Semester Syllabus
for
M. Sc. in Chemistry

With effect from the session 2017-18

SCHOOL OF CHEMISTRY (AUTONOMOUS)
SAMBALPUR UNIVERSITY
Jyoti Vihar, Burla - 768 019

Semester Syllabus for M. Sc. in Chemistry

(with effect from the session 2017-18)

FIRST SEMESTER

Course No	Course Title	Credit	Mark
CH-401	GROUP THEORY AND SOLID STATE CHEMISTRY	03	50
CH -402	TRANSITION METAL CHEMISTRY	03	50
CH -403	STRUCTURE AND REACTIVITY	03	50
CH -404	STEREOCHEMISTRY	03	50
CH -405	THERMODYNAMICS	03	50
CH -406	DYNAMICS	03	50
CH -407	INORGANIC PRACTICAL-I	02	50
CH -408	ORGANIC PRACTICAL-I	02	50
	Total	**22**	**400**

SECOND SEMESTER

Course No	Course Title	Credit	Mark
CH -411	METAL π-COMPLEXES AND CLUSTERS	03	50
CH -412	BIOINORGANIC CHEMISTRY	03	50
CH -413	ORGANIC REACTION MECHANISM - I	03	50
CH -414	ORGANIC REACTION MECHANISM - II	03	50
CH -415	STATISTICAL THERMODYNAMICS & HMO THEORY	03	50
CH -416	SURFACE CHEMISTRY	03	50
CH -417	INORGANIC PRACTICAL-II	02	50
CH -418	ORGANIC PRACTICAL-II	02	50
	Total	**22**	**400**

THIRD SEMESTER

Course No	Course Title	Credit	Mark
CH -501	INSTRUMENTAL METHODS OF ANALYSIS	03	50
CH -502	INORGANIC REACTION DYNAMICS & NUCLEAR CHEMISTRY	03	50
CH -503	ORGANIC REDOX REACTION & SPECTROSCOPY	03	50
CH -504	PERICYCLIC REACTION, PHOTOCHEMISTRY & RETROSYNTHESIS	03	50
CH -505	QUANTUM CHEMISTRY	03	50
CH -506	ATOMIC & MOLECULAR SPECTROSCOPY	03	50
CH -507	PHYSICAL PRACTICAL	03	50
CH -508	REVIEW WORK	02	50
	Total	**23**	**400**

FOURTH SEMESTER

Core Courses

Course No	Course Title	Credit	Mark
CH -511	ADVANCED ORGANOMETALLIC CHEMISTRY	03	50
CH -512	ADVANCED SPECTROSCOPY	03	50
CH -513	COMPUTER APPLICATION IN CHEMISTRY	02	50
CH -514	ANALYTICAL PRACTICAL	02	50
CH -515	PRACTICAL ON COMPUTER IN CHEMISTRY	02	50
CH -516	SEMINAR	02	50
A student is required to choose any three theory elective courses either from Group A or Group B		09	150
	Total	**23**	**450**

Elective Courses

Group A

CH-521	ADVANCED ORGANIC SYNTHESIS	03	50
CH-522	PHOTOPHYSICAL PROCESSES & INSTRUMENTATION	03	50
CH-523	CHEMISTRY OF NANO MATERIALS	03	50
CH-524	INDUSTRIAL PROCESSES	03	50

Group B

CH-531	ADVACED ANALYTICAL CHEMISTRY	03	50
CH-532	SUPRAMOLECULAR CHEMISTRY	03	50
CH-533	ADVANCED SURFCE CHEMISTRY & CATALYSIS	03	50
CH-534	MATERIAL AND ENERGY BALANCE	03	50

FIRST SEMESTER

CH-401: GROUP THEORY & SOLID STATE CHEMISTRY 3 credits

UNIT-I: ***Symmetry and Group Theory***

Symmetry operation, symmetry element, classification of symmetry elements, definition of group, subgroup, cyclic groups, molecular point groups, platonic solids, group multiplication table, group generators, conjugacy relation and classes, matrix representation of symmetry elements, character of a representation, reducible and irreducible representation, the great orthogonality theorem (without proof) and its explanation, properties of irreducible representation.

UNIT-II: ***Symmetry and Spectroscopy***

Character table (explanation and significance), construction of character tables for C_{2v}, C_{3v}, C_{4v} and D_4 point groups, direct product, the standard reduction formula, Applications of group theoretical methods for selection rules in Infrared, Raman and electronic spectroscopy.

UNIT-III: ***Solid State Chemistry***

General idea of crystal lattice, unit cell, classification of crystals, crystal planes, Miller indices, Bragg's law and applications, determination of cubic crystal structure from systematic absences in diffraction pattern, perfect and imperfect crystals, point defects, Schottky defects and Frenkel defects, thermodynamics of Schottky and Frenkel defects, bonding in ionic solids, colour centers, non-stoichiometry defects, general idea of band theory of solids.

***BOOKS*:**

1. *Chemical Applications of Group Theory by F. A. Cotton, Wiley India (P) Ltd., 3rd edn, 2009, New Delhi.*
2. *Symmetry and Spectroscopy of Molecules by K. V. Ready, New Age International Ltd. 2nd edn, 2009, New Delhi.*
3. *Symmetry and Group Theory in Chemistry by R. Ameta, New Age International Ltd., 1st edn, 2013, New Delhi.*
4. *Solid State Chemistry by D. K. Chakravarty, New Age International Limited, 1996, New Delhi.*
5. *Solid State Chemistry and its Applications by A.R. West, Wiley, 1989, 2nd edition, Singapore.*
6. *Principles of the Solid State by H.V. Keer, Wiley Eastern. Limited, 1993, New Delhi.*

CH-402: TRANSTION METAL CHEMISTRY 3 credits

UNIT-I ***Theories of Metal-Ligand Bonding***

a. Crystal field theory (CFT): Splitting of d-orbital under the influence of octahedral, tetrahedral, tetragonal, square planar, trigonal bipyramidal and square pyramidal fields, Streochemical and thermodynamic effect of CF splitting, CFSE and Jahn-Teller effect.

b. Molecular orbital theory (MOT): Sigma bonding in octahedral complexes: Classification of metal valence orbitals into sigma symmetry, formation of ligand group orbitals (LGOs) of sigma symmetry, Formation of molecular orbitals of sigma symmetry, construction of molecular orbital energy level diagram involving only sigma bond contribution from ligands, pi bonding in octahedral complexes, Classification of metal valence orbital into pi symmetry, Formation of LGOs of pi symmetry. Formation of pi MOs and construction of molecular orbital energy level diagram involving sigma and pi contribution from pi donor ligands, Sigma and pi bonding in tetrahedral complexes.

c. Ligand field theory (LFT) and adjusted crystal field theory (ACFT).

UNIT-II ***Complex Equilibria and Term Diagram***

a. Complex Equilibria: Types of complex equilibria in solution and types of complex equilibrium constant (stability constant), The complex formation functions, Determination of stability constant by spectrophotometric method and pH titration method, Stabilization of unusual oxidation state.

b. Term Diagram: Russell-Saunders or L-S coupling scheme, Term symbols and their derivation by Pigeon-Hole diagram especially for p^n and d^n configuration, Inter-electron repulsion parameters and spin-orbit coupling parameters, The effect of weak crystal field on S, P, D, F, G, H and I terms, Orgel diagram for d^1 to d^9 configuration, Term interaction and the energies of the levels.

c. Correlation diagram: Strong field configuration of O_h symmetry, the method of descending symmetry, correlation diagram for d^2 and d^3confuguration, Tanabe-Sugano diagram (qualitative explanation and significance).

Unit-III ***Electronic Spectral and Magnetic Properties of Metal Complexes***

a. Electronic spectral properties of metal complexes: Introduction, types of experimental recording of the spectra, selection rules (mechanism of electronic transition, orbital selection rule, Laporte rule or purity selection rules, spin selection rule), Relaxation of selection rules (departure from cubic symmetry d-p mixing vibronic coupling), Nature of electronic spectral bands with respect to band intensity and bandwidth, Classification of electronic spectra. Ligand field spectra of octahedral and tetrahedral complexes and evaluation of Dq, B' and beta(β) parameters for the complex with T_1 ground state and A_2 ground state, Spectrochemical and nephlelauxetic series, charge transfer spectra.

b. Magnetic properties of metal complexes: Origin of magnetic behavior, concept of magnetic susceptibility, dia, para, ferro and antiferro magnetism, magnetic moments from multiple width cases, quenching of orbital magnetic moment by crystal field, spin-orbit coupling and anomalies magnetic moments, Spin-crossover in coordination compounds.

BOOKS:

1. *Theoretical Inorganic Chemistry by M. C. Day and J. Selbin*
2. *Advanced Inorganic Chemistry by F. A. Cotton and G. Wilkinson*
3. *Introduction to Ligand Field by B. N. Figgs*

CH-403: STRUCTURE AND REACTIVITY **3 credits**

UNIT-I: ***Nature of Bonding in Organic Molecules***

Delocalized chemical bonding, Conjugation, Cross conjugation, Resonance, Hyperconjugation, Bonding in fullerenes, Tautomerism. Aromaticity in benzenoid and non-benzenoid compounds, Alternant and non-alternant hydrocarbons, Huckel's rule, energy levels of pi-molecular orbitals of simple systems, Annulenes, Anti-aromaticity, Homo-aromaticity, Bonds weaker than covalent-addition compounds.

UNIT-II: ***Reaction Mechanism: Structure and Reactivity***

Types of mechanisms, Types of reactions, Thermodynamic and kinetic requirements, Kinetic and thermodynamic control, Hammond's postulate, Potential energy diagrams, Transition states and intermediates, Methods of determining mechanisms, Hard and soft acids and bases,

Effect of structure on reactivity: Resonance and field effects, Steric effect, Quantitative treatment, The Hammett equation and linear free energy relationship, Substituent and reaction constants, Taft equation.

UNIT-III: ***Reagents in Organic Synthesis***

Gilman's reagent, Lithium dimethyl cuprate, Lithium diisopropyl amide, DCC, 1,3-Dithiane, Trimethyl sillyl iodide, Tri-n-butyl tin hydride, Osmium tetroxide, Selenium dioxide, Phase transfer catalysis (Crown ether, Merrifield resin, Wilkinson's catalyst), Dichloro dicyano benzoquinone (DDQ).

BOOKS:

1. *Advanced Organic Chemistry: Reaction Mechanism and Structure by Jerry March (Wiley Eastern Limited)*
2. *Physical Basis of Organic Chemistry by N. Isaac (Wiley Eastern Limited)*
3. *Mechanism and Theory in Organic Chemistry by Lowry and Richardson (Harper Row Publishers, New York)*
4. *Organic Chemistry by Morrison and Boyd*

CH-404: STEREOCHEMISTRY 3 credits

UNIT-I: Chirality, Fischer projection and R and S notations, Threo and erythro nomenclature, E and Z nomenclature, Optical isomerism in biphenyls and allenes, Concept of Prostereoisomerism and Assymetric synthesis (including enzymatic and catalytic nexus), Conformation of a few acyclic molecules (alkanes, haloalkanes), Conformation of cyclic systems having one and two sp2 carbon atoms.

UNIT-II: Dynamic stereochemistry: Conformation and reactivity, Selection of substrates, Quantitative correlation between conformation and reactivity, (Weinstein-Eliel equations and Curtin-Hammett principles), Conformational effects on stability and reactivity in acyclic compounds (ionic elimination, intramolecular rearrangements, NGP) and in cyclic systems, (Nucleophilic substitution reaction at ring carbon, Formation and Cleavage of epoxide rings, Addition reactions to double bonds, Elimination reactions).

UNIT-III: Molecular dissymmetry and chiroptical properties, Linearly and circularly polarised lights, Circular birefringence and circular dicroism, ORD, Plane curves, Cotton effect, Rotatory Dispersion of ketones, Axial haloketone rule, the Octane rule. Helicity rule.

BOOKS:

1. *Stereochemistry of Organic Compounds by D. Nashipuri.*
2. *Stereochemistry by Kalsi*
3. *Stereochemistry by Elliel*

CH-405: THERMODYNAMICS 3 credits

UNIT-I: ***Classical Thermodynamics***

Brief resume of the concepts of laws of thermodynamics, Free energy, chemical potential and entropy, Third law of thermodynamics and determination of entropy, Entropy and probability, Boltzmann-Planck equation, Partial molar properties (partial free energy, molar volume and molar heat content), Their significance and determination. Concept of fugacity and its determination.

UNIT-II ***Thermodynamics of Living Systems***

Bioenergetics and thermodynamics, Phosphate group transfer and ATP, Biological oxidation-reduction reactions.

UNIT-III ***Non-Equilibrium Thermodynamics***

Microscopic reversibility, Entropy productions and irreversible process, Different types of forces and fluxes, Steady states & Cross phenomena, Phenomenological equations, Onsager reciprocity theorem, Chemical Reactions.

BOOKS:

1. *Text Book of Physical Chemistry (Vol-1-4) by K.L. Kapoor*
2. *Physical Chemistry by D.N. Bajpai*
3. *Principles of Physical Chemistry by Puri, Sharma & Pathania*
4. *Physical Chemistry by Atkins*
5. *Physical Chemistry Through Problems by Dogra & Dogra*
6. *Chemical Thermodynamics by Rastogi & Mishra*

7. *Thermodynamics for Chemists by S. Glasstone*
8. *Molecular Thermodynamics by McQuarrir & Simon*
9. *Principle of Biochemistry by A.L. Lehninger*

CH-406: DYNAMICS 3 credits

UNIT-I: ***Chemical Kinetics***

Theories of reaction rates, Collision theory, Transition state theory, Arrehenius equation and the activated complex theory, Reaction between ions, Salt effect, Steady-State Kinetics, Kinetic and Thermodynamic concept of Reactions, Treatment of unimolecular reaction (Lindemann-Hinshelwood and Rice-Ramspeger-Kassel-Marcus (RRKM) theories), Dynamic chain (H_2 + Br_2 reaction, pyrolysis of CH_3CHO, Decomposition of ethane).

UNIT-II: ***Catalytic & Fast Reaction***

Kinetics of Catalytic Reactions: Acid-base Catalysis, Enzyme Catalysis, Homogeneous & Heterogeneous Catalysis.

Fast reactions: General feature, Study of Fast reactions by relaxation, Stopped flow and Flash photolysis.

UNIT-III: ***Electrochemistry***

Interionic attraction theory and Debye-Huckel treatment, Derivation of Onsager limiting law and its verification and modification, Activities, activity coefficients, Debye-Huckel treatment, Debye-Huckel-Bronsted equation, Salt effect, Determination of activity coefficients from solubility method, Ion association, Determination of thermodynamic dissociation constant of weak electrolytes by Shedlovsky method and by EMF method, Nernst equation, redox systems, electrochemical cells.

BOOKS:

1. *Text Book of Physical Chemistry (Vol-1-4) by K.L. Kapoor*
2. *Physical Chemistry by D.N. Bajpai*
3. *Principles of Physical Chemistry by Puri, Sharma & Pathania*
4. *Physical Chemistry by Atkins*
5. *Physical Chemistry Through Problems by Dogra & Dogra*
6. *Electrochemistry by S. Glasstone*
7. *Modern Electrochemistry (Vol-I) by Bookris & Reddy*
8. *Chemical Kinetics by K.J. Laidler*
9. *Reaction Kinetics by Pilling & Seakins*

CH-407: INORGANIC PRACTICAL-I 2 credits

Analysis of an inorganic mixture containing not more than 6 radicals. The mixture will include rare earth like Tungstate, Vanadate, Molybdate and Cerium (IV). Insoluble matters and other interfering radicals will also be included. Organic radicals are excluded.

BOOKS:

1. *Vogel's Qualitative Inorganic Analysis, 7^{th} edition; Revised by G. Svehla.*
2. *Vogel's Text Book of Quantitative Chemical Analysis, 5^{th} Revised by G. H. Jeffery, J. Bassett, J. Mendham and R. C. Denny.*
3. *Advanced Practical Inorganic Chemistry, 22^{nd} edition; By Gurdeep Raj*

CH-408: ORGANIC PRACTICAL-I 2 credits

Isolation and identification of multi-functional compounds in a mixture of two organic compounds.

BOOK: *Advanced Practical Organic Chemistry, 3/e by N K Vishnoi*

SECOND SEMESTER

CH-411: METAL π-COMPLEXES AND CLUSTERS 3 credits

UNIT-I ***Carbon Monooxide Complexes***

Metal carbonyls, structure and bonding, vibrational spectra of metal carbonyls for bonding and structural elucidation, important reaction of metal carbonyls, carbonylate anions and carbonylate hydride, carbonyl halides and related compounds. Nature of M-C bond in carbonyls.

UNIT-II ***Complex of Carbon Monoxide Analogs***

(a) Preparation, bonding and important reaction of transition metal complexes with isocyanide, cyanide, dinitrogen, carbon disulphide and nitrogen monoxides.

(b) Transition metal to carbon multiple bonded: compounds chemistry of carbenes, carbynes.

UNIT-III ***Metal Cluster and Polyacids***

Metal cluster: Occurrence of metal-metal bonds in metal complexes, Bonding in metal cluster. Metal carbonyl type clusters. Anionic and hydride cluster. Method of synthesis, super large cluster, electron counting in medium size cluster (Wade's rule, Capping rule), Isolable relationship, cluster of Fe, Ru, Os groups. Cluster of Co, Rh, Ir groups. Cluster of Ni, Pd, Pt groups. Catalysis by cluster.

Isopoly and heteroply acids and salts.

BOOKS:

1. *Advance Inorganic Chemistry by F.A. Cotton, G. Wilkinson & C. Murillo (6^{th} edition)*
2. *Inorganic Chemistry by J.E. Helay, Harper and Row*
3. *Comprehensive Coordination Chemistry, Eds. by Wilkinson, Gillarsand*
4. *Modern Aspect of Inorganic Chemistry by Emelius and Sharpe*

CH-412: BIOINORGANIC CHEMISTRY 3 credits

UNIT-I ***Biomolecules and their Roles in Metal Ions Storage and Transportation***

Amino acids, peptides and proteins, structures of proteins, Ramachandran's plot, lipids, lipid bilayer, biological membranes, chemistry of biologically relevant molecules like ADP, ATP, FAD, NADP, nucleotides. Biologically important metal ions (Na, K, Mg, Ca, Cu, Fe, Zn, Co and Mo) and their functions, mechanism of transport of metal ions through biological fluids and membranes, different types of passive and active transport processes and their mechanism, Na^+/K^+ pump, calcium pump, and ionophores. Storage and transport of iron, copper and zinc, siderophores, structure and function of ferritin, transferrin in regard to Fe-storage and transportation,

UNIT-II ***Role of Proteins as Oxygen and Electron Carriers***

Chemistry of porphyrin, Iron porphyrins (Heme proteins): Hemoglobin (Hb), Myoglobin (Mb) and their behavior as oxygen carrier, O_2 affinity, cooperativity and Bohr's effect, Heme protein as electron carrier with particular reference to cytochrome-c and cytochrome-450, and cytochrome oxidase. Catalases and peroxidases. Non-heme oxygen uptake protein (hemerythrin and hemocyanin). Magnesium porphyrins (Chlorophyll): Photosynthesis, the light and dark reaction (Calvin cycle). Non-heme iron-sulphur protein as electron carrier, rubredoxins and ferredoxins.

UNIT-III ***Biomolecular Catalysis***

Preliminary idea about enzyme, cofactor, co-enzyme, apoenzyme, prosthetic group, metal-activated enzyme and metalloenzyme. Enzyme-substrate binding problem, carboxypeptidase, carbonic anhydrase and their biological significance, Interchangeability of zinc and cobalt enzyme. Blue-oxidases (ascorbate oxidase, cerulloplasmin, laccase) and non-blue Oxidases (amine oxidase, galactose oxidase, lysyl

oxidase, cytochrome c oxidase), structure and biological functions of molybdenum nitrogenase, superoxide dismutase.

BOOKS:

1. *Bio-Inorganic Chemistry by Asim K Das.*
2. *Bio-Inorganic Chemistry by E. Ochia.*
3. *Bioorganic, BioInorganic and Supramolecular Chemistry by P. S. Kalsi and J. P. Kalsi.*
4. *Inorganic Chemistry (4th Edn) by Huheey, Keiter, Keiter and Medhi.*
5. *Bioinorganic and Suparmolecular Chemistry by A. Bhagi and G. R. Chatwal.*

CH-413: ORGANIC REACTION MECHANISM – I **3 credits**

UNIT-I The S_N2, S_N1, mixed S_N1 and S_N2 and SET mechanisms. The neighbouring group mechanism, Neighboring group participations by sigma and pi bonds, anchimeric assistance. Classical and nonclassical carbocations, phenonium ions, norbornyl system, common carbocation rearrangements, application of NMR spectroscopy in the detection of carbocations. The S_NI mechanism. Nucleophilic substitution at an allylic, aliphatic trigonal and a vinylic carbon. Reactivity effects of substrate structure, attacking nucleophile, leaving group and reaction medium, phase transfer catalysis, ambident nucleophile, regioselectivity.

UNIT-II Alipahatic Electrophilic Substitution mechanism: S_E1, S_E2 and S_E^I mechanisms, Effect of substrate, leaving group and solvent, Reactions (hydrogen exchange, migration of double bonds, keto-enol tautomerism, halogenation, aliphatic diazonium coupling, Stork-enamine reaction).

Aromatic electrophilic substitution mechanism: Structure reactivity relationship in mono-substituted benzene, ring isomer proportions, orientation in benzene ring with one or more than one substituent, Orientation in other ring systems, Vilsmeir - Haack reaction, Pechmann reaction.

UNIT-III Aromatic Nucleophilic Substitution mechanism: Introduction to different mechanisms, Aromatic nucleophilic substitutions (S_NAr, S_N1 aryne), Effect of substrates, leaving groups, and nucleophile, Reactions: Nucleophilic displacement in areno-diazonium salts by different nucleophiles, Chichibabin reaction.

Free radical Substitution: Intermediates, Reaction at sp^2 carbon, Reactivity in aliphatic substrates, Reactivity at bridge head position, Reactivity in aromatic substrates.

BOOKS:

1. *Advanced Organic Chemistry: Reaction Mechanism and Structure by Jerry March (Willey Eastern Limited)*
2. *Organic Reaction Mechanism by Kalsi*

CH-414: ORGANIC REACTION MECHANISM – II **3 credits**

UNIT-I Addition to carbon-carbon multiple bonds, Electrophilic, Nucleophilic and Free radical addition, Orientation and Reactivity, Addition to cyclopropanes, Reactions: Hydroboration, Michael reaction, Sharpless Asymmetric epoxidation.

Addition to carbon-heteroatom multiple bonds: Mechanism and reactivity, Reactions: Mannich reaction, $LiAlH_4$ reduction of carbonyl compounds, acids, esters, nitriles, addition of Grignard reagents - Reformatsky reaction, Aldol condensation, Knoevenagel condensation, Perkin reaction, Tollens reaction, Wittig reaction, Prins reaction, Benzoin condensation.

UNIT-II Elimination mechanism: E_1, E_2, E_1CB and E_2CB mechanisms, Orientation, Effect of substrate, base, leaving group and medium, Orientation of double bond, Sayetzeff and Hoffman rules, Pyrolytic elimination reaction, Oxidative elimination (oxidaton of alcohol by chromium, Moffatt oxidation). Reactions: Cleavage of quaternary ammonium hydroxides, Chugaev reaction, Shapiro reaction.

UNIT-III General mechanistic considerations – nature of migration, migratory aptitude, memory effects.

A detailed study of the following rearrangements, Wagner-Meerwein, Favorskii, Carbene intermediate, Arndt-Eistert synthesis, Neber, Nitrene intermediates (Beckmann, Hofmann, Schmidt, Lossen, Curtius), Baeyer-Villiger, Shapiro reaction, Von-Richter, Sommelet-Hauser rearrangement.

BOOKS:

1. *Advanced Organic Chemistry: Reaction Mechanism and Structure by Jerry March (Willey Eastern Limited),*
2. *Organic Reaction Mechanism by Kalsi*
3. *Physical Basis of Organic Chemistry by N. Isaac (Willey Eastern Limited),*

CH-415: STATISTICAL THERMODYNAMICS & HMO THEORY 3 credits

UNIT-I ***Classical and Quantum Statistical Mechanics***

Concept of probability, Starling approximations, Most probable distribution, System, Phase Space, μ-Space, ϒ-Space, Liouville's Theorem, Statistical Equilibrium, Brief Concepts on Ensembles, Canonical, Grand Canonical and Micro-canonical ensembles.

Bose-Einstien statistics, Fermi-Dirac statistics and Maxwell-Boltzmann statistics

UNIT-II ***Partition Functions & Statistical Thermodynamic Properties of Solids***

Significance of partition function, Calculation of thermodynamic properties and equilibrium constant in terms of partition functions, Evaluation of transnational, vibrational and rotational partition function for monoatomic and polyatomic ideal gases, electronic partition function.

Some thermal characteristics of crystalline solids, Classical treatment of solids, Einstein Model, Debye Modification, Limitation and modification of Debye theory.

UNIT-III ***Huckels Molecular Orbital Theory***

Huckel theory of conjugated systems (Ethylene, Allyl systems, butadiene, cyclopropenyl, cyclobutadiene, bicyclobutadiene, H_3^+, H_3 and H_3^-), Calculation of bond order, charge density, free valence index, Application of group theory for the simplification of MO determinants of 1,4- butadiene and naphthalene.

BOOKS

1. *Physical Chemistry by D.N. Bajpai*
2. *Statistical Thermodynamics by M. C. Gupta*
3. *Introduction to Quantum Chemistry by A.K. Chandra*
4. *Notes on Molecular Orbital Calculations by J.D. Roberts*

CH-416: SURFACE CHEMISTRY 3 credits

UNIT-I ***Phase Rule***

Concept of Equilibrium between phases, Derivation of phase rule, Ideal Solution, Liver Rule, Brief concept on one and two component system, Application of phase rule to three component systems of both solids and liquids.

UNIT-II ***Adsorption***

Surface tension, Capillary action, Adsorption, types of adsorption, Gibbs adsorption isotherm, Freundlich's adsorption isotherm, Langmuir's adsorption isotherm and its limitations, BET adsorption isotherm and its applications, Heat of adsorption, estimation of surface areas of solids from solution adsorption studies.

UNIT-III ***Macromolecules***

Polymer-definition, Classification of polymer, Polymer structure, Number average and molecular weight average, Step growth & chain growth polymerization, Kinetics of polymerization, Stereochemistry of polymerization.

BOOKS:

1. *Text Book of Physical Chemistry Vol-1-4 by K.L. Kapoor*
2. *Physical Chemistry by D.N. Bajpai*
3. *Physical Chemistry by A.W. Atkins*
4. *Introductory Quantum Chemistry by A.K. Chandra*
5. *Polymer Science by Gowariker, Viswanathan & Sreedhar*
6. *Polymer Science & Technology by J. R. Fried*

CH-417: INORGANIC PRACTICAL-II — 2 credits

1. Principle of estimation of the main constituents of Brass and Portland Cement.
   (a) Estimation of Ca and Mg in a given solution prepared from a sample of cement by EDTA method.
   (b) Estimation of Cu and Zn in a given solution prepared from a sample of Brass.
2. Determination of MnO_2 in pyrolusite.
3. Preparation and cheracterisation of the following inorganic compounds:
   (i) Tetramminecupric sulphate $[Cu(NH_3)_4]SO_4 .H_2O$
   (ii) Sodium cobaltinitrite , $Na_3[Co(NO_2)_6]$
   (iii) Potassium chromioxalate , $K_3[Cr(C_2O_4)_3]$.

BOOKS:

1. *Vogel's Qualitative Inorganic Analysis, 7th edition; Revised by G. Svehla.*
2. *Vogel's Text Book of Quantitative Chemical Analysis, 5th Revised by G. H. Jeffery, J. Bassett, J. Mendham and R. C. Denny.*
3. *Advanced Practical Inorganic Chemistry, 22nd edition; By Gurdeep Raj*

CH-418: ORGANIC PRACTICAL-II — 2 credits

1. Preparation of benzoin, benzil and benzillic acid from benzaldehyde.
2. Preparation from p-idotoluene from p-toluidene.
3. Preparation of ethyl acetoacetate from ethyl acetate.
4. Estimation of nitrogen by Kjeldahl method.
5. Estimation of keto group by gravimetric method.
6. Dibenzalacetone from benzaldehyde.
7. Cannizaro reaction – 4-chloro benzaldehyde as substrate.
8. Grignard reaction – synthesis of triphenyl methanol from benzoic acid.

BOOK: *Advanced Practical Organic Chemistry, 3/e by N K Vishnoi*

THIRD SEMESTER

CH-501: INSTRUMENTAL METHOD OF ANALYSIS **3 credits**

UNIT-I ***Spectroscopical Method***

Flame Emission Spectroscopy (FES): Basic Principle, instrumentation-Atomizers, Burners, optical system, Detectors, interference in FES and ways to overcome it, Application of FES – Qualitative and Quantitative Analysis, standard addition method and Internal standard method, Error in FES, Limitation of FES.

Atomic Absorption Spectroscopy (AAS): Basic Principle, difference between FES and AAS, Standard instruments used, Experimental Procedure, Application of AAS, interferences and remedial measures, comparative study between AAS and FES, sensitivity of Instruments.

UNIT-II ***Electroanalyctical Method***

Polarography: Basic principle, instrumentation, theory of current-voltage curve, Theory of diffusion current, Ilkovic equation, polarography wave and half wave potential. Application of polarography. Principle, Application, advantage and disadvantage of Cyclic voltammetry anodic stripping voltammetry, amperometry, conductrometry and ion selective electrodes.

UNIT-III ***Thermo Analytical Methods***

Thermogravimetric analysis (TGA): Principle, instrumentation, factors affecting TGA curve, derivative thermogravimetric analysis (DTGA) and application of thermogravimetric analysis, Differential thermal Analysis (DTA), instrumentation of DTA and application of DTA, Simultaneous study of TGA, DTA with examples. Differential scanning calorimetry (DSC) and thermometric titration.

BOOKS:

1. *Instrumental Method of Analysis by H. Willard, L. Merritt, J. Dean & F. Settle*
2. *Analytical Chemistry (Theory and Practical) by U.N. Dash*
3. *Quantitative Analysis by Vogel*

CHI-502: INORGANIC REACTION DYNAMICS AND NUCLEAR CHEMISTRY **3 credits**

UNIT-I: ***Substitution Reactions of Octahedral Co(III) Compounds***

The nature of substitution reactions, Kinetic Application of Crystal Field Theory, Acid hydrolysis of octahedral Co(III) complexes with reference to effect of charge, chelation, steric crowding & effects of leaving group, Base hydrolysis of octahedral Co(III) complexes: Conjugate base mechanism, Test of conjugate base mechanism, Anation reaction, Substitution reaction without cleavage of metal-ligand bond.

UNIT-II ***Substitution Reactions of Square Planar Pt (II) Complex and Redox Reactions***

Thermodynamic and kinetic stability, Trans effect and its synthetic applications, theories of trans effect (polarization & π -bonding theories), Factors affecting the rate law and reaction profile (leaving group, steric group, charge, electrophillic catalysis, nucleophile and temperature).

Redox reactions: electron tunneling hypothesis, concept of Marcus-Hush theory, atom transfer reactions, one and two electron transfer, complementary and non-complementary reactions, inner sphere and outer sphere reactions, electron transfer through extended bridges, concept of hydrated electron.

UNIT-III ***Nuclear Chemistry***

Atomic nucleus, nuclear stability, magic numbers, Radioactivity, General characteristics of radioactive decay, nature of α- and β-particles, and γ-rays, decay kinetics, nuclear reaction, Bethe's notation, types of nuclear reaction, conservations in nuclear reactions, nuclear cross section, compound nuclear theory, the Brett-Wigner Formula, nuclear fission, Process of nuclear fission, liquid drop model, shell model, hard core preformation theory, Fission fragments and their mass distribution, charge distribution, Ionic charge of fission fragments, fission energy, fission cross-sections, Fission neutrons, concept of nuclear reactor and working principle, concept of nuclear fusion.

BOOKS:

1. *Mechanisms of Inorganic Reactions byF. Basolo and R. G. Pearson*
2. *Inorganic Chemistry by Asim K Das*
3. *Inorganic Chemistry by Cotton and Wilkinson (4^{th} Edn)*
4. *Essentials of Nuclear Chemistry by H. J. Arniker*

CH-503: ORGANIC REDOX REACTION AND SPECTROSCOPY 3 credits

UNIT-I Oxidation: Oxidation of hydrocarbons, oxidation of alcohols by various reagents, and methods, oxidation of carbon-carbon double bonds to diols and epoxides, Chromium (VI), Manganese (VII) oxidants, Oxidation with peracids, oxidation with hydrogen peroxide, with singlet oxygen. Oxidation with ruthenium tetroxide, iodobenzene diacetate, and thallium (III) nitrate, DMSO.

Reduction: Catalytic hydrogenation, selectivity of reduction, Reduction by hydride transfer reagents: Aluminium alkoxid, Lithium aluminium hydride (LAH) and Sodium borohydride ($NaBH_4$), di-isobutylaluminium hydride, Sodium cyanoborodydride, Lithium trialkylborohydride, reduction with hydrazine and diimide, reduction with trialkyltinhydride, the Birch reduction, the Wolff-Kischner reduction, the Cannizarro reduction, the Resenmund reduction.

UNIT-II NMR: Magnetic properties of nuclei, Theory of magnetic nuclear resonance with special reference to proton, Instrumentation, Chemical shift, Simple spin-spin interaction, Shielding effects, Diamagnetic anisotropy, NOE, ^{13}C, ^{15}N, ^{19}F, ^{31}P NMR (preliminary idea).

UNIT-III

(a) Mass spectrometry: Introduction, Mass spectrum, Determination of molecular formulae, Parent peak, Base peak, Use of molecular fragmentation, Mass spectra of some classes of compounds (hydrocarbons, alcohols, phenols, ketones, aldehydes, acids and esters)

(b) Problems involving UV, IR, NMR and Mass spectroscopy.

BOOKS:

1. *Organic Chemistry-II by I.L. Finar*
2. *Spectroscopic Identification of Organic Compounds, Silverstein & Basselr*
3. *Organic Spectroscopy by V.K. Ahluwalia*
4. *Spectroscopy by Donald L. Pavia, Gary M. Lampman, and George S. Kriz*

CH-504: PERICYCLIC REACTION, PHOTOCHEMISTRY AND RETROSYNTHESIS 3 credits

UNIT-I Pericyclic reactions: Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene and allyl system. Classification of pericyclic reactions. Woodward-Hoffmann rules, Correlation diagrams and FMO approaches. Electrocyclic reactions - Conrotatory and disrotatory motions, 4n, 4n+2 and allyl systems. Cycloaddition reactions - suprafacial and antarafacial additions, 4n and 4n+2 systems, [2+2] and [4+2] reactions (thermal and photochemical), 1,3 dipolar cycloadditions and cheletropic reactions. Sigmatropic rearrangements - [*i,j*] shifts of C-H and C-C bonds; Sommelet-Hauser, Claisen, thio-Claisen, Cope and aza-Cope rearrangements. Ene reaction.

UNIT-II First order Photochemical processes Light absorption, Fluorescence and Phosphorescence.

Introduction to photochemical reactions: *Cis-Trans* Isomerization, Dissociation, Reduction of ketones, Paterno-Buchi reaction, Norrish type I and II reactions, Di-pi-methane rearrangement, Photochemistry of arenes, Barton reaction.

UNIT-III Synthetic design: Introduction, Retrosynthetic approach, Terminology in Retro synthetic analysis, One group disconnection, (alcohol, carbonyl compound, olefins and acids), Two group disconnections (β-hydroxy compounds,α, β-unsubstituted carbonyl compounds, 1,3-dicarbonyl compounds, 1,5 dicarbonyl compounds), Synthesis of some organic molecules by disconnection approach.

BOOKS:

1. *Conversion of Orbital Symmetry by Woodward & Hoffman*
2. *Organic Reactions and Orbital Symmetry by Gilchrist and Storr*
3. *Mechanism and Theory in Organic Chemistry by Lowry & Richardson*
4. *Basic Principles of Organic Chemistry by Roberts & Casserio*
5. *Photochemistry and Pericyclic Reactions by Jagdamba Singh*
6. *Organic Synthesis: The Disconnection Approach by Stuart Warren, Paul Wyatt*

CH-505: QUANTUM CHEMISTRY 3 credits

UNIT-I ***Exact Quantum Mechanical Results***

The Schrodinger equation and the postulates of quantum mechanics, Elementary application of the Schrodinger equation, Particle in a box, Harmonic oscillators, Rigid rotator and hydrogen atom.

UNIT-II ***Approximate Methods & Angular Momentum***

The variation theorem, Time independent perturbation of non-degenerate systems, Application of Variation Method and Perturbation Theory to the He atom.

Ordinary angular momentum, generalized angular momentum, Eigen functions for angular momentum, Addition of angular momentum.

UNIT-III ***Chemical Bonding in Diatomics***

Born-Oppenheimer Approximation, Molecular Orbital Theory and its Applications, Valence Bond Theory and its Applications, LCAO-MO Theory.

BOOKS

1. *Introductory Quantum Chemistry, A.K. Chandra*
2. *Fundamentals of Quantum Chemistry, R.K. Prasad*

CH-506: ATOMIC & MOLECULAR SPECTROSCOPY 3 credits

UNIT-I: ***Atomic Spectroscopy***

The electromagnetic spectrum, A general discussion on various molecular excitation processes, Spectra of hydrogen and hydrogen like atoms, alkali metals spectra, L-S coupling, Term symbols, Space quantisation, Zeeman effect, Stark effect, Paschen-Back effect.

UNIT-II ***Vibrational and Rotational Spectroscopy***

Molecular Spectra of Diatomic Gases, Classification of molecules, Rotational Spectra, Vibrational Spectra, Vibrational-Rotational Spectra, P, Q and R Branches.

UNIT-III ***Raman Spectroscopy***

Theory of Raman spectra, Rotational Raman spectra, Vibrational Raman spectra, Rotational-Vibrational Raman spectra, comparison with IR spectra.

BOOKS:

1. *Physical Chemistry by D.N. Bajpai*
2. *Physical Chemistry by A.W. Atkins*
3. *Physical Chemistry Through Problems by Dogra & Dogra*
4. *Spectroscopy Vol. I & II by Walker & Straw*
5. *Fundamentals of Molecular Spectroscopy by C.N. Banwell*
6. *Fundamentals of Molecular Spectroscopy by G.M. Barrow*

CH-507: PHYSICAL PRACTICAL — 3 credits

1. Determination of ionization constants of weak acids and verification of Oswald's Dilution law.
2. Verification of Onsager's limiting law.
3. Conductometric titration of a mixture of HCl+CH_3COOH with NaOH
4. Determination of solubility product of $BaSO_4$.
5. Potentiometric titration of strong acid with strong base.
6. Verification of Beer's Lambert Law and unknown concentration determination.
7. Verification of additivity rule spectrophotometrically.
8. Determination of temperature coefficient and energy of activation of hydrolysis of ethyl acetate.
9. To determine the rate constant of base hydrolysis of ester titrometrically.
10. To study the complex formation between ammonia and Cu^{+2}.
11. To study of an equilibrium $KI + I_2 = KI_3$.
12. To study the simultaneous equilibria in benzoic acid - benzene water system.
13. Determination of unknown dextrose solution by polarimetry
14. Study of inversion of cane sugar in acid medium by polarimetry.

BOOK:

1. *Experimental Physical Chemistry by Das and Behera*
2. *Practical Physical Chemistry by B. Vishwanathan & P.S. Raghavan*
3. *Experimental Physical Chemistry by V.D. Athawale*

CH-507: REVIEW — 2 credits

FOURTH SEMESTER

(Core Courses)

CH-511: ADVANCED ORGANOMETALLIC CHEMISTRY 3 credits

UNIT-I: ***σ- and π-Bonded Organometallic Compounds***

History and perspective, definition of organometallic compound, classifications, nature of metal-carbon bond, nomenclature, the 18-electron rule, general methods of preparation and properties of σ-bonded alkyl and aryl compounds, synthesis, properties and bonding of organometallic complexes of olefinic, acetylenic, allylic, acyclic- and cyclic butadiene ligands. Transition metal π-complexes of η^5-cyclopentadienyl, acyclic pentadienyl, η^5-cyclohexadienyl and η^5-cycloheptadienyl ligands: synthesis and reactions. Davis-Green-Mingos (DGM) rules.

UNIT-II: ***Organometallic Compounds and Unique Reactions***

Transition metal π-complexes of η^6-arene, η^6-cycloheptatriene and η^6-cyclooctatriene ligands: synthesis and reactions. Coordinative unsaturation, oxidative addition reaction, reductive elimination reaction, insertion reaction, mechanism of insertion of CO into $CH_3Mn(CO)_5$, deinsertion reaction, intramolecular hydrogen transfer reaction, Agostic interaction, fluxionality in organometallic compounds, Transition metal compounds with bonds to hydrogen.

UNIT-III: ***Organometallic Compounds in Catalysis***

General idea of catalysis, classification catalysis, hydrogenation of alkenes, Tolman catalytic loop, hydroformylation of alkenes (using cobalt and rhodium catalyst), enantioselective hydrofomylation, Zeigler-Natta polymerization of olefins, reduction of carbon monoxide by hydrogen (Fischer-Tropsch reaction), wacker process, mosanto acetic acid synthesis, hydrosilylation reactions, activation of C-H bond, alkene metathesis reactions, metathesis catalysts, classification of metathesis reactions, Importance of metathesis reactions.

BOOKS:

1. *Basic organometallic Chemistry by B. D. Gupta, A. J. Elias, University Press (India) Pvt. Ltd., 2nd edn, Hyderabad, 2013*
2. *Organometallic Chemistry by R. C. Mehrotra, A. Singh, New Age International Ltd., 1st edn, 2011, New Delhi*
3. *Organometallic Compounds by Indrajeet Kumar, 4th edn, 2013, Pragati Prakashan, Meerut.*
4. *Inorganic Chemistry by G. L. Miessler, D. A. Tarr, 3rd edn., 2004, Pearson Education, Inc.*
5. *Modern Aspects of Inorganic Chemistry by Emelius and Sharpe*
6. *Principle of Organometallic Chemistry by Coutes, Green, Powell and Wade*
7. *Organometallic Chemistry by Pauson*

CH-512: ADVANCED SPECTROSCOPY 3 credits

UNIT-I: ***Electron Spin Resonance Spectroscopy***

Theory, instrumentation, g-values, hyperfine splitting, ESR spectra of systems with more than one unpaired electrons, double resonance, ENDOR and ELDOR techniques.

UNIT-II: ***Photoelectron Spectroscopy***

Basic principle, Instrumentation: the basic design of photoelectron spectrophotometer, X-ray photoelectron spectrophotometer, ultraviolet photoelectron spectrophotometer, chemical information from photoelectron spectroscopy, ultraviolet photoelectron spectra and their interpretation, application of X-ray photoelectron spectroscopy, auger lines.

UNIT-III: ***Mossbauer Spectroscopy***

Principles of Mossbauer spectroscopy, Experimental methods, Theoretical aspects, Quadrupole splitting, Magnetic hyperfine interaction.

BOOKS:

1. *Spectroscopy Vol. I & II, Walker & Straw*
2. *Fundamentals of Molecular Spectroscopy, C.N. Banwell*
3. *Spectroscopy Volume III, Straughan and Walker*
4. *Molecular Spectroscopy, P.S. Sindhu*
5. *Fundamentals of Molecular Spectroscopy, G.M. Barrow*
6. *Physical Chemistry through problems, Dogra & Dogra*

CH-513: COMPUTER APPLICATION IN CHEMISTRY — 2 credits

UNIT-I: ***Introduction to Computers***

Basic structure of a computer: The CPU, the I/O devices, the internal memory, commonly used secondary storage media. Data representation: Overview of binary, octal and hexadecimal number system. The software: Concept of low level and high level languages, Compiler interpreter, editor, operating system concepts, salient features of MS-DOS. Windows operating systems.

UNIT-II: ***Programme Development Process***

Algorithm, Flowchart, Decision-table, elements of high level programming languages. Input-output statements, conditional statements, control structure, concept of data file, file operations like searching, storing, with reference to C Programming.

BOOKS:

1. *Computational Chemistry by A.C. Norris*
2. *C Programming Language by Brian W. Kernighan and Dennis M. Ritchie*
3. *An Introduction to Digital Computer Design by V. Rajaraman & T. Radhakrishnan*

CH-514 ANALYTICAL PRACTICAL — 2 credits

1. Determine the pK value of an acid-base indicator.
2. To estimate metal ions by spectrophotometric titration.
3. To determine the pH of a given solution by spectrphotometrically.
4. Adsorption of CH_3COOH on activated charcoal and verification of Freundlich's & Langumir's adsorption isotherm.
5. Simultaneous estimation of Mn and Cr in a solution of $KMnO_4$ and $K_2Cr_2O_7$.
6. Determination of hydrolysis constant of aniline hydrochloride.
7. Determination of ionisation constants of multibasic acid potentiometrically.
8. Determination of association constants of CH_3COOH by distribution method between water and toluene.
9. To study the rate of acid catalysed iodination of acetone in presence of excess acid and acetone.
10. To study the stability constant of a metal complex.
11. Estimation of Fe ion in a solution of Mhor's salt.

BOOK:

1. *Experimental Physical Chemistry by Das and Behera*
2. *Practical Physical Chemistry by B. Vishwanathan & P.S. Raghavan*
3. *Experimental Physical Chemistry by V.D. Athawale*

CH-515: PRACTICAL ON COMPUTER IN CHEMISTRY — 2 credits

1. Use of computer programmes like EXCEL, Chemdraw.
2. Execution of the Software to solve problems.
3. Development of small programmes for solving chemical problems.

(Elective Courses)

GROUP-A

CH-521 ADVANCED ORGANIC SYNTHESIS 3 credits

UNIT-I Chemistry of some natural products, A study of the following compounds involving their isolation, structure elucidation, synthesis and biogenesis – Alkaloid - morphine, flavonoids - quercetin, cyanidin and genestein, α-terpeneol, α-pinene. coumarins, porphyrins – haemoglobin.

UNIT-II: Systematic nomenclature (Hantzch-Widman system) for monocycle and fused heterocycles. General approach to heterocyclic synthesis-cyclisation and cycloaddition route, Synthesis and reactivity of common heterocyclic compounds containing one or two heteroatoms (O, N, S): furan, pyrrole, thiophene, indole, thiazole, oxazole, imidazole, pyrazole, pyrimidine, seven membered heterocycles (azepine).

UNIT-III: Organometallics Chemistry of Transitional Element and applications in organic synthesis: Preparative structural and characteristic aspects: oxidative insertion, reductive elimination, ligand migration from metal to carbon. Organo lithium, organo copper compounds, organo boranes, organometallic compounds of Zinc, Cadmium, nickel, palladium, mercury and their utilization in chemical reactions. Reactions involving triple bond (Sonogashira reaction), C-C (Kumada, Negishi, Heck, Suzuki and Stille reactions) and C-N (Buchwald-Hartwig reaction) cross-coupling reaction.

BOOKS:

1. *Organic Chemistry II by I. L. Finar*
2. *Principles of Organic Synthesis by R. O. C. Norman*
3. *Creativity in Organic Synthesis by J. S. Bindra and R. Bindra*
4. *Heterocyclic Chemistry by A R Katrizsky*
5. *Recent Literatures and Review Articles*

CH-522: PHOTOPHYSICAL PROCESSES & INSTRUMENTATION 3 credits

UNIT-I: Importance of photochemistry, Laws of photochemistry, photochemistry and spectroscopy, Interaction between light and matter, electronic energy states of atoms, spectroscopic terms for electronic states, orbital symmetry and molecular symmetry, and notation for excited states of organic molecules, Electric dipole transition, Einstein's treatment absorption and emission phenomena, time-dependent Schrödinger equation, the rules governing the transitions between two energy states, Nature of changes on electronic excitation, Electronic, vibrational and rotational energies, potential energy diagram, shapes of absorption band and Frank-Condon principle, emission spectra, environmental effect on absorption and emission spectra, excited state dipole moment, excited state acidity constants-pk^* values, and Wigner spin conservation rule.

UNIT-II: Types of photophysical pathways, radiationless transitions-internal conversion and intersystem crossing, fluorescence emission, fluorescence and structure, delayed fluorescence, Quenching of Fluorescence, Theory of Collisional Quenching, Derivation of the Stern-Volmer Equation, Theory of Static Quenching, Combined Dynamic and Static Quenching, Examples of Static and Dynamic Quenching, Deviations from the Stern-Volmer Equation, Quenching Sphere of Action, Derivation of the Quenching Sphere of Action, Effects of Steric Shielding and Charge on Quenching, Fractional Accessibility to Quenchers, Applications of Quenching to Proteins and Membranes, Characteristics of Resonance Energy Transfer, Theory of Energy Transfer for a Donor–Acceptor Pair, Distance Measurements Using FRET.

UNIT-III: Principles & techniques of Steady State Spectrofluorometers & TCSPC Spectrofluorometers and its Applications, brief concept and applications of Fluorescence Anisotropy & Fluorescence lifetime.

BOOKS

1. *Fundamentals of Photochemistry by K. K. Rohatagi-Mukherjee*
2. *Molecular Photochemistry by N. J. Turro,*
3. *Principles of Photochemistry by J.A. Baltrop & J.D. Coyle*
4. *Principles of Fluorescence Spectroscopy by J. R. Lakowicz*

CH-523: CHEMISTRY OF NANOMATERIALS 3 credits

UNIT-I: ***Semiconductors and Devices***

(a) Conducting and semiconducting organic materials. Synthesis and characterizations of organic semiconductors, band gap engineering. Doping of semiconductors.

(b) Nanostructured Carbon based materials: Fullerene, Carbon nanotube, graphene. Artificial photosynthetic devices, storage-memory and sensors. Electronic devices and coating. High temperature resistant organic/inorganic polymers.

UNIT-II: ***Nanomaterials and Applications***

(a) Nanomaterials for Solar Energy Conversion Systems. Principles of photovoltaic energy conversion (PV), Structural characteristics and concepts. Types of photovoltics Cells, Physical concept of photovoltaic cells, Organic solar cells, Dye-Sensitized Solar Cells, Organic-Inorganic Hybrid solar cells. Current status and future trends.

(b) Conducting and ferroelectric materials, structure and features of ferroelectric materials, ceramic materials, organic/inorganic hybrid materials and their applications.

UNIT-III: ***Structure Properties of Polymers and Applications***

(a) Structure-property relationship, stress-strain behavior, crystalline melting point, effect of chain flexibility and other steric factors, entropy and heat of fusion, glass transition temperature, relationship between Tm and Tg. Effect of molecular weight, property requirements and its utilization.

(b) Synthetic procedure commercial polymers (polycarbonate, polyurethane, polymethylmethacrylate, polyethyethyleneterpthalate, Nylon, polystyrene), Fire retarding and biomedical polymers

BOOKS:

1. *Semiconductor for Solar Cells by H J Moller, Artech House Inc, MA, USA, 1993.*
2. *Solis State Electronic Device by Ben G Streetman, Prentice Hall of India Pvt Ltd., New Delhi.*
3. *Organic Photovoltaics – Materials, Device Physics and Manufacturing Technologies, Eds. By C. Brabec, V. Dyakonov, U. Scherf), 2nd Ed., Wiley-VCH, Germany, 2014.*
4. *Text Book of Polymer Science by F.W. Billmeyer Jr, Wiley.*
5. *Polymer Science by V.R. Gowariker, N.V. Viswanathan and J. Sreedhar, Wiley-Eastern.*

CH-524: INDUSTRIAL PROCESSES 3 credits

UNIT-I: Petroleum and coal based chemicals: Composition of petroleum, cracking processes, Commercial production of ethylene, acetylene, polymerization mechanisms, Addition, condensation, step growth, chain growth, method of polymerization, Distillation of coal.

UNIT-II:

(a) Oil based industries: Oils and fats: Solvent extraction of oils, hydrogenation of oil, use of oil in the manufacturing of soap, paints and varnishes.

(b) Surface active agents: classification and manufacturing of detergents used for cleansing purpose.

(c) Fermentation industries. A general discussion on fermentation conditions, manufacturing of penicillin.

UNIT-III: Pesticides and Pharmaceutical industries: DDT manufacture, BHC manufacture, 2,4-D manufacture, parathion manufacture, Pharmaceutical industry

BOOKS:

1. *Outlines of Chemical Technology by M. Gopala Rao and Marshall Sittig, Affiliated East-West Press Pvt. Ltd.*
2. *Industrial Chemistry by B. K. Sharma*

GROUP-B

CH-531: ADVANCED ANALYTICAL CHEMISTRY 3 credits

UNIT-I: ***Reliability of Analytical Data***

Errors in chemical analysis, classification of errors, significant figures, precision and accuracy, methods of expressing accuracy, absolute error and relative error, methods of expressing precision, average deviation, standard deviation, confidence limits, median value, range, coefficient of variation.

Sampling in analysis definition: Theory of sampling, technique of sampling, statistical criteria of good sampling and required size, stratified sampling, transition and storage samples.

UNIT-II: ***Solvent Extraction and Ion Exchange***

Solvent extraction: basic principles, classification of extraction, mechanism of extraction, extraction equilibria, technique of extraction, applications in analytical chemistry.

Ion exchange: synthesis and characteristics of ion exchange, ion exchange equilibrIa, technique of ion exchange, application of ion exchange for separation.

UNIT-III: ***Ultraviolet and Visible Spectrophotometry***

Introduction, nature of absorbing species, visual colorimetry, photo-electric cell and filters, Photoelectric filter photometry, errors in photoelectric photometry, Spectrophotometry, working of spectrophotometer, simultaneous spectrophotometry, differential spectrophotometry, reflectance spectrophotometry, photometric titrations, composition of coloured complex Sandell's sensitivity, relative concentration and Ringbon's plot, principle of Nephelometry and Turbidimetry, application and factors affecting Nephelometric and Turbidimetric measurement.

BOOKS:

1. *Basic Principle of Analytical Chemistry by S.M. Khopkar*
2. *A Text Book of Quantitative Inorganic Analysis by A.I. Vogal.*

CH-532: SUPRAMOLECULAR CHEMISTRY 3 credits

UNIT-I: ***Fundamentals of Supramolecular Chemistry***

Terminology and definitions in supramolecular chemistry. Intermolecular forces: Ion pairing, ion-dipole and dipole-dipole interactions; hydrogen bonding; cation-pi, anion-pi, pi-pi interactions and Van der Waal forces. Solvent and solution properties, solvation and hydrophobic effect. Binding constants; definition and use, determination of binding constant by physical methods.

UNIT-II: ***Molecular Recognition***

Principle of molecular recognition, host-guest complementarity, preorganisation, chelate effect, cooperativity. Synthesis and applications of supramolecular host (crown ethers, lariat ethers, podands, cryptands, spherands, calix[n]arenes, cyclodextrine) as cation and anion binding receptors and receptors for ion-pair recognition.

UNIT-III: ***Supramolecular Reactivity and Catalysis***

Organocatalysis mediated through hydrogen bonding, preconcentration, self-assembly of catalysts and preorganisation of catalyst-substrate systems. Influence of organisation (effective molarity) on catalysis, Catalytic acyl transfer, acid-base catalysis, catalysis hydrolysis as ATPase mimic

BOOKS:

1. *Supramolecular Chemistry: from Molecules to Nanomaterials Eds. by P.A. Gale and J.W. Steed (2012).*
2. *Modern Supramolecular Chemistry by F. Diederich, P. J. Stang, R. T. Tykwinski (2008). .*

3. *Core Concepts in Supramolecular Chemistry and Nanochemistry by J. W. Steed, D. R. Turner, K. J. Wallace (2007).*
4. *Supramolecular Chemistry by J.W. Steed and J.L. Atwood (2011).*
5. *Supramolecular Chemistry: Concepts and Perspectives by J.-M. Lehn, Wiley VCH, Weinheim (1995).*
6. *Supramolecular Chemistry by V. Balzani (Editor), L. De Cola, Kluwer, Dordrecht (1992).*
7. *Introduction to Supramolecular Chemistry by H. Dodziuk, Kluwer Academic Publishers, The Netherlands (2002).*
8. *Supramolecular Assemblies Y. Murakami (Editor), Mita Press, Tokyo, (1990).*
9. *Advances in Supramolecular Chemistry, Vol 1 (1990), Vol 2 (1992), Vol 3 (1993) by G. W. Gokel (Editor), JAI Press, Greenwich.*
10. *Supramolecular Chemistry – Fundamentals and Applications. Advanced Textbook by T. Kunitake, K Ariga, Berlin: Springer-Verlag Heidelberg, 2006. 208 p. ISBN 978-3-540-01298-6.*

CH-533: SURFACE CHEMISTRY & CATALYSIS 3 credits

UNIT-I: ***Structural Aspects of Organized Molecular Assemblies***

Surfactants, classification of surfactants, micelles, critical micellar concentration, different methods for determination of critical micellar concentration, thermodynamics of micellization, aggregation number, shape & size and their determination, shape transition, reverse micelles, emulsion, microemulsion (oil in water and water in oil), effect of cosurfactants, thermodynamics of microemulsion formation.

UNIT-II: ***Analytical Applications of Organized Assemblies***

Application of micellar systems for UV-Visible/fluorescence spectroscopic detection of ions, micellar enhanced phosphorescence and fluorescence, micellar systems in liquid-liquid extraction, surfactant aggregates in flame and plasma atomic spectrometry, micellar systems in chromatography, recent developments in micellar chromatography, application of surfactants in gel electrophoresis.

UNIT-III: ***Characterization of Industrial and Model Solid Catalysts***

Historical development of catalysis, dividing of catalysis to homogeneous and heterogeneous, enzymatic, phase transfer catalysis. Preparation and characterization of catalysts, influence of heat and mass transport on the rate of catalytic process. Evaluation of activity and selectivity of catalysts. Catalysts acido-basic, hydrogenation-dehydrogenation, oxidation-reduction, zeolite. Mechanisms of catalyzed reactions. Examples of catalysts applications– cracking, alkylation, hydrogenation, hydration and dehydration processes. Modern sorption and spectral methods of characterization of catalysts.

BOOKS:

1. *Introduction to Surface Chemistry and Catalysis by Gábor A. Somorjai (John Wiley & Sons)*
2. *Physical Chemistry of Macromolecules by C. Tanford*

CH-534: MATERIAL AND ENERGY BALANCE 3 credits

UNIT-I: ***Material Balance***

(a) Material Balances Without Chemical Reactions: Process Flow-Sheet, Material Balances, Recycling Operations, Material Balances of Unsteady State Operations.

(b) Material Balances Involving Chemical Reactions, Definition of Terms, Electrochemical Reactions, Recycling, Parallel and Bypassing Operations, Metallurgical Applications.

UNIT-II: ***Energy Balance***

Energy and Thermo-Chemistry, Energy Balances, Heat Capacity, Heat Capacity of Gases at Constant Pressure, Sensible Heat Changes in Liquids, Heat Capacity of Gaseous Mixtures, Latent Heats, Enthalpy Changes During Phase Transfers Accompanied by Sensible Heat Changes, Enthalpy Changes Accompanying Chemical Reactions, Effect of Temperature on Heat of Formation, Heat of Reaction, Adiabatic Reactions, Effect of Pressure on Heat of Reaction, Thermochemistry of Mixing Process, Dissolution of Solids, Liquid-Liquid Mixtures, Heat of Solution by Partial Molal Quantities.

UNIT III: ***Stoichiometry and Unit Operations***

Distillation, Absorption and Stripping, Extraction and Leaching, Crystallisation, Psychrometry, Drying, Evaporation, Less Conventional Operation

BOOK: *Stochiometry by B I Bhatt and S. M. Vora (Tata McGraw Hill, New Delhi)*