

**GOVERNMENT COLLEGE FOR WOMEN (AUTONOMOUS) KUMBAKONAM**  
**(Curriculum – M.Sc., Chemistry– 2023 - 2024)**  
**Programme Code: PSCH**  
**SEMESTER – I**

Department : Chemistry

Part	Course type	Course Code	Title of the Course	Hrs/ Week	Credits	Exam Hrs	Marks		
							CIA	ESE	Total
Part-I	CC- I	P23CHC101	Organic Reaction Mechanism-I	6	5	3	25	75	100
	CC – II	P23CHC102	Structure and Bonding in Inorganic Compounds	6	5	3	25	75	100
	CC – III	P23CHC103P	Organic Chemistry Practical	6	3	3	40	60	100
	EC - I	P23CHDE1	1.Polymer chemistry	5	4	3	25	75	100
			2. Nanomaterials and Nanotechnology						
	EC - II	P23CHDE3	1.Electrochemistry	5	3	3	25	75	100
2.Molecular Spectroscopy									
Part II	SEC- I	P23CH1SE1	Cosmetic Chemistry	2	2	3	25	75	100
<b>Total</b>				<b>30</b>	<b>22</b>				<b>600</b>

**SEMESTER – II**

Part	Course type	Course Code	Title of the Course	Hrs/ Week	Credits	Exam Hrs	Marks		
							CIA	ESE	Total
Part-I	CC- IV	P23CHC204	Organic Reaction Mechanism - II	6	5	3	25	75	100
	CC – V	P23CHC205	Physical Chemistry –I	6	5	3	40	60	100
	CC – VI	P23CHC206	Inorganic Chemistry Practical	6	3	3	25	75	100
	EC - III	P23CHDE5	1. Medicinal Chemistry	5	4	3	25	75	100
			2. Green Chemistry						
	EC - IV	P23CHDE7	1. Bio Inorganic Chemistry	5	3	3	25	75	100
2. Material Science									
Part II	SEC- II	P23CH2SE2	Basic Clinical Chemistry	2	2	3	25	75	100
	ECC-I		MOOCs/ Swayam courses						
			Internship / Industrial training*	--	--	--	--	--	--
<b>Total</b>				<b>30</b>	<b>22</b>				<b>600</b>

**Internship/ Industrial training during summer vacation.The credits shall be awarded in semester III statement of marks**

**SEMESTER – III**

Part	Course type	Course Code	Title of the Course	Hrs/ Week	Credits	Exam Hrs	Marks		
							CIA	ESE	Total
Part-I	CC- VII		Organic synthesis and photochemistry	6	6	3	25	75	100
	CC –VIII		Physical Chemistry - II	6	5	3	25	75	100
	CC – IX		<b>Core Industry Module</b> Industrial Chemistry	6	5	3	25	75	100
	CC - X		Physical chemistry Practical	6	3	6	40	60	100
	EC - V		1.Biomolecules and Heterocyclic Compounds 2.Pharmacognosy and Phyto chemistry	4	3	3	25	75	100
Part II	SEC- III		Food Chemistry	2	2	3	25	75	100
	ECC- II		MOOCS /Swayam courses	-	2/3	-	-	-	-
	AEC		Internship / Industrial training	-	2	-	-	-	-
<b>Total</b>				<b>30</b>	<b>26</b>				

**SEMESTER – IV**

Part	Course type	Course Code	Title of the Course	Hrs/ Week	Credits	Exam Hrs	Marks		
							CIA	ESE	Total
Part-I	CC- XI		Coordination chemistry	6	6	3	25	75	100
	CC – XII		Analytical Instrumentation Techniques- Practical	6	3	3	40	60	100
	CC – XIII		Project with Viva Voce	8	5	-	-	-	100
	EC – VI		Industry / entrepreneurship based 20% theory 80% practical  1. Textile Chemistry practical 2 .Water Analysis Practical	5	4	3	40	60	100
	AEC II		Professional competency skills	5	2	3	25	75	100
Part II	EA		Extension Activity	-	1	-	-	-	-
<b>Total</b>				<b>30</b>	<b>21</b>				<b>500</b>

**Elective courses offered by the Department of Chemistry**

<b>S.no</b>	<b>Title of the Paper</b>	<b>Credits</b>
<b>1.</b>	Polymer chemistry	<b>4</b>
	Nanomaterials and Nanotechnology	<b>4</b>
<b>2.</b>	Electrochemistry	<b>3</b>
	Molecular Spectroscopy	<b>3</b>
<b>3.</b>	Medicinal Chemistry	<b>4</b>
	Green Chemistry	<b>4</b>
<b>4.</b>	Bio Inorganic Chemistry	<b>3</b>
	Material Science	<b>3</b>
<b>5.</b>	Biomolecules and Heterocyclic Compounds	<b>3</b>
	Pharmacognosy and Phyto Chemistry	<b>3</b>
<b>6.</b>	Industry / entrepreneurship based 20% theory 80% practical 1. Textile Chemistry practical 2. Water Analysis Practical	<b>4</b>

<b>SEMESTER I</b> <b>CORE COURSE I -</b> <b>ORGANIC REACTION</b> <b>MECHANISM – I</b>	<b>SUB CODE:P23CHC101</b>
------------------------------------------------------------------------------------------------	---------------------------

**Objectives of the course**

- To understand the feasibility and the mechanism of various organic reactions.
- To comprehend the techniques in the determination of reaction mechanisms.
- To understand the concept of stereochemistry involved in organic compounds.
- To correlate and appreciate the differences involved in the various types of organic reaction mechanisms.
- To design feasible synthetic routes for the preparation of organic compounds.

**UNIT-I: Methods of Determination of Reaction Mechanism:** Reaction intermediates, The transition state, Reaction coordinate diagrams, Thermodynamic and kinetic requirements of reactions: Hammond postulate. Methods of determining mechanism: non-kinetic methods - product analysis, determination of intermediates-isolation, detection, and trapping. Cross-over experiments, isotopic labelling, isotope effects and stereochemical evidences. Kinetic methods - relation of rate and mechanism. Effect of structure on reactivity: Hammett and Taft equations. Linear free energy relationship, partial rate factor, substituent and reaction constants.

**UNIT-II: Aromatic and Aliphatic Electrophilic Substitution:** Aromaticity: Aromaticity in benzenoid, non-benzenoid, heterocyclic compounds and annulenes. Aromatic electrophilic substitution: Orientation and reactivity of di- and polysubstituted phenol, nitrobenzene and halobenzene. Reactions involving nitrogen electrophiles: nitration, nitrosation and diazonium coupling; Sulphur electrophiles: sulphonation; Halogen electrophiles: chlorination and bromination; Carbon electrophiles: Friedel-Crafts alkylation, acylation and arylation reactions. Aliphatic electrophilic substitution Mechanisms:  $S_E2$  and  $S_Ei$ ,  $S_E1$ - Mechanism and evidences.

**UNIT-III: Aromatic and Aliphatic Nucleophilic Substitution:** Aromatic nucleophilic substitution: Mechanisms -  $S_NAr$ ,  $S_N1$  and Benzyne mechanisms -

Evidences - Reactivity, Effect of structure, leaving group and attacking nucleophile. Reactions: Oxygen and Sulphur-nucleophiles, Bucherer and Rosenmund reactions, von Richter, Sommelet- Hauser and Smiles rearrangements.  $S_N1$ , ion pair,  $S_N2$  mechanisms and evidences. Aliphatic nucleophilic substitutions at an allylic carbon, aliphatic trigonal carbon and vinyl carbon.  $S_N1$ ,  $S_N2$ ,  $S_Ni$ , and  $S_E1$  mechanism and evidences, Swain- Scott, Grunwald-Winstein relationship - Ambident nucleophiles.

**UNIT-IV: Stereochemistry-I:** Introduction to molecular symmetry and chirality – axis, plane, center, alternating axis of symmetry. Optical isomerism due to asymmetric and dissymmetric molecules with C, N, S based chiral centers. Optical purity, prochirality, enantiotopic and diastereotopic atoms, groups, faces, axial and planar chirality, chirality due to helical shape, methods of determining the configuration. Racemic modifications: Racemization by thermal, anion, cation, reversible formation, epimerization, mutarotation. D, L system, Cram's and Prelog's rules: R, S-notations, proR, proS, side phase and re phase Cahn-Ingold-Prelog rules, absolute and relative configurations. Configurations of allenes, spiranes, biphenyls, cyclooctene, helicene, binaphthyls, ansa and cyclophanic compounds, exo-cyclic alkylidene-cycloalkanes. Topicity and prostereoisomerism, chiral shift reagents and chiral solvating reagents. Criteria for optical purity: Resolution of racemic modifications, asymmetric transformations, asymmetric synthesis, destruction. Stereoselective and stereospecific synthesis.

**UNIT-V: Stereochemistry-II:** Conformation and reactivity of acyclic systems, intramolecular rearrangements, neighbouring group participation, chemical consequence of conformational equilibrium - Curtin-Hammett Principle. Stability of five and six-membered rings: mono-, di- and polysubstituted cyclohexanes, conformation and reactivity in cyclohexane systems. Fused and bridged rings: bicyclic, poly cyclic systems, decalins and Brett's rule. Optical rotation and optical rotatory dispersion, conformational asymmetry, ORD curves, octant rule, configuration and conformation, Cotton effect, axial haloketone rule and determination of configuration.

**Recommended Text Books**

1. J. March and M. Smith, Advanced Organic Chemistry, 5<sup>th</sup> edition, John-Wiley and Sons.2001.
2. E. S. Gould, Mechanism and Structure in Organic Chemistry, Holt,

Rinehart and Winston Inc., 1959.

3. P.S.Kalsi, Stereochemistry of carbon compounds, 8<sup>th</sup> edition, New Age International Publishers, 2015.
4. P. Y. Bruice, Organic Chemistry, 7<sup>th</sup> edn, Prentice Hall, 2013.
5. J. Clayden, N. Greeves, S. Warren, Organic Compounds, 2<sup>nd</sup> edition, Oxford University Press, 2014

#### Reference Books

1. F.A. Carey and R.J. Sundberg, Advanced Organic Chemistry Part-A and B, 5<sup>th</sup> edition, Kluwer Academic / Plenum Publishers, 2007.
2. D. G. Morris, Stereochemistry, RSC Tutorial Chemistry Text 1, 2001.
3. N.S. Isaacs, Physical Organic Chemistry, ELBS, Longman, UK, 1987.
4. E. L. Eliel, Stereochemistry of Carbon Compounds, Tata-McGraw Hill, 2000.
5. I. L. Finar, Organic chemistry, Vol-1 & 2, 6<sup>th</sup> edition, Pearson Education Asia, 2004.

#### Website & E learning source

1. <https://sites.google.com/site/chemistrybookscollection02/home/organic-chemistry/organic>
2. <https://www.organic-chemistry.org/>

#### Course Learning Outcomes (for Mapping with POs and PSOs)

Students will be able

- CLO1:** To recall the basic principles of organic chemistry.
- CLO2:** To understand the formation and detection of reaction intermediates of organic reactions.
- CLO3:** To predict the reaction mechanism of organic reactions and stereochemistry of organic compounds.
- CLO4:** To apply the principles of kinetic and non-kinetic methods to determine the mechanism of reactions.
- CLO5:** To design and synthesize new organic compounds by correlating the stereochemistry of organic compounds

#### COURSE MAPPING CO -PO

CO /PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO 10
CO 1	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
CO 2	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
CO 3	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
CO 4	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
CO 5	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓

#### COURSE MAPPING CO -PSO

CO /PSO	PSO1	PSO2	PSO3	PSO4	PSO5
CO1	✓	✓	✓	✓	✓
CO2	✓	✓	✓	✓	✓
CO3	✓	✓	✓	✓	✓
CO4	✓	✓	✓	✓	✓
CO5	✓	✓	✓	✓	✓

<b>CORE COURSE II- STRUCTURE AND BONDING IN INORGANIC COMPOUNDS</b>	<b>SUB CODE:P23CHC102</b>
-----------------------------------------------------------------------------	---------------------------

### Objectives of the course

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

**UNIT-I: Structure of main group compounds and clusters:** VB theory – Effect of lone pair and electronegativity of atoms (Bent's rule) on the geometry of the molecules; 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. Structure of silicones, Structural and bonding features of B-N, S-N and P-N compounds; Poly acids – types, examples and structures; Borane cluster: Structural features of closo, nido, arachano and klado; carboranes, hetero and metalloboranes; Wade's rule to predict the structure of borane cluster; main group clusters – zintl ions and mno rule.

**UNIT-II: Solid state chemistry – I:** Ionic crystals: Packing of ions in simple, hexagonal and cubic close packing, voids in crystal lattice, Radius ratio, Crystal systems and Bravais lattices, Symmetry operations in crystals, glide planes and screw axis; point group and space group; Solid state energetics: Lattice energy – Born-Landé equation - Kapustinski equation, Madelung constant.

**UNIT-III: Solid state chemistry – II:** Structural features of the crystal systems: Rock salt, zinc blende & wurtzite, fluorite and anti-fluorite, rutile and anatase, cadmium iodide and nickel arsenide; Spinels -normal and inverse types and perovskite structures. Crystal Growth methods: From melt and solution (hydrothermal, sol-gel methods) – principles and examples.

**UNIT-IV: Techniques in solid state chemistry:** X-ray diffraction technique: Bragg's law, Powder diffraction method – Principle and Instrumentation; Interpretation of XRD data – JCPDS files, Phase purity, Scherrer formula, lattice constants calculation; Systematic absence of reflections; Electron diffraction technique – principle, instrumentation and application. Electron microscopy – difference between optical and electron microscopy, theory, principle, instrumentation, sampling methods and applications of SEM and TEM.

### UNIT-V: Band theory and defects in solids

Band theory – features and its application of conductors, insulators and semiconductors, Intrinsic and extrinsic semiconductors; Defects in crystals – point defects (Schottky, Frenkel, metal excess and metal deficient) and their effect on the electrical and optical property, laser and phosphors; Linear defects and its effects due to dislocations.

### Recommended Text

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

### Reference Books

1. D. E. Douglas, D.H. McDaniel and J. J. Alexander, Concepts and Models in Inorganic Chemistry, 3rd Ed, 1994.
2. R J D Tilley, Understanding Solids - The Science of Materials, 2<sup>nd</sup> edition, Wiley Publication, 2013.
3. C N R Rao and J Gopalakrishnan, New Directions in Solid State Chemistry, 2<sup>nd</sup> Edition, Cambridge University Press, 199.
4. T. Moeller, Inorganic Chemistry, A Modern Introduction; John Wiley: New York, 1982.

5. D. F. Shriver, P. W. Atkins and C.H. Langford; Inorganic Chemistry; 3rd ed.; Oxford University Press: London, 2001.

**Website and e-learning source**

[https://ocw.mit.edu/courses/3-091-introduction-to-solid-state-chemistry-fall-2018/video\\_galleries/lecture-videos/](https://ocw.mit.edu/courses/3-091-introduction-to-solid-state-chemistry-fall-2018/video_galleries/lecture-videos/)

CO3	✓	✓	✓	✓	✓
CO4	✓	✓	✓	✓	✓
CO5	✓	✓	✓	✓	✓

**Course Learning Outcomes (for Mapping with POs and PSOs)**

Students will be able

**CO1:** Predict the geometry of main group compounds and clusters.

**CO2:** Explain about the packing of ions in crystals and apply the radius ratio rule to predict the coordination number of cations.

**CO3:** Understand the various types of ionic crystal systems and analyze their structural features.

**CO4:** Explain the crystal growth methods.

**CO5:** To understand the principles of diffraction techniques and microscopic techniques.

**CO-PO Mapping**

CO/ PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO 10
CO 1	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
CO 2	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
CO 3	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
CO 4	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
CO 5	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓

**CO-PSO Mapping**

CO /PO	PSO1	PSO2	PSO3	PSO4	PSO5
CO1	✓	✓	✓	✓	✓
CO2	✓	✓	✓	✓	✓

<b>CORE COURSE-III - ORGANIC CHEMISTRY PRACTICAL</b>	<b>SUB CODE:P23CHC103P HOURS : CREDITS:</b>
------------------------------------------------------	-----------------------------------------------------

### Objectives of the course

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

### UNIT-I: Separation and analysis:

- A. Two component mixtures
- B. Three component mixtures.

### UNIT-II: Estimations:

- a) Estimation of Phenol (bromination)
- b) Estimation of Aniline (bromination)
- c) Estimation of Ethyl methyl ketone (iodimetry)
- d) Estimation of Glucose (redox)
- e) Estimation of Ascorbic acid (iodimetry)
- f) Estimation of Aromatic nitro groups (reduction)
- g) Estimation of Glycine (acidimetry)
- h) Estimation of Formalin (iodimetry)
- i) Estimation of Acetyl group in ester (alkalimetry)
- j) Estimation of Hydroxyl group (acetylation)
- k) Estimation of Amino group (acetylation)

### UNIT-III: Two stage preparations:

- a) *p*-Bromoacetanilide from aniline
- b) *p*-Nitroaniline from acetanilide
- c) 1,3,5-Tribromobenzene from aniline

- d) Acetyl salicylic acid from methyl salicylate
- e) Benzilic acid from benzoin
- f) *m*-Nitroaniline from nitrobenzene
- g) *m*-Nitrobenzoic acid from methyl benzoate

### Recommended Text

1. A R West, Solid state Chemistry and its applications, 2nd Edition (Students Edition), John Wiley & Sons Ltd., 2014.
2. A K Bhagi and G R Chatwal, A textbook of inorganic polymers, Himalaya Publishing House, 2001.
3. L Smart, E Moore, Solid State Chemistry – An Introduction, 4<sup>th</sup> Edition, CRC Press, 2012.

### Reference Books

1. D. E. Douglas, D.H. McDaniel and J. J. Alexander, Concepts and Models in Inorganic Chemistry, 3rd Ed, 1994.
2. R J D Tilley, Understanding Solids - The Science of Materials, 2<sup>nd</sup> edition, Wiley Publication, 2013.
3. C N R Rao and J Gopalakrishnan, New Directions in Solid State Chemistry, 2<sup>nd</sup> Edition, Cambridge University Press, 199.

### Website and e-learning source

[https://ocw.mit.edu/courses/3-091-introduction-to-solid-state-chemistry-fall-2018/video\\_galleries/lecture-videos/](https://ocw.mit.edu/courses/3-091-introduction-to-solid-state-chemistry-fall-2018/video_galleries/lecture-videos/)

### Course Learning Outcomes (for Mapping with POs and PSOs)

Students will be able:

**CO1:** To recall the basic principles of organic separation, qualitative analysis and preparation.

**CO2:** To explain the method of separation and analysis of separated organic mixtures and convert them as derivatives by suitable preparation method.

**CO3:** To determine the characteristics of separation of organic compounds by various chemical reactions.

**CO4:** To develop strategies to separate, analyze and prepare organic compounds.

**CO5:**To formulate a method of separation, analysis of organic mixtures and design suitable procedure for organic preparations.

**COURSE MAPPING CO -PO**

CO /PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO 10
CO 1	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
CO 2	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
CO 3	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
CO 4	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
CO 5	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓

**COURSE MAPPING CO -PSO**

CO /PSO	PSO1	PSO2	PSO3	PSO4	PSO5
CO1	✓	✓	✓	✓	✓
CO2	✓	✓	✓	✓	✓
CO3	✓	✓	✓	✓	✓
CO4	✓	✓	✓	✓	✓
CO5	✓	✓	✓	✓	✓

<b>ELECTIVE I (CHOICE-I) POLYMER CHEMISTRY</b>	<b>SUB CODE:P23CHDE1 HOURS:5 CREDITS:4</b>
----------------------------------------------------	----------------------------------------------------

### Objectives of the course

- To learn the basic concepts and bonding in polymers.
- To explain various types of polymerization reactions and kinetics.
- To understand the importance of industrial polymers and their synthetic uses.
- To determine the molecular weight of polymers.
- To predict the degradation of polymers and conductivities.

### UNIT-I: Characterization, Molecular weight and its Determination:

Primary and secondary bond forces in polymers; cohesive energy, molecular structure, chemical tests, thermal methods,  $T_g$ , molecular distribution, stability. Determination of Molecular mass of polymers: Number Average molecular mass ( $M_n$ ) and Weight average molecular mass ( $M_w$ ) of polymers. Molecular weight determination of high polymers by physical and methods.

**UNIT-II: Mechanism and kinetics of Polymerization:** Chain growth polymerization: Cationic, anionic, free radical polymerization, Stereo regular polymers: Ziegler Natta polymerization. Reaction kinetics. Step growth polymerization, Degree of polymerization.

**UNIT-III: Techniques of Polymerization and Polymer Degradation:** Bulk, Solution, Emulsion, Suspension, solid, interfacial and gas phase polymerization. Types of Polymer Degradation, Thermal degradation, mechanical degradation, photodegradation, Photostabilizers, Solid and gas phase polymerization.

**UNIT-IV: Industrial Polymers:** Preparation of fibre forming polymers, elastomeric material. Thermoplastics: Polyethylene, Polypropylene, polystyrene, Polyacrylonitrile, Polyvinyl Chloride, Poly tetrafluoro ethylene, nylon and polyester. Thermosetting

Plastics: Phenol formaldehyde and epoxidized resin. Elastomers: Natural rubber and synthetic rubber - Buna - N, Buna-S and neoprene. Conducting Polymers: Elementary ideas; examples: poly sulphur nitriles, polyphenylene, poly pyrrole and polyacetylene. Polymethylmethacrylate, polyimides, polyamides, polyurethanes, polyureas, polyethylene and polypropylene glycols.

**UNIT-V: Polymer Processing:** Compounding: Polymer Additives: Fillers, Plasticizers, antioxidants, thermal stabilizers, fire retardants and colourants. Processing Techniques: Calendaring, die casting, compression moulding, injection moulding, blow moulding and reinforcing. Film casting, Thermofoaming, Foaming. Catalysis and catalysts – Polymerization catalysis, catalyst support, clay compounds, basic catalyst, auto-exhaust catalysis, vanadium, heterogeneous catalysis and active centres.

### Recommended Text

1. V.R. Gowariker, *Polymer Science*, Wiley Eastern, 1995.
2. G.S. Misra, *Introductory Polymer Chemistry*, New Age International (Pvt) Limited, 1996.
3. M.S. Bhatnagar, *A Text Book of Polymers*, vol-I & II, S.Chand & Company, New Delhi, 2004.

### Reference Books

1. F. N. Billmeyer, *Textbook of Polymer Science*, Wiley Interscience, 1971.
2. A. Kumar and S. K. Gupta, *Fundamentals and Polymer Science and Engineering*, Tata McGraw-Hill, 1978.

### Course Learning Outcomes (for Mapping with POs and PSOs)

Students will be able:

- CO1: To understand the bonding in polymers.  
 CO2: To scientifically plan and perform the various polymerization reactions.  
 CO3: To observe and record the processing of polymers.  
 CO4: To calculate the molecular weight by physical and chemical methods.  
 CO5: To interpret the experimental data scientifically to improve the quality of synthetic polymers.

**COURSE MAPPING CO -PO**

CO /PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO 10
CO 1	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
CO 2	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
CO 3	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
CO 4	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
CO 5	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓

**COURSE MAPPING CO -PSO**

CO /PSO	PSO1	PSO2	PSO3	PSO4	PSO5
CO1	✓	✓	✓	✓	✓
CO2	✓	✓	✓	✓	✓
CO3	✓	✓	✓	✓	✓
CO4	✓	✓	✓	✓	✓
CO5	✓	✓	✓	✓	✓

<b>ELECTIVE I (CHOICE-II)</b>	<b>SUB CODE:P23CHDE2</b>
<b>NANO MATERIALS AND NANOTECHNOLOGY</b>	<b>HOURS:5</b>
	<b>CREDITS:4</b>

### Objectives of the course

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

**UNIT-I:** Introduction of nanomaterials and nanotechnologies, Introduction-role of size, classification-0D, 1D, 2D, 3D. Synthesis-Bottom –Up, Top–Down, consolidation of Nano powders. Features of nanostructures, Background of nanostructures. Techniques of synthesis of nanomaterials, Tools of the nanoscience. Applications of nanomaterials and technologies.

**UNIT-II:** Bonding and structure of the nanomaterials, Predicting the Type of Bonding in a Substance crystal structure. Metallic nanoparticles, Surfaces of Materials, Nanoparticle Size and Properties. Synthesis- Physical and chemical methods - inert gas condensation, arc discharge, laser ablation, sol-gel, solvothermal and hydrothermal-CVD-types, metallo organic, plasma enhanced, and low-pressure CVD. Microwave assisted and electrochemical synthesis.

**UNIT-III:** Mechanical properties of materials, theories relevant to mechanical properties. Techniques to study mechanical properties of nanomaterials, adhesion and friction, thermal properties of nanomaterials Nanoparticles: gold

and silver, metal oxides: silica, iron oxide and alumina - synthesis and properties.

**UNIT-IV:** Electrical properties, Conductivity and Resistivity, Classification of Materials based on Conductivity, magnetic properties, electronic properties of materials. Classification of magnetic phenomena. Semiconductor materials – classification-Ge, Si, GaAs, SiC, GaN, GaP, CdS, PbS. Identification of materials as p and n –type semiconductor-Hall effect - quantum and anomalous, Hall voltage - interpretation of charge carrier density. Applications of semiconductors: p-n junction as transistors and rectifiers, photovoltaic and photogalvanic cell.

**UNIT-V:** Nano thin films, nanocomposites. Application of nanoparticles in different fields. Core-shell nanoparticles-types, synthesis, and properties. Nanocomposites-metal-, ceramic-and polymer-matrix composites-applications. Characterization– SEM, TEM and AFM - principle, instrumentation and applications.

### Recommended Text

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

### Reference Books

1. S.Mohan and V. Arjunan, Principles of Materials Science, MJP Publishers, 2016.
2. Arumugam, Materials Science, Anuradha Publications, 2007.
3. Giacavazzo et. al., Fundamentals of Crystallography, International Union

- of Crystallography. Oxford Science Publications, 2010
4. Woolfson, An Introduction to Crystallography, Cambridge University Press, 2012.
  5. James F. Shackelford and Madanapalli K. Muralidhara, Introduction to Materials Science for Engineers. 6<sup>th</sup> ed., PEARSON Press, 2007.

**Website and e-learning source**

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

CO /PSO	PSO1	PSO2	PSO3	PSO4	PSO5
CO1	✓	✓	✓	✓	✓
CO2	✓	✓	✓	✓	✓
CO3	✓	✓	✓	✓	✓
CO4	✓	✓	✓	✓	✓
CO5	✓	✓	✓	✓	✓

**Course Learning Outcomes (for Mapping with POs and PSOs)**

Students will be able:

**CO1:** To explain methods of fabricating nanostructures.

**CO2:** To relate the unique properties of nanomaterials to reduce dimensionality of the material.

**CO3:** To describe tools for properties of nanostructures.

**CO4:** To discuss applications of nanomaterials.

**CO5:** To understand the health and safety related to nanomaterial.

**COURSE MAPPING CO -PO**

CO /PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO 10
CO 1	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
CO 2	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
CO 3	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
CO 4	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
CO 5	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓

**COURSE MAPPING CO -PSO**

<b>ELECTIVE COURSE II (CHOICE-I) ELECTROCHEMISTRY</b>	<b>SUB CODE:P23CHDE3 HOURS: CREDITS:3</b>
-------------------------------------------------------	---------------------------------------------------

### Objectives of the course

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

**UNIT-I: Ionics:** Arrhenius theory -limitations, van't Hoff factor and its relation to colligative properties. Deviation from ideal behavior. Ionic activity, mean ionic activity and mean ionic activity coefficient-concept of ionic strength, Debye Huckel theory of strong electrolytes, activity coefficient of strong electrolytes Determination of activity coefficient ion solvent and ion-ion interactions. Born equation. Debye-Huckel Bjerrum model. Derivation of Debye-Huckel limiting law at appreciable concentration of electrolytes modifications and applications. Electrolytic conduction-Debye-Huckel Onsager treatment of strong electrolyte-qualitative and quantitative verification and limitations. Evidence for ionic atmosphere. Ion association and triple ion formations.

**UNIT-II: Electrode-electrolyte interface:** Interfacial phenomena -Evidences for electrical double layer, polarizable and non-polarizable interfaces, Electrocapillary phenomena - Lippmann equation electro capillary curves. Electro-kinetic phenomena electro-osmosis, electrophoresis, streaming and sedimentation potentials, colloidal and poly electrolytes. Structure of double layer: Helmholtz -Perrin, Guoy- Chapman and Stern models of electrical double layer. Zeta potential and potential at zero charge. Applications and limitations.

**UNIT-III: Electrodicts of Elementary Electrode Reactions:** Behavior of electrodes: Standard electrodes and electrodes at equilibrium. Anodic and Cathodic currents, condition for the discharge of ions. Nernst equation, polarizable and non-polarizable electrodes. Model of three electrode system, over potential. Rate of electro chemical reactions: Rates of simple elementary reactions. Butler-Volmer equation-significance of exchange current density, net current density and symmetry factor. Low and high field approximations. symmetry factor and transfer coefficient Tafel equations and Tafel plots.

**UNIT-IV: Electrodicts of Multistep Multi Electron System:** Rates of multi-step electrode reactions, Butler - Volmer equation for a multi-step reaction. Rate determining step, electrode polarization and depolarization. Transfer coefficients, its significance and determination, Stoichiometric number. Electro-chemical reaction mechanisms-rate expressions, order, and surface coverage. Reduction of  $I^3^-$ ,  $Fe^{2+}$ , and dissolution of Fe to  $Fe^{2+}$ . Overvoltage - Chemical and electro chemical, Phase, activation and concentration over potentials. Evolution of oxygen and hydrogen at different pH. Pourbiach and Evan's diagrams.

**UNIT-V: Concentration Polarization, Batteries and Fuel cells:** Modes of Transport of electro active species - Diffusion, migration and hydrodynamic modes. Role of supporting electrolytes. Polarography-principle and applications. Principle of square wave polarography. Cyclic voltammetry-anodic and cathodic stripping voltammetry and differential pulse voltammetry. Sodium and lithium-ion batteries and redox flow batteries. Mechanism of charge storage: conversion and alloying. Capacitors- mechanism of energy storage, charging at constant current and constant voltage. Energy production systems: Fuel Cells: classification, alkaline fuel cells, phosphoric acid fuel cells, high temperature fuel cells.

### Recommended Text

1. D. R. Crow, Principles and applications of electrochemistry, 4th edition, Chapman & Hall/CRC, 2014.
2. J. Rajaram and J.C. Kuriakose, Kinetics and Mechanism of chemical transformations Macmillan India Ltd., New Delhi, 2011.

- S. Glasstone, Electro chemistry, Affiliated East-West Press, Pvt., Ltd., New Delhi, 2008.
- B. Viswanathan, S. Sundaram, R. Venkataraman, K. Rengarajan and P.S. Raghavan, Electrochemistry-Principles and applications, S. Viswanathan Printers, Chennai, 2007.
- Joseph Wang, Analytical Electrochemistry, 2<sup>nd</sup> edition, Wiley, 2004.

#### Reference Books

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

#### Website and e-learning source

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

#### Course Learning Outcomes (for Mapping with POs and PSOs)

Students will be able:

**CO1:** To understand the behaviour of electrolytes in solution and compare the structures of electrical double layer of different models.

**CO2:** To predict the kinetics of electrode reactions applying Butler-Volmer and Tafel equations

**CO3:** To study different thermodynamic mechanism of corrosion,

**CO4:** To discuss the theories of electrolytes, electrical double layer, electroics and activity coefficient of electrolytes

**CO5:** To have knowledge on storage devices and electrochemical reaction mechanism.

#### COURSE MAPPING CO -PO

CO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO
----	-----	-----	-----	-----	-----	-----	-----	-----	-----	----

/PO											10
CO 1	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
CO 2	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
CO 3	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
CO 4	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
CO 5	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓

#### COURSE MAPPING CO -PSO

CO /PSO	PSO1	PSO2	PSO3	PSO4	PSO5
CO1	✓	✓	✓	✓	✓
CO2	✓	✓	✓	✓	✓
CO3	✓	✓	✓	✓	✓
CO4	✓	✓	✓	✓	✓
CO5	✓	✓	✓	✓	✓

<b>ELECTIVE COURSE II (CHOICE-II) - MOLECULAR SPECTROSCOPY</b>	<b>SUB CODE:P23CHDE4 HOURS:5 CREDITS:3</b>
----------------------------------------------------------------	----------------------------------------------------

#### Objectives of the course

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

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

**UNIT-II: Vibrational Spectroscopy:** Vibrations of molecules, harmonic and anharmonic oscillators- vibrational energy expression, energy level diagram, vibrational wave functions and their symmetry, selection rules, expression for the energies of spectral lines, computation of intensities, hot bands, effect of isotopic substitution. Diatomic vibrating rotor, vibrational-rotational spectra of diatomic molecules, P, R branches, breakdown of the Born-Oppenheimer approximation. Vibrations of polyatomic molecules – symmetry properties, overtone and combination frequencies. Influence of rotation on vibrational spectra of polyatomic molecule, P, Q, R branches, parallel and perpendicular vibrations of linear and symmetric top molecules.

**UNIT-III: Electronic spectroscopy:** Electronic Spectroscopy: Electronic spectroscopy of diatomic molecules, Frank-Condon principle, dissociation and predissociation spectra.  $\pi \rightarrow \pi^*$ ,  $n \rightarrow \pi^*$  transitions and their selection rules. Photoelectron Spectroscopy: Basic principles, photoelectron spectra of simple molecules, X-ray photoelectron spectroscopy (XPS). Lasers: Laser action, population inversion, properties of laser radiation, examples of simple laser systems.

**UNIT-IV: NMR and ESR spectroscopy:** Chemical shift, Factors influencing chemical shifts: electronegativity and electrostatic effects; Mechanism of shielding and deshielding. Spin systems: First order and second order coupling of AB systems, Simplification of complex spectra. Spin-spin interactions: Homonuclear coupling interactions - AX, AX<sub>2</sub>, AB types. Vicinal, germinal and long-range coupling-spin decoupling. Nuclear Overhauser effect (NOE), Factors influencing coupling constants and Relative intensities. <sup>13</sup>C NMR and structural correlations, Satellites. Brief introduction to 2D NMR – COSY, NOESY. Introduction to <sup>31</sup>P, <sup>19</sup>F NMR. ESR spectroscopy Characteristic features of ESR spectra, line shapes and line widths; ESR spectrometer. The g value and the hyperfine coupling parameter (A), origin of hyperfine interaction. Interpretation of ESR spectra and structure elucidation of organic radicals using ESR spectroscopy; Spin orbit coupling and significance of g-tensors, zero/non-zero field splitting, Kramer's degeneracy, application to transition metal complexes (having one to five unpaired electrons) including biological molecules and inorganic free radicals. ESR spectra of magnetically dilute samples.

**UNIT-V: Mass Spectrometry, EPR and Mossbauer Spectroscopy:** Ionization techniques- Electron ionization (EI), chemical ionization (CI), desorption ionization (FAB/MALDI), electrospray ionization (ESI), isotope abundance, molecular ion, fragmentation processes of organic molecules, deduction of structure through mass spectral fragmentation, high resolution. Effect of isotopes on the appearance of mass spectrum. EPR spectra of anisotropic systems - anisotropy in g-value, causes of anisotropy, anisotropy in hyperfine coupling, hyperfine splitting caused by quadrupole nuclei. Zero-field splitting (ZFS) and Kramer's degeneracy. Applications of EPR to

organic and inorganic systems. Structural elucidation of organic compounds by combined spectral techniques. Principle of Mossbauer spectroscopy: Doppler shift, recoil energy. Isomer shift, quadrupole splitting, magnetic interactions. Applications: Mossbauer spectra of high and low-spin Fe and Sn compounds.

### Recommended Text

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

### REFERENCE BOOKS

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

### Website and e-learning source

1. [https://onlinecourses.nptel.ac.in/noc20\\_cy08/preview](https://onlinecourses.nptel.ac.in/noc20_cy08/preview)
2. <https://www.digimat.in/nptel/courses/video/104106122/L14.html>

### Course Learning Outcomes (for Mapping with POs and PSOs)

Students will be able:

**CO1:** To understand the importance of rotational and Raman spectroscopy.

**CO2:** To apply the vibrational spectroscopic techniques to diatomic and polyatomic molecules.

**CO3:** To evaluate different electronic spectra of simple molecules using electronic spectroscopy.

**CO4:** To outline the NMR, <sup>13</sup>C NMR, 2D NMR – COSY, NOESY, Introduction to <sup>31</sup>P, <sup>19</sup>F NMR and ESR spectroscopic techniques.

**CO5:** To develop the knowledge on principle, instrumentation and structural elucidation of simple molecules using Mass Spectrometry, EPR and Mossbauer Spectroscopy techniques.

### COURSE MAPPING CO -PO

CO /PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO 10
CO 1	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
CO 2	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
CO 3	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
CO 4	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
CO 5	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓

### COURSE MAPPING CO -PSO

CO /PSO	PSO1	PSO2	PSO3	PSO4	PSO5
CO1	✓	✓	✓	✓	✓
CO2	✓	✓	✓	✓	✓
CO3	✓	✓	✓	✓	✓
CO4	✓	✓	✓	✓	✓
CO5	✓	✓	✓	✓	✓

<b>SEC-I</b> <b>COSMETIC CHEMISTRY</b>	<b>SUB CODE:P23CHISE1</b> <b>HOURS:2</b> <b>CREDITS:2</b>
-------------------------------------------	-----------------------------------------------------------------

**Objectives of the course**

- To learn the chemistry involved in cosmetics, water purification and food.
- To prepare cosmetics, analyze water samples and identify the adulterants in food samples.

**UNIT-I** History of cosmetics, classification of cosmetics, professional image of self grooming, beauty and wellness.

**UNIT-II** Cosmetics emulsions: cream, cleansers, powders, moisturisers, sun screen, acne and anti aging creams. Chemical peels and peeling agents, lasers and light devices, Electro Chemistry, bath salts, gels, soaps, bubble baths and scrubs

**UNIT-III** Skin Care General Anatomy and Physiology of skin, Structure of skin, Growth and nutrition, dermal fillers Hair Care Structure of hair, growth of hair, Cosmetics used for hair – Shampoos, conditioners, Bleaches, hair dyes, hair gels, hair perms and hair relaxers/straighteners.

**UNIT-IV** Nail Care Structure of nail, cosmetics used for nail – Nail lacquer, nail polish remover, Manicure and Pedicure, nail care techniques.

**UNIT-V** Eye Care Cosmetics used for eye – eye brow pencil, eye liner, eye shadows, mascaras. Eye concealer and eye creams. Practical – Cosmetics Preparations

**Reference Books:-** • Perry Romanowski, Beginning Cosmetic Chemistry, Allured Pub Corp.2009. • Dr. Ramesh Kumari, Chemistry of Cosmetics, Prestige Publishers.

**COURSE OUTCOMES:**

CO1: Identify the types of cosmetics and learn about their chemistry

CO2: Articulate the ingredients present in personal care products and apply it in their preparation.

CO 3: Understand water purification process, food sources and analyze adulterants food.

**COURSE MAPPING CO -PO**

CO /PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO 10
CO 1	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
CO 2	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
CO 3	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓

**COURSE MAPPING CO -PSO**

CO /PSO	PSO1	PSO2	PSO3	PSO4	PSO5
CO1	✓	✓	✓	✓	✓
CO2	✓	✓	✓	✓	✓
CO3	✓	✓	✓	✓	✓

# **SEMESTER -II**

<b>CORE COURSE-IV- ORGANIC REACTION MECHANISM-II</b>	<b>SUB CODE:P23CHC204 HOURS:6 CREDITS:5</b>
------------------------------------------------------	-----------------------------------------------------

### Objectives of the course

- To understand the concept of aromaticity in benzenoid, non-benzenoid, heterocyclic and annulene compounds.
- To understand the mechanism involved in various types of organic reactions with evidences.
- To understand the applications of synthetically important reagents.
- To correlate the reactivity between aliphatic and aromatic compounds.
- To design synthetic routes for synthetically used organic reactions.

**UNIT-I: Elimination and Free Radical Reactions:** Mechanisms: E2, E1, and E1cB mechanisms. Syn- and anti-eliminations. Orientation of the double bond: Hoffmann and Saytzeff rules. Reactivity: Effect of substrate, attacking bases, leaving group and medium. Stereochemistry of eliminations in acyclic and cyclic systems, pyrolytic elimination. Long lived and short-lived radicals – Production of radicals by thermal and photochemical reactions, Detection and stability of radicals, characteristics of free radical reactions and free radical, reactions of radicals; polymerization, addition, halogenations, aromatic substitutions, rearrangements. Reactivity: Reactivity on aliphatic, aromatic substrates, reactivity in the attacking radical, effect of solvent.

**UNIT-II: Oxidation and Reduction Reactions:** Mechanisms: Direct electron transfer, hydride transfer, hydrogen transfer, displacement, addition-elimination, oxidative and reductive coupling reactions. Mechanism of oxidation reactions: Dehydrogenation by quinones, selenium dioxides, ferricyanide, mercuric acetate lead tetraacetate, permanganate, manganese dioxide, osmium tetroxide, oxidation of saturated hydrocarbons, alkyl groups, alcohols, halides and amines. Reactions involving cleavage of C-C bonds - cleavage of double bonds, oxidative decarboxylation, allylic oxidation, oxidation by chromium trioxide-pyridine, DMSO-Oxalyl chloride (Swern oxidation) and Corey-Kim oxidation, dimethyl sulphoxide- dicyclohexyl carbodiimide (DMSO-DCCD). Mechanism of reduction reactions: Wolff-

Kishner, Clemmenson, Rosenmund, reduction with Trialkyl and triphenyltin hydrides, McFadyen-Steven's reduction, Homogeneous hydrogenation, Hydroboration with cyclic systems, MPV and Bouveault-Blanc reduction.

**UNIT-III: Rearrangements:** Rearrangements to electron deficient carbon: Pinacol-pinacolone and semi-pinacolone rearrangements -applications and stereochemistry, Wagner-Meerwein, Demjanov, Dienone-phenol, Baker-Venkataraman, Benzilic acid and Wolff rearrangements. Rearrangements to electron deficient nitrogen: Hofmann, Curtius, Schmidt, Lossen, Beckmann and abnormal Beckmann rearrangements. Rearrangements to electron deficient oxygen: Baeyer-Villiger oxidation and Dakin rearrangements. Rearrangements to electron rich atom: Favorskii, Quasi-Favorskii, Stevens, [1,2]-Wittig and [2,3]-Wittig rearrangements. Fries and Photo Fries rearrangement. Intramolecular rearrangements – Claisen, abnormal Claisen, Cope, oxy-Cope Benzidine rearrangements.

**UNIT-IV: Addition to Carbon Multiple Bonds:** Mechanisms: (a) Addition to carbon-carbon multiple bonds- Addition reactions involving electrophiles, nucleophiles, free radicals, carbenes and cyclic mechanisms-Orientation and reactivity, hydrogenation of double and triple bonds, Michael reaction, addition of oxygen and Nitrogen; (b) Addition to carbon-hetero atom multiple bonds: Mannich reaction, acids, esters, nitrites, addition of Grignard reagents, Wittig reaction, Prins reaction. Stereochemical aspects of addition reactions. Addition to Carbon-Hetero atom Multiplebonds: Addition of Grignard reagents, organozinc and organolithium reagents to carbonyl and unsaturated carbonyl compounds. Mechanism of condensation reactions involving enolates –Stobbe reactions. Hydrolysis of esters and amides, ammonolysis of esters.

**UNIT-V: Reagents and Modern Synthetic Reactions:** Lithium diisopropylamine (LDA), Azobisisobutyronitrile (AIBN), Sodium cyanoborohydride (NaBH<sub>3</sub>CN), *meta*-Chloroperbenzoic acid (m-CPBA), Dimethyl aminopyridine (DMAP), n-Bu<sub>3</sub>SnD, Triethylamine (TEA), Diazobicyclo[5.4.0]undec-7-ene (DBU), Diisopropylazodicarboxylate (DIAD), Diethylazodicarboxylate (DEAD), *N*-bromosuccinimide (NBS), Trifluoroacetic acid (TFA), Tetramethyl piperidin-1-oxyl (TEMPO), Phenyltrimethylammonium tribromide (PTAB). Diazomethane and Zn-Cu, Diethyl maleate (DEM), Copper diacetylacetonate (Cu(acac)<sub>2</sub>), TiCl<sub>3</sub>, NaIO<sub>4</sub>, Pyridinium chlorochromate (PCC), Pyridinium dichromate (PDC),

Meisenheimer complex. Suzuki coupling, Heck reaction, Negishi reaction, Baylis-Hillman reaction.

#### Recommended Text

1. J. March and M. Smith, *Advanced Organic Chemistry*, 5th ed., John-Wiley and Sons, 2001.
2. E. S. Gould, *Mechanism and Structure in Organic Chemistry*, Holt, Rinehart and Winston Inc., 1959.
3. P. S. Kalsi, *Stereochemistry of carbon compounds*, 8<sup>th</sup> edn, New Age International Publishers, 2015.
4. P. Y. Bruice, *Organic Chemistry*, 7<sup>th</sup> edn., Prentice Hall, 2013.
5. R. T. Morrison, R. N. Boyd, S. K. Bhattacharjee *Organic Chemistry*, 7<sup>th</sup> edn., Pearson Education, 2010.

#### Reference Books

1. S. H. Pine, *Organic Chemistry*, 5<sup>th</sup> edn, McGraw Hill International Edition, 1987.
2. L. F. Fieser and M. Fieser, *Organic Chemistry*, Asia Publishing House, Bombay, 2000.
3. E. S. Gould, *Mechanism and Structure in Organic Chemistry*, Holt, Rinehart and Winston Inc., 1959.
4. T. L. Gilchrist, *Heterocyclic Chemistry*, Longman Press, 1989.
5. J. A. Joule and K. Mills, *Heterocyclic Chemistry*, 4<sup>th</sup> ed., John-Wiley, 2010.

#### Website and e-learning source

1. <https://sites.google.com/site/chemistrybookscollection02/home/organic-chemistry/organic>
2. <https://www.organic-chemistry.org/>

#### Course Learning Outcomes (for Mapping with POs and PSOs)

Students will be able:

**CO1:** To recall the basic principles of aromaticity of organic and heterocyclic compounds.

**CO2:** To understand the mechanism of various types of organic reactions.

**CO3:** To predict the suitable reagents for the conversion of selective organic compounds.

**CO4:** To correlate the principles of substitution, elimination, and addition reactions.

**CO5:** To design new routes to synthesis organic compounds.

#### COURSE MAPPING CO -PO

CO /PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO 10
CO 1	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
CO 2	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
CO 3	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
CO 4	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
CO 5	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓

#### COURSE MAPPING CO -PSO

CO /PSO	PSO1	PSO2	PSO3	PSO4	PSO5
CO1	✓	✓	✓	✓	✓
CO2	✓	✓	✓	✓	✓
CO3	✓	✓	✓	✓	✓
CO4	✓	✓	✓	✓	✓
CO5	✓	✓	✓	✓	✓

<b>CORE COURSE-V - PHYSICAL CHEMISTRY-I</b>	<b>SUB CODE:P23CHC205 HOURS:6 CREDITS:5</b>
---------------------------------------------	-----------------------------------------------------

### Objectives of the course

- To recall the fundamentals of thermodynamics and the composition of partial molar quantities.
- To understand the classical and statistical approach of the functions
- To compare the significance of Maxwell-Boltzman, Fermi-Dirac and Bose-Einstein
- To correlate the theories of reaction rates for the evaluation of thermodynamic parameters.
- To study the mechanism and kinetics of reactions.

**UNIT-I: Classical Thermodynamics:** Partial molar properties-Chemical potential, Gibb's- Duhem equation-binary and ternary systems. Determination of partial molar quantities. Thermodynamics of real gases - Fugacity-determination of fugacity by graphical and equation of state methods-dependence of temperature, pressure and composition. Thermodynamics of ideal and non-ideal binary mixtures, Duhem - Margulus equation applications of ideal and non-ideal mixtures. Activity and activity coefficients-standard states - determination-vapour pressure, EMF and freezing point methods.

**UNIT-II: Statistical thermodynamics:** Introduction of statistical thermodynamics concepts of thermodynamic and mathematical probabilities-distribution of distinguishable and non-distinguishable particles. Assemblies, ensembles, canonical particles. Maxwell - Boltzmann, Fermi Dirac & Bose-Einstein Statistics- comparison and applications. Partition functions-evaluation of translational, vibrational and rotational partition functions for monoatomic, diatomic and polyatomic ideal gases. Thermodynamic functions in terms of partition functions-calculation of equilibrium constants. Statistical approach to Thermodynamic properties: pressure, internal energy, entropy, enthalpy, Gibb's function, Helmholtz function residual entropy, equilibrium constants and equipartition principle. Heat capacity of mono and di atomic

gases-ortho and para hydrogen. Heat capacity of solids-Einstein and Debye models.

**UNIT-III: Irreversible Thermodynamics:** Theories of conservation of mass and energy entropy production in open systems by heat, matter and current flow, force and flux concepts. Onsager theory-validity and verification-Onsager reciprocal relationships. Electro kinetic and thermo mechanical effects-Application of irreversible thermodynamics to biological systems.

**UNIT-IV: Kinetics of Reactions:** Theories of reactions-effect of temperature on reaction rates, collision theory of reaction rates, Unimolecular reactions -Lindeman and Christiansen hypothesis- molecular beams, collision cross sections, effectiveness of collisions, Potential energy surfaces. Transition state theory-evaluation of thermodynamic parameters of activation-applications of ARRT to reactions between atoms and molecules, time and true order-kinetic parameter evaluation. Factors determine the reaction rates in solution - primary salt effect and secondary salt effect, Homogeneous catalysis- acid- base catalysis-mechanism of acid base catalyzed reactions-Bronsted catalysis law, enzyme catalysis-Michelis-Menton catalysis.

**UNIT-V: Kinetics of complex and fast reactions:** Kinetics of complex reactions, reversible reactions, consecutive reactions, parallel reactions, chain reactions. Chain reactions-chain length, kinetics of  $H_2 - Cl_2$  &  $H_2 - Br_2$  reactions (Thermal and Photochemical reactions) - Rice Herzfeld mechanism. Study of fast reactions-relaxation methods- temperature and pressure jump methods electric and magnetic field jump methods -stopped flow flash photolysis methods and pulse radiolysis. Kinetics of polymerization-free radical, cationic, anionic polymerization - Polycondensation.

### Recommended Text

1. J. Rajaram and J.C. Kuriacose, Thermodynamics for Students of Chemistry, 2nd edition, S.L.N.Chand and Co., Jalandhar, 1986.
2. I.M. Klotz and R.M. Rosenberg, Chemical thermodynamics, 6th edition, W.A. Benjamin Publishers, California, 1972.
3. M.C. Gupta, Statistical Thermodynamics, New Age International, Pvt. Ltd., New Delhi, 1995.
4. K.J. Laidler, Chemical Kinetics, 3rd edition, Pearson, Reprint - 2013.

5. J. Rajaram and J.C. Kuriokose, Kinetics and Mechanisms of chemical transformation, Macmillan India Ltd, Reprint - 2011.

#### Reference Books

1. D.A. Mcqurie And J.D. Simon, Physical Chemistry - A Molecular Approach, Viva Books Pvt. Ltd., New Delhi, 1999.
2. R.P. Rastogi and R.R. Misra, Classical Thermodynamics, Vikas Publishing, Pvt. Ltd., New Delhi, 1990.
3. S.H. Maron and J.B. Lando, Fundamentals of Physical Chemistry, Macmillan Publishers, New York, 1974
4. K.B. Ytsimiris, "Kinetic Methods of Analysis", Pergamon Press, 1996.
5. Gurdeep Raj, Phase rule, Goel Publishing House, 2011.

#### Website and e-learning source

1. <https://nptel.ac.in/courses/104/103/104103112/>
2. <https://bit.ly/3tL3GdN>

#### Course Learning Outcomes (for Mapping with POs and PSOs)

Students will be able:

**CO1:** To explain the classical and statistical concepts of thermodynamics.

**CO2:** To compare and correlate the thermodynamic concepts to study the kinetics of chemical reactions.

**CO3:** To discuss the various thermodynamic and kinetic determination.

**CO4:** To evaluate the thermodynamic methods for real gases and mixtures.

**CO5:** To compare the theories of reaction rates and fast reactions.

#### COURSE MAPPING CO -PO

CO /PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO 10
CO 1	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
CO 2	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
CO 3	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
CO 4	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓

CO 5	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
------	---	---	---	---	---	---	---	---	---	---

#### COURSE MAPPING CO -PSO

CO /PSO	PSO1	PSO2	PSO3	PSO4	PSO5
CO1	✓	✓	✓	✓	✓
CO2	✓	✓	✓	✓	✓
CO3	✓	✓	✓	✓	✓
CO4	✓	✓	✓	✓	✓
CO5	✓	✓	✓	✓	✓



3										
CO 4	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
CO 5	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓

**COURSE MAPPING CO-PSO**

CO /PSO	PSO1	PSO2	PSO3	PSO4	PSO5
CO1	✓	✓	✓	✓	✓
CO2	✓	✓	✓	✓	✓
CO3	✓	✓	✓	✓	✓
CO4	✓	✓	✓	✓	✓
CO5	✓	✓	✓	✓	✓

<b>ELECTIVE COURSE III (CHOICE-I) MEDICINAL CHEMISTRY</b>	<b>SUB CODE:P23CHDE5 HOURS:5 CREDITS:4</b>
-------------------------------------------------------------------	----------------------------------------------------

### Objectives of the course

- To study the chemistry behind the development of pharmaceutical materials.
- To gain knowledge on mechanism and action of drugs.
- To understand the need of antibiotics and usage of drugs.
- To familiarize with the mode of action of diabetic agents and treatment of diabetes.
- To identify and apply the action of various antibiotics.

**UNIT-I: Introduction to receptors:** Introduction, targets, Agonist, antagonist, partial agonist. Receptors, Receptor types, Theories of Drug – receptor interaction, Drug synergism, Drug resistance, physicochemical factors influencing drug action.

**UNIT-II: Antibiotics:** Introduction, Targets of antibiotics action, classification of antibiotics, enzyme-based mechanism of action, SAR of penicillins and tetracyclins, clinical application of penicillins, cephalosporin. Current trends in antibiotic therapy.

**UNIT-III: Antihypertensive agents and diuretics:** Classification of cardiovascular agents, introduction to hypertension, etiology, types, classification of antihypertensive agents, classification and mechanism of action of diuretics, Furosemide, Hydrochlorothiazide, Amiloride.

**UNIT-IV: Antihypertensive agents and diuretics:** Classification of cardiovascular agents, introduction to hypertension, etiology, types, classification of antihypertensive agents, classification and mechanism of action of diuretics, Furosemide, Hydrochlorothiazide, Amiloride.

**UNIT-V: Analgesics, Antipyretics and Anti-inflammatory Drugs:** Introduction, Mechanism of inflammation, classification and mechanism of

action and paracetamol, Ibuprofen, Diclofenac, naproxen, indomethacin, phenylbutazone and meperidine. Medicinal Chemistry of Antidiabetic Agents Introduction, Types of diabetics, Drugs used for the treatment, chemical classification, Mechanism of action, Treatment of diabetic mellitus. Chemistry of insulin, sulfonyl urea.

### Recommended Text

1. Wilson and Gisvold's textbook of organic medicinal and pharmaceutical chemistry,
2. Wilson, Charles Owens: Beale, John Marlowe; Block, John H, Lipincott William, 12th edition, 2011.
3. Graham L. Patrick, An Introduction to Medicinal Chemistry, 5th edition, Oxford University Press, 2013. JayashreeGhosh, A textbook of Pharmaceutical Chemistry, S.Chand and Co. Ltd, 1999, 1999 edn.
4. O.LeRoy, Natural and synthetic organic medicinal compounds, Ealemi, 1976. S.S.Ashutosh Kar, Medicinal Chemistry, Wiley Eastern Limited, New Delhi, 1993, New edn.

### Reference Books

1. Foye's Principles of Medicinal Chemistry, Lipincott Williams, Seventh Edition, 2012
2. Burger's Medicinal Chemistry, Drug Discovery and Development, Donald J. Abraham, David P. Rotella, Alfred Burger, Academic press, 2010.
3. Wilson and Gisvold's Textbook of Organic Medicinal and Pharmaceutical Chemistry, John M. Beale Jr and John M. Block, Wolters Kluwer, 2011, 12<sup>th</sup> edn.
4. P.Parimoo, A Textbook of Medical Chemistry, New Delhi: CBS Publishers. 1995.
5. S.Ramakrishnan, K.G.Prasannan and R.Rajan, Textbook of Medical Biochemistry, Hyderabad: Orient Longman. 3<sup>rd</sup> edition, 2001.



<b>ELECTIVE COURSE III (CHOICE-II) GREEN CHEMISTRY</b>	<b>SUB CODE:P23CHDE6 HOURS:5 CREDITS:4</b>
----------------------------------------------------------------	----------------------------------------------------

#### Objectives of the course

- To discuss the principles of green chemistry.
- To propose green solutions for chemical energy storage and conversion.  
Propose green solutions for industrial production of Petroleum and Petrochemicals.
- To Propose solutions for pollution prevention in Industrial chemical and fuel production, Automotive industry and Shipping industries.  
To Propose green solutions for industrial production of Surfactants, Organic and inorganic chemicals.

**UNIT-I:** Introduction- Need for Green Chemistry. Goals of Green Chemistry. Limitations/ of Green Chemistry. Chemical accidents, terminologies, International green chemistry organizations and Twelve principles of Green Chemistry with examples.

**UNIT-II:** Choice of starting materials, reagents, catalysts and solvents in detail, Green chemistry in day today life. Designing green synthesis-green reagents: dimethyl carbonate. Green solvents: Water, Ionic liquids-criteria, general methods of preparation, effect on organic reaction. Supercritical carbon dioxide- properties, advantages, drawbacks and a few examples of organic reactions in scCO<sub>2</sub>. Green synthesis-adipic acid and catechol.

**UNIT-III:** Environmental pollution, Green Catalysis-Acid catalysts, Oxidation catalysts, Basic catalysts, Polymer supported catalysts-Poly styrene aluminum chloride, polymeric super acid catalysts, Poly supported photosensitizers.

**UNIT-IV:** Phase transfer catalysis in green synthesis-oxidation using hydrogen peroxide, crown ethers-esterification, saponification, anhydride

formation, Elimination reaction, Displacement reaction. Applications in organic synthesis.

**UNIT-V:** Micro wave induced green synthesis-Introduction, Instrumentation, Principle and applications. Sonochemistry – Instrumentation, Cavitation theory - Ultra sound assisted green synthesis and Applications.

#### Recommended Text

1. Ahluwalia, V.K. and Kidwai, M.R. New Trends in Green Chemistry, Anamalaya Publishers, 2005.
2. W. L. McCabe, J.C. Smith and P. Harriott, Unit Operations of Chemical Engineering, 7<sup>th</sup> edition, McGraw-Hill, NewDelhi, 2005.
3. J. M. Swan and D. St. C. Black, Organometallics in Organic Synthesis, Chapman Hall, 1974.
4. V. K. Ahluwalia and R. Aggarwal, Organic Synthesis: Special Techniques, Narosa Publishing House, New Delhi, 2001.
5. A. K. De, Environmental Chemistry, New Age Publications, 2017.

#### Reference book

1. Anastas, P.T. and Warner, J.K. Oxford Green Chemistry -Theory and Practical, University Press, 1998
2. Matlack, A.S. Introduction to Green Chemistry, Marcel Dekker, 2001
3. Cann, M.C. and Connely, M.E. Real-World Cases in Green Chemistry, American Chemical Society, Washington, 2000
4. Ryan, M.A. and Tinnesand, M., Introduction to Green Chemistry, American Chemical Society Washington, 2002.
5. Chandrakanta Bandyopadhyay, An Insight into Green Chemistry, Books and Allied (P) Ltd, 2019.

#### Website and e-learning source

1. <https://www.organic-chemistry.org/>
2. <https://www.studyorgo.com/summary.php>

### Course Learning Outcomes (for Mapping with POs and PSOs)

Students will be able:

**CO1:** To recall the basic chemical techniques used in conventional industrial preparations and in green innovations.

**CO2:** To understand the various techniques used in chemical industries and in laboratory.

**CO3:** To compare the advantages of organic reactions assisted by renewable energy sources and non-renewable energy sources.

**CO4:** To apply the principles of PTC, ionic liquid, microwave and ultrasonic assisted organic synthesis.

**CO5:** To design and synthesize new organic compounds by green methods.

### COURSE MAPPING CO -PO

CO /PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO 10
CO 1	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
CO 2	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
CO 3	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
CO 4	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
CO 5	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓

### COURSE MAPPING CO -PSO

CO /PSO	PSO1	PSO2	PSO3	PSO4	PSO5
CO1	✓	✓	✓	✓	✓
CO2	✓	✓	✓	✓	✓
CO3	✓	✓	✓	✓	✓
CO4	✓	✓	✓	✓	✓
CO5	✓	✓	✓	✓	✓

<b>ELECTIVE COURSE IV (CHOICE-II) - BIO-INORGANIC CHEMISTRY</b>	<b>SUB CODE:P23CHDE7 HOURS:5 CREDITS:3</b>
-------------------------------------------------------------------------	----------------------------------------------------

### Objectives of the course

- To understand the role of trace elements.
- To understand the biological significance of iron, sulphur.
- To study the toxicity of metals in medicines.
- To have knowledge on diagnostic agents.
- To discuss on various metalloenzymes properties.

**UNIT-I: Essential trace elements:** Selective transport and storage of metal ions: Ferritin, Transferrin and siderophores; Sodium and potassium transport, Calcium signalling proteins. Metalloenzymes: Zinc enzymes–carboxypeptidase and carbonic anhydrase. Iron enzymes–catalase, peroxidase. Copper enzymes – superoxide dismutase, Plastocyanin, Ceruloplasmin, Tyrosinase. Coenzymes - Vitamin-B12 coenzymes.

**UNIT-II: Transport Proteins:** Oxygen carriers -Hemoglobin and myoglobin - Structure and oxygenation Bohr Effect. Binding of CO, NO, CN– to Myoglobin and Hemoglobin. Biological redox system: Cytochromes-Classification, cytochrome a, b and c. Cytochrome P-450. Non-heme oxygen carriers-Hemerythrin and hemocyanin. Iron-sulphur proteins- Rubredoxin and Ferredoxin- Structure and classification.

**UNIT-III: Nitrogen fixation**-Introduction, types of nitrogen fixing microorganisms. Nitrogenase enzyme - Metal clusters in nitrogenase- redox property - Dinitrogen complexes transition metal complexes of dinitrogen - nitrogen fixation via nitride formation and reduction of dinitrogen to ammonia. Photosynthesis: photosystem-I and photosystem-II-chlorophylls structure and function.

**UNIT-IV: Metals in medicine:** Metal Toxicity of Hg, Cd, Zn, Pb, As, Sb. Therapeutic Compounds: Vanadium-Based Diabetes Drugs; Platinum-Containing Anticancer Agents.Chelation therapy; Cancer treatment. Diagnostic Agents: Technetium Imaging Agents; Gadolinium MRI Imaging Agents. temperature and critical magnetic Field.

**UNIT-V:Enzymes** -Introduction and properties -nomenclature and classification. Enzyme kinetics, free energy of activation and the effects of catalysis.Michelis - Menton equation - Effect of pH, temperature on enzymereactions.Factors contributing to the efficiency of enzyme.

### Recommended Text

1. Williams,D.R. –Introduction to Bioinorganic chemistry.
2. F.M. Fiabre and D.R. Williams– The Principles of Bioinorganic Chemistry,Royal Society of Chemistry, Monograph for Teachers-31
3. K.F. Purcell and Kotz., Inorganic chemistry, WB Saunders Co., USA.
4. G.N. Mugherjea and Arabinda Das, Elements of Bioinorganic Chemistry - 1993.
5. R. Gopalan, V. Ramalingam, *Concise Coordination Chemistry*, S. Chand, 2001.

### Reference Books

1. M.Satake and Y.Mido, Bioinorganic Chemistry- Discovery Publishing House, New Delhi (1996)
2. M.N. Hughes, 1982, The Inorganic Chemistry of Biological processes, II Edition, Wiley London.
3. R. W. Hay, Bio Inorganic Chemistry, Ellis Horwood, 1987.
4. R. M. Roat-Malone, Bio Inorganic Chemistry, John Wiley, 2002.
5. T. M. Loehr, Iron carriers and Iron proteins, VCH, 1989.

### Website and e-learning source

1. <https://www.pdfdrive.com/instant-notes-in-inorganic-chemistry-the-instant-notes-chemistry-series-d162097454.html>
2. <https://www.pdfdrive.com/shriver-and-atkins-inorganic-chemistry-5th-edition-d161563417.html>

**Course Learning Outcomes (for Mapping with POs and PSOs)**

Students will be able:

**CO1:** The students will be able to analyse trace elements.

**CO2:** Students will be able to explain the biological redox systems.

**CO3:** Students will gain skill in analyzing the toxicity in metals.

**CO4:** Students will have experience in diagnosis.

**CO5:** Learn about the nitrogen fixation and photosynthetic mechanism.

**COURSE MAPPING CO -PO**

CO /PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO 10
CO 1	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
CO 2	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
CO 3	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
CO 4	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
CO 5	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓

**COURSE MAPPING CO -PSO**

CO /PSO	PSO1	PSO2	PSO3	PSO4	PSO5
CO1	✓	✓	✓	✓	✓
CO2	✓	✓	✓	✓	✓
CO3	✓	✓	✓	✓	✓
CO4	✓	✓	✓	✓	✓
CO5	✓	✓	✓	✓	✓

<b>ELECTIVE COURSE IV (CHOICE-II) MATERIAL SCIENCE</b>	<b>SUB CODE:P23CHDE8 HOURS:5 CREDITS:3</b>
----------------------------------------------------------------	----------------------------------------------------

### Objectives of the course

- To understand the crystal structure, growth methods and X-ray scattering.
- To explain the optical, dielectric and diffusion properties of crystals.
- To recognize the basis of semiconductors, superconductivity materials and magnets.
- To study the synthesis, classification and applications of nanomaterials.
- To learn about the importance of materials used for renewable energy conversion.

**UNIT-I: Crystallography:** symmetry - unit cell and Miller indices -crystal systems - Bravais lattices - point groups and space groups - X-ray diffraction-Laue equations-Bragg's law-reciprocal lattice and its application to geometrical crystallography. Crystal structure-powder and single crystal applications. Electron charge density maps, neutron diffraction-method and applications.

**UNIT-II: Crystal growth methods:** Nucleation-equilibrium stability and metastable state. Single crystal -Low and high temperature, solution growth-Gel and sol-gel. Crystal growthmethods-nucleation-equilibrium stabilityandmetastablestate.Singlecrystal-Lowandhightemperature, solution growth- Gel and sol-gel. Melt growth - Bridgeman-Stockbarger,Czochralskimethods.Fluxtechnique,physicalandchemical vapourtransport. Lorentz and polarization factor - primary and secondary extinctions.

**UNIT-III: Properties of crystals:** Optical studies - Electromagnetic spectrum (qualitative) refractive index – reflectance – transparency, translucency and opacity. Types of luminescence – photo-, electro-, and injection luminescence,

LEDs – organic, Inorganic and polymer LED materials - Applications. Dielectric studies- Polarisation - electronic, ionic, orientation, and space charge polarisation. Effect of temperature. dielectric constant, dielectric loss. Types of dielectric breakdown-intrinsic, thermal, discharge, electrochemical and defect breakdown.

**UNIT-IV: Special Materials:** Superconductivity: Meissner effect, Critical temperature and critical magnetic Field, Type I and II superconductors, BCS theory-Cooper pair, Applications. Soft and hard magnets – Domain theory Hysteresis Loop-Applications. Magneto and gian magneto resistance. Ferro, ferri and antiferromagnetic materials-applications, magnetic parameters for recording applications. Ferro-, Piezo-, and pyro electric materials- properties and applications. Shape memory Alloys-characteristics and applications, Non-linear optics-Second HarmonicGenerators, mixing of Laser wavelengths by quartz, ruby and LiNbO<sub>3</sub>.

**UNIT-V: Materials for Renewable Energy Conversion:** Solar Cells: Organic, bilayer, bulk heterojunction, polymer, perovskite based. Solar energy conversion: lamellar solids and thin films, dye-sensitized photo voltaic cells, coordination compounds anchored onto semiconductor surfaces - Ru(II) and Os(II) polypyridyl complexes. Photochemical activation and splitting of water, CO<sub>2</sub> and N<sub>2</sub>. Manganese based photo systems for water-splitting. Complexes of Rh, Ru, Pd and Pt - photochemical generation of hydrogen from alcohol.

### Recommended Text

1. S. Mohan and V. Arjunan, Principles of Materials Science, MJP Publishers, 2016.
2. Arumugam, Materials Science, Anuradha Publications, 2007.
3. Giacavazzo et. al., Fundamentals of Crystallography, International Union of Crystallography. Oxford Science Publications, 2010
4. Woolfson, An Introduction to Crystallography, Cambridge University Press, 2012.

5. James F. Shackelford and Madanapalli K. Muralidhara, Introduction to Materials Science for Engineers. 6th ed., PEARSON Press, 2007.

#### Reference Books

1. Suggested Readings 1. M.G. Arora, Solid State Chemistry, Anmol Publications, New Delhi, 2001.
2. R.K. Puri and V.K. Babbar, Solid State Physics, S Chand and Company Ltd, 2001.
3. C. Kittel, Solid State Physics, John-Wiley and sons, NY, 1966.
4. H.P. Meyers, Introductory Solid State Physics, Viva Books Private Limited, 1998.
5. A.R. West, Solid State Chemistry and Applications, John-Wiley and sons, 1987.

#### Website and e-learning source

1. <http://xrayweb.chem.ou.edu/notes/symmetry.html>.
2. <http://www.upti.ac.in/classroom-content/data/unit%20cell.pdf>.
3. <https://bit.ly/3QyVg2R>

#### Course Learning Outcomes (for Mapping with POs and PSOs)

Students will be able:

**CO1:** To understand and recall the synthesis and characteristics of crystal structures, semiconductors, magnets, nanomaterials and renewable energy materials.

**CO2:** To integrate and assess the structure of different materials and their properties.

**CO3:** To analyse and identify new materials for energy applications.

**CO4:** To explain the importance of crystal structures, piezoelectric and pyroelectric materials, nanomaterials, hard and soft magnets, superconductors, solar cells, electrodes, LED uses, structures and synthesis.

**CO5:** To design and develop new materials with improved property for energy applications.

#### COURSE MAPPING CO -PO

CO /PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10
--------	-----	-----	-----	-----	-----	-----	-----	-----	-----	------

CO 1	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
CO 2	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
CO 3	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
CO 4	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
CO 5	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓

#### COURSE MAPPING CO -PSO

CO /PSO	PSO1	PSO2	PSO3	PSO4	PSO5
CO1	✓	✓	✓	✓	✓
CO2	✓	✓	✓	✓	✓
CO3	✓	✓	✓	✓	✓
CO4	✓	✓	✓	✓	✓
CO5	✓	✓	✓	✓	✓



**COURSE MAPPING CO-PSO**

CO /PSO	PSO1	PSO2	PSO3	PSO4	PSO5
CO1	✓	✓	✓	✓	✓
CO2	✓	✓	✓	✓	✓
CO3	✓	✓	✓	✓	✓