

**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-Lande equation - Kapustinski equation and Madelung constant	3	Understands lattice energy, Born-Lande equation and Kapustinski equation	Lecture and group discussion	
	4	Representative structures of AB and AB <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-Hammett 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  Formative assessment II
	2	Debye-Hückel limiting law and its applications - diverse ion effect. Van't Hoff factor and its relation to colligative properties	3	Derive Debye Huckel equation	Lecture and group discussion	
	3	Debye-Hückel theory of strong electrolytes. Debye-Huckel length and potential around a central ion - interpretation. Transport of ions in solution	4	Explain the principles and applications of Huckel theory	Lecture	
	4	Electrolytic conduction-. Debye - Huckel-Onsager treatment of strong electrolytes- ionic atmosphere	4	Apply Debye - Huckel-Onsager treatment to strong electrolytes	Lecture	
	5	Anomalous conductance of non-aqueous electrolytes	3	Gain knowledge about the non aqueous electrolytes	Lecture	
<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  Formative assessment II
	2	Structure of electrical double layer - Helmholtz-Perrin - Guoy-Chapmann and Stern models. Butler-Volmer equation for one electron transfer reaction equilibrium	4	Derive Butler-Volmer equation		

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

Course Instructor: Dr. M. Shirly Treasa

HOD: Dr. G. Leema Rose

**Semester I**  
**Analytical Chemistry (Elective I)**

**Subject Code: PG2014**

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

**Objectives**

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

**Course Outcomes (COs)**

CO No.	<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 : III  
 Name of the Course : Organic Chemistry III  
 Subject Code : PG1731

Number of Hours Per week	Number of Credit	Total No. of hours	Marks
6	5	90	100

#### Course Outcome

CO No.	Upon completion of this course, the students will be able to:	PO /PSO Addressed	Cognitive Level
CO-1	Understand the principle and applications of UV, IR, NMR and Mass spectroscopy.	PSO-1	U
CO-2	Predict the structure of organic compounds using spectroscopic techniques.	PSO-4	C
CO-3	Predict the splitting pattern of organic compounds using NMR spectroscopy	PSO-4	C
CO-4	Predict the mass to charge ratio of organic compounds using mass spectroscopy	PSO-4	C
CO-5	Elucidate the structure of heterocyclic compounds.	PSO-2	An
CO-6	Discuss the use of reagents in organic synthesis.	PSO-1	U

#### Teaching Plan

Credit: 4

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

Unit	Module	Topics	Lecture Hours	Learning Outcome	Pedagogy	Assessment/Evaluation
<b>I</b>	<b>UV- Visible spectroscopy and IR spectroscopy</b>					
	1	UV-Visible spectroscopy: Basic principles of electronic transition. Absorption spectra of conjugated dienes, $\alpha,\beta$ -unsaturated carbonyl compounds and aromatic compounds.	3	Understand the principle of UV spectroscopy	Lecture	Evaluation through class test and group discussion  Formative assessment I

	2	Woodward-Fieser rule and Fieser-Khun rule. Effect of solvent polarity on $\lambda_{\max}$ . Applications of UV-Visible spectroscopy.	3	Predict $\lambda_{\max}$ using Woodward-Fieser rule and Fieser-Khun rule.	Lecture and Group discussion	
	3	IR spectroscopy: Principle, instrumentation and sampling techniques, Hooke's law, types of stretching and bending vibrations.	3	Know the principle and instrumentation of IR spectroscopy	Lecture with videos	
	4	Factors influencing the vibrational frequency. Vibrational frequencies of alkane, alkenes, alkynes, aromatic compounds, alcohols, ethers, phenol, amines, acids, esters and amides.	3	Predict the functional groups	Lecture	
	5	Overtone and combination bands. Fermi resonance. Applications of IR spectroscopy.	3	Explain the applications of IR spectroscopy	Lecture	
<b>II</b>	<b>NMR Spectroscopy</b>					
	1	$^1\text{H}$ NMR Spectroscopy: Instrumentation, principle of NMR spectroscopy, Chemical shift and factors affecting chemical shift.	3	Understand the principle and applications of NMR spectroscopy	Lecture with videos	Evaluation through class test and group discussion
	2	Spin-spin splitting. Types of coupling - germinal, vicinal, long range and through space coupling. Coupling constant - AB, AB <sub>2</sub> and A <sub>2</sub> B <sub>3</sub> .	3	Predict the splitting pattern of organic compounds using NMR spectroscopy	Lecture	Formative assessment II
	3	Simplification of complex spectra - chemical exchange, double resonance and NMR shift reagents.	3	Describe the simplification of complex spectra	Lecture	
	4	$^{13}\text{C}$ NMR Spectroscopy: Principle, chemical shift, factors affecting chemical shift, broad band decoupling and OFF - resonance decoupling.	3	Explain the factors affecting chemical shift in $^{13}\text{C}$ NMR Spectroscopy	Lecture	

	5	2D-NMR - COSY-HOMCOR, HETCOR and DEPT Technique.	3	Interpret COSY-HOMCOR and HETCOR	Lecture	
	6	Comparison of $^{13}\text{C}$ NMR and $^1\text{H}$ NMR.	2	Compare of $^{13}\text{C}$ NMR and $^1\text{H}$ NMR.	Lecture and group discussion	
<b>III</b>	<b>Mass Spectroscopy</b>					
	1	Basic principle, instrumentation and production of ions - EI, CI and FAB. Molecular ion peak, base peak, meta stable peak and isotopic peaks.	3	Understand the basic concepts of mass spectroscopy	Lecture with videos	Evaluation through class test and group discussion  Formative assessment III
	2	Nitrogen rule. McLafferty rearrangement. Retro Diels Alder reaction.	2	State and explain nitrogen rule and fragmentation reactions	Lecture	
	3	Fragmentation pattern of simple organic compounds - alkenes, halogens, alkylbenzene, benzene, aliphatic and aromatic alcohols, acids, ketones and aldehydes.	4	Predict the fragmentation pattern of organic compounds	Lecture and group discussion	
	4	Application of mass spectroscopy. Problems related to structural determination using UV, IR, $^1\text{H}$ NMR and Mass spectroscopy.	5	Deduce the structure of organic compounds	Lecture	
	5	Circular birefringence (CB), Circular dichroism (CD), Cotton effect, ORD, Kronig-Kramers relation, applications of axial haloketone rule and octant rule.	4	Understand the applications of axial haloketone rule and octant rule.	Lecture	
<b>IV</b>	<b>Heterocyclic Compounds</b>					
	1	Synthesis, reactions and structure of indole, carbazole, oxazole, imidazole.	2	Understand the synthesis and reactions of some heterocyclic compounds	Lecture	Evaluation through class test and group discussion  Formative assessment II
	2	Synthesis, reactions and structure of thiazole, pyrones, coumarins, chromone.	3	Explain the synthesis and reactions of some heterocyclic compounds	Lecture	

	3	Structural elucidation of flavones, isoflavone.	2	Elucidate the structure of flavones and isoflavones	Lecture	
	4	Anthocyanins, caffeine, theobromine and theopylline.	3	Elucidate the structure of heterocyclic compounds	Lecture	
<b>V</b>	<b>Reagents in organic synthesis</b>					
	1	Oxidation reactions involving SeO <sub>2</sub> , DDQ, DCC, 1,3-dithiane, NBS, m-CPBA and Aluminiumisopropoxide.	3	Understand the oxidation reactions of some reagents	Lecture	Evaluation through class test and group discussion
	2	Reduction involving complex metal hydrides - LiAlH <sub>4</sub> , NaBH <sub>4</sub> , DIBAL, Gilman's reagent.	3	Explain the applications of metal hydrides	Lecture	Formative assessment I
	3	Tri-n-butyl tin hydride, 9-BBN, Wilkinson's catalyst, Vaska's catalyst and Baker yeast.	4	Describe the properties and applications some catalyst	Lecture	
	4	Phase transfer catalysts, crown ether, LDA, Me <sub>3</sub> SiI, Fetizon's reagent.	3	Explain the applications of organic reagents	Lecture	
	5	Lemieux-Von Rudloff reagent and Lemieux-Johnson reagent.	3	Know the applications of Lemieux-Von Rudloff reagent and Lemieux-Johnson reagent	Lecture	

Course Instructor: Y. ChristabelShaji

HOD: G. Leema Rose

**Semester** : **III**  
**Name of the Course** : **Physical Chemistry III**  
**Subject Code** : **PG1732**

Number of Hours Per week	Number of Credit	Total No. of hours	Marks
6	4	90	100

**Course Outcome**

CO No.	Upon completion of this course, the students will be able to:	PO /PSO Addressed	Cognitive Level
CO-1	Construct character table for different point groups	PSO-4	C
CO-2	Apply group theory to normal mode analysis and hybridization	PSO-3	Ap
CO-3	Predict types of electronic transitions in ethylene and formaldehyde	PSO-4	C

CO-4	Infer the characteristics of rotational spectra of diatomic and polyatomic molecules	PSO-1	U
CO-5	Predict the nature of molecules using microwave and photoelectron spectroscopy	PSO-4	C
CO-6	Determine the molecular mass of polymers and kinetics of polymerization	PSO-2	An
CO-7	Explain the experimental techniques related to radiation chemistry	PSO-1	U
CO-8	Apply radiation chemistry in biology and industry	PSO-5	Ap

### Teaching Plan

Credit: 4

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

Unit	Module	Topics	Lecture Hours	Learning Outcome	Pedagogy	Assessment/Evaluation
<b>I</b>	<b>Group Theory - I</b>					
	1	Molecular symmetry elements and symmetry operations, molecular symmetry and point groups.	4	Understand symmetry elements and symmetry operations	Lecture	Evaluation through class test
	2	Group multiplication tables, abelian, non-abelian, cyclic and sub groups, conjugacy relation and classes.	3	Explain the terms in group theory	Lecture	Formative assessment I
	3	Representation of symmetry operations by matrices - representation for the $C_{2v}$ , $C_{3v}$ , $C_{2h}$ .	4	Represent symmetry operations	Lecture	
	4	Reducible and irreducible representations, the great orthogonality theorem and its consequences without proof.	3	Apply orthogonality theorem for the construction of character table	Lecture	
	5	Construction of the character tables $C_{2v}$ , $C_{3v}$ and $C_{4v}$ .	2	Construct character table for different point groups	Lecture	
<b>II</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 $H_2O$ and $NH_3$	Lecture	Evaluation through class test and group discussion
	2	Symmetry properties of integrals and symmetry based selection rule for vibrational spectra. Identification of IR and	4	Identify IR and Raman active vibrations	Lecture	Formative assessment II



		Raman active fundamentals, symmetry of molecular orbitals.				
	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	Group theory applied to determine $\pi$ - 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. Group theory applied to determine hybridization scheme in $\text{CH}_4$ and $\text{BF}_3$ .	2	Determine the hybridization of $\text{CH}_4$ and $\text{BF}_3$		
<b>III</b>	<b>Molecular Spectroscopy - I</b>					
	1	Microwave spectroscopy: Rotation of molecules, rotational spectra of diatomic molecules.	5	Explain microwave spectroscopy	Lecture	Evaluation through class test and group discussion
	2	Intensity of spectral lines, effects of isotopic substitution, non-rigid rotator. Rotational spectra of polyatomic molecules.	3	Infer the characteristics of rotational spectra of polyatomic molecules.	Lecture	Formative assessment III
	3	Chemical analysis by microwave spectroscopy.	2	Analyse compounds microwave spectroscopy	Lecture	
	4	Photoelectron spectroscopy: Principle, photoelectric effect, Ionization process. Applications of photoelectron spectroscopy to simple molecules.	3	Apply photoelectron spectroscopy to simple molecules	Lecture	
	5	PES to $\text{O}_2$ molecule, $\text{N}_2$ molecule, $\text{CO}$ molecule, $\text{NaN}_3$ , Ethyl trifluoro acetate.	3	Apply PES to $\text{O}_2$ , $\text{N}_2$ , $\text{CO}$ , $\text{NaN}_3$ and Ethyltrifluoro acetate	Lecture	
<b>IV</b>	<b>Polymer Chemistry</b>					

	1	General introduction. Determination of molecular mass - osmometry, viscosity, diffusion, light scattering, and sedimentation methods.	4	Determine the molecular mass of polymers by various methods	Lecture	Evaluation through class test and group discussion  Formative assessment II
	2	Visco-elasticity, Rubber elasticity. Kinetics and mechanism of linear stepwise polymerization.	3	Explain the kinetics and mechanism of polymerization	Lecture	
	3	Addition, free radical, cationic and anionic polymerization. Kinetics of co-polymerization.	2	Describe the kinetics of polymerization and co-polymerization	Lecture	
	4	Polymerization in homogeneous and heterogeneous systems.	3	Differentiate Polymerization in homogeneous and heterogeneous systems	Lecture	
	5	Conducting Polymers. Factors affecting the conductivity of conducting polymers. Doping of conducting polymers.	2	Explain conducting polymers	Lecture	
		Polymers processing - compression moulding, injection moulding, transfer moulding and extrusion moulding. Casting extrusion of fibres, spinning.	2	Understand the processing of polymers	Lecture	
<b>V</b>	<b>Radiation Chemistry</b>					
	1	Radioactivity, rate of radioactive disintegration. Sources of high energy radiation. Comparison of radiation chemistry with photochemistry, interaction of high energy radiation with matter. .	4	Compare radiation chemistry with photochemistry	Lecture	Evaluation through class test, group discussion and quiz  Formative assessment I
	2	Nature of radiations from radioactive elements. Detection and measurement of radioactivity - Geiger-Muller counter.	2	Detect and measure radioactivity	Lecture	

3	Wilson Cloud Chamber. G-value, Curie, radiolysis of water, hydrated electron. Radiolysis of some aqueous solutions - Fricke Dosimeter solution.	4	Explain the radiolysis of some aqueous solutions	Lecture
4	Fricke Dosimeter solution and redox reactions using energy transfer from irradiated alkali halides. Radiation dosimetry - Rad, Gray, dose rate and Rontgen. Chemical dosimeters.	3	Understand radiation dosimetry and chemical dosimeters	Lecture with videos
5	Fricke and Ceric sulphate dosimeters. Applications of radiation chemistry in biology and industry.	2	Apply radiation chemistry in biology and industry	Lecture

Course Instructor: S. LizyRoselet

HOD: G. Leema Rose

**Semester** : **III**  
**Name of the Course** : **Advanced Topics in Chemistry**  
**Subject Code** : **PG1733**

Number of Hours Per week	Number of Credit	Total No. of hours	Marks
6	4	90	100

#### Course Outcomes

CO No.	Upon completion of this course, the students will be able to:	PO /PSO Addressed	Cognitive Level
CO-1	Understand the principles of nanotechnology and the properties of nanomaterials	PSO-1	U
CO-2	Synthesize nanoparticles and apply nanotechnology in medical field	PSO-4 and PSO-5	C + Ap
CO-3	Design chemical reactions using green solvents	PSO-4	C
CO-4	Synthesize chemical compounds using solvent free, microwave and sonication assisted techniques	PSO-4	C
CO-5	Apply supramolecular chemistry in organic chemistry and photochemistry	PSO-3	Ap
CO-6	Explain the synthesis and therapeutic action of drugs	PSO-1	U
CO-7	Express the importance and applications of thermodynamics in biology	PSO-1	U

## Teaching Plan

**Credit: 4**

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

Unit	Module	Topics	Lecture Hours	Learning Outcome	Pedagogy	Assessment/Evaluation
<b>I</b>	<b>Nanochemistry</b>					
	1	General principles of nanotechnology Nanoparticles - definition, size relationship and nanoparticles of metals Nanoparticles - semiconductors and oxides.	3	Understand the properties of nanoparticles	Lecture	Evaluation through class test and group discussion  Formative assessment I
	2	Synthesis of nanosized compounds - Reduction methods Synthesis of nanosized compounds - Solgel method Optical and electrical properties of nanoparticles.	3	Synthesis various nanoparticles	Lecture and Seminar	
	3	Introduction, synthesis and purification of Fullerenes, Carbonnanotubes - preparation by Arc method Carbonnanotubes - preparation by chemical vapour deposition method.	2	Synthesis carbon nanotubes and fullerenes	Lecture and Seminar	
	4	Gold and silver nanoshells and its applications.	2	Understand the applications of gold and silver nanoshells	Lecture with videos	
	5	Nanosensors - introduction and nanoscale organization for sensors Nanosensos - characterization and optical properties.	2	Explain nanosensors and its properties	Lecture and Seminar	
		Nanomedicines - introduction and approach to developing nanomedicines Protocol for nanodrug administration Diagnostic and therapeutic applications.	3	Know about the therapeutic applications of nanoparticles		
<b>II</b>	<b>Green Chemistry</b>					
	1	Definition, necessity for green chemistry, Green chemistry and sustainable development. Basic principles and applications of green chemistry.	2	Understand the principle and applications of green chemistry	Lecture and seminar	Evaluation through class test and group discussion  Formative

	2	Atom economy vs. yield in assessing greenness of organic reactions. Prevention of waste/byproducts and Prevention or minimization of hazardous products.	2	Explain the applications of green chemistry	Seminar and group discussion	assessment II
	3	Designing safer chemicals through Sommelet-Hauser and Cope reactions Designing safer chemicals through Wolff, Witting and Bamberger reactions.	2	Design and synthesise compounds using green methods	Lecture	
	4	Energy requirement for synthesis. CFC alternatives – Example for green chemistry in organic synthesis. Selection of appropriate solvent and starting material, use of protecting group and catalyst.	3	Understand the role of solvent, protecting groups and catalyst in green synthesis	Lecture and seminar	
	5	Solvent free reactions, reactions at ambient temperature. Microwave assisted reactions.	2	Synthesise compounds using solvent free and microwave assisted reactions	Lecture and seminar	
	6	Sonication assisted reactions - Reformatsky and Ullmann coupling Sonication assisted reactions – Wurtz and Bouveault reactions	2	Apply sonication method for synthesis	Lecture and seminar	
		Reactions in ionic solvents Reactions in super critical fluids and Tandem reactions.	2	Explain the reactions in ionic solvents	Lecture and seminar	
<b>III</b>	<b>Supramolecular Chemistry</b>					
	1	History and nature of supramolecular interactions Host - guest systems Cation and anion binding host.	3	Understand the host-guest relation in supramolecular chemistry	Lecture with videos	Evaluation through class test and group discussion  Formative assessment I
	2	Crown ethers - synthesis and properties Crown ethers - Applications Lariat ethers.	3	Explain the applications of crown ethers	Lecture with ppt and videos	

	3	Podants - properties 3-dimensional podants Cryptands - synthesis, properties and applications. Spherands - synthesis, structure and uses.	4	Describe the properties and applications of podants, cryptands and spherands	Lecture and group discussion	
	4	Supramolecular chemistry of fullerenes Supramolecular photochemistry.	2	Explain supramolecular photochemistry	Lecture and seminar	
	5	Molecular devices - non- linear optical switches Molecular devices - electrophoto switching Molecular devices - Liquid crystal display.	3	Understand the types and applications of molecular devices	Lecture with videos	
<b>IV</b>	<b>Medicinal Chemistry</b>					
	1	Anti-neoplastic agents - classification and synthesis Assay of cyclophosphamide Assay of chlorambucil.	3	Identify anti-neoplastic agents	Lecture	Evaluation through class test  Formative assessment III
	2	Antimalarial drugs - Classification and synthesis Assay of chloroquine Assay of primaquine.	3	List out the classification and the assay of antimalarial drugs	Seminar	
	3	Diuretics - Classification, synthesis Assay of Frusemide Assay of benzthiazide.	3	Explain the classification and the assay of diuretics	Seminar	
	4	Anti-inflammatory drugs - synthesis and therapeutic action of phenylbutazone Synthesis and therapeutic action of Ibuprofen.	2	Understand the therapeutic action of anti-inflammatory drugs	Lecture	
	5	Antipyretics Non-narcotic analgesics.	2	Know about antipyretics and analgesics	Seminar	
	6	Synthesis and therapeutic action of paracetamol Synthesis and therapeutic action of aspirin.	2	Describe the synthesis and therapeutic action of paracetamol and aspirin		

V	<b>Biophysical Chemistry</b>					
	1	Thermodynamics in biology - limitations of equilibrium thermodynamics Irreversible thermodynamics - Postulates and methodologies. Onsager reciprocal theory Irreversible thermodynamics and biological systems.	4	Explain thermodynamics in biological systems	Lecture	Evaluation through class test  Formative assessment II
	2	Energy flux biochemical standard state ATP ATP Currency of energy - Oxidative phosphorylation.	4	Understand energy flux and oxidative phosphorylation	Lecture and seminar	
	3	Role of Singlet Oxygen in biology Reactions in biomolecules- membrane potential Reactions in biomolecules-ion pumps.	3	Describe the reactions in biomolecules	Lecture	
	4	Photoacoustic effect Photoacoustic effect - Applications in biology.	2	Apply photoacoustic effect in biology	Lecture with ppt	
	5	Biophysical applications of Mossbauer effect NMR imaging - Applications of spin labeling in membrane research.	2	Explain the biophysical application of Mossbauer effect NMR imaging	Lecture with videos	

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