

**DEPARTMENT OF CHEMISTRY**  
**HOLY CROSS COLLEGE (AUTONOMOUS)**  
**NAGERCOIL - 4**

**Nationally Re-Accredited with 'A+' Grade**  
**(CGPA 3.35) by NAAC**



**Syllabus – PG**  
**Semester I & IV**  
**(With effect from the academic year 2020-2021)**

**Master of Science  
Programme Educational Objectives (PEOs)**

<b>PEO No.</b>	<b><i>Upon completion of M.Sc. degree programme, the graduates</i></b>
PEO - 1	apply scientific and computational technology to solve social issues and pursue research
PEO - 2	continue to learn and advance their careers in industry both in public and private sectors, government and academia
PEO - 3	imbibe ethical standards, teamwork, leadership, communication skills and professionalism with global competencies addressing chemistry related issues to the society

**Programme Outcomes (POs)**

<b>PO No.</b>	<b><i>Upon completion of M.Sc. degree programme, the graduates will be able to:</i></b>
PO-1	acquire scientific skills and innovative ideas in their own discipline
PO-2	identify, formulate, perform research and contribute to the developmental needs of the society
PO-3	develop a multidisciplinary perspective and contribute to the knowledge capital of the globe
PO-4	emerge as expressive, ethical and responsible citizens with proven expertise

**M.Sc Chemistry**  
**Programme Specific Outcomes (PSOs)**

<b>PSO No.</b>	<b><i>Upon completion of M.Sc Chemistry programme, the graduates will be able to:</i></b>
PSO-1	impart in-depth knowledge about various aspects of chemistry within an environment committed to excellence
PSO-2	develop critical thinking, technical skills and innovative ideas in analysing and solving problems in the field of chemistry
PSO-3	explore and expedite the recent avenues in chemistry research across the globe with professional competency
PSO-4	inculcate positive approach towards environment and ecology from the chemistry perspective
PSO-5	promote entrepreneurial skills and become self-reliant

**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.	<i>Upon completion of this course, the students will be able to:</i>	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  $\text{BeCl}_2$  -  $\text{BCl}_3$  -  $\text{CCl}_4$  and  $\text{SF}_4$ . Ionic character in a covalent bond and concept of multicentre bonding. Pseudo halogens - structure and bonding in  $\text{ClF}_3$  -  $\text{BrF}_3$  -  $\text{BrF}_5$  -  $\text{IF}_5$  -  $\text{IF}_7$  etc. Oxides and oxyacids of halogens. Bonding in noble gas compounds -  $\text{XeCl}_2$  -  $\text{XeF}_4$  -  $\text{XeOF}_4$  and  $\text{XeF}_6$ .

**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-Landé equation - Kapustinski equation and Madelung constant. Representative structures of AB and  $\text{AB}_2$  types of compounds - rock salt - cesium chloride - wurtzite - zinc blende - rutile - fluorite - antiferite - 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  $\text{Re}_2\text{Cl}_8$  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 -  $\text{S}_4\text{N}_4$  and  $(\text{SN})_x$ .

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<sup>th</sup>ed.). New York: Wiley Interscience.
2. Puri B.R., Sharma, L.R. & Kalia, K.C. (2012). Principles of Inorganic Chemistry. (4<sup>th</sup> ed.). India: Milestone publishers.

3. Kittle, C. (2012). Introduction to Solid State Physics. (8<sup>th</sup>ed.). New York: Wiley Eastern Ltd.
4. Puri, R.K. & Babber, V.K. (2001). Solid State Physics. (1<sup>st</sup> ed.). India: S. Chand and Company Ltd.
5. Lee, J.D. (2008). Concise Inorganic Chemistry. (5<sup>th</sup>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. (4<sup>th</sup>ed.). India: Pearson Education.

**Reference Books:**

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

## Module

**Credit: 5**

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

Unit	Section	Topics	Lecture Hours	Learning Outcome	Pedagogy	Assessment/ Evaluation
<b>I</b>	<b>Chemical Bonding</b>					
	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 <sub>2</sub> - BCl <sub>3</sub> - CCl <sub>4</sub> and SF <sub>4</sub>	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 <sub>3</sub> - BrF <sub>3</sub> - BrF <sub>5</sub> - IF <sub>5</sub> - IF <sub>7</sub> etc.	4	Analyse the types of bonding in pseudohalogens	Lecture	
	5	Oxides and oxyacids of halogens. Bonding in noble gas compounds - XeCl <sub>2</sub> XeF <sub>4</sub> - XeOF <sub>4</sub> and XeF <sub>6</sub>	4	Analyse the bonding in noble gas compounds	Lecture with ppt	
<b>II</b>	<b>Chemistry of Solid State I</b>					
	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-Landé equation - Kapustinski equation and Madelung constant	3	Understands lattice energy, Born-Landé equation and Kapustinski equation	Lecture and group discussion	
	4	Representative structures of AB and AB <sub>2</sub> types of compounds - rock salt - cesium chloride - wurtzite - zinc blende - rutile - fluorite - antiferite - cadmium iodide and nickel arsenide	5	Analyse the types of bonding in AB and AB <sub>2</sub> types of compounds	Lecture	
	5	Structure of graphite and diamond. Spinels - normal and inverse types and perovskite structures.	4	Analyse the structure of graphite and diamond, normal and inverse types of spinels	Lecture with ppt	
<b>III</b>	<b>Chemistry of Solid State II</b>					
	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
	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	Formative assessment II
	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 from melt and solution. Hydrothermal and gel methods	3	Understand electron diffraction and apply crystal growth methods.	Lecture	
<b>IV</b>	<b>Boron Compounds and Clusters</b>					
	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
	2	Borazines - boron nitrides - hydroborate ions - STYX numbers - Wade's rules	4	Understand the structure of borazines, STYX numbers and wade rule	Lecture and group discussion	Formative assessment II
	3	Carboranes - types - preparation - properties and structure of nido - closo and arachno	3	Analyse the structure of carboranes	Lecture	
	4	Metallo-carboranes - general study. Metal clusters - chemistry of low molecularity metal clusters	4	Understand the chemistry of low molecularity metal clusters	Lecture	
	5	Structure of $\text{Re}_2\text{Cl}_8$ and multiple metal-metal bonds	3	Analyse the metal-metal bonds in $\text{Re}_2\text{Cl}_8$	Lecture	
<b>V</b>	<b>Inorganic Chain and Cluster Compounds</b>					
	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
	2	P-N compounds - cyclophosphazenes. S-N compounds - $\text{S}_4\text{N}_4$ and $(\text{SN})_x$	4	Understand the structure of P-N and S-N compounds	Lecture	Formative assessment II

	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.	<i>Upon completion of this course, the students will be able to:</i>	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  $\sigma$  and  $\rho$  - applications of Hammett equation. Taft equation and applications. Reactive intermediates - generation - stability and reactivity - carbocations - carbanions - free radicals - carbenes - benzyne and nitrenes.

**Unit II Aliphatic Nucleophilic Substitution (18 Hours)**

Mechanism of aliphatic nucleophilic substitution reaction -  $S_N1$  -  $S_N2$  and  $S_Ni$  mechanisms. Solvent and leaving group effects on aliphatic nucleophilic 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  $\text{BAC}^2$  -  $\text{AAc}^2$  and  $\text{AAI}^1$ ). 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 complex mechanism and benzyne mechanism. Reactions of aryldiazonium salts. Zeigler alkylation - Vicarious Nucleophilic 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 -  $\text{S}_{\text{N}}^1$  and  $\text{S}_{\text{N}}^2$  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<sup>th</sup> ed.). New York: John Wiley and Sons.
2. Sykes, P. (2003). A Guidebook to Mechanism in Organic Chemistry. (6<sup>th</sup> ed.). India: Pearson.

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

**Reference books:**

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



	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 $AAI^1$ ). 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 nucleophilic substitution reactions	Lecture	
<b>III</b>	<b>Aromatic Electrophilic and Nucleophilic Substitutions</b>					
	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
	2	Synthesis of di- and tri-substituted benzenes from benzene or mono-substituted benzenes. Haworth reaction for naphthalene - Scholl reaction - Vilsmeier-Haack formylation	6	Synthesize benzene derivatives using aromatic electrophilic substitution reactions	Lecture	Formative assessment II
	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 aryl diazonium salts. Zeigler alkylation - Vicarious Nucleophilic Substitution (VNS) - Chichibabin and Schiemann reactions	3	Understand the mechanism of aromatic nucleophilic substitution reactions)	Lecture	
<b>IV</b>	<b>Stereochemistry</b>					
	1	Chirality - symmetry elements - asymmetric and dissymmetric chiral molecules	3	Understand the concept of chirality	Lecture	Evaluation through class test and group discussion
	2	Relative and absolute nomenclature. Newman - Sawhorse - Fischer projections - their conversions	4	Convert Newman, Sawhorse and Fischer projections	Lecture and group discussion	Formative assessment II
	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 - open chain - cyclic and dipolar model. Prelog's rule	3	Illustrate asymmetric synthesis using Cram's rule and prelog's rule	Lecture	
<b>V</b>	<b>Conformational Analysis</b>					
	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 - $S_N^1$ and $S_N^2$ 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.	<i>Upon completion of this course, the students will be able to:</i>	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 coefficient. 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. Photosensitization 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. (3<sup>rd</sup>ed.). New York: Harper and Row.
2. Atkins, P. & Atkins, J.P. (2002). Physical Chemistry. (7<sup>th</sup>ed.). USA: Oxford university press
3. Puri, B.R., Sharma, L.R. & Pathania, M.S.(2016). Principles of Physical Chemistry. (47<sup>th</sup>ed.). India: Vishal Publications.
4. G. W. Castellan, (2004).Physical Chemistry. (4<sup>th</sup> ed.). India: Narosa publishing House.

5. Turro, N.J. (1978). *Modern Molecular Photochemistry*. (1<sup>st</sup> ed.). California: Benjamin/Cummings, Menlo Park.
6. Glastone, S.A. (1969). *Text Book of Physical Chemistry*. (2<sup>nd</sup> ed.). London: Macmillan and Co Ltd.
7. Hamann, C.H., Hamnett, A. & Vielstich, W. (2001). *Electrochemistry*. (4<sup>th</sup> 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*. (1<sup>st</sup> ed.). India: Tata McGraw Hill.
2. Silbey, R.J., Alberty, R.A. & Bawendi, M.G. (2015). *Physical Chemistry*. (4<sup>th</sup> ed.). India: Wiley.
3. Barrow, G.M. (2018). *Physical Chemistry*. (6<sup>th</sup> ed.). New York: Tata McGraw Hill.
4. Rohatgi-Mukherjee, K.K. (1997). *Fundamentals of Photochemistry*. (3<sup>rd</sup> ed.). India: New Age International Ltd.
5. Holze, R. (2009). *Experimental Electrochemistry*. New York: John Wiley and Sons.
6. Rieger, P.H. (2010). *Electrochemistry*. (2<sup>nd</sup> ed.). New York: Chapman and Hall.

## Teaching Module

Credit: 5

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

Unit	Section	Topics	Lecture Hours	Learning Outcome	Pedagogy	Assessment/Evaluation
<b>I</b>	<b>Chemical kinetics</b>					
	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	
<b>II</b>	<b>Catalysis</b>					
	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
	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	Formative assessment I

	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	
<b>III</b>	<b>Photochemistry</b>					
	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
	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	Formative assessment I
	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. Photosensitiation 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	

<b>IV Electrochemistry – I</b>						
	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
	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	Formative assessment II
	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	
<b>V Electrochemistry – II</b>						
	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
	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		Formative assessment II

	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.	<i>Upon completion of this course, the students will be able to:</i>	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 - phosphorimetry - 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. Voltammetry - principle - cyclic voltammetry. 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. (6<sup>th</sup> ed.). India: Prentice Hall.
3. Chatwal, G.R. & Anand, S.K. (2002). Instrumental Methods of Chemical Analysis. (5<sup>th</sup> ed.). India: Himalaya Publishing House.

**Reference Books:**

1. Higson, S. (2003). Analytical Chemistry. (1<sup>st</sup> ed.). USA: Oxford University Press.
2. Christian, G.D. (2007). Analytical Chemistry. (6<sup>th</sup> ed.). New York: John Wiley & Sons.
3. Skoog, D.A, Holler, F.J & Crouch, S.R (2007). Principles of Instrumental Analysis. (6<sup>th</sup> ed.). Australia: Thompson Brooks/Cole.
4. Gopalan, R., Subramanian, P.S. & Rengarajan, K. (2003). Elements of Analytical Chemistry. (3<sup>rd</sup> ed.). 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
<b>I</b>	<b>Error Analysis</b>					
	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	
<b>II</b>	<b>Chromatography</b>					
	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
	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	Formative assessment II
	5	Ion exchange chromatography and high performance liquid chromatography	3	Identify the chemical constituents present in a sample using HPLC	Lecture with videos	
<b>III</b>	<b>Colorimetric and Spectrophotometric Analytical Techniques</b>					
	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 test and group discussion
	2	Principle, instrumentation and applications of spectrophotometry and fluorimetry	3	Identify photoactive fluorescent materials	Lecture and seminar	Formative assessment II
	3	Principle, instrumentation and applications of phosphorimetry and flame photometry	3	Understand the principle and applications of phosphorimetry and flame photometry	Seminar and group discussion	
	4	Principle, instrumentation and applications of nephelometry and turbidimetry. Turbidimetric titrations and applications	4	Differentiate nephelometry and turbidimetry.  Understand the applications of turbidimetric titrations	Lecture and seminar	
<b>IV</b>	<b>Thermoanalytical Techniques</b>					
	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	
<b>V</b>	<b>Electroanalytical Techniques</b>					
	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
	2	Coulometric analysis - coulometric titrations and applications. Potentiostatic coulometry	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	Formative assessment I

	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 II**  
**Coordination Chemistry (Core IV)**  
**Subject Code: PG2021**

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

**Objectives:**

- To understand the thermodynamic and stereochemical aspects of complexes
- To learn about the various mechanisms of substitution and electron transfer reactions.

**Course Outcomes (COs)**

CO No.	<i>Upon completion of this course, the students will be able to:</i>	PSO Addressed	Cognitive Level
CO-1	understand the various theories and reaction mechanisms related to coordination compounds	PSO-1	U
CO-2	apply the theories and reaction mechanisms to determine the properties of complexes	PSO-2	A
CO-3	analyze the reaction mechanism of coordination compounds	PSO-2,3	Y
CO-4	evaluate the magnetic and spectral properties of complexes	PSO-2,3	E
CO-5	create novel complexes and catalyst	PSO-4,5	C

**Unit I Stability of Complexes**

**(18 Hours)**

Stability of complexes - factors affecting stability of complexes - thermodynamic aspects of complex formation - stepwise and overall formation constants - stability correlations - statistical factors and chelate effect. Determination of stability constant and composition of the complexes - spectrophotometric method - ion exchange method - polarographic method and continuous variation method (Job's method).

Stereochemical aspects - stereoisomerism in inorganic complexes - isomerism arising out of ligand distribution and ligand conformation. Chirality - nomenclature of chiral complexes - application of ORD and CD in the identification of complexes.

**Unit II Metal Ligand Bonding**

**(18 Hours)**

Crystal field theory - Splitting of d orbitals under various geometries - factors affecting splitting - CFSE - evidences for CFSE (structural and thermodynamic effects) - spectrochemical series - Jorgensen relation - site preferences - Jahn-Teller distortion - dynamic and static Jahn-Teller - Jahn-Teller effect and chelation. Application of CFT - magnetic properties - spectral properties and kinetic properties - limitations of CFT - evidences for M-L overlap.

Molecular Orbital Theory - energy level diagrams concept of weak and strong fields - sigma and pi bonding - octahedral - square planar and tetrahedral complexes. Nephelauxetic effect. Magnetic properties of complexes. Comparison of CFT and MOT of bonding in octahedral complexes.

### **Unit III Electronic Spectra of Complexes (18 Hours)**

Spectroscopic term symbols for  $d^n$  ions - derivation of term symbols and ground state term symbol - Hund's rule - selection rules - breakdown of selection rules - spin orbit coupling - band intensities - weak and strong field limits - correlation diagram - energy level diagrams. Orgel diagram for weak field  $O_h$  and  $T_d$  complexes - splitting of energy level due to Jahn-Teller distortion. Modified Orgel diagram - limitations of Orgel diagram. Tanabe-Sugano (T-S) diagrams - evaluation of  $Dq$  and  $B$  values for  $d^2$ -  $d^8$  complexes charge transfer spectra. Complications in band classification between LF (d-d) and CT bands. Comparison between d-d bands and CT bands - numerical problems. Lanthanides and Actinides- spectral properties.

### **Unit IV Inorganic Reaction Mechanism (18 Hours)**

Electron transfer reactions - Inner sphere (ISET) and outer sphere (OSET) electron transfer processes. Reaction mechanism of coordination compounds - Types of ligand substitution reactions- mechanism- Dissociative mechanism (D) - Associative mechanism (A) interchange mechanism (I) - labile and inert complexes. Substitution reaction in octahedral complexes - general mechanism - general rate law for A - D and I - distinction between D - ID - IA pathways - replacement of coordinated water - mechanism of acid hydrolysis - base hydrolysis - DCB mechanism - direct and indirect evidences in favour of the mechanism. Ligand substitution reactions without cleavage of M-L Bond. Anation Reactions - substitution in square planar complexes - general mechanism - trans effect- influences of entering and leaving groups - application of trans effect - synthesis of isomers of Pt(II) complexes - theories of trans effect and cis-trans isomerisation reaction. Application of substitution reactions in the synthesis of platinum and cobalt complexes.

## Unit V Catalysis

(18 Hours)

General principles of catalysis - basic reactions involved in the catalysis by organometallic compounds. Hydrogenation of olefins (Wilkinson's catalyst) - Hydroformylation of olefins using cobalt or rhodium catalysts (OXO process) - oxidation of olefins to aldehydes and ketones (wacker process) - Monsanto acetic acid synthesis from methanol. Cyclo oligomerisation of acetylene using Ni catalyst (Reppé's catalyst) - synthetic gasoline by using ZSM-5 catalyst (Fisher-Tropsch and mobil process) - polymerization of olefins (Zeigler-Natta Catalyst) - polymer bound catalyst.

### Text Books:

1. Lee, J.D. (2008). Concise Inorganic Chemistry. (5<sup>th</sup> ed.). India: Wiley India.
2. Huheey, J.E., Keiter, E.A., Keiter, R.L. & Medhi, O.K. (2011). Inorganic Chemistry: Principles of Structure and Reactivity. (4<sup>th</sup> ed.). India: Pearson Education.
3. Puri B.R., Sharma, L.R. & Kalia, K.C. (2012). Principles of Inorganic Chemistry. (4<sup>th</sup> ed.). India: Milestone publishers.
4. Malik, W.U., Tuli, G.D. & Madan, R.D. (2012). Selected topics Inorganic Chemistry. (5<sup>th</sup> ed.). New Delhi: S. Chand Company Ltd.

### Reference Books:

1. Cotton, F.A. & Wilkinson, G. (1988). Advance Inorganic Chemistry. (2<sup>nd</sup> ed.). India: Wiley Eastern Private Ltd.
2. Miessler, G.L. (2004). Inorganic Chemistry. (3<sup>rd</sup> ed.), India: Pearson Education.
3. Purcell, K.F. & Kotz, J.C. (2012). Inorganic Chemistry. (2<sup>nd</sup> ed.). India: Cengage Learning India Pvt. Ltd.
4. Kettle, S.F.A, (1996). Coordination Chemistry-Ari Approach. USA: Spectrum Academic publishers Oxford.
5. Mehrotra, R. C. & Singh, A. (2014). Organometallic Chemistry. (2<sup>nd</sup> ed.) New Delhi: New Age International Ltd.
6. Parkins, A. W. & Poller, R. C. (1987). An Introduction to Organometallic Chemistry. Chennai: Oxford University Press.

## Teaching Module

Credit: 6

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

Unit	Section	Topics	Lecture Hours	Learning Outcome	Pedagogy	Assessment/Evaluation
<b>I</b>	<b>Stability of Complexes</b>					
	1	Stability of complexes - factors affecting stability of complexes-thermodynamic aspects of complex formation	3	Understand the factors affecting the stability of complexes	Lecture and group discussion	Evaluation through class test, online quiz and group discussion Formative assessment I
	2	Stepwise and overall formation constants - stability correlations - statistical factors and chelate effect	3	Apply the theories to determine stepwise and overall formation constants	Lecture	
	3	Determination of stability constant and composition of the complexes - spectrophotometric method - ion exchange method - polarographic method and continuous variation method (Job's method)	5	Apply various methods to determine the stability constants of complexes	Lecture and Seminar	
	4	Stereochemical aspects - stereoisomerism in inorganic complexes - isomerism arising out of ligand distribution and ligand conformation	4	Understand the stereoisomerism in inorganic complexes	Lecture and group discussion	
	5	Chirality - nomenclature of chiral complexes - application of ORD and CD in the identification of complexes	3	Apply ORD and CD in the identification of complexes	Lecture and Seminar	
<b>II</b>	<b>Metal Ligand Bonding</b>					
	1	Crystal field theory - Splitting of d orbitals under various geometries - factors affecting splitting - CFSE - evidences for CFSE (structural and thermodynamic effects)	4	Understand crystal field theory and splitting of d-orbitals under various geometries	Lecture with ppt	Evaluation through class test, online quiz and group discussion

	2	Spectrochemical series - Jorgensen relation - site preferences - Jahn-Teller distortion - dynamic and static Jahn-Teller- Jahn-Teller effect and chelation	4	Analyse dynamic and static Jahn-Teller distortion	Lecture and group discussion	Formative assessment I
	3	Application of CFT - magnetic properties - spectral properties and kinetic properties - limitations of CFT- evidences for M-L overlap.	3	Apply CFT to determine the magnetic, spectral and kinetic properties of coordination compounds	Lecture	
	4	Molecular Orbital Theory - energy level diagrams concept of weak and strong fields - sigma and pi bonding - octahedral - square planar and tetrahedral complexes	4	Apply Molecular Orbital Theory to octahedral, square planar and tetrahedral complexes	Lecture with ppt	
	5	Nephelauxetic effect. Magnetic properties of complexes. Comparison of CFT and MOT of bonding in octahedral complexes	3	Analyse CFT and MOT of bonding in octahedral complexes	Lecture	
<b>III</b>	<b>Electronic Spectra of Complexes</b>					
	1	Spectroscopic term symbols for $d^n$ ions - derivation of term symbols and ground state term symbol	3	Understand spectroscopic term symbols	Lecture	Evaluation through class test and group discussion
	2	Hund's rule - selection rules - breakdown of selection rules - spin orbit coupling - band intensities - weak and strong field limits - correlation diagram - energy level diagrams	4	Apply Hund's rule and selection rules to spin orbit coupling	Lecture and group discussion	Formative assessment II
	3	Orgel diagram for weak field $O_h$ and $T_d$ complexes - splitting of energy level due to Jahn-Teller distortion. Modified Orgel diagram - limitations of Orgel diagram	4	Analyse splitting of energy level due to Jahn Teller distortion in weak $O_h$ and $T_d$ complexes using Orgel diagram	Lecture with ppt	
	4	Tanabe-Sugano (T-S) diagrams - evaluation of $Dq$ and $B$ values for $d^2$ - $d^8$ complexes	4	Evaluate $Dq$ and $B$ values for $d^2$ - $d^8$ complexes	Lecture	

	5	Charge transfer spectra. Complications in band classification between LF (d-d) and CT bands. Comparison between d-d bands and CT bands - numerical problems. Lanthanides and Actinides-spectral properties	3	Evaluate the spectral properties of lanthanides and actinides	Lecture	
<b>IV</b>	<b>Inorganic Reaction Mechanism</b>					
	1	Electron transfer reactions - Inner sphere (ISET) and outer sphere (OSET) electron transfer processes	4	Understand the reaction mechanisms of electron transfer processes	Lecture with ppt	Evaluation through class test, online quiz and group discussion
	2	Reaction mechanism of coordination compounds - Types of ligand substitution reactions-mechanism- Dissociative mechanism (D) - Associative mechanism (A) interchange mechanism (I) - labile and inert complexes	3	Analyse the types of substitution mechanisms in coordination compounds	Lecture and group discussion	Formative assessment II
	3	Substitution reaction in octahedral complexes - general mechanism - general rate law for A - D and I - distinction between D – ID - IA pathways - replacement of coordinated water - mechanism of acid hydrolysis - base hydrolysis – DCB mechanism - direct and indirect evidences in favour of the mechanism	5	Understand the mechanism of substitution reaction in octahedral complexes	Lecture	
	4	Ligand substitution reactions without cleavage of M-L Bond. Anation Reactions - substitution in square planar complexes - general mechanism	3	Apply the mechanism of substitution reaction to square planar complexes	Lecture with ppt	

	5	Trans effect- influences of entering and leaving groups - application of trans effect – synthesis of isomers of Pt(II) complexes – theories of trans effect and cis-trans isomerisation reaction. Application of substitution reactions in the synthesis of platinum and cobalt complexes	3	Apply Trans effect and substitution reactions to synthesise Pt and Co complexes	Lecture	
<b>V</b>	<b>Catalysis</b>					
	1	General principles of catalysis - basic reactions involved in the catalysis by organometallic compounds	4	Understand the general principles and basic reactions involved in the catalysis by organometallic compounds	Lecture	Evaluation through class test, group discussion and quiz  Formative assessment II
	2	Hydrogenation of olefins (Wilkinson's catalyst) - Hydro formylation of olefins using cobalt or rhodium catalysts (OXO process)	3	Understand the mechanism of hydrogenation and hydroformylation of olefins using Co or Rh catalysts	Lecture with ppt	
	3	Oxidation of olefins to aldehydes and ketones (wacker process) - Monsanto acetic acid synthesis from methanol	4	Apply Wackers process to the oxidation of olefins	Lecture and group discussion	
	4	Cyclooligomerisation of acetylene using Ni catalyst (Reppe's catalyst) - synthetic gasoline by using ZSM-5 catalyst (Fisher-Tropsch and mobil process)	4	Apply Reppe's catalyst and ZSM-5 catalyst to the cyclooligomerisation of acetylene and synthetic gasoline	Lecture	
	5	Polymerization of olefins (Zeigler-Natta Catalyst) - polymer bound catalyst	3	Create new polymer catalyst	Lecture	

**Semester II**  
**Reaction Mechanism and Molecular Rearrangements (Core V)**  
**Subject Code: PG2022**

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

**Objectives:**

- To understand the mechanism of organic reactions.
- To get an in-depth knowledge on the various types of oxidation and reduction reactions along with their synthetic utility.

**Course Outcomes (COs)**

CO No.	<i>Upon completion of this course, the students will be able to:</i>	PSO Addressed	Cognitive Level
CO-1	understand the mechanisms of organic reactions	PSO-1	U
CO-2	apply the reaction mechanisms to synthesize organic compounds	PSO-2,3	A
CO-3	analyze the type of reactions in organic compounds	PSO-2,3	Y
CO-4	evaluate nucleophilic, electrophilic substitution and elimination reactions in aromatic and aliphatic compounds	PSO-2	E
CO-5	create novel organic compounds	PSO-3,4	C

**Unit I Addition to Carbon-Carbon Multiple Bond**

**(18 Hours)**

Electrophilic addition to carbon-carbon double and triple bonds. Nucleophilic addition to carbon-carbon multiple bonds. Mechanism and stereochemical factors in reactions - addition of hydrogen halides, hypohalous acids and hydroboration. Hydroxylation of olefinic double bonds - OsO<sub>4</sub> - KMnO<sub>4</sub> - Woodward and Prevost hydroxylation. Epoxidation using peracids - Sharpless epoxidation and ozonolysis.

Mechanism and applications of Michael addition - Robinson annulation sequence - Diels' Alder - Knoevenagel - Mannich - Stork-enamine - Grignard - Darzen's and Reformatsky reactions.

**Unit II Addition to Carbon-Oxygen Multiple Bond**

**(18 Hours)**

Nucleophilic addition to carbon-oxygen double bond - Mannich, benzoin - Darzen's glycidic ester - Stobbe and Knoevenagel condensation reactions. Wittig - Wittig-Horner

olefination reactions. Reactions of sulphur and sulphoniumylides. Julia olefination and Peterson alkene synthesis. Asymmetric reduction of carbonyl functions (Corey's procedure).

### **Unit III Elimination Reactions (18 Hours)**

Elimination reactions - E<sub>1</sub> - E<sub>2</sub> - E<sub>1cb</sub> and E<sub>i</sub> elimination. Effect of solvent - substrate and leaving group in elimination reactions. Hofmann - Saytzeff and Bredt's rule. Saytzeff's Vs Hoffman elimination. Stereochemistry of E<sub>2</sub> elimination. Mechanism of pyrolytic elimination - Chugaev and Cope elimination reactions. Hoffmann exhaustive methylation and pyrolysis of esters.

### **Unit IV Molecular Rearrangements and Name Reactions (18 Hours)**

Molecular rearrangements - classification - electrophilic - nucleophilic and free radical rearrangements. Mechanisms of Wagner Meerwin - Tiffenev-Demyanov - Dienone-Phenol - Favorskii - Fries - Baeyer-Villager - Stevens - Neber - Sommelet-Hauser - Baker-Venkatraman - von-Richter - Ullmann - Pummerer and di- $\pi$  methane rearrangements.

Name reactions - Dieckmann cyclization - Hofmann-Löffler Freytag reaction - Mitsunobu reaction - Shapiro reaction - Eschenmoser-Tanabe and Ramburg-Backlund reactions.

### **Unit V Oxidation and Reduction Reactions (18 Hours)**

Oxidation with Cr - PCC - PDC and Jones. Oxidation with Mn - MnO<sub>2</sub> and BaMnO<sub>4</sub> reagents. Oxidation with LTA - DDQ and SeO<sub>2</sub>. Oxidation using DMSO - DCC - acetic anhydride and oxaloyl chloride. Oxidation using IBX and Dess-Martin Periodinane (DMP) reagent.

Reduction with NaBH<sub>4</sub> - NaCNBH<sub>3</sub> - Zn(BH<sub>4</sub>)<sub>2</sub> - LiAlH<sub>4</sub> - Li(BuO)<sub>3</sub>AlH - DIBAL-H - Red-Al - Et<sub>3</sub>SiH and Bu<sub>3</sub>SnH. Reduction using selectrides - Birch reduction.

#### **Text Books:**

1. March, J. (2006). Advanced organic chemistry. (4<sup>th</sup> ed.). New York: John Wiley and Sons.
2. Ahluwalia, V.K. & Parshar, R.K. (2005). Organic Reaction Mechanism. (2<sup>nd</sup> ed.). India: Narosa, publishing House.
3. Norman, R.O.C. & Coxon, J.M. (1993). Principles of Organic Synthesis, (3<sup>rd</sup>ed.). New York: CRC press, Taylor and Francis Group.
4. Morrison, R.T. & Boyd, R.N. (1997). Organic Chemistry. (6<sup>th</sup> ed.). New Jersey: Prentice Hall.
5. Jain, M.K. & Sharma, S.C. (2014). Modern Principles of Organic Chemistry. India: Vishal publication.

6. Chatwal, G.R. (2016). Reaction Mechanism and Reagents in Organic Chemistry. (5th ed.). India: Himalaya Publishing House.

**Reference books:**

1. Carey, F. & Sundberg, R.J. (2007). Advanced Organic Chemistry-Part A and B. (5<sup>th</sup>ed.). USA: Springer.
2. Smith, M.B. & March, J. (2001). Advanced Organic Chemistry. (5<sup>th</sup>ed.). New York: John Wiley and Sons.
3. Bansal, R.K. (2005). Reaction Mechanism in Organic Chemistry. (3<sup>rd</sup> ed.). Tata McGraw Hill.
4. Clayden, J. Greeves, N & Warren, S. (2012). Organic Chemistry. (2<sup>nd</sup> Ed.). Oxford University Press.
5. Tewari, K.S., Vishnoi, N.K. & Mehrotra, S.N. (2002). A text book of organic chemistry. India: Vikas publishing House Ltd.
6. Kalsi, P.S. (1996). Organic Reactions and Mechanism. (1<sup>st</sup> ed.). India: New Age International Ltd.

## Teaching Module

**Credit: 5**

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

Unit	Section	Topics	Lecture Hours	Learning Outcome	Pedagogy	Assessment/Evaluation
<b>I</b>	<b>Unit I Addition to Carbon-Carbon Multiple Bond</b>					
	1	Electrophilic addition to carbon-carbon double and triple bonds. Nucleophilic addition to carbon-carbon multiple bonds	4	Understand electrophilic addition and nucleophilic addition to carbon-carbon multiple bonds	Lecture	Evaluation through online quiz Formative assessment I
	2	Mechanism and stereochemical factors in reactions - addition of hydrogen halides, hypohalous acids and hydroboration	4	Understand the mechanisms stereochemical factors in organic reactions	Lecture and Group discussion	
	3	Hydroxylation of olefinic double bonds - OsO <sub>4</sub> - KMnO <sub>4</sub> - Woodward and Prevost hydroxylation	3	Synthesize the organic compounds using hydroxylating agents	Lecture and Seminar	
	4	Epoxidation using peracids - Sharpless epoxidation and ozonolysis	3	Understand the Epoxidation reactions	Lecture	
	5	Mechanism and applications of Michael addition - Robinson annulation sequence - Diels' Alder - Knoevenagal - Mannich - Stork-enamine - Grignard - Darzen's and Reformatsky reactions	4	Apply the name reactions to synthesize organic compounds	Lecture	
<b>II</b>	<b>Addition to Carbon-Oxygen Multiple Bond</b>					
	1	Nucleophilic addition to carbon-oxygen double bond - Mannich, benzoin - Darzen's glycidic ester - Stobbe and Knoevenagal condensation reactions	5	Understand the nucleophilic addition to carbon-oxygen double bond	Lecture with models	Evaluation through class test, online quiz and group discussion

	2	Wittig - Wittig-Horner olefination reactions	3	Infer the mechanism of Wittig - Wittig-Horner olefination reactions	Lecture	Formative assessment I
	3	Reactions of sulphur and sulphoniumylides. Julia olefination and Peterson alkene synthesis	5	Know the reactions of sulphur and sulphoniumylides	Lecture and group discussion	
	4	Asymmetric reduction of carbonyl functions (Corey's procedure)	5	Illustrate asymmetric reduction of carbonyl functions	Lecture	
<b>III</b>	<b>Aromatic Electrophilic and Nucleophilic Substitutions</b>					
	1	Elimination reactions - E <sub>1</sub> - E <sub>2</sub> - E <sub>1cb</sub> and E <sub>i</sub> elimination. Effect of solvent - substrate and leaving group in elimination reactions	5	Understand the concept of elimination reaction	Lecture	Evaluation through class test, online quiz and group discussion Formative assessment II
	2	Hofmann - Saytzeff and Bredt's rule. Saytzeff's Vs Hoffman elimination	4	Compare saytzeff's Vs Hoffman elimination	Lecture	
	3	Stereochemistry of E <sub>2</sub> elimination. Mechanism of pyrolytic elimination - Chugaev and Cope elimination reactions	4	Infer the mechanism of pyrolytic elimination reaction.	Lecture and group discussion	
	4	Hoffmann exhaustive methylation and pyrolysis of esters	5	Understand the concept of Hoffmann exhaustive methylation	Lecture	
<b>IV</b>	<b>Molecular Rearrangements and Name Reactions</b>					
	1	Molecular rearrangements - classification - electrophilic - nucleophilic and free radical rearrangements	4	Classify molecular rearrangements	Lecture	Evaluation through class test and group discussion
	2	Mechanisms of Wagner Meerwin - Tiffenev-Demyanov - Dienone-Phenol - Favorskii - Fries - Baeyer-Villager - Stevens and Neber rearrangements	5	Infer the mechanism of molecular rearrangements	Lecture and group discussion	Formative assessment II

	3	Sommelet-Hauser - Baker-Venkatraman - von-Richter - Ullmann - Pummerer and di- $\pi$ methane rearrangements	5	Infer the mechanism of rearrangements	Lecture	
	4	Name reactions - Dieckmann cyclization - Hofmann-Löffler Freytag reaction - Mitsunobu reaction - Shapiro reaction - Eschenmoser- Tanabe and Ramburg- Backlund reactions	4	Understand the mechanism of name reactions	Lecture	
<b>V</b>	<b>Oxidation and Reduction Reactions</b>					
	1	Oxidation with Cr - PCC - PDC and Jones. Oxidation with Mn - MnO <sub>2</sub> and BaMnO <sub>4</sub> reagents	5	Understand and apply oxidising agents in organic synthesis	Lecture with videos	Evaluation through class test, group discussion and quiz
	2	Oxidation with LTA - DDQ and SeO <sub>2</sub>	4	Understand the application of LTA - DDQ and SeO <sub>2</sub>	Lecture	Formative assessment I
	3	Oxidation using DMSO - DCC - acetic anhydride and oxaloyl chloride	4	Understand the application of DMSO - DCC - acetic anhydride and oxaloyl chloride	Lecture	Evaluation through class test, group discussion and quiz
	4	Oxidation using IBX and Dess-Martin Periodinane (DMP) reagent	5	Apply oxidising agents in organic synthesis	Lecture and Group Discussion	Formative assessment II

Course Instructor: Dr. Y. Christabel Shaji

HOD: Dr. G. Leema Rose

**Semester II**  
**Quantum Chemistry and Spectroscopy (Core VI)**  
**Subject Code: PG2023**

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

**Objectives:**

- To learn the principle of quantum mechanics of simple systems.
- To understand the principle, instrumentation, interpretation and applications of various spectroscopic and analytical techniques.

**Course Outcomes (COs)**

CO No.	<i>Upon completion of this course, the students will be able to:</i>	PSO Addressed	Cognitive Level
CO-1	understand the concepts of quantum chemistry, spectroscopy and surface chemistry	PSO-1	U
CO-2	apply the principles of quantum mechanics to simple systems, spectroscopy to characterize compounds and surface chemistry to determine the surface area of surface films and liquids	PSO-2	A
CO-3	analyse molecules using quantum mechanics and spectroscopic techniques	PSO-2,3	Y
CO-4	evaluate eigen values, bond angles, electron density and surface area of simple molecules	PSO-2,3	E

**Unit I Quantum Chemistry-I**

**(18 Hours)**

Black body radiation - Planck's quantum theory - wave particle duality - uncertainty principle. Operators - linear - commutation - Hermitian and Hamiltonian operators. Eigen functions and eigen values. Postulates of quantum mechanics. Derivation of Schrodinger's time-independent wave equation - application - one dimensional box - particle in a three dimensional box - harmonic oscillator and hydrogen atom.

**Unit II Quantum Chemistry - II**

**(18 Hours)**

Born-Oppenheimer approximation - Hydrogen molecule ion. LCAO-MO and VB treatments of the hydrogen molecule. Anti-symmetry and Pauli's exclusion principle. Slater determinant wave function - term symbols and spectroscopic states - Russell Saunders coupling. The variation theorem and perturbation theory - applications of variation method and perturbation theory to the helium atom. Hybridization-determination of bond angles of sp

- $sp^2$  and  $sp^3$  hybridizations. Huckel pi electron (HMO) theory and its applications to ethylene
- butadiene and benzene.

### **Unit III Molecular Spectroscopy - I (18 Hours)**

Electronic Spectroscopy - principle - laws of light absorption - Born-Oppenheimer approximation. Franck-Condon principle - wave-mechanical formulation - dissociation energy - dissociation products and predissociation. Microwave spectroscopy - rotation of molecules - rotational spectra of diatomic molecules - intensity of spectral lines - effects of isotopic substitution - non-rigid rotator. Rotational spectra of polyatomic molecules - chemical analysis by microwave spectroscopy.

### **Unit IV Molecular Spectroscopy - II (18 Hours)**

ESR - theory - hyperfine interactions in ESR - double resonance (ENDOR, ELDOR) - Mc Connell's relation - verification of the relation for cyclic polyene radical - calculation of electron density and experimental techniques.

Laser Raman Spectroscopy - Einstein treatment of absorption and emission phenomena- Einstein's coefficients - probability of induced emission - applications to lasers- conditions for laser action - properties - types of lasers - advantages of lasers in Raman spectroscopy and experimental techniques.

### **Unit V Surface chemistry (18 Hours)**

Electrical aspects of surface chemistry - electrical double layer - zeta potential. BET and Gibbs adsorption isotherms - derivation – applications - determination of surface area (BET equation) - surface films and liquids. Membrane equilibria and dialysis.

Surface active reagents - classification of surface agents - micellization - hydrophilic interactions - critical micellar concentration - factors affecting the CMC of surfaces. Transition state theory of surface reactions - rates of chemisorptions - Hertz-Knudson equation.

#### **Text Books:**

1. Chandra. A.K. (2001). Introductory Quantum Chemistry. (4<sup>th</sup>ed.). India: Tata McGraw-Hill.
2. Prasad, R.K. (2014). Quantum Chemistry. (4<sup>th</sup> ed.). New Delhi: New Age International Publishers.
3. Atkins, P. & Atkins, J.P. (2002). Physical Chemistry. (7<sup>th</sup>ed.).USA: Oxford university press.
4. BanWell, C.N. & Mccash, E.M. (1997). Fundamentals of Molecular Spectroscopy. New Delhi: Tata Mc Grow Hill.

**Reference Books:**

1. Mcquarrie, D.A. (2008). Quantum Chemistry. Sausalito: University Science Books.
2. Puri, B.R., Sharma, L.R. & Pathania, M.S. (2016). Principles of Physical Chemistry (47<sup>th</sup>ed.). India: Vishal Publications.
3. Aruldas, G. (2011). Molecular Structure and Spectroscopy. (2<sup>nd</sup> ed.), India: PHI Learning Pvt. Ltd.

## Teaching Module

Credit: 5

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

Unit	Section	Topics	Lecture Hours	Learning Outcome	Pedagogy	Assessment/Evaluation
<b>I</b>	<b>Quantum Chemistry-I</b>					
	1	Black body radiation- Planck's quantum theory- wave particle duality- uncertainty principle	4	Explain the principle of black body radiation	Lecture	Evaluation through class test and quiz  Formative assessment I
	2	Operators-linear - commutation - Hermitian and Hamiltonian operators	3	Gain knowledge about operators	Lecture	
	3	Eigen functions and eigen values. Postulates of quantum mechanics	3	Understand the postulates of quantum mechanics	Lecture and Seminar	
	4	Derivation of Schrodinger's time-independent wave equation	3	Derive Schrodinger's wave equation	Lecture	
	5	Application - one dimensional box - particle in a three dimensional box - harmonic oscillator and hydrogen atom	5	Apply Schrodinger's wave equation to hydrogen atom	Lecture	
<b>II</b>	<b>Quantum Chemistry - II</b>					
	1	Born-Oppenheimer approximation-Hydrogen molecule ion. LCAO-MO and VB treatments of the hydrogen molecule	4	Compare LCAO-MO and VB treatments of the hydrogen molecule	Lecture	Evaluation through class test, group discussion and online quiz  Formative assessment I
	2	Anti-symmetry and Pauli's exclusion principle. Slater detrimental wave function	4	Apply Slater determinant to construct anti-symmetric wave function	Lecture and group discussion	
	3	Term symbols and spectroscopic states-Russell Saunders coupling	4	Gain knowledge about term symbols	Lecture	

	4	The variation theorem and perturbation theory - applications of variation method and perturbation theory to the helium atom.	3	Apply variation method and perturbation theory to the helium atom	Lecture	
	5	Hybridization-determination of bond angles of sp - sp <sup>2</sup> and sp <sup>3</sup> hybridizations. Huckel pi electron (HMO) theory and its applications to ethylene - butadiene and benzene	3	Determine hybridization and bond angles	Lecture	
<b>III</b>	<b>Molecular Spectroscopy – I</b>					
	1	Electronic Spectroscopy - principle - laws of light absorption - Born-Oppenheimer approximation	4	Understand the principle of electronic spectroscopy	Lecture	Evaluation through class test and group discussion
	2	Franck-Condon principle - wave-mechanical formulation - dissociation energy - dissociation products and predissociation	4	Apply Franck-Condon principle to dissociation.	Lecture and seminar	Formative assessment II
	3	Microwave spectroscopy - rotation of molecules - rotational spectra of diatomic molecules	3	Gain knowledge about microwave spectroscopy	Lecture and group discussion	
	4	Intensity of spectral lines - effects of isotopic substitution - non-rigid rotator	4	Know about the effects of isotopic substitution.	Lecture	
	5	Rotational spectra of polyatomic molecules - chemical analysis by microwave spectroscopy	3	Apply the principle of microwave spectroscopy in chemical analysis	Lecture and seminar	
<b>IV</b>	<b>Molecular Spectroscopy – II</b>					
	1	ESR - theory - hyperfine interactions in ESR - double resonance (ENDOR, ELDOR)	4	Know about hyperfine interactions in ESR	Lecture	Evaluation through class test, group discussion and online quiz
	2	Mc Connell's relation - verification of the relation for cyclic polyene radical	3	Verify Mc Connell's relation for cyclic polyene radical	Lecture and group discussion	Formative

	3	Calculation of electron density and experimental techniques in solution	3	Calculate electron density	Lecture	assessment II
	4	Laser Raman Spectroscopy - Einstein treatment of absorption and emission phenomena- Einstein's coefficients - probability of induced emission - applications to lasers	4	Derive Einstein coefficient	Lecture	
	5	Conditions for laser action - properties types of lasers - advantages of lasers in Raman spectroscopy and experimental techniques	4	Understand different types of lasers	Lecture	
<b>V</b>	<b>Surface chemistry</b>					
	1	Electrical aspects of surface chemistry - electrical double layer - zeta potential.	4	Understand the concepts of surface chemistry	Lecture	Evaluation through class test, group discussion and quiz  Formative assessment II
	2	BET and Gibbs adsorption isotherms - derivation	3	Compare BET and Gibbs adsorption isotherms		
	3	Applications - determination of surface area (BET equation) - surface films and liquids. Membrane equilibria and dialysis	4	Apply BET equation in determination of surface area	Lecture	
	4	Surface active reagents - classification of surface agents - micellization - hydrophilic interactions - critical micellar concentration - factors affecting the CMC of surfaces	4	Gain knowledge about CMC	Lecture with videos	
	5	Transition state theory of surface reactions - rates of chemisorptions - Hertz-Knudson equation	3	Derive Hertz-Knudson equation	Lecture	

Course Instructor: Dr. M. Shirley Treasa

HOD: Dr. G. Leema Rose

**Semester II**  
**Research Methodology (Elective II)**  
**Subject Code: PG2024**

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

**Objectives**

- To understand the importance of research for future development.
- To get information about computation techniques in research

**Course Outcomes (COs)**

CO No.	<i>Upon completion of this course, the students will be able to:</i>	PSO Addressed	Cognitive Level
CO-1	understand the sources of literature survey and analytical techniques for documentation of research and cheminformatics for molecular representation	PSO-1	U
CO-2	apply the features of literature survey in research and analytical techniques to characterize compounds	PSO-2,3	A
CO-3	analyse the sources of research information and chemical compounds	PSO-2,3	Y
CO-4	evaluate the results using analytical techniques	PSO-2,3	E
CO-5	create a journal article	PSO-3	C

**Unit I Literature Survey (12 Hours)**

Source of chemical information - primary - secondary and tertiary sources. Literature survey - indexes and abstracts in science and technology. Applied science and technology index - chemical abstracts - chemical titles - current chemical reactions - current contents and science citation index. Classical and comprehensive reference works in chemistry- synthetic methods and techniques - treatises - reviews - patents and monographs.

**Unit II Chemical Abstracts (12 Hours)**

Current awareness searching - CA weekly issues and CA issue indexes. Retrospective searching - CA volume indexes- general subject index - chemical substance index- formula index - index of ring systems - author index and patent index. CA collective indexes - collective index (CI) and decennial index (DI). Access points for searching CA indexes- index guide - general subject - terms - chemical substance names - molecular formulas - ring

systems - author names - patent numbers. Locating the reference - finding the abstract - finding the original document chemical abstract and service source index.

### **Unit III Research Problem and Scientific Writing (12 Hours)**

Identification of research problem - assessing the status of the problem - guidance from the supervisor - actual investigation and analysis of experimental results - conclusions. Scientific writing - research reports - thesis - journal articles and books. Steps to publishing a scientific article in a journal. Types of publications - communications - articles and reviews. Documenting - Abstracts indicative - descriptive abstracts - informative abstract - footnotes - end notes - referencing styles - bibliography - journal abbreviations - abbreviation used in scientific writing.

### **Unit IV Instrumental Analysis (12 Hours)**

Principle - instrumentation and applications - AFM - SEM - STM - TEM and XRD. Determination of surface morphology and particle size. Sample preparations and applications of UV - IR - NMR and mass spectroscopy.

### **Unit V Cheminformatics (12 Hours)**

Cheminformatics - history and applications. Representing molecules - connection tables and line notation - Inchi - SMILES and WLN canonicalization. Line notation versus connection tables. Query languages - SMARTS. Molecular similarity. 2D topology and 3D configuration. Chemistry softwares - Chemdraw - writing chemical equations and schemes - editing - transporting picture to word and image document. Origin -importing and exporting data - scientific graphing and data analysis - curve fitting and peak analysis - transporting graph to tag image file format.

### **Text Books:**

1. Berg, B.L. (2009). Qualitative Research Methods for the Social Sciences. (7<sup>th</sup> ed.). India: Pearson Education.
2. Patton, M.Q. (2002). Qualitative research and evaluation methods. (3<sup>rd</sup> ed.). India: Sage Publications.
3. Alexis, L. & Mathews, L. (1999). Fundamentals of Information Technology. Chennai: Leon Vikas.
4. Mohan, J. (2001). Organic Spectroscopy Principles and Applications. India: Narosa publishing house.
5. Kemp, W. (1994). Organic Spectroscopy. (3<sup>rd</sup> ed.). New York: Macmillan.
6. Polanski, J. (2009). Cheminformatics. Poland: Elsevier Publications.

## Reference Books:

1. Silverman, D. (2011). Qualitative Research: Issues of Theory, Method and Practice. (3<sup>rd</sup> ed.). India: Sage Publications.
2. Marczyk, G. Dematteo, D. & Festinger, D. (2005). Essential of Research Design and Methodology. New York: John Wiley and Sons.
3. Silverstein, S.M., Bassler, G.V. & Morrill, T.C. (2004). Spectrometric identification of organic compounds. (6<sup>th</sup> ed.). New York: Wiley.
4. Dyer, J.R. (1987). Applications of Absorption spectroscopy of Organic Compounds. New York: Prentice Hall.
5. Dani, V.R. (1995). Organic spectroscopy. India: Tata McGraw Hill.
6. Gasteiger, J. & Engel, T. (2003). Chemoinformatics. New York: John Wiley and Sons.

## Teaching Module

Credit: 3

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

Unit	Section	Topics	Lecture Hours	Learning Outcome	Pedagogy	Assessment/Evaluation
<b>I</b>	<b>Literature Survey</b>					
	1	Source of chemical information - primary - secondary and tertiary sources	2	Understand and identify the sources of information's	Lecture and group discussion	Evaluation through periodic test, class test and group discussion
	2	Literature survey - indexes and abstracts in science and technology	2	Apply the features of literature survey in research	Lecture and seminar	
	3	Applied science and technology index - chemical abstracts - chemical titles - current chemical reactions - current contents and science citation index	3	Understand the terms chemical abstracts and citation index	Lecture with group discussion and seminar	Formative assessment I
	4	Classical and comprehensive reference works in chemistry-synthetic methods and techniques	2	Understand classical and comprehensive reference works in chemistry	Lecture and seminar	
	5	Treatises - reviews - patents and monographs	3	Understand patents and monographs	Lecture with videos	
<b>II</b>	<b>Chemical Abstracts</b>					
	1	Current awareness searching - CA weekly issues and CA issue indexes. Retrospective searching - CA volume indexes and general subject index	2	Understand the importance of current awareness and retrospective searching in research	Lecture and seminar	Evaluation through periodic test, class test, online quiz and class assignment
	2	Chemical substance index- formula index - index of ring systems - author index and patent index	2	Analyzevarious indexes in chemical abstracts	Lecture and seminar	
	3	CA collective indexes collective index (CI) and decennial index (DI)	2	Differentiate CI and DI	Lecture and seminar	Formative assessment II

	4	Access points for searching CA indexes- index guide - general subject - terms - chemical substance names - molecular formulas - ring systems - author names and patent numbers	3	Know how to search CA indexes	Lecture and seminar	
	5	Locating the reference - finding the abstract - finding the original document chemical abstract and service source index	3	Pinpoint chemical abstract and service source index	Lecture and seminar	
<b>III</b>	<b>Research Problem and Scientific Writing</b>					
	1	Identification of research problem - assessing the status of the problem, guidance from the supervisor, actual investigation and analysis of experimental results and conclusions	3	Identify and solve research problems	Lecture with videos and group discussion	Evaluation through periodic test, class test and group discussion Formative assessment II
	2	Scientific writing - research reports, thesis, journal articles and books	2	Know the art of scientific writing in research	Lecture with ppt and seminar	
	3	Steps to publishing a scientific article in a journal. Types of publications - communications, articles and reviews	3	Create journal articles, communication and reviews	Lecture and group discussion	
	4	Documenting - Abstracts indicative - descriptive abstracts and informative abstracts	2	Analyze descriptive and informative abstracts	Lecture and seminar	
	5	Documenting - footnotes, end notes, referencing styles, bibliography, journal abbreviations, abbreviation used in scientific writing	2	Identify the format for documentation of research	Lecture with ppt	

<b>IV Instrumental Analysis</b>						
	1	Principle, instrumentation and applications of AFM - SEM and STM	4	Understand the principle and applications of AFM, SEM and STM	Lecture with videos	Evaluation through periodic test, class test, online quiz and group discussion  Formative assessment I
	2	Principle, instrumentation and applications of TEM and XRD	2	Understand the principle and applications of TEM and XRD	Lecture with videos	
	3	Determination of surface morphology and particle size	2	Determine the surface morphology and particle size of compounds	Seminar and group discussion	Evaluation through periodic test, class test, online quiz and class assignment  Formative assessment II
	4	Sample preparations and applications of UV and IR spectroscopy	2	Apply UV and IR spectroscopy for structural elucidation of compounds	Lecture with ppt and videos	
	5	Sample preparations and applications of NMR and mass spectroscopy	5	Apply NMR and mass spectroscopy for structural elucidation of compounds	Seminar	
<b>V Cheminformatics</b>						
	1	Cheminformatics - history and applications. Representing molecules - line notation - Inchi - SMILES and WLN canonicalization	2	Understand cheminformatics and line notations	Lecture with ppt	Evaluation through periodic test, class test and online quiz and problem solving  Formative assessment I
	2	Connection table and line notation versus connection table. SMARTS	2	Relate line notation and connection tables. Know about the query language SMARTS	Lecture with ppt	
	3	Molecular similarity - 2D topology and 3D configuration	2	Understand the importance of molecular similarity, 2D topology and 3D configuration in cheminformatics	Lecture	

	4	Chemistry softwares - Chemdraw - writing chemical equations and schemes - editing - transporting picture to word and image document	3	Apply Chemdraw software to draw chemical equations and schemes	Lecture with demo using Chemdraw software	
	5	Origin -importing and exporting data - scientific graphing and data analysis - curve fitting and peak analysis - transporting graph to tag image file format	3	Apply Origin software to sketch graph and data analysis	Lecture with demo using Origin software	

Course Instructor: Dr. Sheeba Daniel

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 spectroscopic techniques.
- To elucidate the structure of simple organic compounds using spectral data.

**Course Outcomes (COs)**

CO	<i>Upon completion of this course, the students will be able to:</i>	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  $\lambda_{\max}$  values of conjugated dienes -  $\alpha,\beta$ -unsaturated carbonyl compounds and aromatic compounds. Fieser-Khun rule. Effect of solvent polarity on  $\lambda_{\max}$ .

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)**

**<sup>1</sup>H NMR Spectroscopy**

<sup>1</sup>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<sub>2</sub> and A<sub>2</sub>B<sub>3</sub>. Simplification of complex spectra - chemical exchange, double resonance and NMR shift reagents. Temperature dependent NMR.

### Unit III

(18 Hours)

#### <sup>13</sup>C, <sup>19</sup>F and <sup>31</sup>P NMR Spectroscopy

<sup>13</sup>C NMR spectroscopy: principle - comparison of <sup>13</sup>C NMR and <sup>1</sup>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 - <sup>1</sup>H-<sup>1</sup>H and <sup>13</sup>C-<sup>13</sup>C connectivity. HETCORR - <sup>1</sup>H-<sup>13</sup>C connectivity and MRI.

<sup>19</sup>F NMR spectroscopy: precessional frequency and heteronuclear coupling. Identification of organofluoro compounds CF<sub>3</sub>CO<sub>2</sub>Et and CF<sub>3</sub>CH<sub>2</sub>OH.

<sup>31</sup>P NMR spectroscopy: chemical shift - heteronuclear coupling and P-P bond in NMR. Identification of organophosphorous compounds (Me)<sub>3</sub>P - (EtO)<sub>3</sub>P=O and Ph<sub>3</sub>P.

### 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. (3<sup>rd</sup> ed.). New York: Macmillan.
3. Kalsi, P.S. (2004). Spectroscopy of Organic Compounds. (6<sup>th</sup> ed.). India: New Age International Ltd.
4. Silverstein, S.M., Bassler, G.V. & Morrill, T.C. (2004). Spectrometric identification of organic compounds. (6<sup>th</sup> ed.). New York: Wiley.

### Reference Books

1. Dyer, J.R. (1987). Applications of Absorption spectroscopy of Organic Compounds. New York: Prentice 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. (4<sup>th</sup> ed.). USA: Cengage Learning.
4. Sharma, Y.R. (2013). Elementary Organic Spectroscopy. (5<sup>th</sup> 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
<b>I</b>	<b>UV-Visible and IR spectroscopy</b>					
	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 (quizz), slip test, group discussion and problem solving  Formative assessment I
	2	Woodward-Fieser rules to calculate $\lambda_{\max}$ values of conjugated dienes - $\alpha,\beta$ -unsaturated carbonyl compounds and aromatic compounds. Fieser-Khun rule.	6	Calculate the $\lambda_{\max}$ values of organic compounds	Group discussion and problem solving	
	3	Effect of solvent polarity on $\lambda_{\max}$ .	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	
<b>II</b>	<b><math>^1\text{H}</math> NMR Spectroscopy</b>					
	1	$^1\text{H}$ 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 discussion and 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 and through space coupling. Karplus equation. Coupling constant - AB, AB <sub>2</sub> and A <sub>2</sub> B <sub>3</sub> .	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	
<b>III</b>	<b><sup>13</sup>C, <sup>19</sup>F and <sup>31</sup>P NMR Spectroscopy</b>					
	1	<sup>13</sup> C NMR spectroscopy: principle - comparison of <sup>13</sup> C NMR and <sup>1</sup> H NMR. Chemical shift - factors affecting chemical shift.	3	Understand the concepts of <sup>13</sup> C NMR spectroscopy	Lecture with ppt	Evaluation through class test, quiz and group discussion
	2	Homonuclear and heteronuclear coupling. Broad band decoupling and OFF - resonance decoupling.	3	Analyze the types of coupling and decoupling	Lecture with ppt	Formative assessment II
	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 - <sup>1</sup> H- <sup>1</sup> H and <sup>13</sup> C- <sup>13</sup> C connectivity. HETCORR - <sup>1</sup> H- <sup>13</sup> C connectivity and MRI.	3	Interpret COSY- HOMCOR and HETCOR	Lecture	
	5	<sup>19</sup> F NMR spectroscopy: precessional frequency and heteronuclear coupling. Identification of organofluoro compounds CF <sub>3</sub> CO <sub>2</sub> Et and CF <sub>3</sub> CH <sub>2</sub> OH.	3	Identify organofluoro compounds using <sup>19</sup> F NMR spectroscopy	Lecture with ppt	

	6	<sup>31</sup> P NMR spectroscopy: chemical shift - heteronuclear coupling and P-P bond in NMR. Identification of organophosphorous compounds (Me) <sub>3</sub> P - (EtO) <sub>3</sub> P=O and Ph <sub>3</sub> P.	3	Identification of organophosphorous compounds using <sup>31</sup> P NMR spectroscopy	Lecture with ppt	
<b>IV</b>	<b>Mass Spectrometry</b>					
	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
	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	Formative assessment I
	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	
<b>V</b>	<b>Structural Elucidation using Analytical and Spectral Data</b>					
	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
	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	<i>Upon completion of this course, the students will be able to:</i>	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. Determination of  $\pi$ - 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. (1<sup>st</sup> ed.). Delhi: Shohanlal and Company.
6. Atkins, P. & Atkins, J.P. (2002). Physical Chemistry. (7<sup>th</sup> ed.). USA: Oxford university press.
7. Puri, B.R., Sharma, L.R. & Pathania, M.S. (2016). Principles of Physical Chemistry (47<sup>th</sup> 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. (3<sup>rd</sup> 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. (2<sup>nd</sup> 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
<b>I</b>	<b>Thermodynamics and Non-Ideal Systems</b>					
	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	
<b>II</b>	<b>Irreversible Thermodynamics</b>					
	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	
<b>III</b>	<b>Statistical Thermodynamics</b>					
	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	
<b>IV</b>	<b>Group Theory I</b>					
	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
	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	Formative assessment II
	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	
<b>V</b>	<b>Group Theory – II</b>					
	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	Determination of $\pi$ -electron energy in ethylene. HMO theory - HMO calculations	3	Apply group theory and HMO theory to determine $\pi$ -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	<i>Upon completion of this course, the students will be able to:</i>	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 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 - Wittig 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 cyclophosphamide - 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 - membrane potential and ion pumps. Photoacoustic effect and its application in biology. Biophysical applications of Mossbauer effect. NMR imaging - applications of spin labeling in membrane research.

### **Text Books**

1. Klabunde, K.J. & Richards, R.M. (2009). (2<sup>nd</sup> 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<sup>th</sup> 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. (2<sup>nd</sup> ed.). New York: Taylor and Francis group, CRC Press.
5. Ilango, K. & Valentina, P. (2009). Text Book of Medicinal chemistry. (4<sup>th</sup> ed.). India: Keerthi Publishers.

## Teaching Module

**Credit: 3**

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

Unit	Section	Topics	Lecture Hours	Learning Outcome	Pedagogy	Assessment/ Evaluation
<b>I</b>	<b>Nanochemistry</b>					
	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
	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	Formative assessment II
	3	Designing safer chemicals through Sommelet-Hauser - Cope - Wolff - Wittig 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	<b>Supramolecular Chemistry</b>					

	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
	2	Crown ethers - synthesis - properties and applications. Lariat ethers..	2	Explain the applications of crown ethers	Lecture with ppt and videos	Formative assessment I
	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	
<b>IV</b>	<b>Medicinal Chemistry</b>					
	1	Modern drugs for diseases. Anticancer drugs - classification - synthesis and assay of cyclophosphamide - chlorambucil- cisplatin - vinblastine and vincristine.	2	Identify anti-neoplastic agents	Lecture	Evaluation through class test
	2	Antimalarial drugs - classification - synthesis and assay of chloroquine and primaquine.	2	List out the classification and the assay of antimalarial drugs	Seminar	Formative assessment III

	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		
<b>V</b>	<b>Biophysical Chemistry</b>					
	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 - membrane potential and ion pumps.	2	Describe the reactions in biomolecules	Lecture	
	4	Photoacoustic effect and its application in biology.	2	Apply photoacoustic 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	
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Course Instructor: B.T Delma

HOD: G. Leema Rose

**Semester IV**  
**Inorganic Spectroscopy, Photochemistry and Organometallics (Core IX)**  
**Subject Code: PG2041**

Hours per week	Credits	Total Hours	Marks
6	6	90	100

**Objectives:**

- To understand the principle, interpretation and applications of various spectroscopic techniques to inorganic compounds
- To know the applications of photochemistry, organometallics and bio-inorganic chemistry

**Course Outcomes (COs)**

CO	<i>Upon completion of this course, the students will be able to:</i>	PSO Addressed	CL
CO-1	understand the principles and concepts of inorganic spectroscopy, photochemistry and organometallics.	PSO-1	U
CO-2	apply the principles of spectroscopy, photochemistry and organometallic chemistry to inorganic compounds.	PSO-2	A
CO-3	analyse the structure, reactions and functions of inorganic compounds.	PSO-2	Y
CO-4	evaluate the spectral data and properties of inorganic compounds	PSO-3	E

**Unit I**

**(18 Hours)**

**IR, Raman and NMR Spectroscopy**

IR spectroscopy: introduction - selection rules - stretching frequency of some inorganic ions - effect of coordination on the stretching frequency of sulphato - carbonato - sulphito - aqua - nitro - thiocyanato - cyano - thiourea and DMSO complexes.

Raman spectroscopy: introduction - combined applications of IR and Raman spectroscopy in the structural elucidation of N<sub>2</sub>O - ClF<sub>3</sub> - NO<sub>3</sub><sup>-</sup> - ClO<sub>4</sub> and metal carbonyls.

NMR spectroscopy: introduction - structural assessment of simple inorganic compounds - applications of <sup>1</sup>H - <sup>15</sup>N - <sup>19</sup>F and <sup>31</sup>P NMR spectroscopy in structural problems. Fluxional molecules and effect of quadrupolar nuclei in NMR spectroscopy.

**Unit II**

**(18 Hours)**

**Mössbauer and Photoelectron Spectroscopy**

Mössbauer (MB) spectroscopy: introduction - principle - recoil energy - doppler effect - number of MB signals - isomer shift - quadrupole splitting and magnetic hyperfine splitting. Applications of MB spectroscopy to <sup>57</sup>Fe - <sup>119</sup>Sn and <sup>129</sup>I compounds.

Photoelectron Spectroscopy (PES): theory - types - origin of fine structures - shapes of vibrational fine structures - adiabatic and vertical transitions. PES and evaluation of

vibrational constants of homonuclear diatomic molecules - N<sub>2</sub> and O<sub>2</sub> - heteronuclear diatomic molecules - CO and HCl - polyatomic molecules H<sub>2</sub>O - CO<sub>2</sub> - CH<sub>4</sub> and NH<sub>3</sub>. Koopman's theorem- applications and limitations.

### **Unit III (18 Hours)**

**Inorganic Photochemistry:** Importance of photochemistry. Photochemistry of Co(III) complexes - photosubstitution - photooxidation - photoreduction and photoanation reactions. Photochemistry of Cr(III) complexes - Adamson's rule - photoaquation - photoisomerization - photoracemization - photoanation - photosubstitution in non-aqueous solvents and photoredox reactions. Photochemistry of ruthenium polypyridyls - preparation and characteristics of [Ru(bpy)<sub>3</sub>]<sup>2+</sup> complex. Ground state and excited state properties of [Ru(bpy)<sub>3</sub>]<sup>2+</sup> complex. Reactions of [Ru(bpy)<sub>3</sub>]<sup>2+</sup> complex - photosubstitution - photoredox and reductive quenching reactions.

### **Unit IV (18 Hours)**

**Organometallic Chemistry:** Organometallic compounds - types. EAN rule - 18e- and 16e- rules - determination of oxidation state - configuration - coordination number of the metal centre - types and application 18e- / 16e- rules. Carbonyls - isolated concept - structure of simple and polynuclear carbonyls. Nitrosyls - bridging and terminal nitrosyls - bent and linear nitrosyls. Synthesis, properties and structural features of metal complexes with carbene - alkene - alkyne and arene. Hapticity. Metallocenes - synthesis - properties and bonding in ferrocene. Covalent versus ionic bonding in zirconocene. Reactions of organometallic compounds - substitution - oxidative addition and reductive elimination - insertion and deinsertion (elimination) reactions.

### **Unit V (18 Hours)**

**Bio Inorganic Chemistry:** Photosynthesis - photosystem I and II. Photosynthetic reaction center. Metallo enzymes - Zinc enzymes - structure and functions of carbonic anhydrase and carboxy peptidase. Iron enzymes - catalase and peroxidase. Super oxide dismutase (SOD) - superoxide toxicity - structure and function of Cu,Zn-SOD. Trace elements in biological system. Metal ion toxicity - classes of toxic metal compounds and detoxification. Metals in medicine - anti-arthritis drugs - Au and Cu in rheumatoid arthritis - Li in psychiatry - Pt, Au and metallocenes in anti-cancer drugs. Metals in radiodiagnosis and magnetic resonance imaging.

### **Text Books**

5. Roundhill, D.M. (1994). Photochemistry and Photophysics of Metal Complexes. (1<sup>st</sup> ed.). New York: Plenum Press.
6. Kaur, H. (2006). Spectroscopy. (3<sup>rd</sup> ed.). Meerut: Pragati Prakasan Publications.
7. Banwell, C.N. & Mccash, E.M. (1997). Fundamentals of Molecular Spectroscopy. New Delhi: Tata Mc Grow Hill.
8. Malik, W.U., Tuli, G.D. & Madan, R.D. (2012). Selected topics Inorganic Chemistry. (5<sup>th</sup> ed.). New Delhi: S. Chand Company Ltd.

9. Chatwal, G.R. & Bhagi, A.K. (2005). Bio-inorganic Chemistry. (2<sup>nd</sup> ed.). India: Himalaya Publishing House.

#### **Reference Books**

1. Rohatgi, K.K. & Mukherjee, K.K. (2014). Fundamentals of Photochemistry. (3<sup>rd</sup> ed.). India: New Age International.
2. Iggo, J.A. (2000). NMR Spectroscopy in Inorganic Chemistry. USA: Oxford Scientific Publications.
3. Brisdon, A.K. (1998). Inorganic Spectroscopic Methods. USA: Oxford Scientific Publications.
4. Horwood, E. (2010). NMR, NQR, EPR and Mössbauer Spectroscopy in Inorganic Chemistry. (1<sup>st</sup> ed.). New York: Ellis Horwood Ltd.
5. Puri, B.R., Sharma L.R. & Kalia, K.C. (2012). Principles of Inorganic Chemistry. (4<sup>th</sup> ed.), India: Milestone publishers.
6. Miessler, G.L. (2004). Inorganic Chemistry. (3<sup>rd</sup> ed.), India: Pearson Education.
7. Huheey, J.E., Keiter, E.A., Keiter, R.L. & Medhi, O.K. (2011). Inorganic Chemistry, Principles of Structure and Reactivity. (4<sup>th</sup> ed.). India: Pearson Education.

## Teaching Module

**Credits: 6**

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

Unit	Section	Topics	Lecture Hours	Learning Outcome	Pedagogy	Assessment/Evaluation
<b>I</b>	<b>IR, Raman and NMR Spectroscopy</b>					
	1	IR spectroscopy: introduction - selection rules - stretching frequency of some inorganic ions - effect of coordination on the stretching frequency of sulphato - carbonato - sulphito - aqua - nitro - thiocyanato - cyano - thiourea and DMSO complexes.	5	Understand the principle and applications of IR spectroscopy in structural determination	Lecture and PPT	Evaluation through class test  Formative assessment I
	2	Raman spectroscopy: introduction - combined applications of IR and Raman spectroscopy in the structural elucidation of N <sub>2</sub> O - ClF <sub>3</sub> - NO <sub>3</sub> <sup>-</sup> - ClO <sub>4</sub> and metal carbonyls.	5	Understand the principles of Raman Spectroscopy and compare IR and Raman Spectroscopy in structure elucidation	Lecture and PPT	
	3	NMR spectroscopy: introduction - structural assessment of simple inorganic compounds - applications of <sup>1</sup> H - <sup>15</sup> N - <sup>19</sup> F and <sup>31</sup> P NMR spectroscopy in structural problems	5	Understand the principles of NMR spectroscopy and apply NMR spectroscopy to solve structural problems	Lecture and PPT	
	4	Fluxional molecules and effect of quadrupolar nuclei in NMR spectroscopy.	3	Analyse the effect of quadrupolar nuclei in NMR spectroscopy	Lecture and Seminar	
<b>II</b>	<b>Mössbauer and Photoelectron Spectroscopy</b>					
	1	Mössbauer (MB) spectroscopy: introduction - principle - recoil energy - doppler effect - number of MB signals - isomer shift - quadrupole splitting and magnetic hyperfine splitting. Applications of MB spectroscopy to <sup>57</sup> Fe - <sup>119</sup> Sn and <sup>129</sup> I compounds.	6	Understand the principle of Mössbauer (MB) spectroscopy and apply MB spectroscopy to <sup>57</sup> Fe - <sup>119</sup> Sn and <sup>129</sup> I compounds.	Lecture and PPT	Evaluation through class test and group discussion  Formative assessment II

	2	Photoelectron Spectroscopy (PES): theory - types - origin of fine structures - shapes of vibrational fine structures - adiabatic and vertical transitions.	5	Apply Photoelectron Spectroscopy to predict the origin and shapes of vibrational fine structures	Lecture and demonstration	
	3	PES and evaluation of vibrational constants of homonuclear diatomic molecules - N <sub>2</sub> and O <sub>2</sub> - heteronuclear diatomic molecules - CO and HCl -	4	Evaluate the vibrational constants of homonuclear and heteronuclear diatomic molecules	Lecture and group discussion	
	4	Polyatomic molecules H <sub>2</sub> O - CO <sub>2</sub> - CH <sub>4</sub> and NH <sub>3</sub> . Koopman's theorem - applications and limitations	3	Apply Koopman's theorem	Lecture and group discussion	
<b>III</b>	<b>Inorganic Photochemistry</b>					
	1	Importance of photochemistry. Photochemistry of Co(III) complexes - photosubstitution - photooxidation - photoreduction and photoanation reactions	5	Understand the various photochemical reactions of Co(III) complexes	Lecture and PPT	Evaluation through class test and group discussion
	2	Photochemistry of Cr(III) complexes - Adamson's rule - photoaquation - photoisomerization - photoracemization - photoanation - photosubstitution in non-aqueous solvents and photoredox reactions	5	Compare the types of photochemical reactions in non-aqueous solvents and photoredox reactions	Lecture and seminar	Formative assessment II
	3	Photochemistry of ruthenium polypyridyls - preparation and characteristics of [Ru(bpy) <sub>3</sub> ] <sup>2+</sup> complex.	4	Understand the preparation and characteristics of [Ru(bpy) <sub>3</sub> ] <sup>2+</sup> complex	Lecture and group discussion	
	4	Ground state and excited state properties of [Ru(bpy) <sub>3</sub> ] <sup>2+</sup> complex. Reactions of [Ru(bpy) <sub>3</sub> ] <sup>2+</sup> complex - photosubstitution - photoredox and reductive quenching reactions.	4	Compare the ground state and excited state properties of [Ru(bpy) <sub>3</sub> ] <sup>2+</sup> complex	Lecture and seminar	
<b>IV</b>	<b>Organometallic Chemistry</b>					

	1	Organometallic compounds - types. EAN rule - 18e- and 16e- rules - determination of oxidation state - configuration - coordination number of the metal centre - types and application 18e- / 16e- rules	5	Understand the types of Organometallic compounds and apply EAN rule	Lecture and group discussion	Evaluation through class test and group discussion  Formative assessment I
	2	Carbonyls - isolated concept - structure of simple and polynuclear carbonlys.	2	Compare the structure of simple and polynuclear carbonlys	Lecture and group discussion	
	3	Nitrosyls - bridging and terminal nitrosyls - bent and linear nitrosyls.	2	Classify bridging and terminal nitrosyls - bent and linear nitrosyls	Lecture and discussion	
	4	Synthesis, properties and structural features of metal complexes with carbene - alkene - alkyne and arene.	4	Correlate the structural features of metal complexes	Lecture and project	
	5	Hapticity . Metallocenes - synthesis - properties and bonding in ferrocene. Covalent versus ionic bonding in beryllocene.	3	Compare Covalent versus ionic bonding in beryllocene	Lecture	
	6	Reactions of organometallic compounds - substitution - oxidative addition and reductive elimination - insertion and deinsertion (elimination) reactions	2	Analyse the various reactions of organometallic compounds	Lecture and Discussion	
<b>V</b>	<b>Bio Inorganic Chemistry - II</b>					
	1	Photosynthesis, photosystem I and II and photosynthetic reaction centre.	3	Generalize photosystem I, II and photosynthetic reaction	Lecture	Evaluation through class test, group discussion and quiz  Formative
	2	Metalloenzymes - enzymes in di-oxygen management.	3	Explain metalloenzymes	Lecture	

	3	Super oxide dismutase, superoxide toxicity, structure of Cu, Zn-SOD, enzymatic activity and mechanism.	3	Deduce the structure of Cu, Zn-SOD	Lecture and PPT	assessment I
	4	Peroxidases, catalases, oxidases and mono oxygeneases.	3	Explain the functions of enzymes	Lecture	
	5	Zinc enzymes - the structural role of zinc and zinc constellations of carbonic anhydrase, carboxy peptidase and alcohol dehydrogenase.	3	Understand the role of zinc in zinc enzymes	Lecture	
	6	Metal complexes as probes of nucleic acids. Gold compounds and anti-arthritis agents.	3	Explain the role of metal complexes and its applications	Lecture and group discussion	

Course Instructor: Dr. S. Lizy Roselet

HOD: Dr. G. Leema Rose

**Semester IV**  
**Photochemistry and Natural Products (Core X)**  
**Subject Code: PG2042**

Hours per week	Credits	Total Hours	Marks
6	5	90	100

**Objectives:**

- To understand various organic reactions with their mechanism and synthetic utility.
- To elucidate the structure and synthesise natural products.

**Course Outcomes (COs)**

CO	<i>Upon completion of this course, the students will be able to:</i>	PSO Addressed	CL
CO-1	understand various organic reactions and their mechanism	PSO-1	U
CO-2	apply the reaction mechanism in organic synthesis	PSO-2	A
CO-3	analyze the structure and mechanism of reactions	PSO-2	Y
CO-4	evaluate the synthetic utility of reactions	PSO-2	E

**Unit I** **(18 Hours)**

**Organic Photochemistry:** Introduction - Thermal versus photochemical reactions and Jablonski diagram. Photochemical reactions of ketones - photosensitization - Norrish type - I and Norrish type - II reactions and mechanisms - Paterno-Buchi reaction - photooxidation and photoreduction of ketones. Photochemistry of arenes - Photodimerisation - photoisomerisation. Reactions involving free radicals - Barton - Hundsdiecker - Pschorr and Gomberg-Bauchman reactions.

**Unit II** **(18 Hours)**

**Pericyclic Reactions:** Characteristics and classifications of pericyclic reactions - electrocyclic - cycloaddition and sigmatropic reactions. Woodward Hofmann rule. Retro-Diels Alder reaction - Diels Alder reaction - 2+2 - 2+4 reactions. Cope rearrangements and Claisen rearrangements. Conservation of orbital symmetry. Prediction of reaction conditions using FMO - correlation diagrams and Zimmerman (Möbius-Hückel) approaches.

**Unit III** **(18 Hours)**

**Retrosynthetic Analysis:** Retrosynthetic terminologies - linear and convergent approach - protecting groups - activating groups - synthons and synthetic equivalents. Target molecule - one functional group disconnection - two functional groups disconnection - 1,3- 1,5- and 1,4-dicarbonyl compounds. Functional group addition and interconversions. Umploung synthesis. Latent polarity. Retrosynthetic analysis - bisabolene - cis-jasmone - longifolene and cubane. Synthetic uses of nitrocompounds and alkenes.

**Unit IV****(18 Hours)**

**Alkaloids:** Extraction - general properties - classification and general methods for determining structure. Structural elucidation - atropine - cocaine - dictamnine - reserpine - aconitine and morphine.

**Unit V****(18 Hours)**

**Heterocyclic Compounds:** Synthesis - reactions - structure - carbazole - oxazole - imidazole - thiazole - pyrones - pyrazole - pyrimidine - pyrazine - coumarins and chromone. Structural elucidation - flavones - isoflavone - anthocyanins - caffeine - theobromine and theophylline.

**Text Books**

1. Singh, J & Singh, J. (2012). Photochemistry and Pericyclic Reactions. (3<sup>rd</sup> ed.). India: New Age International Pvt. Ltd.
2. Tewari, K. S., Vishnoi, N. K. & Mehrotra, S.N. (2002). A Text Book of Organic Chemistry. India: Vikas Publishing House Ltd.
3. Warren, S. (2014). Organic Synthesis: The Disconnection Approach. India: Wiley Pvt. Ltd.
4. Finar, I.L. (2002). Organic Chemistry Volume II. (5<sup>th</sup> ed.). India: Pearson Education
5. Bansal, R.K. (2014). Heterocyclic Chemistry. (5<sup>th</sup> ed.). India: New Age International Pvt. Ltd.
6. Clayden, J. Greeves, N& Warren, S. (2012). Organic Chemistry. (2<sup>nd</sup> ed.). Oxford University Press.

**Reference Books**

1. Depuy, C.H., & Chapman, O.S. (1988). Molecular Reactions and Photochemistry. India: Prentice Hall Pvt. Ltd.
2. Gill, G.B. & Wills, M.R. (1974). Pericyclic Reactions. London: Chapman and Hall
3. Agarwal, O.P. (1947). Chemistry of Organic Natural Product Vol. I & II India: Goel Publishing House.
4. Joule, J.A. & Mills, K. (2010). Heterocyclic Chemistry. (5<sup>th</sup> ed.). India: Wiley Pvt. Ltd.
5. Ireland, R.E. (1969). Organic Synthesis. Prentice Hall, Englewood Cliffs, New Jersey, U.S.A.
6. Carruthers, W. (2015). Modern Methods of Organic Synthesis. (4<sup>th</sup> ed), Cambridge University Press.

## Teaching Module

Credit: 5

Total Hours: 90 (Incl. Seminar & Test)

Unit	Section	Topics	Lecture Hours	Learning Outcome	Pedagogy	Assessment/Evaluation
<b>I</b>	<b>Organic Photochemistry</b>					
	1	Introduction - Thermal versus photochemical reactions and Jablonski diagram.	4	Understand the basic concepts of photochemistry	Lecture with ppt	Evaluation through online quiz
	2	Photochemical reactions of ketones - photosensitization - Norrish type - I and Norrish type - II reactions and mechanisms	4	Analyze the photochemical reaction mechanisms of carbonyl compounds	Lecture and Group discussion	Formative assessment I
	3	Paterno-Buchi reaction - photooxidation and photoreduction of ketones.	4	Interpret photooxidation and photoreduction mechanisms in ketones	Lecture and Seminar	
	4	Photochemistry of arenes Photodimerisation - photoisomerisation.	2	Understand the mechanisms of Photodimerisation and photoisomerisation	Lecture	
	5	Reactions involving free radicals - Barton - Hundsdiecker - Pschorr and Gomberg-Bauchman reactions.	4	Understand various name reactions involving free radicals	Lecture with ppt	
<b>II</b>	<b>Pericyclic Reactions</b>					
	1	Characteristics and classifications of pericyclic reactions - electrocyclic - cycloaddition and sigmatropic reactions.	4	Classify the types of pericyclic reactions	Lecture and Seminar	Evaluation through class test, online quiz and group discussion
	2	Woodward Hofmann rule. Retro-Diels Alder reaction - Diels Alder reaction - 2+2 - 2+4 reactions.	5	Differentiate Retro-Diels Alder and Diels Alder reaction	Lecture	Formative assessment I
	3	Cope rearrangements and Claisen rearrangements. Conservation of orbital symmetry.	4	Compare Cope and Claisen rearrangements	Lecture and group discussion	

	4	Prediction of reaction conditions using FMO - correlation diagrams and Zimmerman (Mobius-Huckel) approaches.	5	Predict FMO - correlation diagrams and Zimmerman (Mobius-Huckel) approaches	Lecture	
<b>III</b>	<b>Retrosynthetic Analysis</b>					
	1	Retrosynthetic terminologies - linear and convergent approach - protecting groups - activating groups - synthons and synthetic equivalents.	4	Understand the basic terminologies of retero synthesis	Lecture with models	Evaluation through class test, online quiz and group discussion
	2	Target molecule - one functional group disconnection - two functional groups disconnection - 1,3- 1,5- and 1,4- dicarbonyl compounds.	6	Interpret one and two functional groups disconnections	Lecture	Formative assessment II
	3	Functional group addition and interconversions. Umploung synthesis. Latent polarity.	5	Illustrate functional interconversions in retro synthesis	Lecture and group discussion	
	4	Retrosynthetic analysis - bisabolene - cis-jasmone - longifolene and cubane.	3	Interpret the retrosynthetic analysis of bisabolene - cis-jasmone - longifolene and cubane.	Lecture	
	5	Synthetic uses of nitrocompounds and alkenes.		Describe the synthetic uses of nitrocompounds		
<b>IV</b>	<b>Alkaloids</b>					
	1	Extraction and general properties of alkaloids	3	Understand the general properties of alkaloids	Lecture	Evaluation through class test and group discussion
	2	Classification of Alkaloids	3	Classify the types of alkaloids		
	3	General methods for determining structure of alkaloids	4	Understand the methods for determining structure of alkaloids	Lecture	Formative assessment II

	4	Structural elucidation - atropine and cocaine	4	Elucidate the structure of atropine and cocaine	Lecture	
	5	dictamnine - reserpine - aeronycine and morphine.	3	Elucidate the structure of various alkaloids	Lecture	
<b>V</b>	<b>Heterocyclic Compounds</b>					
	1	Synthesis - reactions - structure - carbazole - oxazole - imidazole	5	Understand the synthesis and reactions of heterocyclic compounds	Lecture with videos	Evaluation through class test, group discussion and quiz
	2	Synthesis of thiazole - pyrones - pyrazole - pyrimidine	5	Understand the synthesis and reactions of heterocyclic compounds	Lecture	Formative assessment I
	3	Pyrazine - coumarins and chromone	2	Understand the synthesis and reactions of heterocyclic compounds	Lecture	Evaluation through class test, group discussion and quiz
	4	Structural elucidation - flavones - isoflavone - anthocyanins	3	Elucidate the structure of flavones, isoflavone and anthocyanins	Lecture and Group Discussion	Formative assessment II
	5	Caffeine - theobromine and theopylline.	3	Elucidate the structure of caffeine, theobromine and theopylline		

Course Instructor: Dr. Y. Christabel Shaji

HOD: Dr. G. Leema Rose

**Semester IV**  
**Polymer chemistry (Core XI)**  
**Subject Code: PG2043**

Hours per week	Credits	Total Hours	Marks
6	5	90	100

**Objectives:**

- To gain knowledge about applications of polymers.
- To know the importance of various polymerization techniques.
- To study about synthetic polymers.

**Course Outcome (COs)**

CO	Upon completion of this course, the students will be able to:	PSO Addressed	CL
CO -1	Understand the concept of polymer chemistry	PSO - 1	U
CO -2	Apply the processing techniques in the manufacture of synthetic polymer	PSO - 5	A
CO -3	Analyze glass transition temperature, crystallinity and degradation in polymers.	PSO - 3	Y
CO -4	Evaluate molecular weight and size of the polymer	PSO - 3	E

**Unit I**

**(18 hours)**

**Chemistry of Polymerization:** Basic concepts of polymer chemistry - repeat unit - degree of polymerization - classification - chain polymerization - free radical polymerization - ionic polymerisation - coordination polymerisation: Zeigler- Natta catalyst - stereo regulating polymerization - step polymerization - ring opening polymerization - copolymerisation - types - free radical copolymerisation - ionic copolymerization - copolycondensation - block and graft copolymers.

**Unit II**

**(18 hours)**

**Polymerisation Techniques Molecular Weight and Size:** Polymerisation techniques - bulk - solution - suspension - emulsion - polymerizations -melt polycondensation - solution polycondensation interfacialcondensation - solid and gas phase polymerization - molecular weight and size -number average and weight average molecular weights - sedimentation and viscosity average molecular weights -polydispersity and molecular weight distribution in polymers - practical significance of polymer molecular weight.

**Unit III**

**(18 hours)**

**Polymer Processing:** Processing techniques - calendering - die casting - rotational casting - film casting - compression moulding - injection moulding - blow moulding - extrusion moulding - thermoforming, foaming and reinforcing techniques - hand lay-up technique - filament winding technique - spray-up technique. Fibre spinning - dry spinning - wet spinning - uniaxial orientation - post treatment for fibres.

#### **Unit IV**

**(18 hours)**

**Synthetic Polymers:** Synthetic resins - plastics - manufacture - applications - polyethylene - PVC - teflon - polystyrene - polymethylmethacrylate - polyurethane - phenol-formaldehyde resins - urea- formaldehyde and melamine- epoxy polymers. Synthetic fibers - rayon -nylons -polyesters -acrylics – modacrylics. Natural rubber -production -constitution - vulcanization (hot and cold) - fillers and accelerators - antioxidants - synthetic rubber - SBR - butyl rubber - nitrile rubber -neoprene - silicone rubber and polysulphides.

#### **Unit V**

**(18 hours)**

**Polymer Degradation and Additives:** Polymer degradation - types - thermal degradation - mechanical degradation - photo degradation – degradation by ultrasonic waves - degradation by high energy radiation - hydrolytic and oxidative degradations - additives for polymers - fillers - plasticisers - thermal stabilizers - photo stabilizers - antioxidants and colourants.

#### **Text Books**

1. Billmeyer, F. (1971). Textbook of Polymer Science. ( 2<sup>nd</sup> ed), New York : John Wiley and Sons.
2. Gowariker, V.R (2009). Polymer Science. ( 2<sup>nd</sup> ed), New Age international .). India: New Age International Pvt. Ltd.
3. Braun, D. (1982). Simple Methods for Identification of Plastics. New York : Macmillan Publishing Co.
4. Robert Weast, C. (1985). Handbook of Chemistry and Physics. ( 65<sup>th</sup> ed), Boca Raton, FL : CRC Press.
5. Hightstown, N.J. (1990). Modern Plastics, Encyclopedia, Volume 67: McGraw Hill.

#### **Reference Books**

1. Odian, G. (2004). Principles of Polymerization. ( 4<sup>th</sup> ed): John Wiley and Sons
2. Manas Chanda. (2000). Advanced Polymer Chemistry: Marcel Dekker Inc.
3. Malcolm. P. Stevens. (1999). Polymer Chemistry: An Introduction. (3<sup>rd</sup> edition) : USA : Oxford University Press
4. Misra .G.S. (1993). Introductory Polymer Chemistry : New York : J. Wiley and Sons.
5. Charles E. Carraher Jr. ( 2017). Introduction to Polymer Chemistry. ( 4<sup>th</sup> ed):CRC Press.
6. Rodriguez, F., Cohen, C., Ober, C.K. & Archer, L. (2015). Principles of Polymer Systems. (6<sup>th</sup> ed), CRC Press.

## Teaching Module

Credit: 5

Total Hours: 90 (Incl. Seminar & Test)

Unit	Section	Topics	Lecture Hours	Learning Outcome	Pedagogy	Assessment/Evaluation
<b>I</b>	<b>Chemistry of Polymerization</b>					
	1	Basic concepts of polymer chemistry - repeat unit - degree of polymerization - classification	4	Understand the basic concepts of polymer chemistry	Lecture and group discussion	Evaluation through class test  Formative assessment I
	2	stereochemistry of polymers -nomenclature of stereo regular polymers	3	Discuss the nomenclature of stereo regular polymers	Lecture and group discussion	
	3	chain polymerization - free radical polymerization - ionic polymerisation coordination polymerisation: Zeigler-Natta catalyst - step polymerization - ring opening polymerization	8	Explain the different types of polymerization	Lecture and ppt	
	4	copolymerisation - block and graft copolymers - preparation.	3	Describe copolymers preparation	Lecture	
<b>II</b>	<b>Polymerisation Techniques Molecular Weight and Size</b>					
	1	Polymerisation techniques -bulk - solution -suspension - emulsion – polymerizations	4	Explain various polymerization techniques	Lecture	Evaluation through class test and group discussion  Formative assessment II
	2	melt polycondensation - solution polycondensation interfacial condensation	4	Compare different types of poly condensation processes	Lecture and group discussion	

	3	solid and gas phase polymerization.	4	Analyse solid and gas phase polymerization processes	Lecture	
	4	polydispersity and molecular weight distribution in polymers	3	Evaluate the poly dispersity index and molecular weight of polymers	Lecture	
	5	the practical significance of polymer molecular weight.	3	Explain the practical significance of polymer molecular weight.		
<b>III</b>	<b>Polymer Processing</b>					
	1	Processing -Calendering - die casting - rotational casting - film casting	5	Explain the various polymer casting processes	Lecture	Evaluation through class test and group discussion  Formative assessment III
	2	compression moulding - injection moulding - blow moulding - extrusion moulding	5	Compare the moulding processes in polymers.	Lecture and field visit	
	3	thermoforming, foaming and reinforcing techniques	2	Explain the techniques of polymer processes.	Lecture	
	4	synthetic resins – plastics- manufacture and applications of polyethylene -PVC - Teflon -polystyrene - polymethylmethacrylate -polyurethane - phenol- formaldehyde resins - urea-formaldehyde and melamine- epoxy polymers.	6	Describe the manufacture and application of synthetic resins	Videos and industrial visit	
<b>IV</b>	<b>Synthetic Polymers</b>					

	1	Synthetic fibres -rayon -nylons -polyesters -acrylics -modacrylics	5	Describe the manufacture and application of synthetic fibres	Lecture and video	Evaluation through class test and group discussion
	2	spinning techniques	2	Explain the spinning techniques of polymer process	Lecture and video	Formative assessment II
	3	natural rubber - production -constitution -vulcanization (hot and cold)	3	Discuss the production and vulcanization of rubber	Lecture and field visit	
	4	fillers and accelerators – antioxidants	3	Compare the functions of fillers accelerators and antioxidants	Lecture and group discussion	
	5	Synthetic rubber -SBR - butyl rubber - nitrile rubber -neoprene - silicone rubber and polysulphides.	5	Describe the manufacture and application of synthetic rubber	Lecture	
<b>V</b>	<b>Polymer Degradation and Additives</b>					
	1	Polymer degradation	1	Describe polymer degradation	Lecture	Evaluation through class test, group discussion and quiz
	2	types of degradation - thermal -mechanical photo - hydrolytic and oxidative degradations	7	Classify the types of polymer degradation	Lecture	
	3	additives for polymers - fillers -plasticizers	5	Discuss the role of additives in polymers	Lecture and group discussion	Formative assessment I
	4	thermal stabilizers - photo stabilizers - antioxidants and colorants.	5	Differentiate thermal and photo stabilizers	Lecture and group discussion	

Course Instructor: M.Shirly Treasa

HOD: G. Leema Rose

## Teaching Module

Credits: 3

Total Hours: 60 (Incl. Seminar & Test)

Unit	Section	Topics	Lecture Hours	Learning Outcome	Pedagogy	Assessment/Evaluation
<b>I</b>	<b>Introduction to Energy Sources</b>					
	1	Introduction, conventional energy sources like coal, oil, gas, agricultural and organic wastes, water power, thermal power and nuclear power.	3	Recall the sources of conventional energy	Lecture with videos	Evaluation through class test and seminar  Formative assessment I
	2	Non-conventional energy sources like solar energy and wind energy.	3	Explain non-conventional energy sources	Lecture and group discussion	
	3	Energy from bio-mass and bio-gas, ocean thermal energy, tidal energy.	3	Understand various sources of energy	Lecture	
	4	Geothermal energy and hydrogen energy. Advantages of renewable energy.	3	Discuss the advantages of renewable energy	Lecture and PPT	
<b>II</b>	<b>Solar Energy</b>					
	1	Solar radiation and its measurement - Introduction, solar constant, solar radiation at the earth's surface, solar radiation geometry and solar radiation data.	3	Explain solar radiations and its measurement	Lecture and videos	Evaluation through class test and seminar  Formative assessment II
	2	Solar energy collectors - Introduction, physical principles of the conversion of solar radiation into heat, flat plate and concentration collectors.	3	Understand the principle of solar energy conversion and collectors	Lecture and PPT	
	3	Advantages and disadvantages of concentration collectors over flat collectors.	2	Compare the concentration collectors and flat collectors	Lecture	
	4	Energy balance equation and collector efficiency.	4	Determine energy balance and collector efficiency	Lecture	
<b>III</b>	<b>Wind Energy</b>					

	1	Introduction, basic principles of wind energy conversion, power of the wing, forces on the blades.	2	Understand the basis of wind energy	Lecture with videos	Evaluation through class test and seminar
	2	Wind energy conversion, wind data and estimation, site selection.	2	Illustrate wind energy conversion	Lecture with ppt and videos	Formative assessment II
	3	Types of wind machines - Horizontal axis and vertical axis machines.	2	Classify the types of wind machine	Lecture and seminar	
	4	Analysis of aerodynamic forces acting on the blade, performance of wind machines.	2	Analyse the forces acting on the blade	Lecture and group discussion	
	5	Generating systems - Introduction, schemes of electric generation, generator control, load control, energy storage. Application of wind energy.	4	Explain generating system and applications of wind energy	Lecture with videos	
<b>IV</b>	<b>Bio-energy</b>					
	1	Introduction, biomass conversion techniques - wet processes and dry processes.	2	Explain biomass and its conversion	Lecture and PPT	Evaluation through class test and quiz
	2	Biogas generation. Classification of biogas plants - floating drum plant and fixed dome type plant. Biogas from plant waste.	3	List out the classification of biogas plants	Lecture and seminar	Formative assessment I
	3	Materials used for biogas generation, selection of site for a biogas plant, digester design. Problems related with biogas plants.	3	Describe the biogas generation and identify the problems related to biogas plant	Lecture and seminar	
	4	Fuel properties of biogas and utilization of biogas.	4	Understand the properties of biogas	Lecture and seminar	
<b>V</b>	<b>Chemical energy sources</b>					
	1	Fuel cells - Introduction, conversion efficiency of fuel cells, types of electrodes, work output.	2	Understand the basis of fuel cells	Lecture and seminar	Evaluation through class test and quiz

	2	EMF of fuel cells. Applications of fuel cells.	2	Determine the EMF of fuel cells and explain the applications of it	Lecture and seminar	Formative assessment I
	3	Hydrogen energy: Hydrogen production – electrolysis, thermo-chemical, fossil fuel and solar energy methods.	3	Explain hydrogen production by various methods	Lecture and Seminar	
	4	Hydrogen storage and hydrogen transportation.	2	Explain the hydrogen storage and hydrogen transportation	Lecture and seminar	
	5	Utilization of hydrogen gas. Hydrogen as an alternative fuel for motor vehicles. Safety and management.	3	Describe the utilization and safety measures of hydrogen gas	Lecture and PPT	

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