to qualitative and quantitative analysis. Concept of pulse polarography. Voltametry - principle - cyclic voltametry. Amperometric titrations - principle and applications.

Text Books:

1. Kaur, H. (2016). Instrumental Methods of Chemical Analysis. India: Pragati Prakashan Publishing Ltd.
2. Day, R.A. & Underwood, A.L. (1998). Quantitative Analysis. (6th ed.). India: Prentice Hall.
3. Chatwal, G.R. & Anand, S.K. (2002). Instrumental Methods of Chemical Analysis. (5th ed.). India: Himalaya Publishing House.

Reference Books:

1. Higson, S. (2003). Analytical Chemistry. (1sted.). USA: Oxford University Press.
2. Christian, G.D. (2007). Analytical Chemistry. (6th ed.). New York: John Wiley & Sons.
3. Skoog, D.A, Holler, F.J & Crouch, S.R (2007). Principles of Instrumental Analysis. (6thed.). Australia: Thompson Brooks/Cole.
4. Gopalan, R., Subramanian, P.S. & Rengarajan, K. (2003). Elements of Analytical Chemistry. (3rded.). New Delhi: Sultan Chand & Sons.

Teaching Module

Credit: 3 ***Total Hours: 60 (Incl. Seminar & Test)**

Unit	Section	Topics	Lecture Hours	Learning Outcome	Pedagogy	Assessment/ Evaluation
I	**Error Analysis**					
	1	Significant figures - rounding off the values - accuracy and precision	2	Understand accuracy and precision	Lecture and group discussion	Evaluation through periodic test, class test, online quiz and problem solving Formative assessment I
	2	Errors - classification of errors. Expression and calculation of errors in different forms. Precision and accuracy with respect to random errors	3	Classify and evaluate errors with accuracy and precision	Lecture and Seminar	
	3	Minimization of errors - calibration of apparatus - analysis of standard samples - running a blank determination and independent analysis	3	Analyze and minimize errors	Seminar	
	4	Confidence limits. Tests of significance - F-test - t-test - chi square test and annova. Correlation and regression analysis	4	Calculate F-test, t-test and chi square test. Evaluate correlation and regression analysis	Lecture and Seminar	
II	**Chromatography**					
	1	General principle - classification of chromatographic methods - nature of partition forces and chromatographic behaviour of solutes	2	Understand the principle and classification of chromatography	Lecture with videos	Evaluation through periodic test, class test, online quiz and group discussion Formative assessment I
	2	Plate and rate theories. Normal and reversed phase liquid chromatography	2	Understand the theories and concepts in liquid chromatography	Lecture with videos	
	3	Column chromatography - principle -	2	Apply column chromatographic technique to	Seminar and group discussion	Evaluation through periodic test,

		experimental technique and applications		separate chemical compounds		class test, online quiz and class assignment Formative assessment II
	4	Gas chromatography - gas-solid and gas-liquid chromatography. Thin layer chromatography	3	Apply gas and thin layer chromatographic techniques to separate chemical compounds	Seminar and group discussion	
	5	Ion exchange chromatography and high performance liquid chromatography	3	Identify the chemical constituents present in a sample using HPLC	Lecture with videos	
III	**Colorimetric and Spectrophotometric Analytical Techniques**					
	1	Colorimetry - fundamental laws, instrumentation and applications	2	Apply colorimetry to determine the concentration of unknown sample	Seminar with ppt	Evaluation through periodic test, class testand group discussion Formative assessment II
	2	Principle, instrumentation and applications of spectrophotometry and fluorimetry	3	Identify photoactive fluorescent materials	Lecture and seminar	
	3	Principle, instrumentation and applications ofphsophorimetry and flame photometry	3	Understand the principle and applications of phsophorimetry and flame photometry	Seminar and group discussion	
	4	Principle, instrumentation and applications of nephelometry and turbidimetry. Turbidimetric titrations and applications	4	Differentiate nephelometry and turbidimery. Understand the applications of turbidimetric titrations	Lecture and seminar	
IV	**Thermoanalytical Techniques**					
	1	Thermogravimetric analysis (TGA) - principle and instrumentation. Factors affecting thermogram - decomposition of calcium oxalate	3	Analyze the purity and thermal stability of compounds using TGA	Lecture with videos and seminar	Evaluation through periodic test, class test, online quiz and class assignment

		monohydrate and copper sulphate pentahydrate				Formative assessment II
	2	Differential thermal analysis (DTA) - principle and instrumentation. Thermal behaviour of copper sulphate pentahydrate by DTA	3	Understand DTA and analyse the thermal behaviour of compounds	Lecture with videos and seminar	
	3	Differential scanning calorimetry (DSC) - principle and instrumentation. Phase transition studies by DSC	3	Apply DSC to detect the phase transitions of compounds	Lecture with videos and seminar	
	4	Thermometric titrations - principle, working and applications	3	Understand the principle and applications of thermometric titrations	Lecture with videos and seminar	
V	**Electroanalytical Techniques**					
	1	Electrogravimetric analysis - Theory, instrumentation and applications	2	Understand the applications of electrogravimetric analysis	Lecture with ppt and seminar	Evaluation through periodic test, class test, group discussion and online quiz Formative assessment I
	2	Coulometric analysis - coulometric titrations and applications. Potentiostaticcoulometry	3	Understand the application of coulometry	Lecture with videos and seminar	
	3	Polarography - principle - current-voltage relationship - dropping mercury electrode (DME) - experimental assembly - polarogram - half-wave potential and Ilkovic equation	3	Understand the principle of polarography	Lecture with videos and seminar	

	4	Polarography - applications to qualitative and quantitative analysis. Concept of pulse polarography	2	Apply polarographic techniques for qualitative and quantitative analysis	Seminar and group discussion	
	5	Voltametry - principle - cyclic voltametry. Amperometric titrations - principle and applications	2	Understand the principle of voltametry and amperometric titrations	Lecture with videos and seminar	

Course Instructor: Dr. B.T Delma HOD: Dr. G. Leema Rose

Semester III
Organic Spectroscopy (Core VII)
Course Code: PG2031

No. of hours per week	Credit	Total no. of hours	Marks
6	5	90	100

Objectives

- To understand the principle and applications of UV, IR, NMR and Mass spectroscopictechniques.
- 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	CL
CO-1	understand the principle and applications of various spectroscopic techniques	PSO-1	U
CO-2	apply the spectroscopic concepts to determine the structure of organic compounds	PSO-2,3	A
CO-3	analyze the functional groups, molecular formula, structure and spectral data of compounds	PSO-2,3	Y
CO-4	evaluate the purity, structure and molecular mass of compounds using various spectroscopic methods	PSO-2,3	E
CO-5	create and characterize novel organic compounds	PSO-3,4	C

Unit I **(18 Hours)**

UV-Visible and IR spectroscopy

UV-Visible spectroscopy: principle - types of electronic excitations - chromophore - auxochrome - bathochromic - hypsochromic - hypochromic and hyperchromic shifts. Woodward-Fieser rules to calculate λ_{max} values of conjugated dienes - α,β-unsaturated carbonyl compounds and aromatic compounds. Fieser-Khun rule. Effect of solvent polarity on λ_{max}.

IR spectroscopy: principle - Hooke's law - types of molecular vibrations. Factors influencing the vibrational frequency. Identification of functional groups in organic compounds. Finger print region. Fermi resonance - overtones and combination bands.

Unit II **(18 Hours)**

^{1}H NMR Spectroscopy

^{1}H NMR Spectroscopy: principle - instrumentation - shielding and deshielding. Chemical shift - factors affecting chemical shift - electronegativity - hybridization - hydrogen bonding - anisotropic effect - double bond - triple bond - aromatic compounds - carbonyl compounds and annulenes. Spin-spin splitting pattern of simple organic compounds. Types of coupling - germinal - vicinal - long range and through space coupling. Karplus equation. Coupling

constant - AB, AB_2 and A_2B_3. Simplification of complex spectra - chemical exchange, double resonance and NMR shift reagents. Temperature dependent NMR.

Unit III **(18 Hours)**

^{13}C, ^{19}F and ^{31}P NMR Spectroscopy

^{13}C NMR spectroscopy: principle - comparison of ^{13} C NMR and ^{1}H NMR. Chemical shift - factors affecting chemical shift. Homo nuclear and heteronuclear coupling. Broad band decoupling and OFF - resonance decoupling. Distortionless Enhancement by Polarization Transfer (DEPT) spectrum - DEPT-45 - DEPT-90 and DEPT-135. 2D Correlation spectroscopy (COSY) - HOMCORR - ^{1}H-^{1}H and ^{13}C-^{13}C connectivity. HETCORR - ^{1}H-^{13}C connectivity and MRI.

^{19}F NMR spectroscopy: precessional frequency and heteronuclear coupling. Identification of organofluoro compounds CF_3CO_2Et and CF_3CH_2OH.

^{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.

Unit IV **(18 Hours)**

Mass Spectrometry: principle - production of ions - Electronic Ionization (EI), Chemical Ionization (CI) and Fast Atom Bombardment (FAB). Molecular ion peak - base peak - meta stable peak and isotopic peaks. Nitrogen rule. McLafferty rearrangement and Retro Diels Alder reaction. 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.

Unit V **(18 Hours)**

Structural Elucidation using Analytical and Spectral Data: Determination of molecular formula of organic compounds using elemental (CHN) analysis data. Structural determination of simple organic compounds using UV - IR - NMR and Mass spectral data.

Text Books

1. Mohan, J. (2001). Organic Spectroscopy Principles and applications. India: Narosa publishing house.
2. Kemp, W. (1991). Organic Spectroscopy. (3rd ed.). New York: Macmillan.
3. Kalsi, P.S. (2004). Spectroscopy of Organic Compounds. (6th ed.). India: New Age International Ltd.
4. Silverstein, S.M., Bassler, G.V. &Morril, T.C. (2004). Spectrometric identification of organic compounds. (6th ed.). New York: Wiley.

Reference Books

1. Dyer, J.R. (1987). Applications of Absorption spectroscopy of Organic Compounds. New York: Prientice Hall.
2. Dani, V.R. (1995). Organic spectroscopy, India: Tata McGraw Hill.
3. Pavia, D.L., Lampman, G.M.,Kriz, G.S. & Vyvyan, J.R. (2009). Introduction to Spectroscopy. (4th ed.). USA: Cengage Learning.
4. Sharma, Y.R. (2013). Elementary Organic Spectroscopy. (5th ed.). New Delhi: S. Chand Publishing.

Teaching Module

Credit: 5 **Total Hours: 90 (Incl. Seminar & Test)**

Unit	Section	Topics	Lecture Hours	Learning Outcome	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	Recognize the concepts of UV-Visible spectroscopy	Flipped Lecture	Evaluation through online quiz (quizizz), slip test, group discussion and problem solving Formative assessment I
	2	Woodward-Fieser rules to calculate λ_{max} values of conjugated dienes - α,β-unsaturated carbonyl compounds and aromatic compounds. Fieser-Khun rule.	6	Calculate the λ_{max} values of organic compounds	Group discussion and problem solving	
	3	Effect of solvent polarity on λ_{max}.	1	Describe the role of solvent polarity in electronic transitions	Lecture with ppt	
	4	IR spectroscopy: principle - Hooke's law - types of molecular vibrations.	2	Recollect the concepts of IR spectroscopy	Lecture with videos	
	5	Factors influencing the vibrational frequency. Identification of functional groups in organic compounds.	3	Identify the functional groups in organic compounds	Lecture and Group discussion	
	6	Finger print region. Fermi resonance - overtones and combination bands.	3	Depict various bands in IR spectroscopy	Lecture with ppt	
II	**^{1}H NMR Spectroscopy**					
	1	^{1}H NMR Spectroscopy: principle - instrumentation - shielding and deshielding.	3	Understand the concepts and instrumentation of NMR spectroscopy	Lecture with videos	Evaluation through class test, quiz, group discussionand problem solving Formative assessment I
	2	Chemical shift - factors affecting chemical shift - electronegativity - hybridization - hydrogen bonding - anisotropic effect - double bond - triple bond - aromatic compounds - carbonyl compounds and	4	Explain the factors which affect the chemical shift	Lecture with ppt	

		annulenes.				
	3	Spin-spin splitting pattern of simple organic compounds	3	Predict the splitting pattern of organic compounds	Group discussion and problem solving	
	4	Types of coupling - germinal - vicinal - long range andthrough space coupling. Karplus equation. Coupling constant - AB, AB_2 and A_2B_3.	4	Analyse the types of coupling	Lecture with ppt	
	5	Simplification of complex spectra - chemical exchange, double resonance and NMR shift reagents. Temperature dependent NMR.	4	Describe the methods used for the simplification of complex spectrum	Lecture with ppt	
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	Understand the concepts of ^{13}C NMR spectroscopy	Lecture with ppt	Evaluation through class test, quiz and group discussion Formative assessment II
	2	Homonuclear and heteronuclear coupling. Broad band decoupling and OFF - resonance decoupling.	3	Analyze the types of coupling and decoupling	Lecture with ppt	
	3	Distortionless Enhancement by Polarization Transfer (DEPT) spectrum - DEPT-45 - DEPT-90 and DEPT-135.	3	Illustrate DEPT spectrum	Lecture with videos	
	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	Interpret COSY-HOMCOR and HETCOR	Lecture	
	5	^{19}F NMRspectroscopy: precessional frequency and heteronuclear coupling. Identification of organofluoro compounds CF_3CO_2Et and CF_3CH_2OH.	3	Identify organofluoro compounds using ^{19}F NMRspectroscopy	Lecture with ppt	

	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	Identification of organophosphorous compounds using ^{31}P NMR spectroscopy	Lecture with ppt	
IV	**Mass Spectrometry**					
	1	Principle - production of ions - Electronic Ionization (EI), Chemical Ionization (CI) and Fast Atom Bombardment (FAB).	4	Understand the principle and production of ions in mass spectroscopy	Lecture with videos	Evaluation through class test, quiz, group discussion and problem solving Formative assessment I
	2	Molecular ion peak - base peak - meta stable peak and isotopic peaks.	2	Identify the peaks in mass spectrum	Lecture with ppt	
	3	Nitrogen rule. McLafferty rearrangement and Retro Diels Alder reaction.	2	State and explain nitrogen rule and fragmentation reactions	Lecture	
	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	Predict the fragmentation pattern of organic compounds	Lecture and group discussion	
V	**Structural Elucidation using Analytical and Spectral Data**					
	1	Determination of molecular formula of organic compounds using elemental (CHN) analysis data.	4	Determine the molecular formula of chemical compounds	Group discussion and problem solving	Evaluation through class test, group discussion and problem solving Formative assessment II
	2	Structural determination of simple organic compounds using UV - IR - NMR and Mass spectral data.	14	Elucidate the structure of chemical compounds	Group discussion and problem solving	

Course Instructor: Dr. Sheeba Daniel HOD: Dr. G. Leema Rose

Semester III
Thermodynamics and Group Theory (Core VIII)
Course Code: PG2032

Hours per week	Credits	Total Hours	Marks
6	5	90	100

Objectives:

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

Course Outcomes (COs)

CO	*Upon completion of this course, the students will be able to:*	PSO Addressed	CL
CO-1	understand the concepts and applications of thermodynamics and group theory	PSO-1	U
CO-2	apply thermodynamics and group theory to determine thermodynamic parameters, vibrations and hybrid orbitals	PSO-2	A
CO-3	analyze the thermodynamic functions, point groups and normal mode of vibration of molecules	PSO-2	Y
CO-4	evaluate the thermodynamic parameters and delocalization energy in molecules	PSO-2	E

Unit I (18 Hours)

Thermodynamics and Non-Ideal Systems: Concepts of partial molar properties - 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. Fugacity - determination of fugacity of gases by graphical method - variation of fugacity with temperature and pressure - Lewis Randal rule and Duhem-Margules equation. Determination of activity and activity coefficient of non-electrolyte by e.m.f method - excess functions.

Unit II (18 Hours)

Irreversible Thermodynamics: Nernst heat theorem - Third law of thermodynamics - applications of third law - entropy change -calculation of absolute entropies - apparent exceptions to third law. Non-equilibrium thermodynamics - basic concepts - forces and fluxes - entropy of irreversible processes - entropy production - Clausius inequality - phenomenological equations - Onsager reciprocity relations and coupled reactions. Principle of microscopic reversibility - the Onsager reciprocal relations - verification. Entropy production.

Unit III (18 Hours)

Statistical Thermodynamics: Statistical thermodynamics - concept of distributions - types of particles (bosons, fermions, mesons) - types of ensembles. Thermodynamic probability -

most probable distribution law - classical statistics - Maxwell-Boltzmann (MB) statistics - Quantum statistics - Bose-Einstein (BE) and Fermi-Dirac (FD) statistics - derivation of distribution function - MB, BE and FD statistics - comparison. Partition functions - translational - rotational - vibrational and electronic partition function - calculation of thermodynamic parameters and equilibrium constants in terms of partition function. Debye and Einstein heat capacity of solids.

Unit IV **(18 Hours)**

Group Theory I: Molecular symmetry elements - symmetry operations - molecular symmetry and point groups. Group multiplication tables - abelian - non-abelian - cyclic and sub groups - conjugacy relation and classes. Representation of symmetry operations by matrices - representation for C_{2v} - C_{3v} and C_{2h} point groups. Reducible and irreducible representations. The great orthogonality theorem and its consequences. Construction of the character tables - C_{2v} - C_{3v} and C_{2h} point groups.

Unit V **(18 Hours)**

Group Theory II: 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. Symmetry properties of integrals and symmetry based selection rule for vibrational spectra. Identification of IR and Raman active fundamentals - symmetry of molecular orbitals and symmetry based selection rule for electronic transition - prediction of electronic transitions in ethylene and formaldehyde. Determinationof π- electron energy in ethylene. HMO theory - HMO calculations and delocalization energy in trans-1,3-butadiene and benzene. Application of Determination of hybridization in CH_4 and BF_3.

Text Books

5. Kuriacose, J.C. & Rajaram, J. (1986). Thermodynamics. (1st ed.). Delhi: Shohanlal and Company.
6. Atkins, P. & Atkins, J.P. (2002). Physical Chemistry. (7th ed.). USA: Oxford university press.
7. Puri, B.R., Sharma, L.R. & Pathania, M.S. (2016). Principles of Physical Chemistry (47th ed.). India: Vishal Publications.
8. Bhattacharya,P.K. (1986). Group Theory and its Chemical Applications. India: Himalaya Publishing house.
9. Cotton, F.A. (2008). Chemical Applications of Group Theory. (3rd ed.). New York: Wiley.

Reference Books

1. Glasstone, S. (1969). Thermodynamics for chemistry. New York: Van Nostrand Company
2. Glasstone, S.A. (1969). Text Book of Physical Chemistry. (2nd ed.). London: Macmillan and Co Ltd.
3. Kapoor, K.L. (1986). Text Book of Physical Chemistry. Delhi: MacMillan India Ltd.
4. Ramakrishnan, V. & Gopinathan, M.S. (1998). Group Theory in Chemistry. India: Vishal Publications.
5. Raman, K.V. (1990). Group Theory and its Applications to Chemistry. India: Tata Mcgraw Hill Publishing Co.

Teaching Module

Credit: 5 **Total Hours: 90 (Incl. Seminar & Test)**

Unit	Section	Topics	Lecture Hours	Learning Outcome	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	Recognize the concepts of partial molar properties.	Lecture	Evaluation through class test Formative assessment I
	2	Chemical potential - variation of chemical potential with temperature and pressure - Van't Hoff isotherm and solution.	4	Explain the effect of pressure and temperature on chemical potential	Lecture and Seminar	
	3	Fugacity - determination of fugacity of gases by graphical method - variation of fugacity with temperature and pressure .	4	Determine the fugacity of gases	Lecture and Seminar	
	4	Lewis Randal rule and Duhem-Margules equation	3	Deduce the relationship between fugacity and mole fraction	Lecture and group discussion	
	5	Determination of activity and activity coefficient of non-electrolyte by e.m.f method - excess functions.	3	Determine the activity and activity coefficient of non-electrolyte	Lecture	
II	**Irreversible Thermodynamics**					
	1	Nernst heat theorem - Third law of thermodynamics - applications of third law.	4	Discuss the effect of temperature on entropy change of reactions.	Lecture and group discussion	Evaluation through class test and group discussion

	2	entropy change - calculation of absolute entropies - apparent exceptions to third law.	3	Calculate the absolute entropies of various reactions	Group discussion and problem solving	Formative assessment II
	3	Non-equilibrium thermodynamics - basic concepts - forces and fluxes - entropy of irreversible processes - entropy production	3	Explain the - basic concepts of non-equilibrium thermodynamics	Lecture	
	4	Clausius inequality - phenomenological equations - Onsager reciprocity relations and coupled reactions.	4	Deduce Onsager reciprocity relations	Lecture	
	5	Principle of microscopic reversibility - the Onsager reciprocal relations - verification. Entropy production.	4	Verify Onsager reciprocity relations	Lecture and group discussion	
III	**Statistical Thermodynamics**					
	1	Statistical thermodynamics - concept of distributions - types of particles (bosons, fermions, mesons) - types of ensembles.	4	Classify the types of particles and ensembles	Lecture and group discussion	Evaluation through class test and group discussion Formative assessment III
	2	Thermodynamic probability - most probable distribution law - classical statistics - Maxwell-Boltzmann (MB) statistics	3	Derive Maxwell-Boltzmann distribution equation	Lecture	
	3	Quantum statistics - Bose-Einstein (BE) and Fermi-Dirac (FD) statistics - derivation of distribution function -	5	Compare MB, BE and FD statistics	Lecture and group discussion	

		MB, BE and FD statistics - comparison.				
	4	Partition functions - translational - rotational - vibrational and electronic partition function	3	Describe various partition functions	Lecture	
	5	calculation of thermodynamic parameters and equilibrium constants in terms of partition function. Debye and Einstein heat capacity of solids.	3	Calculate equilibrium constant in terms of partition function	Group discussion	
IV	**Group Theory I**					
	1	Molecular symmetry elements - symmetry operations - molecular symmetry and point groups.	4	Understand symmetry elements and symmetry operations	Lecture	Evaluation through class test and group discussion Formative assessment II
	2	Group multiplication tables - abelian - non-abelian - cyclic and sub groups - conjugacy relation and classes.	3	Explain the terms in group theory	Lecture and group discussion	
	3	Representation of symmetry operations by matrices - representation for C_{2v} - C_{3v} and C_{2h} point groups.	4	Represent symmetry operations	Lecture	
	4	Reducible and irreducible representations. The great orthogonality theorem and its consequences.	3	Apply orthogonality theorem for the construction of character table	Lecture and PPT	

	5	Construction of the character tables C_{2v}, C_{3v} and C_{2h}.	4	Construct character table for different point groups	Lecture	
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	Apply group theory to normal mode analysis of H_2O ,NH_3 and CO_2	Lecture and group discussion	Evaluation through class test and group discussion Formative assessment II
	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	Identify IR and Raman active vibrations	Lecture and group discussion	
	3	symmetry based selection rule for electronic transition - prediction of electronic transitions in ethylene and formaldehyde.	4	Predict the electronic transitions in ethylene and formaldehyde	Lecture	
	4	Determinationof π-electron energy in ethylene.HMO theory - HMO calculations	3	Apply group theory and HMO theoryto determine π-electron energy	Lecture	
	5	delocalization energy in trans-1,3-butadiene and benzene. Application of Determination of hybridization in CH_4 and BF_3.	3	Determine the hybridization of CH_4 and BF_3	Lecture and videos	

Course Instructor: M.Shirly Treasa HOD: G. Leema Rose

Semester III
Advanced Topics in Chemistry (Elective III (a))
Course Code: PG2033

No. of hours per week	Credit	Total no. of hours	Marks
4	3	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	CL
CO-1	understand the principles and application of advanced areas in chemistry	PSO-1	U
CO-2	apply the principle of nanochemistry and green chemistry to design and synthesise novel compounds	PSO-2,3	A
CO-3	analyze the properties of nanoparticles, supramolecular interactions, therapeutic action of drugs and reactions in biomolecules	PSO-2,3	Y
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	E
CO-5	create novel nanoparticles and compounds using green chemistry techniques	PSO-3,4	C

Unit I **(12 Hours)**

Nanochemistry: General principles of nanotechnology. Nanoparticles - definition - size relationship - nanoparticles of metals - semiconductors and oxides. Synthesis of nanosized compounds - reduction methods and solgel methods. Optical and electrical properties of nanoparticles. Nanosystems - introduction - synthesis and purification of fullerenes. Carbonnanotubes - types - preparation - Arc and chemical vapour deposition methods. Nanoshells - gold and silver nanoshells and its applications. Nanosensors - introduction - nanoscale organization - characterization and optical properties. Nanomedicines - introduction - approach to developing nanomedicines - protocol for nanodrug administration -diagnostic and therapeutic applications.

Unit II **(12 Hours)**

Green Chemistry: Green chemistry and sustainable development - principles andapplications 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. Energy requirement for synthesis. CFC alternatives - green chemistry in organic synthesis.

Selection of appropriate solvent and starting material. Use of protecting groups and catalyst. Methods of greening organic reactions - solvent free reactions and reactions at ambient temperature. Microwave assisted reactions. Sonication assisted reactions - Reformatsky - Ullmann coupling - Wurtz and Bouveault reaction. Reactions in ionic solvents and super critical fluids. Tandem reactions.

Unit III **(12 Hours)**

Supramolecular Chemistry: Supramolecular interactions - discussion of host-guest systems - cation and anion binding host. Crown ethers - synthesis - properties and applications. Lariat ethers. Podants - properties and 3-dimensional podants. Cryptands - synthesis - properties and applications. Spherands - synthesis - structure and uses. Supramolecular chemistry of fullerenes and cyclodextrins. Molecular devices - non-linear optical switches and electrophotoswitching, Liquid crystal display. Supramolecular photochemistry.

Unit IV **(12 Hours)**

Medicinal Chemistry: 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. Diuretics - classification - synthesis and assay of Frusemide and benzthiazide. Anti-inflammatory drug - synthesis and therapeutic action of phenylbutazone and ibuprofen. Antipyretics and non-narcotic analgesics - synthesis and therapeutic action of paracetamol and aspirin

Unit V **(12 Hours)**

Biophysical Chemistry: Thermodynamics in biology and limitations of equilibrium thermodynamics. Irreversible thermodynamics - postulates and methodologies. Irreversible thermodynamics and biological systems. Biochemical standard state - ATP. Currency of energy - oxidative phosphorylation. Role of singlet oxygen in biology. Reactions in biomolecules - membrate potential and ion pumps. Photoacoustic effect and its application in biology. Biophysical applications of Moss-bauer effect. NMR imaging - applications of spin labeling in membrane research.

Text Books

1. Klabunde, K.J. & Richards, R.M. (2009). (2^{nd} ed.). Nanoscale Materials in Chemistry. New York: Wiley.
2. Ozin, G. & Arsenault, A. (2005). Nanochemistry: A Chemical Approach to Nanomaterials. USA: Elsevier.
3. Rao, C.N.R. (2001). Nanochemistry. New York: Wiley.
4. Ahluwalia, V.K. (2006). Green chemistry-Environmentally benign reactions. India: Ane Books Publications.
5. Kar, A. (2007). Medicinal Chemistry. (4^{th} ed.), New Age International Publishers.

Reference Books

1. Brechignac, C., Houdy, P. & Lahmani, M. (2006). Nanomaterials and Nano chemistry. New York: Springer.
2. Nalwa, H. (1998). Nanostructured Materials and Nanotechnology. New York: Academic Press.
3. Ahluwalia, V. K. (2012). Strategies for Green Organic Synthesis. New York: Taylor and Francis group, CRC Press.
4. Matlack, A. (2010). Introduction to Green Chemistry. (2nd ed.). New York: Taylor and Francis group, CRC Press.
5. Ilango, K. & Valentina, P. (2009). Text Book of Medicinal chemistry. (4th ed.). India: Keerthi Publishers.

Teaching Module

Credit: 3 **Total Hours: 60 (Incl. Seminar & Test)**

Unit	Section	Topics	Lecture Hours	Learning Outcome	Pedagogy	Assessment/ Evaluation
I	**Nanochemistry**					
	1	General principles of nanotechnology. Nanoparticles - definition - size relationship - nanoparticles of metals - semiconductors and oxides.	2	Understand the properties of nanoparticles	Lecture	Evaluation through class test and group discussion Formative assessment I
	2	Synthesis of nanosized compounds - reduction methods and solgel methods. Optical and electrical properties of nanoparticles	2	Explain the synthesis of various nanoparticles	Lecture and Videos	
	3	Nanosystems - introduction - synthesis and purification of fullerenes. Carbonnanotubes - types - preparation - Arc and chemical vapour deposition methods	2	Describe the synthetic methods involved in carbon nanotubes and fullerenes	Lecture and Videos	
	4	Nanoshells - gold and silver nanoshells and its applications. Nanosensors - introduction - nanoscale organization - characterization and optical properties	1	Understand the applications of gold and silver nanoshells	Lecture with PPT	
	5	Nanosensors - introduction - nanoscale organization - characterization and optical properties	3	Explain nanosensors and its properties	Lecture and Seminar	
	6	Nanomedicines - introduction - approach to developing nanomedicines - protocol for nanodrug administration - diagnostic and therapeutic applications.	2	Describe the therapeutic applications of nanoparticles	Lecture and group discussion	

II	**Green Chemistry**					
	1	Green chemistry and sustainable development - principles and applications of green chemistry	2	Understand the principle and applications of green chemistry	Lecture	Evaluation through class test and group discussion Formative assessment II
	2	Atom economy - atom economy vs. yield. Prevention of waste/byproducts. Prevention or minimization of hazardous products.	2	Explain the applications of green chemistry	Lecture and group discussion	
	3	Designing safer chemicals through Sommelet-Hauser - Cope - Wolff - Witting and Bamberger reactions	2	Design and synthesize compounds using green methods	Lecture	
	4	Energy requirement for synthesis. CFC alternatives - green chemistry in organic synthesis. Selection of appropriate solvent and starting material. Use of protecting groups and catalyst.	2	Understand the role of solvent, protecting groups and catalyst in green synthesis	Lecture and seminar	
	5	Methods of greening organic reactions - solvent free reactions and reactions at ambient temperature. Microwave assisted reactions	1	Explain the synthesis of compounds using solvent free and microwave assisted reactions	Lecture and videos	
	6	Sonication assisted reactions - Reformatsky - Ullmann coupling - Wurtz and Bouveault reaction	2	Apply sonication method for synthesis of nanoparticles	Lecture and seminar	
		Reactions in ionic solvents and super critical fluids. Tandem reactions.	1	Explain the reactions in ionic solvents	Lecture and seminar	
III	**Supramolecular Chemistry**					

	1	Supramolecular interactions - discussion of host-guest systems - cation and anion binding host.	2	Understand the host-guest relation in supramolecular chemistry	Lecture with videos	Evaluation through class test and group discussion Formative assessment I
	2	Crown ethers - synthesis - properties and applications. Lariat ethers..	2	Explain the applications of crown ethers	Lecture with ppt and videos	
	3	Podants - properties and 3-dimensional podants. Cryptands - synthesis - properties and applications. Spherands - synthesis - structure and uses.	3	Describe the properties and applications of podants, cryptands and spherands	Lecture and group discussion	
	4	Spherands - synthesis - structure and uses. Supramolecular chemistry of fullerenes and cyclodextrins.	2	Explain supramolecular photochemistry	Lecture and seminar	
	5	Molecular devices - non-linear optical switches and electrophotoswitching, Liquid crystal display. Supramolecular photochemistry.	3	Understand the types and applications of molecular devices	Lecture with videos	
IV	**Medicinal Chemistry**					
	1	Modern drugs for diseases. Anticancer drugs - classification - synthesis and assay of cyclophoshamide - chlorambucil- cisplatin - vinblastine and vincristine.	2	Identify anti-neoplastic agents	Lecture	Evaluation through class test Formative assessment III
	2	Antimalarial drugs - classification - synthesis and assay of chloroquine and primaquine.	2	List out the classification and the assay of antimalarial drugs	Seminar	

	3	Diuretics - Classification, synthesis Assay of Frusemide Assay of benzthiazide.	2	Explain the classification and the assay of diuretics	Seminar	
	4	Anti-inflammatory drug - synthesis and therapeutic action of phenylbutazone and ibuprofen	2	Understand the therapeutic action of anti-inflammatory drugs	Lecture	
	5	Antipyretics and non-narcotic analgesics	2	Know about antipyretics and analgesics	Seminar	
	6	Synthesis and therapeutic action of paracetamol and aspirin	2	Describe the synthesis and therapeutic action of paracetamol and aspirin		
V	**Biophysical Chemistry**					
	1	Thermodynamics in biology and limitations of equilibrium thermodynamics. Irreversible thermodynamics - postulates and methodologies. Irreversible thermodynamics and biological systems	3	Explain thermodynamics in biological systems	Lecture	Evaluation through class test Formative assessment II
	2	Biochemical standard state - ATP. Currency of energy - oxidative phosphorylation.	3	Understand energy flux and oxidative phosphorylation	Lecture and seminar	
	3	Role of singlet oxygen in biology. Reactions in biomolecules - membrate potential and ion pumps.	2	Describe the reactions in biomolecules	Lecture	
	4	Photoacoustic effect and its application in biology.	2	Apply photo acoustic effect in biology	Lecture with ppt	

	5	Biophysical applications of Moss-bauer effect. NMR imaging - applications of spin labeling in membrane research.	2	Explain the biophysical application of Moss-bauer effect NMR imaging	Lecture with videos	

Course Instructor: B.T Delma HOD: G. Leema Rose