



# **Vidyasagar University**

## **Midnapore-721102, West Bengal**

**The SYLLABUS for  
POST-GRADUATE Programme**

**in**

# **CHEMISTRY**

**Under Choice Based Credit System (CBCS)  
(Semester Programme)**



**[w.e.f. 2022-23]**

**M.Sc. in CHEMISTRY**

SEMESTER	COURSE NO.		Marks	Lecture hours	Credit (L+T+P)
I	CEM 101	PHYSICAL CHEMISTRY - I	40 + 10	40	4 (3-1-0)
	CEM 102	ORGANIC CHEMISTRY- I	40 + 10	40	4 (3-1-0)
	CEM 103	INORGANIC CHEMISTRY- I	40 + 10	40	4 (3-1-0)
	CEM 104	FOOD PROCESSING AND PRESERVATION AND COMPUTER BASICS	40 + 10	40	4 (3-1-0)
	CEM 195	INORGANIC CHEMISTRY (practical)	50	100	4 (0-0-4)
	CEM 196	FOOD PROCESSING AND PRESERVATION (practical)	50	100	4 (0-0-4)
	<b>TOTAL</b>		<b>300</b>	<b>360</b>	<b>24</b>
II	CEM 201	PHYSICAL CHEMISTRY-II	40 + 10	40	4 (3-1-0)
	CEM 202	ORGANIC CHEMISTRY-II	40 + 10	40	4 (3-1-0)
	CEM 203	INORGANIC CHEMISTRY-II	40 + 10	40	4 (3-1-0)
	C-CEM 204	NANOTECHNOLOGY:PRINCIPLES AND PRACTICES(CBCS)	40 + 10	40	4 (3-1-0)
	CEM 295	ORGANIC CHEMISTRY (practical)	50	100	4 (0-0-4)
	CEM 296	PHYSICAL CHEMISTRY (practical)	50	100	4 (0-0-4)
	<b>TOTAL</b>		<b>300</b>	<b>360</b>	<b>24</b>
III	CEM 301	ADVANCED SPECTROSCOPY-I (Organic specialization + Inorganic specialization + Physical specialization)	40 + 10	40	4 (3-1-0)
		<i>PHYSICAL CHEMISTRY SPECIALISATION</i>			
	CEM 302	ADVANCED PHYSICAL CHEMISTRY-I	40 + 10	40	4 (3-1-0)
	CEM 303	ADVANCED PHYSICAL CHEMISTRY-II	40 + 10	40	4 (3-1-0)
		<i>INORGANIC CHEMISTRY SPECIALISATION</i>			
	CEM 302	ADVANCED INORGANIC CHEMISTRY-I	40 + 10	40	4 (3-1-0)
	CEM 303	ADVANCED INORGANIC CHEMISTRY-II	40 + 10	40	4 (3-1-0)
		<i>ORGANIC CHEMISTRY SPECIALISATION</i>			
	CEM 302	ADVANCED ORGANIC CHEMISTRY-I	40 + 10	40	4 (3-1-0)
	CEM 303	ADVANCED ORGANIC CHEMISTRY-II	40 + 10	40	4 (3-1-0)
	CEM 304	<i>INTRODUCTION TO PHARMACEUTICAL CHEMISTRY(CBCS)</i>	40 + 10	40	4 (3-1-0)
	CEM 395	CHEMISTRY PROJECT-I (PHYSICAL SPL/ORGANIC SPL/INORGANIC SPL)	100	200	8 (0-0-8)
	<b>TOTAL</b>		<b>300</b>	<b>360</b>	<b>24</b>
IV	CEM 401	ADVANCED SPECTROSCOPY-II (Organic specialization + Inorganic specialization + Physical specialization)	40 + 10	40	4 (3-1-0)
		<i>PHYSICAL CHEMISTRY SPECIALISATION</i>			
	CEM 402	ADVANCED PHYSICAL CHEMISTRY-III	40 + 10	40	4 (3-1-0)
	CEM 403	ADVANCED PHYSICAL CHEMISTRY-IV	40 + 10	40	4 (3-1-0)

CEM 404	CHEMISTRY IN TECHNOLOGY	40 + 10	40	4 (3-1-0)
<i>INORGANIC CHEMISTRY SPECIALISATION</i>				
CEM 402	ADVANCED INORGANIC CHEMISTRY-III	40 + 10	40	4 (3-1-0)
CEM 403	ADVANCED INORGANIC CHEMISTRY-IV	40 + 10	40	4 (3-1-0)
CEM 404	CHEMISTRY IN TECHNOLOGY	40 + 10	40	4 (3-1-0)
<i>ORGANIC CHEMISTRY SPECIALISATION</i>				
CEM 402	ADVANCED ORGANIC CHEMISTRY-III	40 + 10	40	4 (3-1-0)
CEM 403	ADVANCED ORGANIC CHEMISTRY-IV	40 + 10	40	4 (3-1-0)
CEM 404	CHEMICAL PRINCIPLES IN FOOD SCIENCE AND TECHNOLOGY	40 + 10	40	4 (3-1-0)
CEM 495		100	200	8 (0-0-8)
<b>TOTAL</b>		300	360	24
<b>ALL TOTAL</b>		1200	1240	96

### Overview of the Syllabus

Semester	Paper	No of Papers	Full Marks of Each Paper	Credit Point of Each Paper	Total Marks	Credit Points	Total Credit Point
1 <sup>st</sup>	Theoretical	4	40+10 = 50	4	200	16	24
	Practical	2	50	4	100	8	
2 <sup>nd</sup>	Theoretical	4	40+10 = 50	4	200	16	24
	Practical	2	50	4	100	8	
3 <sup>rd</sup>	Theoretical	4	40+10 = 50	4	200	16	24
	Practical (Project)	1	100	8	100	8	
4 <sup>th</sup>	Theoretical	4	40+10 = 50	4	200	16	24
	Practical (Project)	1	100	8	100	8	
Grand Total 96 Credit Points							

#### **Program outcome (P.O):**

The purpose of the postgraduate chemistry at Vidyasagar University is to provide the key knowledge base and laboratory resources to prepare students for careers as professional in the field of Chemistry.

After completion of the program students will be ready for:

- i. Global level research opportunities to pursue Ph.D. program in Chemistry, Biochemistry and allied fields.
- ii. Job opportunities in chemical, pharmaceuticals, food products, life oriented material industries, etc.
- iii. Discipline specific competitive examinations conducted by different central and state agencies.
- iv. Acquired knowledge for the solution of natural and individual problems.
- v. Attend profound knowledge to identify, formulate, review of research literature, and to analyze complex problems to reach substantiated conclusions.
- vi. Attain the ability to design solutions for the public health and safety including the cultural, societal, and environmental considerations.

### **Programme Specific Outcomes (PSOs):**

1. Upon completing their M.Sc. in Chemistry, students will develop a strong sense of human and social values within the framework of their chemical education.
2. Graduates will cultivate a proactive stance on environmental and ecological issues through the lens of chemistry.
3. Equipped with comprehensive knowledge in advanced chemistry, students will sharpen their critical thinking and analytical abilities.
4. Graduates will leverage their chemistry expertise to address and resolve pertinent social challenges.
5. The program will foster entrepreneurial skills, enabling students to establish their ventures in key areas of chemistry-related industries and businesses.

1 <sup>st</sup> Semester: General Course				
Paper	Course	Marks	Lecture hours	Credit (L+T+P)
<b>CEM-101</b>	<b>Physical Chemistry-I</b>	40 + 10	40	4 (3-1-0)
Unit I	Mathematical preliminaries & Quantum Mechanics-I			
Unit II	Thermodynamics			
Unit III	Statistical Mechanics I			
Unit IV	Rotational Spectroscopy			
Unit V	Vibrational Spectroscopy			
<b>CEM-102</b>	<b>Organic Chemistry-I</b>	40 + 10	40	4 (3-1-0)
Unit I	Pericyclic reaction-1			
Unit II	Organic transformations / synthesis /reagents			
Unit III	Natural products- terpenoids			
Unit IV	Natural products- alkaloids			
Unit V	Retro-synthesis I	40 + 10	40	4 (3-1-0)
<b>CEM-103</b>	<b>Inorganic Chemistry-I</b>			
Unit I	Symmetry and Group theory-I			
Unit II	Solid state chemistry and Crystallography	40 + 10	40	4 (3-1-0)
Unit III	Bioinorganic chemistry-I			
<b>CEM 104</b>	<b>Food processing and preservation and Computer basics</b>			
Unit I	Constituents of food, food pigments and flavouring agents			
Unit II	Introduction to food microbiology	50	100	4 (3-1-0)
Unit III	Food preservation: Principles and methods			
Unit IV	Computer basics I			
Unit V	Computer basics II; data manipulation	50	100	4 (0-0-4)
<b>CEM-195</b>	<b>Inorganic Chemistry Practical</b>			
<b>CEM-196</b>	<b>Food processing preservation and packaging Practical</b>	300	360	24

2 <sup>nd</sup> Semester: General Course				
Paper	Course	Marks	Lecture hours	Credit (L+T+P)
<b>CEM-201</b>	<b>Physical Chemistry-II</b>	40 + 10	40	4 (3-1-0)
Unit I	Quantum Mechanics-II			
Unit II	Chemical kinetics-I			
Unit III	Electronic Spectroscopy			
Unit IV	Raman Scattering			
Unit V	Surface chemistry			
<b>CEM-202</b>	<b>Organic Chemistry-II</b>	40 + 10	40	4 (3-1-0)
Unit I	Pericyclic reaction-2			
Unit II	Organic transformations/synthesis/reagents chemistry-2			
Unit III	Retrosynthetic analysis II			
Unit IV	Stereochemistry-I			
Unit V	Stereochemistry-II			
<b>CEM-203</b>	<b>Inorganic Chemistry-II</b>	40 + 10	40	4 (3-1-0)
Unit I	Organometallic chemistry -I			
Unit II	Group theory-II			
Unit III	Chemistry of p and d-block elements			
<b>CEM 204</b> (Elective Course)	<b>Nanotechnology: Principles and Practices</b> Introduction, synthesis of nanomaterials, analysis techniques, application of nanotechnology	40 + 10	40	4 (3-1-0)
<b>CEM-295</b>	<b>Organic Chemistry Practical</b>	50	100	4 (0-0-4)
<b>CEM-296</b>	<b>Physical Chemistry Practical</b>	50	100	4 (0-0-4)
<b>Total</b>		300	360	24

3 <sup>rd</sup> Semester: Physical Chemistry Spl.				
Paper	Course	Marks	Lecture hours	Credit (L+T+P)
<b>CEM-301</b>	<b>Advanced Spectroscopy-I</b>	40 + 10	40	4 (3-1-0)
Unit I	Photophysical Processes			
Unit II	LASERs and its applications			
Unit III	EPR spectroscopy			
Unit IV	PES and NQR spectroscopy			
<b>CEM-302</b>	<b>Advanced Physical Chemistry-I</b>	40 + 10	40	4 (3-1-0)
Unit I	Matrix mechanics			
Unit II	Stationary perturbation theory			
Unit III	Semiclassical radiation – matter interaction			
Unit IV	Semiempirical methods in quantum chemistry			
Unit V	Group theory & quantum mechanics			
<b>CEM-303</b>	<b>Advanced Physical Chemistry-II</b>	40 + 10	40	4 (3-1-0)
Unit I	Solid state chemistry I			
Unit II	Solid state chemistry II			
Unit III	Statistical mechanics II			
Unit IV	Statistical mechanics III			
Unit V	Non equilibrium thermodynamics			
<b>CEM 304</b>	<b>Introduction of Pharmaceutical Chemistry (CBCS) : Classification and nomenclature of drugs, Theory of drug action and factors affecting the drugs, Types of drugs, Antimalarial drugs</b>	40 + 10	40	4 (3-1-0)
<b>CEM-395</b>	<b>Project I</b>	100	200	8 (0-0-8)
<b>Total</b>		300	360	24

3 <sup>rd</sup> Semester: Inorganic Chemistry Spl.				
Paper	Course	Marks	Lecture hours	Credit (L+T+P)
<b>CEM-301</b>	<b>Advanced Spectroscopy-I</b>	40 + 10	40	4 (3-1-0)
Unit I	Photophysical Processes			
Unit II	LASERs and its applications			
Unit III	EPR spectroscopy			
Unit IV	PES and NQR spectroscopy			
<b>CEM-302</b>	<b>Advanced Inorganic Chemistry-I</b>	40 + 10	40	4 (3-1-0)
Unit I	Organometallic chemistry – II and catalysis			
Unit II	Chemical applications of group theory			
<b>CEM-303</b>	<b>Advanced Inorganic Chemistry-II</b>	40 + 10	40	4 (3-1-0)
Unit I	Bioinorganic chemistry – II			
Unit II	Inorganic photochemistry			
<b>C-CEM 304</b>	<b>Introduction of Pharmaceutical Chemistry (CBCS):</b> Classification and nomenclature of drugs, Theory of drug action and factors affecting the drugs, Types of drugs, Antimalarial drugs	40 + 10	40	4 (3-1-0)
<b>CEM-395</b>	<b>Project I</b>	100	200	8 (0-0-8)
<b>Total</b>		300	360	24

3 <sup>rd</sup> Semester: Organic Chemistry Spl.				
Paper	Course	Marks	Lecture hours	Credit (L+T+P)
<b>CEM 301</b>	<b>Advanced Spectroscopy-I</b>	40 + 10	40	4 (3-1-0)
Unit I	Photophysical Processes			
Unit II	LASERs and its applications			
Unit III	EPR spectroscopy			
Unit IV	PES and NQR spectroscopy	40 + 10	40	4 (3-1-0)
<b>CEM 302</b>	<b>Advanced Organic Chemistry-I</b>			
Unit I	Pericyclic Reaction-III			
Unit II	Linear free energy relationship I			
Unit III	Linear free energy relationship II	40 + 10	40	4 (3-1-0)
Unit IV	Organometallic Chemistry			
<b>CEM 303</b>	<b>Advanced Organic Chemistry II</b>			
Unit I	Bioorganic and Supramolecular Chemistry-I			
Unit II	Bioorganic and Supramolecular Chemistry-II	40 + 10	40	4 (3-1-0)
Unit III	Bioorganic and Supramolecular Chemistry-III			
Unit IV	Peptides and Nucleic acids			
Unit V	Green Chemistry.			
<b>C-CEM 304</b>	<b>Introduction of Pharmaceutical Chemistry (CBCS):</b> Classification and nomenclature of drugs, Theory of drug action and factors affecting the drugs, Types of drugs, Antimalarial drugs	40 + 10	40	4 (3-1-0)
<b>CEM-395</b>	<b>Project I</b>	100	200	8 (0-0-8)
<b>Total</b>		300	360	24

4 <sup>th</sup> Semester: Physical Chemistry Spl.					
Paper	Course	Marks	Lecture hours	Credit (L+T+P)	
<b>CEM 401</b>	<b>Advanced Spectroscopy-II</b>	40 + 10	40	4 (3-1-0)	
Unit I	NMR spectroscopy I				
Unit II	NMR spectroscopy II				
Unit III	Mass spectroscopy				
Unit IV	Combined applications of spectroscopic techniques				
Unit V	CD, ORD, MossBauer spectroscopy				
<b>CEM 402</b>	<b>Advanced Physical Chemistry III</b>	40 + 10	40	4 (3-1-0)	
Unit I	Quantum mechanics of many electron systems I				
Unit II	Atomic Spectroscopy				
Unit III	Application of perturbation theory				
Unit IV	QM of many electron systems I				
Unit V	QM of many electron systems II				
<b>CEM 403</b>	<b>Advanced Physical Chemistry IV</b>	40 + 10	40	4 (3-1-0)	
Unit I	Chemical kinetics II				
Unit II	Chemical kinetics III				
Unit III	Macromolecules				
Unit IV	Biopolymers				
Unit V	Advanced electrochemistry				
<b>CEM 404</b>	<b>Chemistry in Technology</b>	40 + 10	40	4 (3-1-0)	
Unit I	Biophysical Chemistry				
Unit II	Instrumental analysis: theory and practices				
Unit III	Chemical toxicology				
Unit IV	Fundamentals of Nanoscience and technology				
<b>CEM 495</b>	<b>Project II</b>	100	200	8 (0-0-8)	
<b>Total</b>		300	360	24	

4 <sup>th</sup> Semester: Inorganic Chemistry Spl.				
Paper	Course	Marks	Lecture hours	Credit (L+T+P)
<b>CEM 401</b>	<b>Advanced Spectroscopy-II</b>	40 + 10	40	4 (3-1-0)
Unit I	NMR spectroscopy I			
Unit II	NMR spectroscopy II			
Unit III	Mass spectroscopy			
Unit IV	Combined applications of spectroscopic techniques			
Unit V	CD, ORD, MossBauer spectroscopy	40 + 10	40	4 (3-1-0)
<b>CEM 402</b>	<b>Advanced Inorganic Chemistry III</b>			
Unit I	Magnetochemistry			
Unit II	Metal carbonyls and clusters	40 + 10	40	4 (3-1-0)
<b>CEM 403</b>	<b>Advanced Inorganic Chemistry IV</b>			
Unit I	Inorganic reaction mechanism			
Unit II	Analytical chemistry	40 + 10	40	4 (3-1-0)
<b>CEM 404</b>	<b>Chemistry in technology</b>			
Unit I	Biophysical Chemistry			
Unit II	Instrumental analysis: theory and practices			
Unit III	Chemical toxicology	100	200	8 (0-0-8)
Unit IV	Fundamentals of Nanoscience and technology			
<b>CEM 495</b>	<b>Project II</b>	300	360	24
<b>Total</b>				

<b>4<sup>th</sup> Semester: Organic Chemistry Spl.</b>				
<b>Paper</b>	<b>Course</b>	<b>Marks</b>	<b>Lecture hours</b>	<b>Credit (L+T+P)</b>
<b>CEM 401</b>	<b>Advanced Spectroscopy-II</b>	40 + 10	40	4 (3-1-0)
Unit I	NMR spectroscopy I			
Unit II	NMR spectroscopy II			
Unit III	Mass spectroscopy			
Unit IV	Combined applications of spectroscopic techniques			
Unit V	CD, ORD, MossBauer spectroscopy			
<b>CEM 402</b>	<b>Advanced Organic Chemistry III</b>	40 + 10	40	4 (3-1-0)
Unit I	Organic photochemistry I & II			
Unit II	Biologically active molecules			
Unit III	Vitamins and coenzymes			
Unit IV	Heterocyclic chemistry			
<b>CEM 403</b>	<b>Advanced Organic Chemistry IV</b>	40 + 10	40	4 (3-1-0)
Unit I	Stereochemistry III			
Unit II	Stereochemistry IV			
Unit III	Stereochemistry V			
Unit IV	Stereochemistry VI			
<b>CEM 404</b>	<b>Chemical principles in food science and technology:</b> Storage and handling of fresh and processed food and vegetables, dairy processing, cereal processing, fats and oils, quality control and food safety.	40 + 10	40	4 (3-1-0)
<b>CEM 495</b>	<b>Project II</b>	100	200	8 (0-0-8)
<b>Total</b>		<b>300</b>	<b>360</b>	<b>24</b>

### **Distinctive features of course content :**

- **Employability / entrepreneurship/ skill development:** CEM-195, CEM-196, CEM-204, CEM-295, CEM-296, CEM-395, CEM-495, CEM-401, C404.
- **Digital content:** CEM-101, CEM-102, CEM-201, CEM-202, CEM-203, CEM-204, CEM-401, CEM-403, CEM-404
- **Ethics, human values, environment & sustainability:** CEM-104, CEM-196, CEM-204, CEM-404.

## **SEMESTER-I**

### **CEM – 101: Physical Chemistry-I**

Marks: 40 + 10; Lecture hours: 40; Credit (L+T+P): 4 (3-1-0)

#### **Unit-1: Mathematical Preliminaries & Quantum Mechanics-I**

Elements of Calculus, Extremum Principles, Constrained Extremization, powerer Series, Fourier transformation, Vectors and vector space, Differential equations. Postulates and their analysis, Properties of Operators and Commutators, angular momentum operator, Equation of Motion, Stationary States, Ehrenfest's Theorems, Bound states: box with infinite and finite walls, rigid rotator problem.

#### **Unit-2: Thermodynamics:**

Chemical potential, Thermodynamic properties of gases with special reference to real gases in pure state and mixtures. Thermodynamics of ideal and non-ideal binary solutions: excess functions; partial molar properties. Gibbs Duhem equation: uses. Fugacity, Different scales of activity co-efficients for solutes and solvents, Nernst heat theorem, Third law of entropy.

#### **Unit-3: Statistical Mechanics - I:**

Phase cell, macrostate, microstate, thermodynamical probability and entropy, Maxwell-Boltzmann, Bose-Einstein and Fermi-Dirac statistics. PF for atoms and diatoms (translational, rotational, vibrational and electronic), Determination of molar energy and molar entropy using molecular partition function, Gibbs paradox.

#### **Unit-4: Rotational Spectroscopy:**

Rotational spectroscopy of diatomic molecules (Rigid rotator model), polyatomic molecules (linear, spherical to, symmetrical top, asymmetric top molecules), Non-rigid rotator model, Effect of electric field on rotational spectra: Stark effect, Applications of Rotational spectroscopy.

#### **Unit-5: Vibrational Spectroscopy:**

Diatomc molecules: Lagrange equation of motion, normal co-ordinate and linear transformations, simultaneous diagonalization.

Quantum mechanical treatment of vibrational motion, Morse potential energy diagram, Vibrational dependence of rotational spectra, symmetries of normal modes, higher vibrational wave functions, combination bands.

#### **Course Outcome (C.O.)**

The students will gain understanding on the basics of Quantum Mechanics, Thermodynamics, Statistical Mechanics and Principles of molecular spectroscopy.

## **CEM 102: Organic Chemistry –I**

Marks: 40 + 10; Lecture hours: 40; Credit (L+T+P): 4 (3-1-0)

### **Unit-01**

#### **Pericyclic reaction I:**

Pericyclic reactions characteristic features, conservation of orbital symmetry MO of different polyenes, electrcyclic, cycloaddition, sigmatropic reactions, Rationalisation of different example with the basis of frontier orbital interaction, Woodward Hofmann symmetry rules for pericyclic reactions, exceptions to symmetry rules, correlation diagram of different perecyclic reactions. Problems relating to these reactions.

### **Unit-02**

#### **Organic transformations/ Reagent Chemistry/Synthesis-I:**

Cation-olefin cyclization reaction: application to the synthesis of triterpenes: biogenetic isoprene rule: monocyclic, bicyclic, tricyclic, tetracyclic and pentacyclic ring systems. Fragmentation reaction, Remote functionalization: biomimetic reactions / template effect, examples. Functional groups inter conversion. Multicomponent reactions: Definition, early examples, Passerine reaction, Ugi reaction. Olefin metathesis reaction: Definition, Ring closing metathesis reaction, examples. Phase transfer catalysis.

### **Unit-03**

#### **Natural products-Terpenoids:**

Terpenoids: Isoprene rules, acyclic monoterpenoids, cetrat geraniol neral, linalool monocyclic monoterpenoids; -terpineol, structure elucidation, synthesis and biogenesis. Higher terpenoids: sesqui-, di-, sester-, tri-, tetra- terpenoids.

### **Unit - 04**

#### **Natural Products - Alkaloids:**

Alkaloids: Phenyl ethyl amine, quinine, nicotine, indole: structure, synthesis, biogenesis.

### **Unit - 05**

#### **Retrosynthetic analysis-I:**

Organic Synthesis Strategy, the disconnection approach.

### **Course Outcome (C.O.)**

The students will gain understanding on Pericyclic reaction, Organic transformations, Natural products like terpenoids, alkaloids and Retro-synthesis

## CEM 103: Inorganic Chemistry-I

Marks: 40 + 10; Lecture hours: 40; Credit (L+T+P): 4 (3-1-0)

### Unit- 1: Symmetry and Group theory-I

Groups and their properties- the concept of groups; subgroups, classes and the related theorems; commutative (abelian) groups and cyclic groups and their examples; group multiplication tables and the rearrangement theorem. Symmetry elements and operations, products of symmetry operations, equivalent symmetry elements and equivalent atoms, symmetry in platonic solids, identification of point groups, Symmetry of  $C_{60}$  fullerenes, Crystallographic symmetry: 32 crystal classes, Hermann–Mauguin (HM) notations, optical activity and dipole-moment on the basis of point group symmetry; similarity transformation and the invariance of characters; block diagonalisation; direct product of matrices and their characters etc. Matrix representation of symmetry operations, characters of symmetry operations in a representation, invariance of character under similarity transformation, the row / column orthogonality of characters, reducible and irreducible representations, the “Great Orthogonality Theorem” (without derivation) and its corollaries.

### Unit- 2: Solid state Chemistry and crystallography

Defects in solids, line and plane defects. Determination of equilibrium concentration of Schottky and Frenkel defects, Stoichiometric imbalance in crystals and non-stoichiometric phases, Color centres in ionic crystals. Band theory, band gap, metals, insulators, semiconductors (intrinsic and extrinsic), hopping semiconductors, rectifiers and transistors. Bonding in metal crystals: Free electron theory, electronic specific heat, Hall effect, electrical and thermal conductivity of metals, Superconductivity, Meissner effect, basic concepts of BCS (Bardeen-Copper-Schriffer) theory.

Crystalline solid: single crystal and polycrystal (twinning problem) lattice, unit cell-primitive and non-primitive unit cells, unit cell parameters and crystal systems. Space group- Hermann–Mauguin notations, space group in triclinic and monoclinic system. Indexing of lattice planes, Miller indices. Bragg's equation, reciprocal lattice and its relation to direct lattice; Bragg's reflection in terms of reciprocal lattice-sphere of reflection and limiting sphere; relation between  $d_{hkl}$  and lattice parameters.

**Unit 3: Bioinorganic chemistry-I:** Essential elements in Biology (major and trace); Beneficial and toxic elements; Role of metal ions; Biomolecules; Metal-protein interaction; Bioenergetic principle and role of ATP; Oxygen–uptake proteins: haemoglobin, myoglobin, hemerythrin and hemocyanin: structure, function and model study; Metal ions in electron transport proteins: Fe-S proteins, cytochromes; Metal ions transport and storage proteins: ferritin, transferrin, ceruloplasmin; Transport across biological membrane: Ion pumps, ionophores; Hydrolytic enzymes: carbonic anhydrase, carboxy peptidase, urease; Toxic effects of metal: Copper toxicity and Wilson's disease, Arsenic poisoning, Aluminium toxicity and Alzheimer disease; Transition metal complexes as drugs.

### Course Outcome (C.O.)

The students will gain understanding on Symmetry and Group theory, Solid state chemistry, Crystallography and Bioinorganic chemistry.

## **CEM 104: FOOD PROCESSING AND PRESERVATION-I and COMPUTER BASICS**

Marks: 40 + 10; Lecture hours: 40; Credit (L+T+P): 4 (3-1-0)

### **UNIT-I:**

**Constituents of Food:** Water; Water in foods and its properties, **Carbohydrates;** Sources and physico-chemical and functional properties, **Proteins;** Sources and physico-chemical and functional properties, Purification of proteins, Common food proteins, **Lipids;** Sources and physico chemical and functional properties, PUFA (Poly-unsaturated Fatty Acids), Lipids of biological importance like cholesterol and phospholipids, Hydrogenation and rancidity of lipids, Saponification number, iodine value of lipids, **Vitamins and Minerals;** Sources, classification and structures of minerals & vitamins, Effect of processing and storage of vitamins, Pro vitamins A & D; Vitamins as antioxidants

**Food Pigments & Flavouring Agents:** Importance, types and sources of pigments, their changes during processing and storages

### **UNIT-II:**

**Introduction to food microbiology-** definition, historical development and significance, Factors influencing the growth and survival of microorganisms in foods, Role of microbes in fermented foods and genetically modified foods, Food spoilage, Types and causes of food spoilage.

Microbiology of milk & milk products like cheese, butter, ice-cream, Microbiology of meat, fish, poultry & egg and their products, Microbiology of cereal and cereal products like bread, confectionary etc.

### **UNIT-III:**

**Food preservation:** Principles and methods: **Canning;** Preservation principle of canning of food items, thermal process time calculations for canned foods, spoilage in canned foods; **Dehydration and drying of food items;** Water activity of food and its significance in food preservation, IMF, **Low temperature preservation;** freezing and cold storage, cold chain, **Preservation by fermentation;** curing and pickling, **Use of preservative in foods;** chemical preservative, biopreservatives, antibiotics, lactic acid bacteria, **Hurdle technology**

### **Unit -IV:**

**Computer Basics-I:** Block diagram of a computer, Functions of the Different Units, Input unit, Output unit, Memory unit, CPU (ALU+CU), Input Devices: Keyboard, Mouse, Data Scanning devices image scanner, OCR, OMR, MICR, Barcode reader, card reader. Output Devices: Monitor, Printer- laser printer, dot-matrix printer, inkjetprinter, Projector. Memories, Registers, Cache Memory, Primary memory, RAM, ROM, Secondary Memories - Hard disk, Structure of a hard disk, concept of tracks, sectors, clusters, cylinders. Software: System Software - Operating System - Functions of O/S, Types of O/S, Program Language Translators, Assembler, Compiler, Interpreter, Utility Programs, Application Software, Computer Languages - Machine language, . Assembly language, High-level language, Data storage: The decimal number system, the binary number system, hexadecimal notation, octal number system. Conversion from one number system to another number system, Codes, ASCII, BCD etc. Arithmetic Operation for Binary Numbers. Representation of numbers in 1"s and 2"s Complement method. Subtraction using 1"s and 2"s Complement method.

### **Unit V:**

**Computer Basics – II: Data Manipulation:** Logical Operations: AND, OR, NOT, NAND, NOR, EX-OR, EX-NOR. Logic gates with the truth table, Universal Gates, Representation of function using gates. Boolean Algebra & Logical Gates- Basic Definitions Boolean Algebra, Theorems of Boolean Algebra. Boolean Functions. Simplification of Boolean Function- Karnaugh Map Method 3 variable, 4 variable, 5 variable Map. Sum Of Product Product of Sum, Don't care Combinational Circuits-Design Procedure Adders. Sequential Circuits - Flip-flops.

## **Course Outcome (C.O.)**

The students will gain understanding on Constituents of food, food pigments, flavouring agents, food microbiology, Food preservation, Computer basics and Data Manipulation.

### **Text Books/References:**

1. Food Science, 5<sup>th</sup> Ed, 1997, B. Srilakshmi, New Age International (P) Ltd, New Delhi.
2. N.N. Potter CBS Publishers and Distributors, Delhi, 5th Ed, 1996 Food Science.
3. Food Processing and Preservation by B. Sivasankar

**CEM 195: Inorganic Chemistry (Practical)**  
Marks: 50; Lecture hours: 100; Credit (L+T+P): 4 (0-0-4)

**1. Quantitative analysis**

- 1A. Gravimetric estimation of Zn(II) as  $Zn(NH_4)(PO_4)$
- 1B. Gravimetric estimation of Cu(II) as  $CuSCN$
- 1C. Gravimetric estimation of Ni(II) as  $Ni(DMGH)_2$
- 1D. Gravimetric estimation of Ba(II) as  $BaSO_4$
- 1E. Gravimetric estimation of Pb(II) as  $(Pb)_3(PO_4)_2$
- 1F. Volumetric estimation of Mn(II)/Fe(III)
- 1G. Volumetric estimation of Cr(VI)/ Fe(III)
- 1H. Volumetric estimation of Cu(II)/ Fe(III)
- 1I. Volumetric estimation of Cu(II)/Cr(VI)

**2. Analysis of Metals and Alloys**

- 2A. Quantitative estimation of Zn(II) and Cu(II) in brass sample by volumetry and gravimetry
- 2B. Quantitative estimation of iron in cast iron and steel.

**3. Analysis of Ores and Minerals**

- 3A. Quantitative estimation of manganese in pyrolusite
- 3B. Quantitative estimation of  $CaCO_3$  and  $CaCO_3$  in dolomite

**4. Equilibrium studies on inorganic reactions**

- 4A. Determination of composition of Fe(III)-sulfosalicylate complex in solution by Mole-Ratio method.
- 4B. Determination of composition of Fe(II)-1,10-phenanthroline complex in solution by Mole-Ratio method.
- 4C. Determination of composition of Fe(III)-sulfosalicylate complex in solution by Slope-Ratio method.
- 4D. Determination of composition of Fe(II)-1,10-phenanthroline complex in solution by Slope-Ratio method.
- 4E. Determination of composition of Fe(III)-sulfosalicylate complex in solution by Job's method of continuous variation.

4F. Determination of composition of Fe(II)-1,10-phenanthroline complex in solution by Job's method of continuous variation.

### **5. Spectrophotometric Estimation**

- 5A. Colourimetric estimation of Fe(III) (as thiocyanate complex)
- 5B. Colourimetric estimation of Fe(II) and Fe(III) in a mixture as Fe(II)-1,10-phenanthroline complex.

### **6. Synthesis and Characterization of inorganic compounds**

- 6A. Reinkey's salt
- 6B.  $[\text{Co}(\text{NH}_3)_6]\text{Cl}_3$
- 6C.  $[\text{Cu}(\text{NH}_3)_4(\text{SO}_4)(\text{H}_2\text{O})]$
- 6D.  $[\text{Co}(\text{NH}_3)_5\text{Cl}]\text{Cl}_2$
- 6E.  $[\text{Ni}(\text{en})_2]\text{Cl}_2$
- 6F.  $\text{K}_3[\text{Fe}(\text{ox})_3]$
- 6G.  $\text{K}_3[\text{Cr}(\text{ox})_3]$
- 6H.  $[\text{Co}(\text{NH}_3)_6]\text{Cl}_3$
- 6I.  $[\text{Cu}(\text{NH}_3)_4(\text{SO}_4)(\text{H}_2\text{O})]$
- 6J. Crome alum  $[\text{K}_2\text{SO}_4, \text{Cr}_2(\text{SO}_4)_3, 24\text{H}_2\text{O}]$

## **CEM 196: FOOD PROCESSING, PRESERVATION & PACKAGING LAB (Practical)**

Marks: 50; Lecture hours: 100; Credit (L+T+P): 4 (0-0-4)

### **EXPERIMENTS**

- I: Preparation of jams, jellies, syrups, squashes
- II: Preparation of mixed fruit juices: Aloe vera mixed with lichi, mango, pine apple, water melon, etc.
- III: Estimation of Food Values (carbohydrate, fat, protein, vitamins) and Food Safety Test.
- IV: Preservation of processed food
- V: Packaging of processed and preserved food
- VI: Study of Rheology of Jam, Jelly and sauce
- VII: Value addition in food products

### **REFERENCES**

1. Rahman, M.S. "Handbook of Food Preservation", Marcel Dekker, 1999.
2. Ranganna, S. "Handbook of Canning and Aseptic Packaging" Vol. I, II & III, Tata McGraw – Hill, 2000.

## **SEMESTER-II**

### **CEM 201: Physical Chemistry –II**

Marks: 40 + 10; Lecture hours: 40; Credit (L+T+P): 4 (3-1-0)

#### **Unit-1: Quantum Mechanics-II**

Harmonic Oscillator (Operator method), Hydrogen atom Problem: Cartesian and Polar coordinates. Approximate method: Variational principle, Linear variation method, Applications of linear variational theory. Perturbation theory: Derivation of time independent non-degenerate perturbation equations, first order correction to energy and wave function and its applications.

#### **Unit-2: Chemical Kinetics-I**

Kinetics of Fast reactions: flow method, relaxation method, flash photolysis. Oscillatory reactions: Observation and mechanism. Autocatalytic reaction.

Kinetics of redox reaction: inner sphere and outer sphere mechanism.

Reactions between ions: influence of solvent dielectric constant (double sphere model), single sphere activated complex model, influence of ionic strength, Enzyme catalysis and Enzyme inhibition (Competitive inhibition, Uncompetitive inhibition, mixed inhibition)

#### **Unit-3: Electronic Spectroscopy**

Electronic Spectroscopy: Born-Oppenheimer approximation, Franck-Condon principle, Quantum mechanical treatment of Frank-Condon factor, electronic energy and electronic angular momentum of diatomic molecules, rotational fine structure of electronic-vibrational transitions, Forrat diagram, Electronic spectroscopy of polyatomic molecules.

#### **Unit-4: Raman Scattering:**

Introduction. Classical Theory of Raman Scattering, Q.M Picture of Raman Scattering, Characteristic parameters of Raman lines, Pure Rotation and Vibrational Raman spectra, Basic Principles of a Raman spectrometer, Application of Raman Spectroscopy.

#### **Unit-5: Surface Chemistry**

Curved surfaces: Young-Laplace and Kelvin equations, Adsorption on solids: BET eqn. Micelles, reverse micelles; micellization equilibrium; thermodynamics of micellization; micro and macro emulsions.

#### **Course Outcome (C.O.)**

The students will gain understanding on Quantum Mechanics, Chemical kinetics, Molecular spectroscopy and Surface chemistry.

## CEM 202: Organic Chemistry – II

Marks: 40 + 10; Lecture hours: 40; Credit (L+T+P): 4 (3-1-0)

### Unit - 01

#### Pericyclic reaction I:

Perturbation molecular orbital theory (PMO), energy diagram of ethylene and butadiene system with different substitutions and study of their cycloaddition reactions, FMO approach and correlation diagram, Regioselectivity, Periselectivity and Site selectivity, secondary interactions in pericyclic reactions, cheletropic reactions. Problems relating to these reactions.

### Unit-02

#### Organic transformations/ Reagent Chemistry/Synthesis-II:

Oxidations reactions: Hydroxylation reagents, use of peroxy acids, Woodward prevost hydroxylation, Sharpless asymmetric expoxidation, AD-mix, Transformation of epoxides. Organophosphorus reagents, organo sulfer reagents, organo boranes, organo silanes, organostannanes, Organo catalytic reaction, metal hydrides, Birch reduction, Bayer Villiger reactions, chichibabin reaction, Merrifield resin: solid phase synthesis.

### Unit 03

Retro synthetic analysis-II: disconnection approach. Examples to illustrate disconnection approach in organic synthesis.

### Unit 04

#### Stereochemistry I:

Different projection formulae and their interconversions. Conformational and configurational enantiomers. Stereochemical nomenclatures : (E, Z), chiral centre, chiral axis, chiral plane, helicity, threo-erythro, pref-parf, chiral simplex. Stereogenicity and chirotopicity. Symmetry and molecular chirality. Stereochemical features : cyclohexane and its derivatives conformation and physical properties. Computation of stereoisomers of different systems. Conformation and relative reactivity of diastereomers. 2-, 3-, and 4- Alkyl ketone effects.

### Unit 05

#### Stereochemistry II:

Prochirality and Prostereoisomerism. Topicity and Reactivity. A symmetric synthesis : Addition of a chiral reagents to chiral ketones and aldehydes, models of stereochemical control : Cram, Felkin and Karabatsos. Atropisomerism Molecular rearrangements with Neighbouring group participations. Stereospecific and stereoselective reactions. Enantioselective reactions.

### Course Outcome (C.O.)

The students will gain understanding on Pericyclic reaction, Organic transformations, Retro synthetic analysis and Stereochemistry.

## CEM 203: Inorganic Chemistry – II

Marks: 40 + 10; Lecture hours: 40; Credit (L+T+P): 4 (3-1-0)

**Unit 1: Organometallic chemistry –I:** Application of 18-electron and 16-electron rules to transition metal organometallic complexes; Ligands in organometallic chemistry; Synthesis, structure, bonding and chemistry of Metal-alkyl, -alkene, -alkyne, - allyl, -carbene, -carbyne and -carbide complexes; Agostic interaction; Stereochemical non-rigidity and fluxional behaviour of organometallic compounds with typical examples.

### Unit: 2: Group theory-II

Character tables ( $C_{2v}$ ,  $C_{3v}$ ,  $C_{4v}$ ,  $D_4$ ), representation for cyclic groups, wave functions as bases for Irreducible Representations, the standard reduction formula; the direct product representation and its decomposition, identifying nonzero matrix elements, spectral transition probabilities, allowedness - forbiddenness of  $n-\pi^*$  and  $\pi-\pi^*$  transitions, symmetry of normal modes, normal mode analysis, selection rules for IR and Raman transitions. Projection operator (without derivation), use of the projection operator to form symmetry adapted linear combination (SALC) of simple system.

### Unit: 3: Chemistry of p and d-block elements

Boron cluster classification, skeletal electron counting. Boron hydrides: boranes, structure, bonding (MO description of  $B_2H_6$  and  $B_2H_6^{2-}$ ) and Lipscomb's topology, styx' system of numbering, nomenclature; carboranes, metalloboranes, metallocarboranes-synthesis and structure; Wade's rules, boroncompounds of potential medicinal interest; boron neutron capture theory (BNCT).

Chemistry of Ti -Zr- Hf, V-Nb-Ta, Cr-Mo- W, Mn-Tc-Re, Ru-Rh-Pd, Os-Ir-Pt with reference to electronic configuration, oxidation states, coordination number, aqueous chemistry, redox behavior. Iso- and heteropolyoxometalates with respect of V, Mo and W: synthesis, reactions, structures, uses. Dinitrogen and dioxygen complexes: synthesis, structure, bonding and reactivity. Bonding and properties of molybdenum blue, tungsten blue, ruthenium blue, platinum blue, tungsten bronze, ruthenium red. Creutz-Taube complex, Vaska's complex. Nb, Ta halide clusters. Electronic configuration, oxidation state and comparative study Stabilization of uncommon oxidation states of transition metals by complex formation -Fe(IV), Co(IV), Ni(III), Ru(IV), Os(IV), Pd(III / IV), Pt(III), synthesis and structures.

### Course Outcome (C.O.)

The students will gain understanding on Organometallic chemistry, Group theory, Chemistry of p and d-block elements.

## **CEM 204: Nanotechnology: Principles and Practices (Elective Course)**

Marks: 40 + 10; Lecture hours: 40; Credit (L+T+P): 4 (3-1-0)

### **Unit I:**

**Introduction:** Bulk vs. Nano, Geometric structure, Magic numbers, co-ordination number of small clusters.

### **Unit II:**

**Synthesis of Nanomaterials:** Physical methods, Chemical methods, Biological methods.

**Properties of Nanomaterials:** Mechanical properties, structural properties, melting of nanoparticles, electrical conductivity, optical properties, magnetic properties.

### **Unit III:**

#### **Analysis techniques:**

Microscopes: Optical microscopes, Electron microscopes, Scanning electron microscope, Transmission electron microscope, Scanning probe microscope, Scanning tunneling microscope, Atomic force microscope, XRD, Spectroscopies: UV-VIS-NIR, Infrared (FTIR), Photo luminescence, XPS (X-ray photo electron spectroscopy), Anger electron spectroscopy.

### **Unit IV:**

#### **Application of Nanotechnology:**

Electronics, Energy, Automobiles, Sports and Toys, Textiles, Cosmetics, Domestic applications, Biotechnology and medical field, space and Defense, Nanotechnology and environment.

### **Course Outcome (C.O.)**

The students will gain understanding on synthesis of nanomaterials, analysis techniques, applications of nanotechnology.

## **CEM 295: Organic Chemistry Practical**

Marks: 50; Lecture hours: 100; Credit (L+T+P): 4 (0-0-4)

### **1. Liquid Sample**

Qualitative analysis (color, odour, solubility etc.); Thin Layer Chromatography (TLC, preparation of TLC plates, analysis), boiling point determination, Assign  $^1\text{H-NMR}$ ,  $^{13}\text{C-NMR}$  spectra, Identify the liquid substance.

[15]

### **2. Extraction of Renewable chemicals**

Take a particular part of a plant such as fruit, leaf, bark, heavy wood, etc. Weight it. Extract with a particular solvent. Remove the volatiles. Purify. Weigh the product. Calculate % yield, Analyze the product by Thin Layer Chromatography, calculate  $R_f$  value. UV-VIS spectral characterizations: Measure  $\lambda_{\text{max}}$ ,  $\epsilon_{\text{max}}$  and explain. Submit the product with proper label.

[15]

**OR**

### **2. Preparation**

Preparation of pure organic compound single-step or two step procedure and submission of crystallized product: Table Preparation; Weigh the compound, calculate theoretical yield, prepare the compound, weigh the product, calculate % yield, crystallize, check M.P., submit crystallized product.

### **3. Sessional Work**

To be awarded by the class teacher on the basis performance of the students during the course work.

[10]

### **4. Viva Voce**

To be jointly conducted by the external and internal examiners during the examination.

[10]

**CEM 296: Physical Chemistry Practical**  
Marks: 50; Lecture hours: 100; Credit (L+T+P): 4 (0-0-4)

<b>1. List of Experiments:</b>	<b>35</b>
<p>1. Kinetics of Inversion of Cane-sugar by Polarimeter /</p> <p>2. Determination of concentration of Glucose-fructose in a mixture using polarimeter</p> <p>3. Conductometric determination of concentrations of KCl, HCl and NH<sub>4</sub>Cl in a mixture.</p> <p>4. Verify the Onsagar equation using KCl, K<sub>2</sub>SO<sub>4</sub> and BaCl<sub>2</sub> as electrolytes and determine their <math>\Lambda_0</math> values.</p> <p>5. Determination of CMC of a surfactant in aqueous solution by conductometric method.</p> <p>6. Potentiometric titration of halide mixture (Chloride, Bromide and Iodide).</p> <p>7. Determine the E<sub>0</sub> value of Ag<sup>+</sup>/Ag electrode and activity coefficients of different aqueous AgNO<sub>3</sub> solutions potentiometrically.</p> <p>8. Determine the standard potential of *Fe(CN)<sub>6</sub><sup>3-</sup> / *Fe(CN)<sub>6</sub><sup>4-</sup> electrode by potentiometer.</p> <p>9. Determine the dissociation constants (K<sub>1</sub>, K<sub>2</sub>, and K<sub>3</sub>) of H<sub>3</sub>PO<sub>4</sub> by pH meter.</p> <p>10. Study the kinetics of Iodination of acetone spectrophotometrically.</p> <p>11. Determination of composition of complexes (Ferric-salicylate complex/Ferrous-orthophenanthroline complex) by Job's method.</p> <p>12. Determine the rate constant and the order of the reaction of KBrO<sub>3</sub> &amp; KI in acid medium.</p> <p>13. Determine the order and rate constant of the reaction between K<sub>2</sub>S<sub>2</sub>O<sub>8</sub> &amp; KI and study the influence of ionic strength on the rate constant.</p> <p>14. Study of the kinetic of alkaline hydrolysis of crystal violet. Determine the order with respect to alkali and salt effect on the system.</p> <p>15. Spectroscopic experiments relating to quenching of fluorescence.</p> <p>16. Experiment for the measurements of activation barrier of some model chemical reactions.</p> <p>17. Synthesis of metal/semiconducting nanoparticle and their photophysical study.</p>	

**2. Sessional Work:**

To be awarded by the class teacher on the basis performance of the students during the practical classes.

5

**3. Viva Voce:**

To be jointly conducted by the external and internal examiners during the examination.

10

## **SEMESTER-III**

### **CEM 301: Advanced Spectroscopy-I (Common Paper: Physical/Inorganic/Organic)**

Marks: 40 + 10; Lecture hours: 40; Credit (L+T+P): 4 (3-1-0)

#### **Unit: 1**

##### **Photophysical processes:**

Photophysical processes of unimolecular processes, Delayed fluorescence, Kinetics of bimolecular processes: collision quenching, Stern-Volmer equation, Concentration dependence of quenching and excimer formation, Excited state electron transfer processes: Exciplex, Twisted intramolecular charge transfer processes, proton couple electron transfer processes (both intra and intermolecular).

#### **Unit: 2**

##### **Laser and its applications:**

General feature and properties of LASER, Method of obtaining population inversion, Laser cavity modes, Q-switching, Mode locking, Example of LASER: Ruby laser, Nd-YAG laser, diode laser, He-Ne laser, N<sub>2</sub> laser, Ar laser, excimer and exciplex laser, Dye laser.

#### **Unit: 3**

##### **EPR spectroscopy**

Principle, spin Hamiltonian (comparison to NMR spectra), energy of spinning electron in a magnetic field, EPR-instrumentation, representation of EPR spectrum, X-band and Q-band spectra, line width, hyperfine splitting, magnetically equivalent and nonequivalent sets of nuclei, g-anisotropy, spectra of simple organic free radicals: expected number of lines, intensities. Spectra of transition metal complexes, metal hyperfine anisotropic spectra, zero-field splitting, application: determination of oxidation state of metal ion in samples.

#### **Unit: 4**

##### **PES and NQR spectroscopy**

Photoelectron spectroscopy: Photoexcitation and photoionization, core level (XPS, ESCA) and valence level (UPS) photoelectron spectroscopy, XPS and UPS experiments, chemical shift, detection of atoms in molecules and differentiation of same elements in different environments from XPS, information about the nature of molecular orbitals from UPS, UPS of simple diatomic molecules e.g. N<sub>2</sub>, O<sub>2</sub>, CO, HCl etc. Principle of NQR, nuclear quadrupole coupling constant, structural information from NQR spectra.

#### **Course Outcome (C.O.)**

The students will gain understanding on Photophysical Processes, LASERs and its applications, EPR, PES and NQR spectroscopy.

## **CEM 302: Advanced Physical Chemistry-I (Physical Spl.)**

Marks: 40 + 10; Lecture hours: 40; Credit (L+T+P): 4 (3-1-0)

### **Unit-1: Matrix mechanics:**

Basis and representations, Elementary matrix properties, Unitary and similarity transformation in quantum mechanics, Energy representations, angular momentum matrices, the pauli spin matrices. Matrix eigen value problem. Linear variational principle and matrix.

### **Unit-2: Perturbation theory**

Perturbation theory: Derivation of time independent degenerate perturbation theory and its applications. independent non-degenerate perturbation equations, first order non-degenerate and degenerate perturbation theory, Applications: anharmonic oscillator, non-rigid rotator, He atom, Stark effect, Zeeman effect

### **Unit-3: Semi-classical treatment of radiation-matter interaction**

Theoretical basis of interaction of radiation with matter: time dependent perturbation theory, Harmonic perturbation and transition probabilities, Einstein's A & B co-efficient, LASER and MASER

### **Unit-4: Semiempirical methods of Quantum Chemistry:**

The Hückel Molecular orbital Theory: Mathematical formalism of Hückel theory, Hückel MO's and orbital of 1,3-Butadiene, Nodal properties of the  $\pi$ -MO of butadiene, Alternate and non-alternate conjugated hydrocarbons, Analytical expression for Hückel MO's and orbital energies in linear and cyclic polyenes. Delocalization energy, excitation energy and Ionization energy of conjugated hydrocarbons, charge density, Bond order and free valence index derived from Hückel MO's.

### **Unit-5: Group Theory and Quantum Mechanics:**

Quantum mechanics and group representation theory, Direct product representation, Vanishing of quantum mechanical integral, Transition probability, Selection Rules, Projection operation, symmetry adapted linear combination of atomic orbitals. Application of group theory to molecular vibrations, Normal modes, Vibrational transitions, IR and Raman Spectra and Selection rule, Application of group theory to Ligand and crystal field theory, Symmetry and chemical reactions; Woodward –Hoffmann Rule.

### **Course Outcome (C.O.)**

The students will gain understanding on advanced level quantum mechanics like Matrix mechanics, Perturbation theory, Semi classical approach to radiation – matter interaction, Semi-emperical methods in quantum chemistry, Group theory & quantum mechanics.

## **CEM 302: Advanced Inorganic Chemistry-I (Inorganic Spl.)**

Marks: 40 + 10; Lecture hours: 40; Credit (L+T+P): 4 (3-1-0)

**Unit 1: Organometallic Chemistry II:** Chemistry of transition metal complexes with cyclic polyenes: 3-6 membered ring systems; Sandwich and non-sandwich complexes; Organometallic chemistry of heterocyclic ligands (N, B, O); Multidecker sandwich complexes; Bioorganometallic chemistry; Organometallic polymers; Main group organometallic chemistry;

**Unit 2: Catalysis:** Terminology in catalysis: TO, TON, TOF; Chemical engineering fundamentals in catalysis; Catalytic cycle; Sequences in catalysed reactions; Unique reactions in organometallic chemistry and catalysis: Coordinative unsaturation, Substitution, Oxidative addition, Insertion (migration), Isomerization, Reductive elimination; Catalytic converters; Alkene hydrogenation; Water gas shift reaction; Fischer Tropsch process; Hydroformylation (Oxo process); Methanol carbonylation and Oxidation of Olefins: Monsanto's acetic acid synthesis; Celanese process with LiI modified Rhodium catalyst; Tennessee Eastman acetic anhydride process, Cativa process, Wacker process; Polymerization of olefins; Ziegler-Natta catalyst.

### **Unit: 3**

#### **Chemical applications of group theory**

Splitting of orbitals and free ion terms in weak crystal fields, symmetries and multiplicities of energy levels in strong crystal fields, correlation diagram, Orgel diagram, Tanabe-Sugano diagrams, Effect of lowering of symmetry on the orbitals and energy levels, correlation table. Vanishing of quantum mechanical integral, transition probability, selection rules. Justification of Laporte selection rule, vibronic coupling and vibronic polarization, polarization of electronically allowed transitions.

Symmetry adapted linear combination of atomic orbitals, construction of  $\square \square$  MO for different system; LCAO-MO approximations Huckel theory for conjugated system. Symmetry of hybrid orbitals. Determine the symmetry and combinations of Ligand group Orbitals (LGO) and metal orbitals in octahedral, square planar, tetrahedral and other ligand environments using of projection operator. Construction of qualitative MO energy level and interaction diagram on the basis of symmetry considerations only. Drawing of LGO and MO diagrams. Application to IR and Raman spectra. Symmetry and chemical reactions; Woodward-Hoffmann rule.

### **Course Outcome (C.O.)**

The students will gain understanding on advanced level Organometallic chemistry catalysis and Chemical applications of group theory

## **CEM 302: Advanced Organic Chemistry-I (Organic Spl.)**

Marks: 40 + 10; Lecture hours: 40; Credit (L+T+P): 4 (3-1-0)

### **Unit-01: Pericyclic reaction III:**

Pericyclic reactions and applications of MO theory to Organic Chemistry: Electrocyclic reactions, cycloaddition and cycloreversion reactions, Sigmatropic rearrangement, chelotropic reactions, ene reaction.

Frontier Molecular Orbital theory, concept of aromaticity of Transition States, orbital correlation diagrams, Huckel MO theory- MO's of chains and rings alternants and nonalternants.

### **Unit 02: Linear Free Energy Relationship-I**

Linear Free Energy Relationship: Quantitative correlations of rate and equilibria. Linear free energy relationships with special reference to Hammett, Yukawa-Tauno and Grunwald-Weinstein equations.

### **Unit-03: Linear Free Energy Relationship-II**

Application of Linear Free Energy Relationship to aromatic, aliphatic, polynuclear and hetero-aromatic systems. Multiparameter correlation reactions (elementary ideas). Electrophilic substitutions in aliphatic systems.

### **Unit-04: Organometallic Chemistry**

Preparation and reactions of pi-complexes, haptonumbers, rules for nucleophilic addition to complexes, applications to typical synthesis, use of transition metals: organometallics in organic synthesis.

### **Course Outcome (C.O.)**

The students will gain understanding on advanced level Pericyclic Reaction, Linear free energy relationship in organic reaction and Organometallic Chemistry.

## **CEM 303: Advanced Physical Chemistry-II (Physical Spl.)**

Marks: 40 + 10; Lecture hours: 40; Credit (L+T+P): 4 (3-1-0)

### **Unit-1: Solid state chemistry- I**

Electrical conductivity of metals; free electron theory of metals (classical and quantum theory), X-ray diffraction, Laue's diffraction, atomic scattering factor and geometrical structure factor, Hall effect, Lattice vibration: phonon and exciton, superconductors.

### **Unit-2: Solid state chemistry- II**

Defects in solids: Point, line and plane defects. Determination of equilibrium concentration of schottky defect and Frenkel defects, stoichiometric imbalance in crystals. Band theory: band gap, metal, insulators, semiconductors (intrinsic and extrinsic), hopping semiconductors; rectifiers and transistors.

### **Unit-3: Statistical mechanics-II**

Concept of ensemble and phase space, ergodic hypothesis, Liouville's theorem, Concept of different ensembles, microcanonical ensembles: partition function, temperature, Canonical ensemble, distribution, probability and partition function. Partition function and different thermodynamic state functions. Black body radiation.

### **Unit-4: Statistical mechanics III**

Principle of equipartition of energy, chemically equilibrium system of interacting particles, imperfect gas. Grand canonical ensemble: nature of quantum particle, Bose- Einstein and Fermi-Dirac statistics, specific heat of electron gas, Bose-Einstein condensation, quantum statistics, density matrix.

### **Unit-5: Non-equilibrium thermodynamics**

Characterization of non-equilibrium states: entropy production rate; Onsager reciprocal relations, principle of microscopic reversibility and detailed balancing, thermonuclear pressure difference and thermonuclear effect, cyclic and oscillatory reactions, non-linear region, higher order symmetries.

### **Course Outcome (C.O.)**

The students will gain understanding on advanced level Solid state chemistry, Statistical mechanics and nonequilibrium thermodynamics.

## **CEM 303: Advanced Inorganic Chemistry-II (Inorganic Spl.)**

Marks: 40 + 10; Lecture hours: 40; Credit (L+T+P): 4 (3-1-0)

### **Unit: 1: Bioinorganic chemistry-II**

Electron transfer (redox) enzyme: Catalase Peroxidase, Cytochrome P<sub>450</sub>, Super oxide dismutase, Ascorbate oxidase. Molybdenum containing enzymes: Nitrate reductase, Xanthine oxidase, Sulphate oxidase. Vanadium containing protein: Amavadin, Vanadium bromo peroxidase. Vitamin B<sub>12</sub>, Chlorophil (Photosystem). Metal ions in genetic information transfer: Replication, transcription and translation process. Interaction of metal ions with nucleic acids and their monomeric constituents-metal complexes of nucleosides and nucleotide.

### **Unit: 2: Inorganic photochemistry**

Introduction to inorganic photochemistry, photophysical and photochemical process, characteristics of the electronically excited states of inorganic compounds, ligand field states, charge transfer states, Frank Condon (FC) states, THEXI and DOSENCO states, kinetics of photochemical process, photosensitization. Transition probabilities, Transition moment integral and its applications. Selections rules. Jablonski diagram, Fluorescence and phosphorescence, delayed fluorescence, quantum yield, mechanism and decay kinetics of photophysical processes. Fluorescence quenching (dynamic and static), Stern-Volmer equation. Photochromism; chemical actinometry, photochemical reaction of coordination compounds. Photochemical splitting of water, photochemical conversion and storage of solar energy, organometallic photochemistry.

### **Course Outcome (C.O.)**

The students will gain understanding on advanced level Bioinorganic chemistry and Inorganic photochemistry.

## **CEM 303: Advanced Organic Chemistry-II (Organic Spl.)**

Marks: 40 + 10; Lecture hours: 40; Credit (L+T+P): 4 (3-1-0)

### **Unit-01: Bioorganic and Supramolecular Chemistry-I**

Crown ethers: discovery, nomenclature, synthesis, properties and applications. Cryptands: structures and applications. molecular recognition: definition, examples of molecular recognition utilizing H-bonding, electrostatic, solvophobic, pi-pi interaction, etc., application of molecular recognition. H-bonding in molecular organization, chiral recognition, Introduction to molecular mechanics calculation and its use in the design of molecular receptors.

### **Unit-02: Bioorganic and Supramolecular Chemistry-II**

Cyclodextrins: Structure, property, applications. Enzymes: enzyme kinetics, mechanism; application of enzymes in organic synthesis, model enzymes based on cyclodextrins.

### **Unit 03: Bioorganic and Supramolecular Chemistry-III**

Self-assembling systems: micelles, reverse micelles; vesicles, fibers and tubules; amphiphiles, bola-amphiphiles, Self-replication. Gels: definition, classification, examples, study of the morphology and rheology of gels, applications Chemical sensors. Photo-responsive systems, Dye sensitized solar cell, Liquid Crystals, Molecular Electronic devices, organic conductors.

### **Unit-04: Peptides and Nucleic acids**

Peptides and Proteins: Structure and Functions;  $\alpha$ -helix,  $\beta$ -pleated sheet,  $\beta$ -turn, 3.10 helix, Ramachandran plot. Nucleic acids: Structure and functions; replication of nucleic acids.

### **Unit-05: Green Chemistry**

The current status of chemistry and the environment. What is green chemistry? How Green and Renewables are related to sustainability. Principles, methodologies and techniques in Green Chemistry. Synthesis in aqueous media, Catalytic methods in synthesis, Examples of green chemistry. Future trends in green chemistry. Unconventional energy sources in synthesis: solar energy.

### **Course Outcome (C.O.)**

The students will gain understanding on advanced level Bioorganic and Supramolecular Chemistry, Peptides and Nucleic acids synthesis and Green Chemistry.

## **CEM 304: Pharmaceutical Chemistry (CBCS)**

Marks: 40 + 10; Lecture hours: 40; Credit (L+T+P): 4 (3-1-0)

### **1. Introduction of Pharmaceutical Chemistry**

Important aspects of pharmaceutical chemistry, importance of chemistry in pharmaceuticals, some important terms used in chemistry of drugs, pharmacopeia.

### **2. Classification and nomenclatures of drugs**

Classification of drugs and their nomenclature.

### **3. Theory of drug action and factors affecting the drugs**

Theory of drug action and structure activity relation, drug receptors: isolation, modification and localization, theories related to drug action.

### **4. Types of drugs**

- A. Hyponotics and sedative drugs, Anticonvulsivant and analgesic drugs, general anaesthetics and local anaesthetics, expectorant, psychoactive and nervous system stimulant drugs, antiperkinson, antihistamine, anti-inflammatory and antipyretic drugs.
- B. Antiamoebic, antifungal and antiviral drugs, disinfectant and antiseptic, Vitamins, sulfonamides and antibiotics.

### **5. Antimalarial drugs**

Malaria parasite and its life cycle, chemotherapy of malaria using antimalarial drugs.

### **Course Outcome (C.O.)**

The students will gain understanding on Classification and nomenclature of drugs, theory of drug action and factors affecting the drugs, types of drugs, Antimalarial drugs etc.

## **CEM 395: Project (Physical/Inorganic Spl.)**

Marks: 100; Lecture hours: 200; Credit (L+T+P): 8 (0-0-8)

### **Unit 01:**

Visit to an Industry and submission of a Work-Report (approximately 10 pages) on the Industry Visit **OR Review** in an area of contemporary interest: Topic to be finalized in consultation with the Incharge and a Review-Report (approximately 10 pages) has to be submitted **OR Internship** (Without hampering regular classes and subject to approval of the authority)

[20]

### **Unit 02:**

**Research** problem has to be finalized in consultation with the Incharge. The work has to be carried out under the supervision of the Incharge and Research Report of approximately 25 pages has to be submitted.

[60]

### **Unit 03**

**Seminar Lecture** has to be delivered on the total work carried out. It will involve Power Point Presentation (Industry visit: 2 slides/ Review: 2 slides, Research work: 5 slides; total presentation time = 10 minutes (max.)).

[20]

## **CEM 395: Project (Organic Spl.)**

Marks: 100; Lecture hours: 200; Credit (L+T+P): 8 (0-0-8)

### **Review work / Industry Visit / Field work:**

**Review** in an area of contemporary interest: Topic to be finalized in consultation with the Incharge and a Review-Report (approximately 10 pages) has to be submitted.

**OR**

Industry Visit:

It will involve visit to an **Industry** and submission of a Work-Report (approximately 10 pages) on the Industry Visit

**OR**

Field Work, Sample Collection and submission of a Work-Report (approximately 10 pages) on the Field Work.

**OR**

Internship (Without hampering regular classes and subject to approval of the authority)

[30]

### **Research Work:**

#### **Unit 01:**

**Research** problem has to be finalized in consultation with the Incharge. The work has to be carried out under the supervision of the Incharge and Research Report of approximately 25 pages has to be submitted.

[50]

#### **Unit 02**

**Seminar Lecture** has to be delivered on the total work carried out. It will involve Power Point Presentation (Industry visit: 2 slides, Review: 2 slides, Research work: 5 slides; total presentation time = 10 minutes (max.)).

[20]

## **SEMESTER-IV**

### **CEM 401: Advanced Spectroscopy-II (Common Paper: Physical/Inorganic/Organic)**

Marks: 40 + 10; Lecture hours: 40; Credit (L+T+P): 4 (3-1-0)

#### **Spectroscopy for Structure Elucidation**

##### **Unit-01**

Detailed study of  $^1\text{H}$  NMR and preliminary aspects of  $^{13}\text{C}$  NMR, CW and FT techniques. Ring current: Aromaticity, Antiaromaticity, Homoaromaticity, Annulene systems.

##### **Unit-02**

NMR spectroscopy: Principles, Relaxation phenomenon, factors influencing chemical shifts and coupling constants, simplification of complex spectrum, NOE, Rotating frame of reference.

##### **Unit-03**

Mass-spectrometry combined applications of spectroscopical methods to organic molecules : Principles of Mass spectrometry, Different techniques, fragmentation modes.

##### **Unit-04**

Combined application of spectroscopic techniques (UV, IR, NMR, MS) in elucidation of structure and study of reactions of organic compounds.

##### **Unit 05:**

CD ORD and Mossbauer Spectroscopy

#### **Course Outcome (C.O.)**

The students will gain understanding on advanced level NMR spectroscopy, Mass spectroscopy, combined applications of spectroscopic techniques and CD, ORD and Moss Bauer spectroscopy.

## **CEM 402: Advanced Physical Chemistry-III (Physical Spl.)**

Marks: 40 + 10; Lecture hours: 40; Credit (L+T+P): 4 (3-1-0)

### **Unit-1: Quantum mechanics of many electron systems-I:**

Identical particle and Pauli's Antisymmetry principle, Slater determinant for system with more than two electrons, Eigen functions of many electron spin operator: Pure spin states, Energy expectation value of pure spin states; Orbitals in many electron atoms: The Hartree-Fock Theory, Koopman's theorem, The Hartree-Fock-Roothaan method for closed cell systems, Roothaan equation, Brillouin's theorem.

### **Unit-2: Atomic Spectroscopy:**

Ground state electronic configuration of elements, Spectroscopic term symbol: LS coupling scheme, j-j coupling scheme, Electronic spectrum of many electron atoms, Zeeman Effect in many electron atoms, Electron correlation and method of configuration interaction.

### **Unit-3: Applications of perturbation theory:**

The Hellmann-Feynman theorem, Electrical responsive properties, perturbation treatment to, NMR spectroscopy: A-X, A2 Spin system, more than two spin system; ESR spectroscopy: total magnetic Hamiltonian of an electron, magnetic interaction in atoms, application of perturbation theory on the splitting of ESR lines on some model system.

### **Unit-4: Computational Chemistry-I**

Exteded Huckel theory, CNDO formalism, INDO formalism, Basic NDDO formalism: MNDO, AM1, PM3.

Ab Initio HF theory: Basis set: Gaussian functions, single Zeta, multiple Zeta and split valence functions, polarization and diffuse functions.

Electron correlation in MO theory: Configuration interaction: single determinant reference, multi reference.

### **Unit-5: Computational Chemistry-II**

Density Functional Theory (DFT): Philosophy, early approximations, Hohenberg-Kohn existence theorem, Hohenberg-Kohn variational theorem, Kohn-Sham SCF methodology, Exchange correlation functionals: Local density approximation, density gradient and kinetic energy corrections.

Advantages and dis-advantages of DFT compare to MO theory, General performance of DFT.

### **Course Outcome (C.O.)**

The students will gain understanding on advanced level Quantum mechanics of many electron systems, Atomic Spectroscopy and Computational Chemistry.

## **CEM 402: Advanced Inorganic Chemistry-III (Inorganic Spl.)**

Marks: 40 + 10; Lecture hours: 40; Credit (L+T+P): 4 (3-1-0)

### **Unit: 1: Magnetochemistry**

Magnetic properties of substances, orbital and spin angular momentum of electrons, paramagnetic moment and magnetic susceptibility. Paramagnetic and diamagnetic materials, ferromagnetism, ferrimagnetism, antiferromagnetism, magnetic permeability, magnetic susceptibility, magnetization, classical theory of diamagnetism (Langevin's theory), classical theory of paramagnetism (Langevin's theory), diamagnetism and Pascal's constants, zero-field splitting, spin-orbit coupling.

Magnetic properties and temperature – The Curie and Curie-Weiss law, derivation of Curie law. Microstates, hole formalism, multiplet, multiplet width, Lande interval rule, magnetic moments for different multiplet widths, crystal field diagram, quenching of orbital contribution, high spin/low spin equilibrium. Antiferromagnetic interactions in inorganic compounds: Mechanism like – direct interaction, super exchange interactions and elucidation with poly nuclear metal complexes as well as oxide and halide salts of transition metals. Magnetic behaviour of lanthanides and actinides.

**Unit: 2: Metal carbonyls and clusters:** Carbonyl ligand; Binding in carbonyl ligands; Synthesis, structure and reactivity of metal carbonyls; Metal carbonyl anions; Metal carbonyl halides; Low nuclearity (M3-M4) and high nuclearity (M5-M10) carbonyl clusters (LNCC and HNCC); Capping rule; Total valence electron counts in d-block organometallic clusters; Condensed cages; TVE count in condensed clusters, Halide clusters of Nb, Ta, Mo, W, Re. Synthesis, structure and bonding; Interstitial Clusters-hydrides; Carbides and nitrides;

**Unit: 3: Metal-Metal Bonding:** Metal -metal bonds, Metal-metal multiple bonds: Examples, synthesis, structures, bonding; Electronic transition; Metal-metal quadruple bond; Metal-metal quintuple bond

### **Course Outcome (C.O.)**

The students will gain understanding on advanced level Magnetochemistry, Metal carbonyls and clusters.

## **CEM 402: Advanced Organic Chemistry-III (Organic Spl.)**

Marks: 40 + 10; Lecture hours: 40; Credit (L+T+P): 4 (3-1-0)

### **Unit-01: Organic Photochemistry-I**

Organic Photochemistry: Fundamental concepts, Jablonski diagram, Photochemistry of carbonyl compounds, Norrish type- I and type II processes, Paterno Buchi reaction, Barton reaction, Hofmann-Löffler-Freytag reaction, photolysis of hypohalites, addition reaction, oxidation reaction.

### **Unit-02: Organic Photochemistry-II**

Photochemical reduction, photorearrangements, substitution reaction, cis-trans isomerism, photochemistry of butadiene, di-pi methane rearrangement and related processes, dimerization of alkenes, photochromism.

### **Unit-03: Biological Active Molecules**

Antibiotics, Penicillin, Structure, Synthesis and biological activity to bacteria.

### **Unit-04: Vitamins and co-enzymes**

Vitamins, coenzymes, NAD, FAD and reactivity of different Vitamin in biological reactions.

### **Unit-05: Heterocycles**

Heterocycles: Synthesis and Reactions: Generalized approach to the synthesis of heterocycles possessing 5-,6-, and 7- membered rings with one or two or three heteroatoms per ring. Reactions of heterocycles: oxidation and reduction reactions with electrophiles, nucleophiles and other reactive intermediates with typical monocyclic and fused ring systems as examples.

### **Course Outcome (C.O.)**

The students will gain understanding on advanced level Organic photochemistry, biologically active molecules, Vitamins, coenzymes and Heterocyclic chemistry.

## **CEM 403: Advanced Physical Chemistry-IV (Physical Spl.)**

Marks: 40 + 10; Lecture hours: 40; Credit (L+T+P): 4 (3-1-0)

### **Unit-I: Chemicals Kinetics-II**

Thermodynamics formulation of reaction rates, Potential energy surface, reaction co-ordinates and reaction path, BEBO method. Absolute rate theory by using partition function; statistical formulation of chemical kinetics, equilibrium formulation, derivation of expression for specific rate, entropy of activation, volume of activation. Rates of chemisorptions, rates of desorption.

### **Unit- II: Chemical Kinetics-III**

Rate processes and some physical phenomena. Statistical approach to rate theory: Hinshelwood, RRK and RRKM theories. Reaction in molecular beams and shockwaves. Application of absolute reaction rate theory in viscosity. Diffusion controlled reaction (full and partial microscopic diffusion controlled). Bimolecular surface reaction: reaction between two adsorbed molecules, reaction between a gas molecule and an adsorbed molecule, inhibition, exchange reactions. TST of surface reaction.

### **Unit-III: Macromolecules:**

Classification of polymers, kinetics of polymerization, Molecular weight of polymers, molecular weight determination by viscosity, osmometry, light scattering, diffusion and ultracentrifugation methods. Thermodynamics of polymer solutions. Polymer conformation.

### **Unit-IV: Biopolymers**

Structure of biomolecules i) Protein-building, peptide bonds, primary, secondary, tertiary, quaternary structure. Phi-Psi map 2) Nucleic acids- A,B,Z conformations, t-RNA conformation, carbohydrates and lipids biomembranes. a) SDS-PAGE (for proteins) b) agarose gel method (for nucleic acids). Techniques to study biomolecules: CD, ORD, Flurescence, IR and Raman spectroscopy.

### **Unit –V: Advanced electrochemistry**

Debye Huckel theory, its modifications and extensions, mean ionic activity co-efficients, ion association, and precise determination of dissociation constants of weak electrolytes by method of emf and conductance measurements, ion-solvent interaction and solvation number. Non stationary processes in electrolytic solutions, Onsager conductance equation, effect of high electric field and frequency on ion conductance.

Overvoltage, polarography, amperometric titration, basic principles of cyclic voltammetry and coulometry, polyelectrolyte. Mechanism of multi-step electrochemical reactions, hydrogen overvoltage, thermodynamics of ideally polarized electrodes, structures of metal and semiconductor-electrolyte junctions, fuel cell, photoelectrochemical cells.

### **Course Outcome (C.O.)**

The students will gain understanding on advanced level Chemical kinetics, Macromolecules, Biopolymers and electrochemistry.

## **CEM 403: Advanced Inorganic Chemistry-IV(Inorganic Spl.)**

Marks: 40 + 10; Lecture hours: 40; Credit (L+T+P): 4 (3-1-0)

### **Unit: 1: Inorganic reaction mechanism**

Energy profile of reactions, discussion on general reactivity of metal complexes, inert and labile complexes, different types of mechanisms („D“, „A“, „I<sub>a</sub>“ and „I<sub>d</sub>“). Techniques for experimental measurements of reaction rates, techniques for fast reaction. Substitution reactions: Application of CFT, mechanism of ligand substitution in octahedral complexes, mechanism of isomerisation and racemisation, substitution reactions in square planar complexes. *Cis*- and *trans*- effects.

Mechanism of redox reactions with reference to metal complexes. Electron transfer reactions – outer sphere and inner sphere, atom transfer, induced electron transfer reactions, two electron transfer reactions, complementary and non-complementary reactions, synthetic implications of electron transfer reactions, solid state electron transfer reactions. Electroprotic reactions. Twist mechanism of racemisation, inversion of configuration and associated process.

### **Unit: 2: Analytical chemistry**

Electroanalytical methods: Basic principles-polarised and depolarized electrodes; diffusion current, *dropping mercury electrode (DME)*, *polarographic wave*; Ilkovic equation (simplified derivation) and its significance; half-wave potential and its applications in identification of elements. Ilkovic-Heyrovsky equation, Cottrell equation. Stripping voltammetry, amperometric titration. Modern developments in polarographic techniques: Lingane’s method.

Cyclic voltammetry and Coulometry: Basic principle, three electrode configuration. Solvents and supporting electrolytes. Representation of cyclic voltammogram, half wave potential, irreversible, reversible and quasi-reversible redox processes. Electron transfer at a constant potential, no. of electron transfer. Application in coordination chemistry (characterization, determination of redox potential), e.g. ferrocene, Co(II)/Co(III); Ni(II)/Ni(III); Cu(I)/Cu(II); Ru(II)(bpy)<sub>3</sub>

Thermal methods of analysis: Basic principles of Differential Thermal Analysis, Thermo Gravimetric Analysis. Application in coordination chemistry.

### **Course Outcome (C.O.)**

The students will gain understanding on advanced level Inorganic reaction mechanism and Analytical chemistry.

## **CEM 403: Advanced Organic Chemistry-IV (Organic Spl.)**

Marks: 40 + 10; Lecture hours: 40; Credit (L+T+P): 4 (3-1-0)

### **Unit-01: Stereochemistry-III**

Conformation and Chemical Reactivity : Curtin-Hammett principle, its derivation under different conditions and applications; quantitative treatment of mobile systems, Winstein Holness equation and Eliel equation - their applications ;  $\alpha$  -Strain and  $\beta$  -strain, allylic 1,2 -and 1, 3-strain (in pseudoallylic systems also), their applications.

### **Unit-02: Stereochemistry-IV**

Fused ring systems, *trans* and *cis* declains, conformation, steroid and nonsteroid conformation, symmetry, torsion angle enthalphy, entropy, free energy, substituted declains q-methyldecalins and 9,10 dimethyldecalins, decalones; conformation of cis-octalins and trans-octalins.

### **Unit 03: Stereochemistry-V**

Stereochemistry of 4-10 membered rings, transannular reactions; perhydrophenanthrenes and perhydroanthracenes conformation, energy, symmetry and optical activity, relative stability, stereochemistry of perhydrodiphenic acids and perhydrophenanthrenes, conformations of some triterpenes.

### **Unit- 04: Stereochemistry-VI**

Modern concepts of nucleophilic addition to carbonyl compounds, Felkin model (torsional strain) Burz Dunitz trajectory, Cieplak model, examples.

### **Unit- 05: Stereochemistry-VII**

Optical rotation, specific and molecular rotations-their units, Brewster rule, Lowe's rule, origin of optical rotation, circular birefringence, optical rotatory dispersion (ORD) octant rule, axial haloketone rule-application (octant projection diagrams) ; circular dichroism (CD) differential dichroic absorption, specific ellipticity and molar ellipticity, applications of CD-helicity rule, exciton chirality (dibenzoate chirality rule) Davydov splitting-applications with different steroidal glycals.

### **Course Outcome (C.O.)**

The students will gain understanding on advanced level organic Stereochemistry.

## **CEM 404: Chemistry in Technology (Common Paper: Physical/Inorganic Spl.)**

Marks: 40 + 10; Lecture hours: 40; Credit (L+T+P): 4 (3-1-0)

### **Unit 01:**

**Biophysical Chemistry:** Structure and function of biomolecules: protein, nucleic acid, carbohydrates and lipids. Membrane structure, biomolecular complexes: protein-ligand, enzyme-substrate and drug-DNA. Examples, techniques for study of biomolecular structure and function.

### **Unit 02:**

**Instrumental Analysis: Theory and Practices:** Electron Microscopy, atomic force microscopy, Polarizing optical microscopy, Circular dichroism, Calorimetry, Phase contrast microscope, dynamic light scattering, epi Fluorescence microscopy.

### **Unit 03:**

**Chemical Toxicology:** Toxic Chemicals in the environment, Impact of toxic chemicals on enzymes, Biochemical effects of arsenic, cadmium, sulphur dioxide, ozone and PAN, Cyanide, pesticides, Carcinogens.

### **Unit 04:**

**Fundamentals of Nanoscience and technology:** Introduction and fundamentals of nanoscience and technology; synthesis, Characterization and properties of nanomaterials; Application of nanomaterials.

## **Course Outcome (C.O.)**

The students will gain understanding on advanced level Biophysical Chemistry, Instrumental analysis: theory and practices, Chemical toxicology and Corrosion technology.

## **CEM 404: Chemical Principles in Food Science and Technology (Organic Spl.)**

Marks: 40 + 10; Lecture hours: 40; Credit (L+T+P): 4 (3-1-0)

### **Unit 01:**

Storage and handling of fresh fruits and vegetables, pre and post harvest changes, thermal and osmotic dehydration of fruits and vegetables, canning and bottling, CAP and MAP storage, juice extraction and preparation of drinks, syrups, squashes, cordials, nectars, jam, jelly, marmalade, ketchup, pickles, chutneys, sauces, fruits juice concentrates and powders, fermented fruit and vegetable products,

### **Unit 02:**

**Science and technology of dairy processing** Definition, composition of milk, Quality standards for milk, Pasteurization of milk; standardization, toning, homogenization and cream separation. Technology of dried whole milk, butter, ghee, margarine, condensed milk, fermented milk products, UHT milk, ice-cream, cheese (cheddar, cottage)

### **Unit 03:**

**Science and technology of Cereal Processing** Production of milled rice, Parboiling and parboiled rice, wheat processing - classification of wheat; milling of wheat, dough mixing, types of dough and its rheology testing, production of wheat products such as bread, biscuits and cakes;

### **Unit 04:**

**Science and technology of Fats and Oils Processing:** Chemical composition, nutritional importance of dietary oils and fats, Effect of processing and storage on fats and oils (oxidative and hydrolytic rancidity), fat micelles, soap and detergency , essential fatty acids, extraction, physical and chemical refining of oils from oilseed such as mustard including winterization, bleaching and deodorization; Hydrogenation and catalysis. margarine, analytical techniques for fat and oil analysis (saponification number, acid number, iodine value, acetyl value, Reichert-Meissl number and Polenski value. Smoke, fire, flash point of oils) .

### **Unit 05:**

**Quality control and Food Safety:** Quality definition of different food products according to food laws :especially FSSAI, PFA, FPO, Essential Commodities Act, 1955, BIS, AGMARK, Classifications and functions and safety limits of food additives such as preservatives, antioxidants, colors, emulsifiers, sweeteners, buffering salts , Voluntary quality standards and certification - GMP, HACCP, GAP, ISO 9000, ISO 14000, ISO 22000; Misbranding. Adulteration in oil, dairy items and spices.

### **Course Outcome (C.O.)**

The students will gain understanding on Storage and handling of fresh and processed food and vegetables, dairy processing, cereal processing, fats and oils, quality control and food safety.

### **Text books/ References:**

1. Robinson RK; 1996; Modern Dairy Technology, Vol 1 & 2; Elsevier Applied Science Pub.
2. Developments in Dairy Chemistry – Vol 1 & 2; Fox PF; Applied Science Pub Ltd.
3. Outlines of Dairy Chemistry, De S; Oxford.
4. Processing Fruits: Science and Technology, Vol. I, Biology Principles and Applications, L. Somogyi, Woodhead Publishing, 1st Edition, 1996.
5. Food oils and their uses; Weiss TJ;1983,AVI 6.Modern Technology in the Oils and Fats industry by S.C.Singhal, OTA(I)

## **CEM 495: Project (Physical/Inorganic Spl.)**

Marks: 100; Lecture hours: 200; Credit (L+T+P): 8 (0-0-8)

### **Research Work (extension from Semester III):**

#### **Unit 01:**

##### **Skill to Read Research Articles:**

A recent research article will be supplied and the students will have to answer some questions on the article **OR** Internship (Without hampering regular classes and subject to approval of the authority)

[20]

#### **Unit 02:**

**Research** problem has to be finalized in consultation with the Incharge. The work has to be carried out under the supervision of the Incharge and Research Report of approximately 25 pages has to be submitted.

[60]

#### **Unit 03**

**Seminar Lecture** has to be delivered on the total work carried out. It will involve Power Point Presentation (Total number of slides = 10; total presentation time = 10 minutes (max.)).

[20]

## **CEM 495: Project (Organic Spl.)**

Marks: 100; Lecture hours: 200; Credit (L+T+P): 8 (0-0-8)

### **Review work / Industry Visit / Field work:**

**Review** in an area of contemporary interest: Topic to be finalized in consultation with the Incharge and a Review-Report (approximately 10 pages) has to be submitted.

**OR**

### **Industry Visit:**

It will involve visit to an **Industry** and submission of a Work-Report (approximately 10 pages) on the Industry Visit

**OR**

Field Work, Sample Collection and submission of a Work-Report (approximately 10 pages) on the Field Work.

**OR**

Internship (Without hampering regular classes and subject to approval of the authority)

[30]

### **Research Work:**

#### **Research Work (extension from Semester III):**

##### **Unit 01:**

**Research** problem has to be finalized in consultation with the Incharge. The work has to be carried out under the supervision of the Incharge and Research Report of approximately 25 pages has to be submitted.

[50]

##### **Unit 02**

**Seminar Lecture** has to be delivered on the total work carried out. It will involve Power Point Presentation (Industry visit: 2 slides, Review: 2 slides, Research work: 5 slides; total presentation time = 10 minutes (max.)).

[20]

### **Suggested Reading (Organic Chemistry):**

1. Photochemistry and Pericyclic Reactions, Jagdamba Singh and Jaya Singh
2. Advanced Organic Chemistry, Part-A, F.A. Carey and R.J. Sundburg
3. Advanced Organic Chemistry, Part-B, F.A. Carey and R.J. Sundburg
4. March's Advanced Organic Chemistry, Michael B. Smith and Jerry March
5. Organic Chemistry, T.W. Graham, Solomons and Craig B. Fryhle
6. Organic Chemistry, Paula Yurkanis Bruice
7. Green Chemistry, Paul T. Anastas and Tracy C. Williamson
8. Green Chemistry: Theory and Practice, Paul T. Anastas and John C. Warner
9. Molecular Gels: Materials with Self-Assembled Fibrillar Networks, Richard G. Weiss and P. Terech.
10. Spectroscopic Identification of Organic Compounds, Robert M. Silverstein and Francis X. Webster
11. Organic Synthesis: The Disconnection Approach, Stuart Warren
12. Modern Methods of Organic Synthesis: William Carruthers and Iain Coldham

### **Suggested Reading (Inorganic Chemistry):**

1. Chemical Application of Group Theory – F.A. Cotton
2. Group Theory – Robert L. Carter
3. Symmetry in Chemistry – Jeffe & Archin
4. Symmetry in Molecules – J. M. Hollar
5. Symmetry Orbitals & Spectra – Jeffe & Archin
6. Physical Methods in Inorganic Chemistry – R. S. Drago
7. Electron Spin Resonance – Assculieien
8. Fundamentals of Molecular Spectroscopy – C. W. Banwell
9. Introduction to Molecular Spectroscopy – G. M. Barrow
10. Advanced Inorganic Chemistry – F. A. Cotton & G. Wilkinson
11. Inorganic Chemistry – J. E. Huheey, E. A. Keiter & R. L. Keiter
12. Chemistry of The Elements – N. N. Greenwood & A. Earnshaw
13. An Introduction to Inorganic Chemistry – K. F. Pucell & J. C. Kotz
14. Concept and Model in Inorganic Chemistry – Douglass, McDanniel & Alexander
15. Coordination Chemistry – S. F. A. Kettle
16. Valence Theorū – S. F. A. Kettle, J. N. Murrall & S. Teddler

17. Valence – C. A. Coulson
18. Theoretical Approach to Inorganic Chemistry – A. F. Williams
19. Theoretical Inorganic Chemistry M. C. Dey and I. Selbin
20. Introduction to Ligand Field Theory – C. J. Ballhausen
21. Introduction to Ligand Field – B. N. Figgis
22. Inorganic Electronic Spectroscopy – A. B. P. Lever
23. Elements in Magnetochemistry – R. L. Dutta and A. Shyamal
24. Organo Transition Metal Chemistry – S. G. Davies
25. Principles and Application of Organotransition Metal Chemistry – J. P. Collman, L. S. Hegedus, Borton & R. G. Finke
26. Organometallic Chemistry – An Introduction – R. C. Mahrotra & A. Singh
27. Principles of Organometallic Chemistry – G. E. Coats, H. L. H. Green, P. Powell & K. Wade
28. Basic Organometallic Chemistry – J. J. Zuckerman and I. Haiduc
29. The Organometallic Chemistry of Transition Metals – R. H. Carbtree
30. Bioinorganic Chemistry – R. W. Hay
31. Introduction to Bioinorganic Chemistry - D.R. Williams
32. Elements of Bioinorganic Chemistry – G. N. Mukherjee & A. Das
33. Inorganic Chemistry – D. F. Shriver, P. W. Atkins & C. H. Langford
34. Instrumental Methods Analysis – Williard, merit, Dean & Sett
35. Electroanalytical Techniques for Inorganic Chemistry – J. B. Headri
36. Comprehensive Coordination Chemistry – G. Wilkinson, R. A. Gillard & J. A. McCleverty (eds)
37. Inorganic Chemistry – A. G. Sharpe
38. Inorganic Chemistry – Modern Introduction
39. Fundamentals of Analytical Chemistry – D. A. Skoog, D. M. West and F. J. Holler
40. Analytical Chemistry – G. D. Christian
41. Analytical Chemistry, Principles – J. H. Kennedy

### **Practical (Inorganic):**

1. Spot Tests of Inorganic Analysis – F. Feigel & V. Anger (translated by R. Oesper)
2. Macro and Semi Macro Qualitative Inorganic Analysis - A. J. Vogel
3. Quantitative Inorganic Analysis - G. Charlot & D. Bezier (translated by R. C. Murray)
4. Quantitative Chemical Analysis - I. M. Kolthoff, E. B. Sandel, J. Meehan and S. Bruckenstein
5. Advanced Experiments in Inorganic Chemistry – G. N. Mukherjee.

## **Suggested Reading (Physical Chemistry):**

1. Elementary Quantum Chemistry – F. I. Pilar
2. Quantum Chemistry – I. N. Levine
3. Molecular Quantum Mechanics – P. W. Atkins
4. Quantum Mechanics – J. I. Powel, B. Crasemann
5. Introduction to Quantum Mechanics – D. J. Griffiths
6. The Feynman Lectures in Physics, Vol. 3 – R. P. Feynman, R. B. Leighton, M. Sands
7. Chemical Applications of Group Theory – F. A. Cotton
8. Group Theory and Chemistry – D. M. Bishop
9. Coulson's Valance - R. McWeeny
10. Thermodynamics and an Introduction to Thermodynamics – H. B. Callen
11. Theories of chemical reaction rates – K. J. Laider
12. Theory of Rate Processes – S. Glaasstone, K. J. Laidler, H. Eyring
13. Principles of Physical Biochemistry – K. E. van Holde, C. Johnson, P. S. Ho
14. Modern Electrochmistry – J. O'M. Bockris, A. K. N. Reddy
15. Physical Chemistry of Macromolecules – C. Tanford
16. Polymer Chemistry – P. J. Flory
17. Molecular Spectroscopy – I. N. Levine
18. Molecular Spectroscopy – J. D. Graybeal
19. Principles of Fluorescence Spectroscopy – J. R. Lakowicz
20. Introduction to Magnetic Resonance – A. Carrington, A. D. McLachlan
21. Statistical and Thermal Physics – F. Reif
22. Statistical Mechanics – D. A. McQuarrie
23. Statistical Mechanics – S. K. Ma
24. Statistical Mechanics – K. Huang
25. Statistical Mechanics – R. K. Patharia
26. Statistical Mechanics – B. B. Laud
27. Chemical Kinetics and Dynamics – J. I. Steinfeld, J. S. Francisco, W. L. Hase
28. Molecular Reaction Dynamics – R. D. Levine
29. Molecular Reaction Dynamics and Chemical Reactivity – R. D. Levine, R. B. Bernstein
30. Introduction to Solid State Physics – C. Kittel
31. Introduction to Solid State Theory – O. Madelung
32. Solid State Physics – A. J. Dekker
33. Molecular Modelling Principles and Application – A. R. Leach
34. Genetic Algorithm in Search Optimization and Machine Learning-D.E. Goldberg
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