Vidyasagar University



Dept. of Chemistry and Chemical Technology

Syllabus 2018

For

M.Sc. in Chemistry

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

[w. e. f. 2018-19 session]

SEMESTER	COURSE	COURSE TITLES	Full	Credit
	NO.		Marks	
	CEM 101	PHYSICAL CHEMISTRY - I	50	4
	CEM 102	ORGANIC CHEMISTRY- I	50	4
	CEM 103	INORGANIC CHEMISTRY- I	50	4
Ι	CEM 104	FOOD PROCESSING AND PRESERVATION AND COMPUTER BASICS	50	4
	CEM 195	INORGANIC CHEMISTRY (practical)	50	4
	CEM 196	FOOD PROCESSING AND PRESERVATION (practical)	50	4
		TOTAL	300	24
	CEM 201	PHYSICAL CHEMISTRY-II	50	4
	CEM 202	ORGANIC CHEMISTRY-II	50	4
	CEM 203	INORGANIC CHEMISTRY-II	50	4
	C-CEM 204	NANOTECHNOLOGY: PRINCIPLES AND PRACTICES(CBCS)	50	4
	CEM 295	ORGANIC CHEMISTRY (practical)	50	4
	CEM 296	PHYSICAL CHEMISTRY (practical)	50	4
		TOTAL	300	24
	CEM 301	ADVANCED SPECTROSCOPY-I	50	
		PHYSICAL CHEMISTRY SPECIALISATION		
	CEM 302	ADVANCED PHYSICAL CHEMISTRY-I	50	4
п	CEM 303	ADVANCED PHYSICAL CHEMISTRY-II	50	4
II		INORGANIC CHEMISTRY SPECIALISATION		
	CEM 302	ADVANCED INORGANIC CHEMISTRY-I	50	4
	CEM 303	ADVANCED INORGANIC CHEMISTRY-II	50	4
		ORGANIC CHEMISTRY SPECIALISATION		1
	CEM 302	ADVANCED ORGANIC CHEMISTRY-I	50	4
	CEM 303	ADVANCED ORGANIC CHEMISTRY-II	50	4
	C-CEM 304	INTRODUCTION TO PHARMACEUTICAL CHEMISTRY(CBCS)	50	4
	CEM 395	CHEMISTRY PROJECT-I(PHYSICAL SPL/ORGANIC SPL/INORGANIC	100	8
		SPL)		
		TOTAL	300	24
	CEM 401	ADVANCED SPECTROSCOPY-II	50	4
		PHYSICAL CHEMISTRY SPECIALISATION		
	CEM 402	ADVANCED PHYSICAL CHEMISTRY-III	50	4
	CEM 403	ADVANCED PHYSICAL CHEMISTRY-IV	50	4
	CEM 404	CHEMISTRY IN TECHNOLOGY	50	4
		INORGANIC CHEMISTRY SPECIALISATION	1	
	CEM 402	ADVANCED INORGANIC CHEMISTRY-I	50	4
** *	CEM 403	ADVANCED INORGANIC CHEMISTRY-II	50	4
IV	CEM 404	CHEMISTRY IN TECHNOLOGY	50	4
		ORGANIC CHEMISTRY SPECIALISATION		
	CEM 402	ADVANCED ORGANIC CHEMISTRY-III	50	4
	CEM 403	ADVANCED ORGANIC CHEMISTRY-IV	50	4
	CEM 404	CHEMICAL PRINCIPLES IN FOOD SCIENCE AND TECHNOLOGY	50	4
	CEM 495	CHEMISTRY PROJECT-II (PHYSICAL SPL/ORGANIC SPL/ INORGANIC	100	8
		SPL)		
		TOTAL	300	24
		ALL TOTAL	1200	96

M.Sc. in CHEMISTRY

Overview

Semester	Paper	No of	Full Marks	Credit Point	Total Marks	Credit	Total
		Papers	of Each	of Each		Points	Credit
			Paper	Paper			Point
				-			
1 st	Theoretical	4	40+10 = 50	4	200	16	24
	Practical	2	50	4	100	8	
2 nd	Theoretical	4	40+10 = 50	4	200	16	24
	Practical	2	50	4	100	8	
3rd	Theoretical	4	40+10 = 50	4	200	16	24
	Practical (Project)	1	100	8	100	8	
4 th	Theoretical	4	40+10 = 50	4	200	16	24
	Practical (Project)	1	100	8	100	8	
			·	·	Grand T	otal 96 Crec	lit Points

	1 st semester: General	Course		
Paper	Course	Duration	Marks	Credit Point
CEM 101	Physical Chemistry-I	45L	50	4
Unit I Unit II Unit IV Unit V Unit V CEM-102 Unit I Unit II Unit III Unit IV Unit V	Mathematical preliminaries & Quantum Mechanics-I Thermodynamics Statistical Mechanics I Fundamentals of Nanoscience and Technology Principles of molecular spectroscopy-I Organic Chemistry-I Pericyclic reaction-1 Organic transformations / synthesis / reagents Natural products- terpenoids Natural products- alkaloids Retro-synthesis I	45L	50	4
CEM-103	Inorganic Chemistry-I	45L	50	4
Unit I Unit II Unit III	Symmetry and Group theory-I Solid state chemistry and Crystallography Bioinorganic chemistry-I			
CEM-104	Food processing and preservation and Computer basics	45L	50	4
Unit I Unit II Unit III Unit IV	Constituents of food, food pigments and flavouring agents Introduction to food microbiology Food preservation: Principles and methods Computer basics I			
Unit V	Computer basics I; data manipulation			
CEM-195	Inorganic Chemistry Practical	8 Weeks	50	4
CEM-196	Food processing preservation and packaging Practical	8 Weeks	50 Total Marks	4 5 30
			Total Credit	24

	2 nd Semester: General Course					
Paper	Course	Duration	Marks	Credit Point		
CEM-201 Unit I Unit II Unit III Unit IV Unit V	Physical Chemistry-II Quantum Mechanics-II Chemical kinetics-I Electrochemistry Molecular spectroscopy-II Surface chemistry	45L	50	4		
CEM-202 Unit I Unit II Unit III Unit IV Unit V CEM-203	Organic Chemistry-II Pericyclic reaction-2 Organic transformations/synthesis/reagents chemistry-2 Retrosynthetic analysis II Stereochemistry-1 Stereochemistry-2, Inorganic Chemistry-II	45L 45L	50	4		
Unit I Unit II Unit III CEM-204 (Elective Course)	Organometallic chemistry -I Group theory-II Chemistry of p and d-block elements Nanotechnology: Principles and Practices Introduction, synthesis of nanomaterials, analysis techniques, application of nanotechlogy	45L	50	4		
CEM-295	Organic Chemistry Practical	8 Weeks	50	4		
CEM-296	Physical Chemistry Practical	8 Weeks	50	4		
		Тс	otal Marks	300		
		Το	otal Credit	24		

	3rd Semester: Physical Chemistry Spl.						
Paper	Course	Duration	Marks	Credit Point			
CEM-301	Advanced Spectroscopy-I	45L	50	4			
Unit I	Photophysical Processes						
Unit II	LASERs and its applications						
Unit III	EPR spectroscopy						
Unit IV	PES and NQR spectroscopy						
CEM-302	Advanced Physical Chemistry-I	45L	50	4			
Unit I	Matrix mechanics						
Unit II	Stationary perturbation theory						
Unit III	Semiclassical radiation – matter interaction						
Unit IV	Semiemperical methods in quantum chemistry						
Unit V	Group theory & quantum mechanics						
CEM-303	Advanced Physical Chemistry-II	45L	50	4			
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 theromodynamics						
C-CEM 304	Introduction of Pharmaceutical Chemistry (CBCS) : Classification and nomenclature of drugs,Theory of drug action and factors affectingthe drugs, Types of drugs, Antimalarial drugs	45L	50	4			
		16					
CEM-395	Physical Chemistry Project I	Weeks	100	8			
	Total Marks		300				
	Total Credit			24			

	3rd Semester: Inorganic Chemistry Spl.				
Paper	Course	Duration	Marks	Credit Point	
CEM-301	Advanced Spectroscopy-I	45L	50	4	
Unit I	Photophysical Processes				
Unit II	LASERs and its applications				
Unit III	EPR spectroscopy				
Unit IV	PES and NQR spectroscopy				
CEM-302	Advanced Inorganic Chemistry-I	45L	50	4	
Unit I	Organometallic chemistry – II and catalysis				
Unit II	Chemical applications of group theory				
CEM-303	Advanced Inorganic Chemistry-II	45L	50	4	
Unit I	Bioinorganic chemistry – II				
Unit II	Inorganic photochemistry				
C-CEM 304	Introduction of Pharmaceutical Chemistry (CBCS): Classification and nomenclature of drugs, Theory of drug action and factors affecting the drugs, Types of drugs, Antimalarial drugs	45L	50	4	
		16			
CEM-395	Inorganic Chemistry Project I	Weeks	100	8	
	Total Marks		300		
	Total Credit			24	

	3rd Semester: Organic Chemistry Spl.			
Paper	Course	Duration	Marks	Credit Point
CEM 301	Advanced Spectroscopy-I	45L	50	4
Unit I	Photophysical Processes			
Unit II	LASERs and its applications			
Unit III	EPR spectroscopy			
Unit IV	PES and NQR spectroscopy			
CEM 302	Advanced Organic Chemistry-I	45L	50	4
Unit I	Pericyclic Reaction-III			
Unit II	Linear free energy relationship I			
Unit III	Linear free energy relationship II			
Unit IV	Organometallic Chemistry			
CEM 303	Advanced Organic Chemistry II	45L	50	4
Unit I	Bioorganic and Supramolecular Chemistry-I			
Unit II	Bioorganic and Supramolecular Chemistry-II			
Unit III	Bioorganic and Supramolecular Chemistry-III			
Unit IV	Peptides and Nucleic acids			
Unit V	Green Chemistry.			
C-CEM 304	Introduction of Pharmaceutical Chemistry (CBCS): Classification and nomenclature of drugs, Theory of drug action and factors affecting the drugs, Types of drugs, Antimalarial drugs	45L	50	4
		16		
CEM-395	Organic Chemistry Project I	Weeks	100	8
	Total Marks		300	
	Total Credit			24

	4th Semester: Physical Chemistry Sp	l.		
Paper	Course	Duration	Marks	Credit Point
CEM 401	Advanced Spectroscopy-II	45L	50	4
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			
CEM 402	Advanced Physical Chemistry III	45L	50	4
Unit I	Quantum mechanics of many electron systems I			
Unit II	Atomic Spectroscopy			
Unit III	QM of diatomic molecules			
Unit IV	QM of many electron systems II			
Unit V	Application of perturbation theory			
CEM 403	Advanced Physical Chemistry IV	45L	50	4
Unit I	Chemical kinetics II			
Unit II	Chemical kinetics III			
Unit III	Macromolecules			
Unit IV	Bioploymers			
Unit V	Advanced electrochemistry			
CEM 404	Chemistry in technology	45L	50	4
Unit I	Biophysical Chemistry			
Unit II	Instrumental analysis: theory and practices			
Unit III	Chemical toxicology			
Unit IV	Corrosion technology			
		16		
CEM 495	Physical Chemistry Project II	Weeks	100	8
	Total Marks		300	
	Total Credit			24

	4th Semester: Inorganic Chemistry Spl.				
Paper	Course	Duration	Marks	Credit Point	
CEM 401	Advanced Spectroscopy-II	45L	50	4	
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				
CEM 402	Advanced Inorganic Chemistry III	45L	50	4	
Unit I	Magnetochemistry				
Unit II	Metal carbonyls and clusters				
CEM 403	Advanced Inorganic Chemistry IV	45L	50	4	
Unit I	Inorganic reaction mechanism				
Unit II	Analytical chemistry				
CEM 404	Chemistry in technology	45L	50	4	
Unit I	Biophysical Chemistry				
Unit II	Instrumental analysis: theory and practices				
Unit III	Chemical toxicology				
Unit IV	Corrosion technology				
CEM 495	Inorganic Chemistry Project II	16 Weeks	100	8	
	Total Marks		300		
	Total Credit			24	

	4th Semester: Organic Chemistry S	Spl.		
Paper	Course	Duration	Marks	Credit Point
CEM 401	Advanced Spectroscopy-II	45L	50	4
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			
CEM 402	Advanced Organic Chemistry III	45L	50	4
Unit I	Organic photochemistry I & II			
Unit II	Biologically active molecules			
Unit III	Vitamins and coenzymes			
Unit IV	Heterocyclic chemistry			
CEM 403	Advanced Organic Chemistry IV	45L	50	4
Unit I	Stereochemistry III			
Unit II	Stereochemistry IV			
Unit III	Stereochemistry V			
Unit IV	Stereochemistry VI			
Unit V	Stereochemistry VII			
CEM 404	Chemical principles in food science and technology:Storage and handling of fresh and processed food and vegetables, dairy processing, cereal processing, fats and oils, quality control and food 	45L	50	4
CEM 495	Organic Chemistry Project II	16 Weeks	100	8
	Total Marks		300	
	Total Credit			24

SEMESTER-I

CEM – 101: Physical Chemistry-I Marks: 50 Credits: 4 Classes: 45L

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 status: box with infinite and finite walls.

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.

Unit-3: Statistical Machanics - 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), Gibbs paradox.

Unit: 4: Fundamentals of Nanoscience and technology

Introduction and fundamentals of nanoscience and technology; synthesis, Characterization and properties of nanomaterials; Application of nanomaterials.

Unit: 5: Principle of Molecular Spectroscopy-I

General introduction, nature of electromagnetic radiation, shapes & width of spectral lines, Intensity of spectral lines, Fourier transform.

Microwave Spectroscopy: Moment of Inertia and Classification of molecules, Diatomic molecule as rigid rotator, non rigid rotator, Hyperfine Structures, Stark Effect and determination of Dipole moment. Infrared Spectroscopy: Vibrational Spectra of diatomic Molecules, Harmonic Oscillator model, Anhermonic oscillator model, Rotational Vibrational spectra of diatomic molecules.

CEM 102: Organic Chemistry –I Marks: 50 Credits: 4 Classes: 45L

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, Wood Word 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 tritepenes: 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, cetral geraniol neral, linalool monocyclic monoterpenoids; -terpeinol, structure elucidation, synthesis and biogenesis. Higher terpenoids: sesqui-, di-, sester-, tri-, tetra- terpenoids.

Unit - 04

Natural Products - Alkaloids:

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

Unit - 05

Retrosynthetic analysis-I: Organic Synthesis Strategy, the disconnection approach.

CEM 103: Inorganic Chemistry-I Marks: 50 Credits: 4 Classes: 45L

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, <u>Hermann–Mauguin (HM) notations</u>, 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. Deterination of equilibrium concentration of Schottky and Frenkel defects, Stoichimetric 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. Bioenergetic principle and role of ATP. O_2 – uptake proteins: hemoglobin, myoglobin, hemerythrin and hemocyanin, structure, function and model study. Electron transport protein: Fe-S proteins, cytochromes. Metal ions transport and storage proteins: ferritin, transferin, ceruloplasmin. Transport across biological membrane - Na⁺-K⁺-ATPase, ionophores. Hydrolytic enzymes: carbonic anhydrase, carboxy peptidase, urease. Metal dependent diseases: Wilson's disease, Alzheimer disease. Transition metal complexes as drugs.

CEM 104: FOOD PROCESSING AND PRESERVATION-I and COMPUTER BASICS Marks: 50 Credits: 4 Classes: 45L

UNIT-I:

Constituents of Food: Water; Water in foods and its properties, **Carbohydrates**; Sources and physicochemical 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.

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.

Text Books/References:

- 1. Food Science, 5th 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) 8 weeks

1. Quantitative analysis

- 1A. Gravimetric estimation of Zn(II) as Zn(NH₄)(PO₄)
- 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 BaSO₄
- 1E. Gravimetric estimation of Pb(II) as (Pb)₃(PO₄)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 CaCO₃ and CaCO₃ 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. $[Co(NH_3)_6]Cl_3$ 6C. $[Cu(NH_3)_4(SO_4)(H_2O)]$ 6D. $[Co(NH_3)_5Cl]Cl_2$ 6E. $[Ni(en)_2]Cl_2$ 6F. $K_3[Fe(ox)_3]$ 6G. $K_3[Cr(ox)_3]$ 6H. $[Co(NH_3)_6]Cl_3$ 6I. $[Cu(NH_3)_4(SO_4)(H_2O)]$ 6J. Crome alum $[K_2SO_4, Cr_2(SO_4)_3, 24H_2O]$

CEM 196: FOOD PROCESSING, PRESERVATION & PACKAGING LAB (Practical) (8 weeks)

Full Marks : 50

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: 50 Credits: 4 Classes: 45L

Unit-1: Quantum Mechanics-II

Harmonic Oscillator (Wave function and Operator methods), Hydrogen atom Problem: Cartesian and Polar coordinates. Centre of Mass and relative coordinate, Spherical harmonics. Real and complex orbital, Role of constant of motion.

Approximate method: Variational principle

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: 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.

Unit-4: Molecular Spectroscopy-II

Raman Spectroscopy: 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.

Electronic Spectroscopy: Fluorescence, Phosphorescence and nonradiative processes.

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.

CEM 202: Organic Chemistry - II Marks: 50 Credits: 4 Classes: 45L

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, orbital coefficient and diagram of polyene systems with various substitutions. 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, Sharpness asymmetric expoxidation, AD-mix, Transformation of expoxides. Organophosphorus reagents, organo sulfer reagents, organo boranes, organo silanes, organostannanes, metal hydrides, Birch reduction, Bayer Villiger reactions, chichibabin reaction, Merrifield resin: solid phase synthesis.

Retro synthetic analysis: disconnection approach. Examples to illustrate disconnection approach in organic 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, threoerythro, pref-parf, chiral simplex. Stereogencity 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- Alkyle 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. Sharpless expoxidation.

CEM 203: Inorganic Chemistry - II Marks: 50 Credits: 4 Classes: 45L

Unit: 1: Organometallic chemistry –I

Application of 18-electron and 16-electron rules to transition metal organometallic complexes, Ligands in organometallic chemistry; Synthesis, bonding and reactivity 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- π^* and π - π^* 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, boron compounds 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. Isoand 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.

CEM 204: Nanotechnology: Principles and Practices (Elective Course) Marks: 50 Credits: 4 Classes: 45L

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.

Syllabus: Department of Chemistry and Chemical Technology

CEM 295: Organic Chemistry Practical Marks: 50 Credits: 4

1. Liquid Sample

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

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 λ_{max} , ε_{max} and explain. Submit the product with proper label.

<u>OR</u>

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.

4. Viva Voce

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

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CEM 296: Physical Chemistry Practical Marks: 50 Credits: 4

(One day examination - duration 6 hours, Full Marks = 50)

1. List of Experiments:

1. Kinetics of Inversion of Cane-sugar by Polarimeter /

2. Determination of concentration of Glucose-fructose in a mixture using polarimeter

3. Conductometric determination of concentrations of KCl, HCl and NH4Cl in a mixture.

4. Verify the Onsagar equation using KCl, K_2SO_4 and $BaCl_2$ as electrolytes and determine their Λ_0 values.

5. Determination of CMC of a surfactant in aqueous solution by conductometric method.

6. Potentiometric titration of halide mixture (Chloride, Bromide and Iodide).

7. Determine the E0 value of Ag+/Ag electrode and activity coefficients of different aqueous AgNO3 solutions potentiometrically.

8. Determine the standard potential of *Fe(CN)6+3-/ *Fe(CN)6+4- electrode by potentiometer.

9. Determine the dissociation constants (K1, K2, and K3) of H3PO4 by pH meter.

10. Study the kinetics of Iodination of acetone spectrophotometrically.

11. Determination of composition of complexes (Ferric-salicylate complex/Ferrous-orthophenanthroline complex) by Job's method.

12. Determine the rate constant and the order of the reaction of KBrO3 & KI in acid medium.

13. Determine the order and rate constant of the reaction between K2S2O8 & KI and study the influence of ionic strength on the rate constant.

14. Study of the kinetic of alkaline hydrolysis of crystal violet. Determine the order with respect to alkali and salt effect on the system.

14. Spectroscopic experiments relating to quenching of fluorescence

15. Experiment for the measurements of activation barrier of some model chemical reactions

2. Sessional Work:

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

3. Viva Voce:

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

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SEMESTER-III

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

Marks: 50 Credits: 4 Classes: 45L

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_2 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 form XPS, information about the nature of molecular orbitals from UPS, UPS of simple diatomic molecules e.g. N_2 , O_2 , CO, HCl etc. Principle of NQR, nuclear quadrupole coupling constant, structural information from NQR spectra.

CEM 302: Advanced Physical Chemistry-I (Physical Spl.) Marks: 50 Credits: 4

Classes: 45L

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: Stationary perturbation theory

Perturbation theory: Derivation of time 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: Semiclasical 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-Butadine, Nodal properties of the π -MO of butadiene, Alternate and nonalternate 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.

CEM 302: Advanced Inorganic Chemistry-I (Inorganic Spl.) Marks: 50 Credits: 4

Classes: 45L

Unit: 1

Organometallic chemistry –II and catalysis

Chemistry of transition metal complexes with cyclic polyenes: 3-6 membered ring systems. Sandwitch and non sandwitch complexes. Organometallic chemistry of heterocyclc ligands (N,B,O). Multidecker sandwitch complexes. Bioorganometallic chemistry, Organometallic polymers, Main group organometallic chemistry.

Terminology in catalysis: TO, TON, TOF. 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), Carbonylation of olefins, Monsanto's acetic acid synthesis, Wacker oxidation (Pd-catalysed), Polymerization of olefins, Ziegler-Natta catalyst.

Unit: 2

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 \Box 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.

CEM 302: Advanced Organic Chemistry-I (Organic Spl.) Marks: 50 Credits: 4

Classes: 45L

Unit-01: Pericyclic reaction III:

Pericyclic reactions and applications of MO theory to Organic Chemistry: Electrocyclic reactions, Sigmatropic rearrangement, cycloaddition and cycloreversion reactions, cheletropic 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, Taft, Yukawa-Tauno and Grunwald-Weinstein equations.

Unit-03: Linear Free Energy Relationship-II

Application of Linear Free Energy Relationship to aromatic, aliphatic, polynuclear and heteroaromatic systems. Multiparameter correlation reactions (elementary ideas). Electrophilic substitutions in aliphatic systems (SE1 and SE2 reactions).

Unit-04: Organometallic Chemistry

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

CEM 303: Advanced Physical Chemistry-II (Physical Spl.) Marks: 50 Credits: 4 Classes: 45L

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, Cannonical 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.

CEM 303: Advanced Inorganic Chemistry-II (Inorganic Spl.) Marks: 50 Credit:4 Classes: 45L

Unit: 1: Bioinorganic chemistry-II

Electron transfer (redox) enzyme: Catalase Peroxidase, Cytochrome P_{450} , Super oxide dismutase, Ascorbate oxidase. Molybdenum containing enzymes: Nitrate reductase, Xanthine oxidase, Sulphate oxidase. Vanadium containing protein: Amavadin, Vanadium bromo peroxidase. Vitamin B₁₂, 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. Photochemical splitting of water, photochemical conversion and storage of solar energy, organometallic photochemistry.

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CEM 303: Advanced Organic Chemistry-II (Organic Spl.) Marks: 50 Credit:4 Classes: 45L

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; α -helix, β -pleated sheet, β -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 sustainabilty. 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.

C-CEM 304: Pharmaceutical Chemistry (CBCS) Marks: 50 Credit: 4 Classes: 45L

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, antineoplastic agents, disinfectant and antiseptic, thyroid hormones and antithyroid drugs, Vitamins, sulfonamides and antibiotics.

5. Antimalarial drugs

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

CEM 395: Project (Physical/Inorganic Spl.) Full Marks = 100 Credits: 8 Duration: 16 Week

<u>Unit 01:</u>

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.

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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]

<u>Unit 03</u>

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.)).

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CEM 395: Project (Organic Spl.) Full Marks = 100 Credits: 8 Duration: 16 Week

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. [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.

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<u>Unit 02</u>

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.)).

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SEMESTER-IV

CEM 401: Advanced Spectroscopy-II (Common Paper: Physical/Inorganic/Organic) Marks: 50 Credits: 4 Classes: 45L Spectroscopy for Structure Elucidation

Unit-01

Detailed study of ¹H NMR and preliminary aspects of ¹³C 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

CEM 402: Advanced Physical Chemistry-III (Physical Spl.) Marks: 50 Credits: 4 Classes: 45L

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 Hatree-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: QM of diatomic molecules:

Born – Oppenheimer approximation, Solution of electronic Schrodinger equation for molecules, Valence bond method, The molecular orbital theory, MO term symbols, Comparison of MO and VB theory.

Unit-4: QM of many electron system-II:

Basis sets for the molecular orbital calculations of polyatomic molecules, Configuration interaction. Density function theory; global reactivity descriptors: polarizability, chemical hardness, Electrophilicity; Local reactivity descriptors: Fukui functions. Calculations of polyatomic molecules, Illustrative examples of Ab initio HF and Post HF calculations, Atomic charge and bonding Indices in polyatomic molecules.

Unit-5: 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.

CEM 402: Advanced Inorganic Chemistry-III (Inorganic Spl.) Marks: 50 Credits: 4 Classes: 45L

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, superexchange 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

Metal carbonyls: Synthesis, structure and reactivity. Low nuclearity (M_3-M_4) and high nuclearity (M_5-M_{10}) carbonyl clusters. Metal-metal bonding(MO), skeletal electron counting. Wade-Mingos-Lauher rule, isolobal analogy. Halide clusters of Nb, Ta, Mo, W, Re. Synthesis, structure and bonding. Interstitial Clusters-hydrides, carbides and nitrides. Metal-metal multiple bond. Examples, synthesis, structures and bonding(MO). Electronic transition.

CEM 402: Advanced Organic Chemistry-III (Organic Spl.) Marks: 50 Credits: 4 Classes: 45L

Unit-01: Organic Photochemistry-I

Organic Photochemistry: Fundamental concepts, Jablonski diagram, Photochemistry of organic compounds, Norrish type- I and type II processes, Patterno Buchi reacgtion, Barton reaction, addition reaction, oxidation reaction.

Unit-02: Organic Photochemistry-II

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

Unit-03: Biological Active Molecules

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

Unit-04: Vitamins and co-enzymes

Vitamins A1, B1, C, K coenzymes, NAD, FAD and reactivity of different Vitamin in biological reactions. Chemistry of nucleosides, nucleotides and ATP, elementary structure and role of DNA and various types of RNA"s in protein biosynthesis.

Unit-05: Hetercycles

Heterocycles: Synthesis and Reactions: Generalized approach to the synthesis of heterocycles possessing 5-,6-, and 7- membered rings with one or two 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.

CEM 403: Advanced Physical Chemistry-IV (Physical Spl.) Marks: 50 Credits: 4 Classes: 45L

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

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.

CEM 403: Advanced Inorganic Chemistry-IV(Inorganic Spl.) Marks: 50 Credits: 4 Classes: 45L

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_a' and 'I_d'). 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 voltametry 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)₃

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

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CEM 403: Advanced Organic Chemistry-IV (Organic Spl.) Marks: 50 Credits: 4 Classes: 45L

Unit-01: Stereochemistry-III

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

Unit-02: Stereochemistry-IV

Fused ring systems, *trans* and *cis* declaims, 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

Sterochemistry of 4-10 membered rings, transanular reactions; perhydrophenanthrenes and perhydroanthracenesconformation, energy, symmetry and optical activity, relative stability, sterochemistry 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) Burzi 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 birefrigence, optical rotatory dispersion (ORD) octant rule, axial haloketone rule-application (octant projection diagrams) ; circular dichroism (CD) differential dichronic absorption, specific ellipticity and molar ellipticity, applications of CD-helicity rule, exciton chirality (dibenzoate chirality rule) Davydor splitting-applications with different steroidal glycols.

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

Marks: 50 Credits: 4 Classes: 45L

Unit 01:

Biophysical Chemistry: Structure and function of biomolecules: protein, nuclic 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:

Corrosion Technology: Introduction, What is corrosion, Corrosion principles: Electrochemical and other aspects of corrosion, corrosion prevention.

CEM 404: Chemical Principles in Food Science and Technology (Organic Spl.) Marks: 50 Credits: 4 Classes: 45L

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 Fats and Oils : 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.

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.) Full Marks = 100

Credits: 8 Duration: 16 Week

Research Work (extension from Semester III):

<u>Unit 01:</u>

Skill to Read Research Articles:

A recent research article will be supplied and the students will have to answer some questions on the article.

[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]

<u>Unit 03</u>

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.) Full Marks = 100 Credits: 8 Duration: 16 Week

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. [30]

Research Work:

Research Work (extension from Semester III):

<u>Unit 01:</u>

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]

<u>Unit 02</u>

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 Chemmistry, Paula Yurkanis Bruice
- 7. Green Chemistry, Paul T. Anantas 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. Puecell & J. C. Kotz
- 14. Concept and Model in Inorganic Chemistry Douglass, McDanniel & Alexander
- 15. Coordination Chemistry S. F. A. Kettle
- 16. Valence Theoru S. F. A. Kettle, J. N. Murral & 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 Organomtallic 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. Bruckenstei 5. Advanced Experiments in Inorganic Chemistry G. N. Mukkheriee
- 5. Advanced Experiments in Inorganic Chemistry G. N. Mukkherjee.

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
- 35. Computational Intelligence-A. Konar
- 36. Photodissociation Dynamics-R. Schinke

- 37. Modern Spectroscopy-J. M. Hollas
- 38. Symmetry and Spectroscopy-D. C. Harris, M. D. Bertolucci
- 39. Molecular Vibrations-E. B. Wilson Jr., J. C. Decius, P. C. Cross
- 40. Microwave Spectroscopy- C. H. Townes and A. L. Schawlow
- 41. Laser Spectroscopy- W. Demtroder
- 42. Practical Physical Chemistry- A. M. James, F. F. Prichard
- 43. Findlay"s Practical Physical Chemistry- B. P. Levitt
- 44. Experimental Physical Chemistry- Shoemaker and Garland