

Vidyasagar University



Post Graduate Syllabus
in
Chemistry & Chemical Technology

under Choice Based Credit System
(CBCS)

[w.e.f. : 2016-2017]



Vidyasagar University

Dept. of Chemistry and Chemical Technology

Syllabus

For

M.Sc. in Chemistry

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

[w. e. f 2016-2017]

Overview

Semester	Paper	No of Papers	Full Marks of Each Paper	Credit Point of Each Paper	Total Marks	Credit Points	Total Credit 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	
3 rd	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 Total 96 Credit Points							

1 st semester: General Course				
Paper	Course	Duration	Marks	Credit Point
CEM-101	Physical Chemistry	45L	50	4
	Mathematical preliminaries & Quantum Mechanics-I, statistical thermodynamics and mechanics, electrochemistry-I, principles of molecular spectroscopy-I			
CEM-102	Organic Chemistry	45L	50	4
	Pericyclic reaction-1, Organic transformations/synthesis/reagents chemistry-1, natural products-terpenoids, Natural products-alkaloids, Retro-synthesis I			
CEM-103	Inorganic Chemistry	45L	50	4
	Symmetry and Group theory-I, Crystallography, Bioinorganic chemistry-I , Chemical toxicology			
CEM-104	Food processing and preservation-I and Computer basics	45L	50	4
	Constituent of food, Introduction to food microbiology, Food preservation, Computer basics I and II			
CEM-105	Inorganic Chemistry Practical	8 Weeks	50	4
CEM-106	Food processing preservation and packaging Practical	8 Weeks	50	4
Total Marks 300				
Total Credit 24				

2nd Semester: General Course				
Paper	Course	Duration	Marks	Credit Point
CEM-201	Physical Chemistry	45L	50	4
	Quantum Mechanics-II, Chemical kinetics, electrochemistry-II, molecular spectroscopy-II			
CEM-202	Organic Chemistry	45L	50	4
	Pericyclic reaction-2, Organic transformations/synthesis/reagents chemistry-2, Retrosynthesis II, Stereochemistry-1, Stereochemistry-2,			
CEM-203	Inorganic Chemistry	45L	50	4
	Organometallic chemistry –I, Allotropes of carbon and boron compounds, Group theory-II, Chemistry of d-block elements			
CEM-204 (Elective Course)	Nanotechnology: Principles and Practices	45L	50	4
	Introduction, synthesis of nanomaterials, analysis techniques, application of nanotechnology			
CEM-205	Organic Chemistry Practical	8 Weeks	50	4
CEM-206	Physical Chemistry Practical	8 Weeks	50	4
Total Marks				300
Total Credit				24

3rd Semester: Physical Chemistry spl.				
Paper	Course	Duration	Marks	Credit Point
CEM-301	Approximate method in QM-I, Approximate method in QM-II, Group theory-I & Group theory-II	45L	50	4
CEM-302	Statistical mechanics, Chemical kinetics-I, Chemical Kinetics-II, Advanced Electrochemistry	45L	50	4
CEM-303	NMR, ESR, LASER, PES, NQR, Photophysical Processes	45L	50	4
CEM-304 (Elective Course)	Introduction of Pharmaceutical Chemistry, Classification and nomenclature of drugs, Theory of drug action and factors affecting the drugs, Types of drugs, Antimalarial drugs	45L	50	4
CEM-305	Project work: Physical Chemistry spl.	16 Weeks	100	8
Total Marks				300
Total Credit				24

3rd Semester: Inorganic Chemistry spl.				
Paper	Course	Duration	Marks	Credit Point
CEM-301	Organometallic chemistry – II, Application of organometallic compounds and catalysis, Chemical application of group theory – I, Chemistry of f-block elements	45L	50	4
CEM-302	Bioinorganic chemistry – II, Nuclear chemistry, Inorganic photochemistry Solid state chemistry	45L	50	
CEM-303	NMR, ESR, LASER, PES, NQR, Photophysical Processes	45L	50	4
CEM-304 (Elective Course)	Introduction of Pharmaceutical Chemistry, Classification and nomenclature of drugs, Theory of drug action and factors affecting the drugs, Types of drugs, Antimalarial drugs	45L	50	4
CEM-305	Project work: Inorganic Chemistry spl.	16 Weeks	100	8
Total Marks				300
Total Credit				24

3rd Semester: Organic Chemistry spl.				
Paper	Course	Duration	Marks	Credit Point
CEM-301	Pericyclic reaction-III, Linear free energy relationship I and II, Organometallic chemistry	45L	50	4
CEM-302	Bioorganic and supramolecular Chemistry- 1,2, and 3, Peptides and nucleic acids, Green chemistry.	45L	50	4
CEM-303	NMR, ESR, LASER, PES, NQR, Photophysical Processes	45L	50	4
CEM-304 (Elective Course)	Introduction of Pharmaceutical Chemistry, Classification and nomenclature of drugs, Theory of drug action and factors affecting the drugs, Types of drugs, Antimalarial drugs	45L	50	4
CEM-305	Project work: Organic Chemistry spl.	16 Weeks	100	8
Total Marks				300
Total Credit				24

4 th Semester: Physical Chemistry spl.				
Paper	Course	Duration	Marks	Credit Point
CEM-401	Quantum mechanics of many electron atoms, Atomic Spectroscopy, QM of diatomic molecules, QM of polyatomic molecules	45L	50	4
CEM-402	Non-equilibrium thermodynamics, Macromolecules & Biopolymers, Solid state-I, Solid state-II	45L	50	4
CEM-403	Detailed ¹ H NMR, ¹³ C NMR, CW and FT techniques, Principles of relaxation, NOE, Mass spectroscopy, Combined applications of spectroscopic techniques for structure elucidation, CD ORD, Moss-Bauer.	45L	50	4
CEM-404	Milk products, Cereals, Legumes and nuts, Fats and oils, food safety, fruits and vegetables	45L	50	4
CEM-405	Project work: Physical Chemistry spl.	16 Weeks	100	8
Total Marks				300
Total Credit				24

4th Semester: Inorganic Chemistry spl.				
Paper	Course	Duration	Marks	Credit Point
CEM-401	Molecular magnetism-I, Molecular magnetism-II, Metal carbonyls, clusters and metal-metal bonded compounds Supramolecular chemistry and designing of molecular materials	45L	50	4
CEM-402	Reaction mechanism of transition metal complexes, Electron transfer reactions and twist mechanism, Analytical chemistry-I Analytical chemistry-II	45L	50	4
CEM-403	Detailed ^1H NMR, ^{13}C NMR, CW and FT techniques, Principles of relaxation, NOE, Mass spectroscopy, Combined applications of spectroscopic techniques for structure elucidation, CD ORD, Moss-Bauer.	45L	50	4
CEM-404	Milk products, Cereals, Legumes and nuts, Fats and oils, food safety, fruits and vegetables	45L	50	4
CEM-405	Project work: Inorganic Chemistry spl	16 Weeks	100	8
Total Marks 300				
Total Credit 24				

4th Semester: Organic Chemistry spl.				
Paper	Course	Duration	Marks	Credit Point
CEM-401	Organic photochemistry-1 & 2, Biological active molecules, Vitamins & co-enzymes, Heterocycles-2	45L	50	4
CEM-402	Stereochemistry-3, Stereochemistry-4, Stereochemistry-5, Stereochemistry-6, Stereochemistry-7,	45L	50	4
CEM-403	Detailed ^1H NMR, ^{13}C NMR, CW and FT techniques, Principles of relaxation, NOE, Mass spectroscopy, Combined applications of spectroscopic techniques for structure elucidation, CD ORD, Moss-Bauer.	45L	50	4
CEM-404	Milk products, Cereals, Legumes and nuts, Fats and oils, food safety, fruits and vegetables	45L	50	4
CEM-405	Project work: Organic Chemistry spl.	16 Weeks	100	8
Total Marks				300
Total Credit				24

Semester-I**CEM – 101 (Physical Chemistry)****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, Barrier problems.

Unit-2: Statistical Thermodynamics and Mechanics

Thermodynamic equation of state, Partial molar quantities, thermodynamics of mixing, activity and fugacity-applications in real systems, Nernst heat theorem, third law of thermodynamics, Phase cell, macrostate, microstate, thermodynamical probability and entropy, Maxwell-Boltzmann, Bose-Einstein and Fermi-Dirac statistics. Partition functions of diatoms (translational, rotational, vibrational and electronic).

Unit-3: Electrochemistry-I

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.

Unit: 4: 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.

Semester-I
CEM 102 (Organic Chemistry)

Unit-01**Pericyclic reaction 1 :**

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 pericyclic 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 nerol, 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, peptides, nucleoside and nucleotide structure, synthesis, biogenesis.

Unit - 05

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

Semester-I
CEM 103 (Inorganic Chemistry)

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**Crystallography**

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.

Unit: 4**Chemical Toxicology**

Trace elements and their chemical speciation with special reference to Cu, Zn, Cd, Hg, Pb , Ag, Sb, Se, Ti, Si, Be etc. Toxic chemical in air, water, soil, diet, fertilizer, their effects and remedial measures. Metal ion toxicity, metal dependent diseases, remedial measures, Bio-mineralogy.

Semester – I**CEM-104****FOOD PROCESSING AND PRESERVATION-I and Computer Basics****UNIT-01:**

Constituents of Food: Water, carbohydrates, Lipids, Proteins, Vitamins and Minerals; Mineral water: natural and with added minerals. (8 Lectures)

UNIT-02:

Introduction to food microbiology, Factors influencing microbial activity, Food spoilage, Types and causes of food spoilage. (8 Lectures)

UNIT-03:

Food preservation: Principles and methods; Drying, Refrigeration, Freezing, chemical additives, evaporation, Fermentation. (8 Lectures)

Unit –04:

Computer Basics-I : Hardware, Software, Memory, Storage devices, **Data storage** : The decimal number system, the binary number system, hexadecimal notation, octal number system. Conversaion 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.

(8 Lectures)

Unit 05:

Computer Basics – II: Data Manipulation: Logical Operations : AND, OR, NOT, NANT, NOR, EXOR, EX-NOR. Logic gates with truth table, Universal Gates, Representation of function using gates. Boolean algebra: Postulates, Minimization of functions.

(8 lectures)

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.

Semester-I CEM 105: Inorganic Practical

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. $[Co(NH_3)_6]Cl_3$
- 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 $[K_2SO_4, Cr_2(SO_4)_3, 24H_2O]$

Semester I**CEM 106:****FOOD PROCESSING, PRESERVATION & PACKAGING LAB**

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

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

Bound States, Box with infinite and finite walls. 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.

Unit-2: Chemical Kinetics

Flow and relaxation methods of measurements of reaction rates, flash photolysis, Kinetics of fast reaction, Homogeneous and heterogeneous catalysis, Enzyme catalysis and inhibition, autocatalysis, oscillatory reactions (general introduction only), redox reactions, Preliminary idea of Transition State Theory.

Unit-3: Electrochemistry-II

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.

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.

Semester-II CEM 202 (Organic Chemistry)**Unit – 01: Pericyclic reaction 2 :**

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, Sharpless asymmetric expoxidation, AD-mix, Transformation of epoxides. Organophosphorus reagents, organo sulfer reagents, organo boranes, organo silanes, organostannanes, metal hydrides, Birch reduction, Bayer Villiger reactions, chichibabin reaction, Merrifield resin: solid phase synthesis.

Unit 03: Retro synthetic analysis-II:

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

Unit 04: Stereochemistry 1 :

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. Stereogency 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 2 :

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.

Semester-II CEM 203 (Inorganic Chemistry)

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

Allotrops of carbon and boron compounds

Allotropes of Carbon: C_{60} and compounds (fullerenes), Intercalation compounds of Graphite, Carbon nanotubes, synthesis, properties, structure-single walled, multi-walled, applications, Graphene.

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).

Unit: 3

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: 4

Chemistry of d-block elements

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

Semester-II CEM-204 (Elective Course)
Nanotechnology: Principles and Practices

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.

Semester – II
CEM 205
Physical Practical Syllabus
(Full Marks = 50)

(Two days examination - 6 hours per day, Full Marks = 50)

1. List of Experiments:

1. Kinetics of Inversion of Cane-sugar by Polarimeter.
2. Determination of dissociation constant and Λ_0 of a weak monobasic acid conductometrically and verification of Ostwald's Dilution Law.
3. Conductometric determination of concentrations of KCl, HCl and NH4Cl in a mixture (one day).
4. Verify the Onsagar equation using KCl, K2SO4 and BaCl2 as electrolytes and determine their Λ_0 values (one and half day).
5. Determine the solubility product of BaSO4 conductometrically (one day).
6. Determination of CMC of a surfactant in aqueous solution by conductometric method (one day).
7. Determination of strength of supplied KCl and K_{sp} of AgCl by a potentiometer.
8. Potentiometric titration of halide mixture (Chloride, Bromide and Iodide).
9. Determine the E_0 value of Ag+/Ag electrode and activity coefficients of different aqueous AgNO3 solutions potentiometrically (one day).
10. Determine the standard potential of $[Fe(CN)_6]^{3-}$ / $[Fe(CN)_6]^{4-}$ electrode by potentiometer (one day).
11. Determine the dissociation constants (K1, K2, and K3) of H3PO4 by pH meter (one day).
12. Determination of pKa, pK and pK2 of a weak monobasic and dibasic acid pH-metrically.
13. Determine the indicator constant of bromocresol green spectrophotometrically (one and half day).
14. Study the kinetics of Iodination of acetone spectrophotometrically.
15. Determination of composition of complexes (Ferric-salicylate complex/Ferrous-orthophenanthroline complex) by Job's method (one day).
16. Determine the rate constant and the order of the reaction of KBrO3 & KI in acid medium (one and half day).
17. Determine the order and rate constant of the reaction between K2S2O8 & KI and study the influence of ionic strength on the rate constant (two days).
18. Study of the kinetic of alkaline hydrolysis of crystal violet. Determine the order with respect to alkali and salt effect on the system (two days).
19. Determination of critical solution temperature (CST) and critical composition of two component system.

2. Sessional Work:

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

10

3. Viva Voce:

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

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Semester – II
CEM 206
Organic Practical Syllabus
(Full Marks = 50)

1. Liquid Sample: Qualitative analysis (color, odour, solubility etc.); *Thin Layer Chromatography (TLC, preparation of TLC plates, analysis)*, boiling point determination; functional groups tests, UV-VIS spectral characterizations: (Measure λ_{max} , ϵ_{max} and explain), 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 λ_{max} , ϵ_{max} and explain. Submit the product with proper label.

[15]

OR

2. 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]

Semester-III

CEM – 301
(Physical Special)

Unit-1: Approximate method in QM-I

Approximate methods in quantum mechanics, variational principle, Eckart's Rule, Linear variation theorem, Hückel Theory and its applications, analytical methods for linear and cyclic polyenes, Hückel Theory of systems containing hetero atoms, Extended Hückel Theory and its application.

Unit-2: Approximate method in QM-II

Perturbation theory, derivation of perturbation equations, first order non-degenerate and degenerate perturbation theory, applications, anharmonic oscillator, non rigid rotator, Hydrogen molecule ion, Stark effect.

Unit-3: Group Theory-I

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.

Unit-4: Group Theory-II

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.

Semester-III CEM – 302
(Physical Special)

Unit-1: Statistical mechanics-II

Concept of ensemble and phase space, ergodic hypothesis, temperature, canonical ensemble, distribution, 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-2: Chemical Kinetics-I

Transition State Theory, thermodynamic formulation of reaction rates, Potential Energy Surface and contour reaction path, valley and Saddle point-activation energy; quantitative treatment of TST by using partition function; statistical formulation of chemical kinetics, equilibrium formulation, derivation of expression for specific reaction rate, entropy of activation.

Unit-3: Chemical Kinetics-II

Reaction in Molecular Beams, reactions in Shock Waves, Application of absolute reaction rate theory in viscosity, Reaction between ions, influence of solvent dielectric constant (double sphere model), pre exponential factors, single sphere activated complex model, influence of ionic strength. Diffusion controlled reactions (full and partial microscopic diffusion controlled).

Unit-4: Advanced Electrochemistry

Mechanism of multi-step electrochemical reactions, hydrogen overvoltage, thermodynamics of ideally polarized electrodes, structures of metal and semiconductor-electrolyte junctions, fundamentals of fuel cells, photoelectrochemical cells and corrosion.

Semester-III
CEM-303 (Common Paper)
(Physical Special)

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, N₂ 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. N₂, O₂, CO, HCl etc. Principle of NQR, nuclear quadrupole coupling constant, structural information from NQR spectra.

Semesterester – III
Physical Special
CEM 304 (Elective Course)
Pharmaceutical Chemistry

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. Hypnotics and sedative drugs, Anticonvulsant 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.

Semesterester – III
CEM 305
Project (Physical Special) Full Marks = 100

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. [20]

Research Work:

Unit 01:

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.

[10]

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.

[50]

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]

Semester-III CEM 301
(Inorganic Chemistry Spl)

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

Application of organometallic chemistry and catalysis

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: 3

Chemical applications of group theory

(a) 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.

(b) 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.

Unit: 4

Chemistry of f-block elements

Lanthanides. Actinides and Super heavy elements. Electronic structure, differences between 4f and 5f orbitals. Stable oxidation states. Lanthanide and Actinide construction, separation and isolation. Absorption spectra and magnetic properties. Comparative chemistry of d and f block elements, Comparative chemistry of Lanthanides and Actinides. Aqueous chemistry, coordination chemistry. Organic metallic compounds. trans actinide elements, nuclear instability and synthesis chemistry of U and Pu. Periodicity of trans Lawrencium elements, superactinides.

Semester-III CEM 302
(Inorganic Chemistry Spl)

Unit: 1**Bioinorganic chemistry-II**

Electron transfer (redox) enzyme: Catalase Peroxidase, Cytochrome P₄₅₀, 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.

Unit: 2**Nuclear chemistry**

Nuclear models-nuclear forces, liquid drop model, Fermi gas model, Magic numbers. Nuclear spin and nuclear isomerism. Nuclear reactions-energetics, mechanism and models, nuclear fission and nuclear fusion. Nuclear reactors and particle accelerators. Interaction of radiation with matter.

Unit: 3**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.

Unit: 4**Solid state chemistry**

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.

Semester-III
CEM-303 (Common Paper)
(Inorganic Special)

Unit: 1**Photophysical processes:**

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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, N₂ laser, Ar laser, excimer and exciplex laser, Dye laser.

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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.

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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. N₂, O₂, CO, HCl etc. Principle of NQR, nuclear quadrupole coupling constant, structural information from NQR spectra.

Semester – III
CEM 304 (Elective Course)
Pharmaceutical Chemistry

1. Introduction of Pharmaceutical Chemistry

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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

C. Hyponotics and sedative drugs, Anticonvulsant and analgesic drugs, general anaesthetics and local anaesthetics, expectorant, psychoactive and nervous system stimulant drugs, antiperkinson, antihistamine, anti-inflammatory and antipyretic drugs.

D. 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.

Semester – III**CEM 305****Project (Inorganic Special) Full Marks = 100****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. [20]

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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]

Semester - III
Chemistry: Organic Special

CEM 301

Unit-01: Pericyclic reaction 3:

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-1

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-2

Application of Linear Free Energy Relationship to aromatic, aliphatic, polynuclear and hetero-aromatic 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.

Semester - III
Chemistry: Organic Special
CEM 302

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 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.

Semester – III
CEM-303 (common paper)
(Organic Special)
Spectroscopy Fundamentals

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, N₂ 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. N₂, O₂, CO, HCl etc. Principle of NQR, nuclear quadrupole coupling constant, structural information from NQR spectra.

Semester – III**(Organic Special)****CEM 304 (Elective Course)****Pharmaceutical Chemistry****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.

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4. Types of drugs

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F. 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.

Semester – III**CEM 305****Project****(Organic Special)****Full Marks = 100****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. [20]

Research Work:**Unit 01:**

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.

[10]

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.

[50]

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]

Sem-IV
CEM – 401
(Physical Special)

Unit-1: Quantum mechanics of many electron atoms:

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.

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 polyatomic molecules:

Separation of electronic and nuclear motion, Basis sets for the molecular orbital calculations of polyatomic molecules, Configuration interaction calculations of polyatomic molecules, Illustrative examples of Ab initio HF and Post HF calculations, Atomic charge and bonding Indices in polyatomic molecules.

Sem-IV
CEM – 402
(Physical Special)

Unit-1 : Non-equilibrium thermodynamics

Entropy production in irreversible processes, onsagar reciprocal relation, principle of microscopic reversibility, thermonuclear pressure difference and thermonuclear effect, cyclic and oscillatory reactions, non-linear region, higher order symmetries.

Unit-2: Macromolecular & Biopolymers

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

Structures of biomolecules: 1) proteins –building, peptide bonds, primary, secondary, tertiary, quaternary structures. Phi-psi map. 2) Nucleic acids-A, B, Z conformations, t-RNA conformation, carbohydrates and lipids biomembrances. Methods for determination of molecular weight of biopolymers: a) SDS-PAGE (for proteins), b) agarose gel methods (for nucleic acids). Techniques to study biomolecules: CD, ORD, fluorescence, IR and Raman Spectroscopy (simple applications).

Unit-3: Solid State – 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, Lattice vibration, Phonons and Excitons, Hall Effect.

Unit-4: Solid State – II

Band theory of solids, conductors, semiconductors (n-type, p-type and n-p junction), superconductors and insulators. Lattice defects (Schottky defect and Frenkel defect). Color centre: F-centre, V-centre, F'-centre etc.

Semester - IV
(Physical Special)

CEM 403
(Common Paper)

Spectroscopy for Structure Elucidation

Unit-01

Detailed study of ^1H NMR and preliminary aspects of ^{13}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

Sem IV
(Physical Special)
CEM-404
(Common Paper)
(FOOD PROCESSING AND PRESERVATION-II)

Unit 01:

Milk Products: Definition, composition of milk, Quality standards for milk, Pasteurization of milk; HTST and UHT techniques, Fermentation of milk, Manufacture of milk products like evaporated milk, Milk powder, Condensed milk, Cheese, Yoghurt, and Cream Butter.

(8 Lectures)

Unit 02:

Cereals legumes and nuts: Production of milled rice, Parboiling and parboiled rice, Processing of wheat, pulses, Corn, maize and malting.

(8 Lectures)

Unit 03:

Fats and Oils: Chemical composition, nutritional importance of dietary oils and fats, Production and processing of Edible vegetable oils and fat, hydrogenated fat.

(8 Lectures)

Unit 04:

Food Safety: Introduction, PFA, FPO, FSSA, HACCP, and Hygienic Design.

(8 Lectures)

Unit 05:

Fruits and Vegetables: Pre and post-harvest changes, Principles of fruits and vegetables processing, Storage of fresh fruits and Vegetables, Fruits and vegetables products like Jam, Jelly, Marmalades, Juices, Pickles, Sauces, Ketchup, Chutneys etc.

(8 Lectures)

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)
7. N.N. Potter CBS Publishers and Distributors, Delhi, 5th Ed, 1996 Food Science.

Semester – IV**CEM 405****Project****(Physical Special)****Full Marks = 100****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.

[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]

Semester - IV
Inorganic Chemistry Special
CEM 401

Unit: 1**Magnetochemistry-I**

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. Determination of magnetic susceptibility by these methods: Gouy, Faraday and SQUID.

Unit: 2**Magnetochemistry-II**

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 materials, long range ordering, superparamagnetism, molecular magnets, metamagnetism, single chain magnet, magnetic ordering, magnetic behaviour of lanthanides and actinides.

Unit: 3**Metal carbonyls, clusters and metal-metal bonded compounds**

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.

Unit: 4**Supramolecular chemistry and designing of molecular materials**

Origin of supramolecular chemistry-“Chemistry beyond the molecules”. Concepts and terminology of supramolecular chemistry. Natural types of supramolecular interactions (Hydrogen bonding, van der Waal's interaction, π -stacking, CH --- π interaction. supramolecular chemistry in inorganic perspective. Inorganic crystal engineering and design principle of metal organic framework (MOF) and inorganic-organic hybrid material. Application of MOFs in material science.

Semester - IV
Inorganic Chemistry Special
CEM 402

Unit: 1**Reaction mechanism of transition metal complexes**

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.

Unit: 2**Electron transfer reactions and twist mechanism**

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, 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: 3**Analytical chemistry-I**

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.

Unit: 4**Analytical chemistry-II**

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)₃

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

Semester - IV
Inorganic Chemistry Special

CEM 403
(Common Paper)

Spectroscopy for Structure Elucidation

Unit-01

Detailed study of ^1H NMR and preliminary aspects of ^{13}C NMR, CW and FT techniques.

Ring current: Aromaticity, Antiaromaticity, Homoaromaticity, Annulene systems.

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Principles of Mass spectrometry, Different techniques, fragmentation modes.

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CD ORD and Mossbauer Spectroscopy

Semester - IV
Inorganic Chemistry Special

CEM-404
(Common Paper)
(FOOD PROCESSING AND PRESERVATION-II)

Unit 01:

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(8 Lectures)

Unit 02:

Cereals legumes and nuts: Production of milled rice, Parboiling and parboiled rice, Processing of wheat, pulses, Corn, maize and malting. (8 Lectures)

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8. 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)
7. N.N. Potter CBS Publishers and Distributors, Delhi, 5th Ed, 1996 Food Science.

Semester – IV
CEM 405
Project (Inorganic Special) Full Marks = 100

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.

[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]

Semester – IV**Chemistry: Organic Special****CEM 401****Unit-01: Organic Photochemistry-1**

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

Unit-02: Organic Photochemistry-2

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: Heterocycles-2

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.

Semester - IV
Chemistry: Organic Special
CEM 402

Unit-01: Stereochemistry-3

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 ; α -Strain and β -strain, allylic 1,2 - and 1, 3-strain (in pseudoallylic systems also), their applications.

Unit-02: Stereochemistry-4

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

Unit 03: Stereochemistry-5

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-6

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

Unit- 05: Stereochemistry-7

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) Davydon splitting-applications with different steroid glycols.

Semester - IV
Chemistry: Organic Special
CEM 403 (Common Paper)

Spectroscopy for Structure Elucidation

Unit-01

Detailed study of ^1H NMR and preliminary aspects of ^{13}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

Sem-IV
(Organic Special)
CEM-404 (Common Paper)
(FOOD PROCESSING AND PRESERVATION-II)

Unit 01:

Milk Products: Definition, composition of milk, Quality standards for milk, Pasteurization of milk; HTST and UHT techniques, Fermentation of milk, Manufacture of milk products like evaporated milk, Milk powder, Condensed milk, Cheese, Yoghurt, and Cream Butter.

(8 Lectures)

Unit 02:

Cereals legumes and nuts: Production of milled rice, Parboiling and parboiled rice, Processing of wheat, pulses, Corn, maize and malting. (8 Lectures)

Unit 03:

Fats and Oils: Chemical composition, nutritional importance of dietary oils and fats, Production and processing of Edible vegetable oils and fat, hydrogenated fat. (8 Lectures)

Unit 04:

Food Safety: Introduction, PFA, FPO, FSSA, HACCP, and Hygienic Design.

(8 Lectures)

Unit 05:

Fruits and Vegetables: Pre and post-harvest changes, Principles of fruits and vegetables processing, Storage of fresh fruits and Vegetables, Fruits and vegetables products like Jam, Jelly, Marmalades, Juices, Pickles, Sauces, Ketchup, Chutneys etc.

(8 Lectures)

Text books/ References:

9. Robinson RK; 1996; Modern Dairy Technology, Vol 1 & 2; Elsevier Applied Science Pub.
10. Developments in Dairy Chemistry – Vol 1 & 2; Fox PF; Applied Science Pub Ltd.
11. Outlines of Dairy Chemistry, De S; Oxford.
12. 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)
7. N.N. Potter CBS Publishers and Distributors, Delhi, 5th Ed, 1996 Food Science.
8. Desroiser and Desroiser, CBS Publishers and Distributors, New Delhi, 4th Ed, 1987 Technology of Food preservation.

Semester – IV**CEM 405****Project****(Organic Special)****Full Marks = 100****Research Work (extension from Semester III):****Unit 01:****Skill to Read Research Articles:**

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Unit 03

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[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. Puecell & J. C. Kotz
14. Concept and Model in Inorganic Chemistry – Douglass, McDanniel & Alexander
15. Coordination Chemistry – S. F. A. Kettle
16. Valence Theorou – 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. Carptree
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. 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