**Department of Chemistry**

**Course Structure**

**M.Sc. Chemical Sciences**

**SEMESTER I**

| S. No. | | COURSE TITLE | COURSE CODE | L T P | CREDIT |
|---|---|---|---|---|---|
| 1 | PCC | Inorganic Chemistry I | **BCY551** | 3 0 3 | 4 |
| 2 | PCC | Physical Chemistry I | **BCY553** | 3 0 3 | 4 |
| 3 | PCC | Organic Chemistry I | **BCY555** | 3 0 3 | 4 |
| 4 | PCC | Analytical Chemistry I | **BCY557** | 3 0 3 | 4 |
| 5 | ESC | Waste Management Technology | **BCY559** | 3 1 0 | 4 |
| | Total Credits (A) | | | | **20** |

**SEMESTER- II**

| S. No. | | COURSE TITLE | COURSE CODE | L T P | CREDIT |
|---|---|---|---|---|---|
| 1 | PCC | Inorganic Chemistry II | BCY550 | 3 0 3 | 4 |
| 2 | PCC | Physical Chemistry II | BCY552 | 3 0 3 | 4 |
| 3 | ESC | Material Characterization Techniques | BCY558 | 3 1 0 | 4 |
| 4 | PCC | Organic Chemistry II | BCY554 | 3 0 3 | 4 |
| 5 | PCC | Analytical Chemistry II | BCY556 | 3 0 3 | 4 |
| | Total Credits (B) | | | | **20** |

**SEMESTER- III**

| S. No. | | COURSE TITLE | COURSE CODE | L T P | CREDIT |
|---|---|---|---|---|---|
| 1 | PCC | Physical Chemistry III | BCY 651 | 3 0 3 | 4 |
| 2 | PCC | Organic Chemistry III | BCY 653 | 3 0 3 | 4 |
| 3 | ESC | Bioinorganic Chemistry | BCY 655 | 3 1 0 | 4 |
| 4 | ISC | Internship | BCY 657 | 0 0 4 | 2 |
| 5 | PEC | Elective-1 | BCY 659 | 3 1 0 | 4 |
| 6 | PCC | Minor Project | BCY 661 | 0 0 4 | 2 |
| | Total Credits (C) | | | | **20** |

**SEMESTER- IV**

| S. No. | | COURSE TITLE | COURSE CODE | L T P | CREDIT |
|---|---|---|---|---|---|
| 1 | PCC | Analytical Chemistry III | BCY650 | 3 0 3 | 4 |
| 2 | ESC | Energy and Environmental Sustainability | BCY652 | 3 1 0 | 4 |
| 3 | PEC | Elective II | BCY654 | 3 1 0 | 4 |
| 4 | PCC | Capstone Project | BCY656 | 0 0 16 | 8 |
| | Total Credits (D) | | | | **20** |
| | Grand Total Credits (A+B+C+D) | | | | **80** |

# SEMESTER-I

L T P C
3 0 3 4

**Unit I**

**Metal-Ligand Bonding in Transition Metal Complexes:**

Crystal field splitting diagrams in complexes of low symmetry; Spectrochemical and Nephelauxetic series; thermodynamic and structural effects; site selection in spinels, Jahn-Teller distortions; experimental evidence for metal-ligand orbital overlap; ligand field theory, molecular orbital theory as applied to metal complexes.

(10-12 lectures)

**Unit II**

**Molecular Symmetry and Character Tables:**

Symmetry elements and symmetry operations, symmetry groups, defining properties of a group, Character tables and its application.

(6-8 lectures)

**Unit III**

**Electronic Spectra of Transition Metal Complexes:**

Spectroscopic ground states; Orgel energy level and Tanabe-Sugano diagrams for transition metal complexes; Charge transfer spectra; electronic spectra of octahedral and tetrahedral Co(II) and Ni(II) complexes and calculation of ligand-field parameters.

(6-8 lectures)

**Unit IV**

**Chemistry of Inner Transition Elements:**

Special features of f-block elements, introduction, occurrence, separation, oxidation states, lanthanide contraction, coordination number, structures, and simple reactions. Spectral, Magnetic properties and Analytical applications.

(4-6 lectures)

**Unit V**

**Cluster Compounds:**

Introduction, clusters in elemental states, cluster classification, skeletal electron (Elm0 counting, higher boron hydrides-structures and reactions, equation of balance, Lipscomb topological diagrams, polyhedral skeletal electron pair theory (PSEPT), carboranes, metalloboranes and heteroboranes, metallocarboranes, zintl ions, chevral compounds, infinite metal chains, cluster-surface analogy.

(6-8 lectures)

**Books Recommended**


1. F.A. Cotton and G. Wilkinson Advanced Inorganic Chemistry, 6th Edn. (1999), John Wiley & Sons, New York.
2. James E. Huheey, Inorganic Chemistry, 4th Edn. (1993), Addison-Wesley Pub. Co., New York.
3. R. S. Drago, Physical Methods in Inorganic Chemistry, International Edn. (1971), Affiliated East-West Press, New Delhi.
4. Keith F. Purcell and John C. Kotz, Inorganic Chemistry, W. B. Sauders Com. (1987), Hong Kong.




Shaili Pal

5. K. Veera Reddy, Symmetry and Spectroscopy of Molecules, New Age International Pvt. Ltd., New Delhi (1999).

**List of Experiments:**

1. Qualitative analysis of inorganic mixture.
2. Qualitative analysis of insoluble- oxides, sulphates and halides.
3. Gravimetrically estimation of Zn, Ba in the given solution.
4. Separation of cations and anions by Paper Chromatography.
5. Estimation of Nickel as Nickel (+2) dimethylglyoximate in the given Ni(+2) sulfate.

## BCY553: Physical Chemistry-I

**L T P C**
**3 0 3 4**

**Unit I**

**Electrochemistry:**

Metal/Electrolyte interface: OHP and IHP, potential profile across double layer region, potential difference across electrified interface; Structure of the double layer: Helmholtz-Perrin, Gouy Chapman, and Stern models. Butler-Volmer equation under near equilibrium and non-equilibrium conditions, exchange current density, Tafel plot. Polarizable and non-polarizable interfaces.

(8-10 lectures)

**Unit II**

**Chemical Kinetics:**

**Theories of reaction rates:** Collision theory, Potential energy surfaces (basic idea), Transition state theory, Theory of unimolecular reactions, Lindemann mechanism, Hinshelwood treatment, RRKM model.

**Solution Kinetics:** Factors affecting reaction rates in solution. Effect of solvent and ionic strength (primary salt effect) on the rate constant, Secondary salt effects.

(8-10 lectures)

**Unit III**

**Surface Chemistry and Catalysis:**

Catalytic activity at surfaces (volcano curve), transition state theory of surface reactions: rates of chemisorption and desorption, Unimolecular and bimolecular surface reactions ( reaction between a gas molecule and an adsorbed molecule, reaction between two adsorbed molecules, inhibition and activation energy of such reactions) comparison of homogeneous and heterogeneous reaction rates, surface heterogeneity, lateral interaction.

(4-6 lectures)

**Unit IV**

**Quantum Chemistry:**

Shaili Pal

Review of essential mathematical concepts, Origin of quantum theory, Black body radiation, Wien and Rayleigh-Jeans laws, Planck's law and energy of harmonic oscillator, Postulates of quantum mechanics, Three dimensional time independent Schrodinger, wave equation, Eigen functions and eigen values, Normalization and Orthogonality conditions, One dimensional harmonic oscillator, Tunnel effect, Eigen function and eigen value of H-atom (Solutions not required), shapes of s, p, d and f- orbitals. **Approximate Methods-** Variation principle and its application to ground state H-atom, Radial and Angular distribution curves for H-atom

(8-10 lectures)

**Unit V**

**Spectroscopy:**

**Molecular Spectra-** Basic Concepts of molecular spectroscopy, classification of spectra, characterization of electromagnetic radiations, regions of the spectrum.

**Rotational Spectra-** Rigid and non-rigid rotation spectra-selection rule, centrifugal distortion, isotopic shift, spectra of polyatomic molecules, rotational constant, Experimental techniques.

(6-8 lectures)

**Books Recommended:**


1. Modern Electrochemistry, Vol. 2 A & B, J.O'M. Bockris and A. K. N. Reddy, 2nd Ed. Plenum Press, New York (1998).
2. Chemical Kinetics, K. J. Laidler, 3rd Ed. (1987), Harper & Row, New York.
3. Physical Chemistry, P. W. Atkins, 7th& 8th Eds., Oxford University Press, New York.
4. Physical Chemistry, I.N. Levine, 5th Ed., Tata McGraw Hill Pub. Co. Ltd., New Delhi.
5. Physical Chemistry by Puri, Sharma & Pathania, Vishal Publishing Company, Jalandhar.


**List of Experiments:**

1. Potentiometric titration of weak/strong acid and strong /weak base.
2. Conductometric study of the kinetics of saponification of ethyl acetate.
3. Potentiometric titration of a redox system (Ferrous ammonium sulphate with $K_2Cr_2O_7$).
4. Determination of the partition coefficient of benzoic acid between water and benzene.
5. Determine the cell constant of a given conductivity cell at a given temp.
6. Determine the equivalent conductance of a strong electrolyte at several concentration at a given temperature.

**BCY555: Organic Chemistry-I**

**L T P C**
**3 0 3 4**

**Unit I**

**Aromaticity:**

Benzenoid and nonbenzenoid systems, antiaromaticity, homoaromaticity, alternant and nonalternant hydrocarbons.



Shaili Pal

(5-6 lectures)

**Unit II**

**Stereochemistry:**

Elements of symmetry, chirality, molecules with more than one chiral centre, threo and erythro isomers, optical purity, enantiotropic and diastereotropic atoms, group and faces, stereospecific and stereoselective synthesis, optical purity in the absence of chiral carbon (biphenyl allenes and spiranes), chirality due to helical shape, R/S nomenclature, chiral centres and chiral molecules.

(8-10 lectures)

**Unit III**

**Nucleophilic Substitution at Saturated Carbon:**

Mechanism and Stereochemistry of $S_N1$, $S_N2$, $S_Ni$ and $S_N2'$ reactions. The reactivity effects of substrate structure, solvent effects, competition between $S_N1$ and $S_N2$ mechanisms

**Nucleophilic Aromatic substitution:** The Aromatic $S_N1$, $S_N2$ and benzyne mechanisms. Reactivtiy–effect of substrate structure, leaving group, and attacking nucleophile

(8-10 lectures)

**Unit IV**

**Neighbouring Group Participation:**

Evidences of N.G.P.; the phenonium ion, participation by $\pi$ and $\sigma$ bonds, Anchimeric assistance. Classical versus non-classical carbonium ions–the present status.

(6-8 lectures)

**Unit V**

**Reaction Intermediates:**

Generation, stability and reactivity of carbocations, carbanions, carbenes, free radicals, benzyne and nitrene

(6-8 lectures)

**Books recommended**


1. M.B. Smith & Jerry March, March's Advanced Organic Chemistry, 5th Edition (2001), John Wiley & Sons, New York.
2. Peter Sykes, A Guide book to Mechanism in Organic Chemistry, 6th Edition (1997), Orient Longman Ltd., New Delhi.
3. S. M. Mukherjee and S.P. Singh, Reaction Mechanism in Organic Chemistry, Ist Edition (1990), Macmillan India Ltd., New Delhi.
4. T.H. Lowry and K.S. Richardson, Mechanism and Theory in Organic Chemistry, 3rd Edition (1998), Addison – Wesley Longman Inc. (IS Edition)
5. P.S. Kalsi, Organic Reactions and their Mechanisms, 1st Edition (1996), New Age International Publication, New Delhi.


**List of Experiments:**

1. Separation and identification of binary mixtures of organic compounds.
2. Synthesis of organic compounds involving Bromination, reactions
3. Synthesis of organic compounds involving Nitration reactions

Shaik Pal

4. Estimation of glucose, aldehydes and ketones by chemical and spectroscopic methods.
5. Spectrophotometric identification of simple organic compounds (IR and UV vis).

## BCY557: Analytical Chemistry-I

**L T P C**
**3 0 3 4**

**Unit I**

**Introduction:**

Scope & objectives, Analytical chemistry and chemical analysis, Classification of analytical methods, Method selection, Sample processing, Steps in a quantitative analysis, Quantitative range (bispartite classification), Data organisation, Analytical validations, Limit of detection and limit of quantitation, The tools of analytical chemistry and good lab practices.

(6-8 lectures)

**Unit II**

**Standard Data and Data Processing:**

Determinant, constant and indeterminate errors, minimization of errors, accuracy and precision, central limit theory. Distribution of random errors. Average deviation and standard deviation, variance and confidence limit. Significant figures and computation rules, Least square method, polynomial regression and correlation analysis, mean deviation and standard deviation, Gaussian distribution. Validation Qualification, validation and calibration of equipments. Harmonised protocols for the adoption of standardized analytical methods and for the presentation of their performance characteristics. Methods of sampling: sample size

(8-10 lectures)

**Unit III**

**Treatment of Equilibria:**

Solvents and solutions, general treatment of equilibria in aqueous medium involving monoprotic weak acid and weak base, and salts of weak acids and weak bases. Activity and concentration, Effect of electrolytes on chemical equilibria, Calculation of pH, Constructing titration curves from charge balance and mass balance equations, Acid-base titrations and theory of pH indicators, Complexation equilibria and complexometric titrations, Redox equilibria and redox titration, Theory of redox indicators, Precipitation reaction and precipitation titrations and theory of adsorption indicators.

(8-10 lectures)

**Unit IV**

**Spectrophotometric Determination of Stoichiometry of Complexes:**

Job's method of continuous variation, mole ratio and slope ratio analysis, Advantages and limitations, typical examples

(5-6 lectures)

**Unit V**

Shaili Pal

Principles of automation, Process control through automated instruments, Autoanalyzers (single channel and multi-channel), Basic sequences of multi-fold operational analyzers in segmented and non-segmented flows.

(6-8 lectures)

**Books Recommended**


1. R. L. Pecsok, L. D. Shields, T. Cairns and L.C. Mc William, Modern Methods of Chemical Analysis, 2nd Edition (1976), John Wiley, New York.
2. G. D. Christian, Analytical Chemistry, 5th Edition (1994), John Wiley & Sons, New York.
3. D. A. Skoog, D.M. West, F.J. Holler, S.R. Crouch, Analytical Chemistry - An Introduction, 7th Edition (2000), Saunders College Publishing, Philadelphia, London.
4. J. H. Kennedy, Analytical Chemistry: Principles, 2nd Edition (1990), Saunders Holt, London.


**List of Experiments:**

1. Determination of $Na_2CO_3$ content (in %) of washing soda using a pH meter.
2. Determination of hardness of water using EDTA.
3. Determination of % of Chlorine in Bleaching powder.
4. Determination of iron content in the given ore sample.
5. Determination of chloride content in supplied water sample by Mohr's method.

## BCY559: Waste Management Technology

**L T P C**
**3 1 0 4**

**UNIT I**

Sources, classification and composition of solid, liquid and gaseous wastes, hazardous and nonhazardous wastes, special waste materials.

(8-10 Lecture)

**UNIT II**

Storage and transport of wastes. Transportation and collection systems.

(5-6 Lecture)

**UNIT III**

Management of wastes, minimization, reuse and recycling.

(5-6 Lecture)

**UNIT IV**

Waste utilization and materials recovery: Food waste, Biowaste/marine waste, Plastic waste, Carbondioxide.

(8-10 Lecture)

**UNIT V**

Treatment of wastes; biological treatment, composting, anaerobic digestion, combustion, incineration and landfills, ultimate disposal.

(8-10 Lecture)

**Books Recommended:**

1. H. S. Peavy, D.R. Rowe and G. Techbanoglous, Environmental Engineering, Mcgraw Hill Books Co., 1985.

2. R. A. Corbitt, Started Handbook A Environmental Engineering; Mcgraw Hill New Y ork,1990.

3. A. M. Martin (ed), Bio-conservation of waste Materials to Industrial Products; Elsevier, Amsterdam,1991.

4. O.P. Kharbanda and E. A. Stellworthy, Waste Management- towards a Sustainable Society, Gower, 1990.



Shaili Pal

# SEMESTER-II

L T P C
3 0 3 4

**Unit I**

**Reaction Mechanism in Transition Metal Complexes:**

Inert and labile complexes, Mechanism of octahedral substitution, acid hydrolysis, factors affect acid hydrolysis, base hydrolysis, conjugate base mechanism, direct indirect evidence in favour of conjugate mechanism.

(6-8 lectures)

**Unit II**

**Electron Transfer Reactions:**

Mechanism and rate laws; various types of electron transfer reactions, Marcus-Husch theory, correlation between thermal and optical electron transfer reactions; identification of intervalence transfer bands in solution.

(6-8 lectures)

**Unit III**

**Organometallic Chemistry:** Introduction, classification, nomenclature, valence electron count, oxidation number and formal ligand charge; structure and bonding of carbonuls, nitrosyls and related pi-acids, alkyl, alkene, alkyne, π-allyl, polyene and cyclopolyene compounds; metal carbenes and carbines, isolobal analogy, Dewar-Chatt model, oxophilicity, Agostic interaction.

(6-8 lectures)

**Unit IV**

**(a)Inorganic π-Acid Ligands**: Dioxygen and dinitrogen, nitrosyl, tertiary phosphines and arsines as ligands.

**(b) Complexes of σ-donor ligands**: Transition metal alkenyls, alkynyls, carbenes and carbynes

**(c) π-complexes of unsaturated molecules**: Preparation, bonding and structure of alkene, alkyne, allyl, dienyl and trienyl complexes; reactions with special reference to organic synthesis

(8-10 lectures)

**Unit V**

**Transition metal compounds in homogenous catalysis and compound with M-H bond:**

Hydrogenation, hydroformylation and polymerization; Waker Process, hydrocarbanylation of olefins, oxopalladation reactions, activation of C-H bond. Metal hydrides (Classical and Non-classical). Agostic interaction. Application of NMR in studying hydrido complexes.

(8-10 lectures)

**Books Recommended**


1. F. Basalo and R. G. Pearson, Mechanism of Inorganic Reactions, 2nd Edn (1967), Wiley Eastern Ltd., New Delhi.
2. D. F. Shriver and P. W. Atkins, Inorganic Chemistry, 3rd Edn. (1999), ELBS, London.
3. F. A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry, 6th Edn. (1999), John Wiley & Sons, New York.
4. D.N. Sathyanarayana, Electronic Absorption Spectroscopy and Related Techniques, UniversitiesPress (India) Ltd., Hyderabad (2001).
5. Keith F. Purcell and John C. Kotz, Inorganic Chemistry, W. B. Sauders Com. (1987), Hong Kong.
6. Martin L. Tobe and John Burgess, Inorganic Reaction Mechanisms, Longmans Ist Edn. (1999).




Shaili Pal

**List of Experiments:**

1. Qualitative Mixture analysis of inorganic mixture. Containing one or two the less common metals: Tl, Mo, W, Zr, Th, V, U
2. Separation and determination of two metal ions Cu-Ni, Ni-Zn, Cu-Fe using volumetric and gravimetric methods.
3. Synthesis and identification of inorganic coordination compounds.
4. Separation of $Co^{2+}$ + $Ni^{2+}$ present in a sample using anion exchange resin and estimation of each metal ion separated by EDTA titration.
5. To prepare potassium trioxalatochromate (+3) tihydrate $K_3[Cr(C_2O_4)_3].3H_2O$.

## BCY552: Physical Chemistry-II

**L T P C**
**3 0 3 4**

**Unit I**
**Photochemistry:**
Primary and secondary processes in photochemistry, Fate and properties of excited states, Photoluminesence and Photostationary state, Photosensitiztion, Rice-Herzfeld mechanisms, photochemical chain reactions (hydrogen and chlorine, hydrogen and bromine) Non-chain photochemical reactions (formation of phosgene, decomposition of $H_2O_2$ in presence of CO.

(4-6 lectures)

**Unit II**
**Statistical Thermodynamics:**
Concept of ensembles, Canonical ensembles, Boltzmann distribution, Thermodynamic quantities and canonical partition function. Grand canonical ensemble, Fermi-Dirac and Bose-Einstein distributions. Molecular partition functions, Translational, rotational and vibrational partition functions. Ideal monoatomic and diatomic gases, classical partition functions, thermodynamic properties, equipartition theorem. Debye and Einstein theory of heat capacity of solids. Structure and Thermal properties of liquids, Pair correlation functions. Linear response theory, Irreversible processes, Onsager's Law, Entropy production, Non-equilibrium stationary states.

(8-10 lectures)

**Unit III**
**Polymer:**
Definition, types of polymers, Molecular mass – number and mass average molecular mass, determination of molecular mass by Osmometry, viscosity, light scattering and size exclusion chromatography.

(4-6 lectures)

**Unit IV**
**Nuclear Chemistry:**

Classification of nuclides, nuclear stability, Atomic energy, Types of nuclear reactions-fission and fusion, Conservation in nuclear reactions-linear momentum and mass-energy, Reaction cross-section, Bohr's compound nucleus theory of nuclear reaction. Szilard-Chalmers reactions. General characteristics of radioactive decay, decay kinetics, parent-daughter decay growth relationships, artificial radioactivity. Application of radioactivity- radiochemical principles, Isotope dilution and neutron activation analysis.

(8-10 lectures)

**Unit V**

**Equilibrium and Non- equilibrium Thermodynamics:**

Properties of non-ideal solutions - deviations (negative and positive) from ideal behavior, excess functions for nonideal solutions, Third Law of thermodynamics: Nernst heat theorem, variation of entropy with temperature, determination of absolute entropy of liquids and gases, residual entropy. Entropy production in irreversible processes, fluxes and forces, linear phenomenological relations, Onsager's reciprocity relations, thermodynamic theory of membrane permeability, reverse osmosis and electrokinetic phenomena.

(8-10 lectures)

**Books Recommended**


1. Modern Electrochemistry, J.O'M. Bockris and A. K. N. Reddy,Vol. 2 A & B, 2nd Edition, Plenum Press, New York (1998).
2. Electrochemical Methods: Fundamentals and Applications; A.J. Bard and L.R. Faulkner,2nd edition (2001), John Wiley & Sons, New York.
3. Micelles: Theoretical and Applied Aspects, Y. Moroi, , Plenum Press, New York (1992).
4. Text Book of Polymer Science, F.W. Billmayer, Jr., 3rd Edition (1984), Wiley-Interscience, New York.
5. Essentials of Nuclear Chemistry, H.J. Arnikar, 4th Edition (1995), Wiley-Eastern Ltd., New Delhi.
6. Physical Chemistry, P. W. Atkins, 7th& 8thEditions, Oxford University Press, New York.
7. Introduction of Thermodynamics of irreversible Processes, I. Prigogine.


**List of Experiments:**

1. Determination of viscosity and density of aqueous solution of glucose/ Sucrose/Urea at different temperatures.
2. Determination of the surface tension of a given liquid by drop number method.
3. Adsorption of acetic acid on charcoal to verify Freundlich adsorption isotherm and Langmuir isotherm.
4. Determination of molecular weight of acetanilide by Rast method using camphor as solvent.
5. Determination of the molecular weight of a volatile substance by Victor Meyer's method.
6. Determination of dissociation constant k for a weak acid using conductometry.
7. Determination of viscosity average molecular weight of given polymer.

## BCY554 Organic Chemistry-II

L T P C
3 0 3 4

**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 correlation diagram, FMO and PMO approach, Electrocyclic reactions-conrotatory and disrotatory motions, [4n], [4n+2] and allyl systems. Cycloadditions-antrafacial and suprafacial additions, [4n], [4n+2] systems, [2+2] addition of ketenes, 1,3-dipolar cycloadditions and cheleotropic reactions. Sigmatropic rearrangement.

(8-10 lectures)

**Conservation of Orbital Symmetry in Pericyclic Reactions**

Woodward-Hoffmann rules; cycloaddition [2+2] and [4+2], and electrocylic reactions. Prototropic and Sigmatropic rearrangements, Ene reactions and Cheletropic reactions; 1,3-Dipolar cycloaddition

(6-8 lectures)

**Unit II**

**Addition to Carbon–Carbon Multiple Bonds:**

Electrophilic, free-radical and nucleophilic addition: Mechanistic and Stereochemical aspects. Orientation and reactivity. Hydroboration and Michael reaction

(4-6 lectures)

**Unit III**

**Electrophilic Aromatic Substitution:**

The arenium ion mechanism, orientation and reactivity in monosubstituted benzene rings, ortho/ para ratio. **Esterification and Hydrolysis of Esters:** Evidence for tetrahedral intermediate in BAc2 and AAc2 mechanisms, steric and electronic effects. The AAc1 and other pathways involving alkyl to oxygen bond cleavage

(6-8 lectures)

**Unit IV**

**Elimination reactions:**

The E1, E2 and E1cB mechanisms, Orientation of the double bond. Hoffmann versus Saytzeff elimination, Pyrolytic syn-elimination, Competition between substitution and elimination reactions

(4-6 lectures)

**Unit V**

**Kinetic Isotope Effects:**

Its origin and importance in determining reaction mechanism. Solvent isotope effects.

(3-4 lectures)

**Books Recommended**


1. M.B. Smith & Jerry March, March's Advanced Organic Chemistry, 5th Edition (2001), John Wiley & Sons, New York.
2. Peter Sykes, A Guide Book to Mechanism in Organic Chemistry, 6th Edition (1997), Orient Longman Ltd., New Delhi.


Shaili Pal 14

3. S. M. Mukherjee and S.P. Singh, Reaction Mechanism in Organic Chemistry, 1st Edition 1990), Macmillan India Ltd., New Delhi.
4. T.H. Lowry and K.S. Richardson, Mechanism and Theory in Organic Chemistry, 3rd Edition (1998), Addison – Wesley Longman Inc. (IS Edition).
5. P. S. Kalsi, Organic Reactions and Their Mechanisms, 1st Edition (1996), New Age International Pub., New Delhi.
6. S.M. Mukherjee and S.P. Singh, Pericyclic Reactions, MacMillan India, New Delhi.
7. I. Fleming, Pericyclic Reactions, Oxford University Press, Oxford (1999).

**List of Experiments:**

1. Separation and identification of ternary mixtures of organic compounds.
2. Synthesis of organic compounds involving Acetylation.
3. Synthesis of organic compounds involving Diazotization.
4. Synthesis of organic compounds involving Benzoylation.
5. Isolation of Caffeine from tea leaves and eugenol from cloves.

## BCY556: Analytical Chemistry-II

**L T P C**
**3 0 3 4**

**Unit I**

**Polarography:**

Origin of polargraphy, Current-voltage relationship, Theory of polarographic waves (DC and sampled DC (tast) polarograms), Instrumentation, Ilkovic equation, Qualitative and quantitative applications.

(6-8 lectures)

**Unit II**

**Spectroscopic Techniques:**

Theory, Instrumentation and applications of X-rays (emission, absorption, diffraction and fluorescence methods), Atomic absorption Spectroscopy, Atomic fluorescence spectrometry, Atomic emission spectrometry

(6-8 lectures)

**Unit III**

**Spectroscopy:** UV-visible molecular absorption spectrometry (instrumentation and application), Molecular luminescence spectroscopy (fluorescence, phosphorescence, chemiluminescence).

(6-8 lectures)

**Unit IV**

**Separation Methods:**

Principle of chromatography, Classifications of chromatography, Techniques of TLC, Paper and column chromatography, Gas chromatography, High-performance liquid chromatography and hyphenated techniques.

(8-10 lectures)

**Unit V**

**Thermal Analysis:**

Theory, methodology and applications of thermogravimetric analysis (TGA), Differential Thermal Analysis (DTA), and Differential scanning calorimetry (DSC). Principles, techniques and applications of thermometric titration methods

(6-8 lectures)

**Books Recommended**


1. D.A. Skoog, Principles of Instrumental Analysis, 5th Edition (1998), Saunders College Publishing, Philadelphia, London.
2. G.W. Ewing, Instrumental Methods of Chemical Analysis, 5th Edition (1978), McGraw Hill Books Co., New York.
3. R.L. Pecsok, L. D. Shields, T. Cairns and L.C. Mc William, Modern Methods of Chemical Analysis, 2nd Edition (1976), John Wiley, New York.
4. J.H. Kennedy, Analytical Chemistry: Principles, 2nd Edition (1990), Saunders Holt, London.


**List of Experiments:**

1. Spectrophotometric identification of simple organic compounds (IR and UV-Vis)
2. Colorimetric determination of Chromium (VI) (in ppm) using 1,5- diphenyl carbazide as a reagent for color development.
3. Separation of metal ions by paper chromatography.
4. Separation of amino acids by thin layer chromatography.
5. Estimation of carbohydrates, protein, amino acids, ascorbic acid, blood cholesterol and aspirin in APC tablets by UV-Visible spectrophotometric method.

## BCY558: Material Characterization Techniques

**L T P C**
**3 1 0 4**

**Unit I**

**Introduction:** Need of materials characterization and available techniques.

(2 Lectures)

**Unit II**

**Optical Microscopy:** Optical microscopy techniques including polarized light and phase contrast; Quantitative microscopy and its applications.

(4 Lectures)

**Unit III**

**Scanning Electron Microscopy and Scanning Probe Microscopy:** Working principle of SEM, image formation methods in SEM, including voltage contrast, electron back scattered diffraction. Scanning Probe Microscopy-Scanning Tunneling Microscopy (STM) & Atom Force Microscopy (AFM). Applications.

(10-12 Lectures)

**Unit IV**

**Transmission Electron Microscopy:** Working principle of TEM, formation of image and selected area diffraction pattern, interpretation of electron diffraction patterns, theories of image contrast and

their application to study of perfect and imperfect crystalline specimens. High resolution electron microscopy. Convergent Beam Electron Diffraction (CBED), Electron Energy Loss Spectroscopy (EELS) and Scanning Transmission Electron Microscopy (STEM). Specimen preparation techniques.

(10-12 Lectures)

**Unit V**

**X-ray Diffraction:** X-ray diffraction techniques, factors affecting diffracted intensity, application of X-ray diffraction to phase identification, order-disorder transformation, phase diagram evaluation and introduction to texture determination, dislocation density. Comparison of X-ray and neutron diffraction.

(10-12 Lectures)

**Recommended Books:**


1. Li, Lin, Ashok Kumar Materials Characterization Techniques Sam Zhang; CRC Press, (2008).
2. Cullity, B.D., and Stock, R.S., "Elements of X-Ray Diffraction", Prentice-Hall, (2001).
3. D.B. Williams and C.B. Carter, Transmission Electron Microscopy, V ol 1-4, Plenum Press.
7. W. Zhou and Z. Lin W ang, Scanning Microscopy for Nanotechnology Techniques and Applications, Springer.
8. J.I. Goldstein, D.E. Newbury, P. Echlin, D.C. Joy, C.E. Lyman, E. Lifshin, L. Sawyer, J.R. Michael, Kluwer Scanning Electron Microscopy and X-Ray Microanalysis, Academic/Plenum.

# SEMESTER-III

## BCY651: Physical Chemistry-III

L T P C
3 0 3 4

**Unit I**

**Electrode Kinetics:**

Multistep reactions- a near equilibrium relation between current density and over potential, Concept of rate determining step, Determination of reaction order, stochiometric number, and transfer coefficient. Electrocatalysis-comparison of electrocatalytic activity. Importance of hydrogen evolution reaction and its mechanism.

(6-8 lectures)

**Unit II**

**Statistical thermodynamics-II**

Distribution Law (Barometric formula), Sedimentation equilibrium, Maxwell's law of distribution of velocity and energy, Maxwell's law and Gaussian density function, R, M,S, Mean and most probable velocities, Collision frequency, Collision between like and unlike molecules, Triple collision.

(6-8 lectures)

**Unit III**

**Atomic structure:**

Many electron wave functions. Pauli Exclusion Principle. Helium atom. Atomic term symbols. The self-consistent field method. Slater-type orbitals.

(4-6 lectures)

**Unit IV**

**Group Theory:**

The Great Orthogonality theorem, construction of character tables. Symmetry adapted atomic basis sets. Construction of molecular orbitals. The direct product representation.

(5-6 lectures)

**Unit V**

**Molecular Structure:** Born-Oppenheimer approximation. Molecular orbital treatment for $H_2^+$. MO treatment of homo- and hetero nuclear diatomic molecules. Hückel MO treatment of simple and conjugated polyenes. Alternant hydrocarbons.

(5-6 lectures)

**Books Recommended**


1. Physical Chemistry, P. W. Atkins, 7th& 8thEditions, Oxford University Press, New York.
2. Physical Chemistry: A Molecular Approach, D.A. Mc Quarrie And J.D. Simon, (1998) Viva Books, New Delhi.
3. Valence Theory, J.N. Murrell, S.F.A. Kettle And J. M. Tedder, 2nd Edition (1965), John Viley, New York.
4. Physical Chemistry by Puri, Sharma & Pathania, Vishal Publishing Company, Jalandhar.


**List of Experiments:**



Shaili Pal

1. Verify Beer's Law and apply it to find the concentration of the given unknown solution.
2. Determination of solubility and solubility product of sparingly soluble salts ($PbSO_4$, $BaSO_4$) conductometrically, Potentiometry, pHmetry:
3. Kinetics analysis of Ru(III) catalysed oxidation of alcohols/diols by Ce(IV) sulphate in acidic medium.
4. Kinetics of oxidation of aliphatic/cyclic alcohols/glycols by alkaline hexacyanoferrate(III) catalyzed by ruthenium (III) chloride.
5. Determination of $R_f$ value of Methyl Orange and Phenolphthalein using paper/ thin layer chromatography.

## BCY653: Organic Chemistry-III

**L T P C**
**3 0 3 4**

**Unit I**

**Photochemistry:**

Photophysical processes: Jablonskii diagram, energy pooling, exciplexes, excimers, photosensitization, quantum yield, solvent effects, Stern-Volmer plot, delayed fluorescence, etc. Photochemistry of alkenes: cis-trans isomerization, non-vertical energy transfer; photochemical additions; reactions of 1,3-, 1,4- and 1,5-dienes; dimerizations. Photochemistry of carbonyl compounds: Norrish type I & II reactions (cyclic and acyclic); α,β-unsaturated ketones; β,γ-unsaturated ketones; cyclohexenones (conjugated); cyclohexadienones (cross-conjugated & conjugated); Paterno–Buchi reactions; photoreductions. Photochemistry of aromatic compounds: Isomerizations, skeletal isomerizations, Dewar and prismanes in isomerization. Singlet oxygen reactions; Photo Fries rearrangement of ethers and anilides; Barton reaction, Hoffman-Loefller-Freytag reaction.

(8-10 lectures)

**Unit II**

**Rearrangement Reactions:**

Migration to electron deficient carbon atom: Pinacole- Pinacolane rearrangement, Wagner- Meerwein rearrangement, Triffeneau- Demjanov ring expantion, Dienone- Phenol rearrangement, Benzil Benzillic acid rearrangement, Favorski rearrangement.

(6-8lectures)

**Unit III**

**Migration to Electron Deficient Nitrogen Atom:** Wolf, Hoffmann, Curtius, Losen, Schmidt, Beckmann Rearrangement.; Migration to Electron Deficient Oxygen Atom: Bayer-Villiger Rearrangement

(6-8 lectures)

***Unit IV***

***Bio-polymers:***

*Polysaccharides-starch, sucrose, cellulose, Chitin and Chitosan, amino acids and polypeptides, proteins.*

(6-8 lectures)

***Unit V***

***Reagents and Organic Synthesis:***

Shaili Pal 20 Verma

(i) Gilman reagent-Lithium dimethylcuprate, (ii)Lithium diisopropylamide (LDA), (iii) Dicyclohexyl carbodimide (DCC), (iv) 1,3-Dithiane (Umplong reagent), (v) Peterson Synthesis, (vi) Bakers yeast, (vii) Palladium catalysed reactions, (viii) Woodward and Prevost hydroxylation, (ix) Iodotrimethyl silane and (x) Ionic Liquids.

(7-10 lectures)

**Books Recommended**


1. Yescombe, Sources of information on rubber, plastic and allied industries, Press, 1968.
2. Peter Bernfeld,Biogenesis of Natural compounds,2nd edition, Pergamon press,1967.
3. J. Clayden, N. Greeves, S. Warren and P. Wothers, Organic chemistry, Oxford University press INC, New York, 2001
4. Harry R. Allcock, Frederick W. Lampe and James E. Mark, Contemporary Polymer Chemistry,3rd edition, Pearson Prentice Hall,2005


**List of Experiments:**

1. Chromatographic Separation
   a. Paper Chromatography: identification of alpha amino acids.
   b. Column Chromatography: separation of mixture of ortho and para- Nitroanilines.
   c. Thin Layer Chromatography: separation of mixture of ortho and para- Nitroanilines.
2. Preparation and Characterization of two steps organic compounds.
3. Preparation and Characterization of three steps organic compounds.
4. Synthesis of azo-dye and find its $\lambda_{max}$ by UV-Visible spectrophotometric method.
5. To prepare Glucosazone, $C_6H_{10}O_4(N.NHC_6H_5)_2$ .

**BCY655: Bio-inorganic Chemistry**

**L T P C**
**3 1 0 4**

**Unit I**

**Role of Metal Ions in Biological Systems:** Basics of chemical biology, Photosystems; nitrogen fixation, $Na^+/ K^+$ pump. Transition elements in Biology – their occurrence and function, active site structure and function of metalloproteins and metalloenzymes. $O_2$ binding properties of heme (hemoglobin and myoglobin) and non-heme proteins (hemocyanin & hemerythrin) their coordination, geometry and electronic structure.

(8-10 lectures)

**Unit II**

**Electron Transfer Proteins**: Active site structure and functions of ferredoxin, rubredoxin and cytochromes and their comparison. Vitamin $B_{12}$ and cytochrome $P_{450}$ and their mechanism of actions. Metals in medicine- therapeutic applications of cis-platin, radio-isotopes and MRI agents. Toxicity of metals, Cd, Hg and Cr toxic effects with specific examples.

(6-8 lectures)

**Unit III**

**Metallo-Enzymes**: **Mo-containing enzymes-** Nitrogenase; Xanthine Oxidase, sulphite, oxidase and nitrate reductase

(6-8 Lectures)

**Unit IV**

**Iron- Containing Enzymes-** Cytochrome-c-oxidase, catalases, peroxidases, cytochrome $P_{450}$.

(6-8 Lectures)

**Unit V**

**Copper-Containing enzymes-** Superoxide dismutase (SOD), Bovine Superoxide dismutase (BOD), ascorbic acid oxidase and Zinc containing enzymes.

(6-8 Lectures)

**Books Recommended**


1. Ivano Bertini, Harry B. Gray, Edward I. Stiefel, Joan Selverstone Valentine, Biological Inorganic Chemistry – Structure & Reactivity"
2. S. J. Lippard, The Inorganic Side of Chemical Biology, Nat. Chem. Biol., 2006, 2, 504-507.
3. Bioinorganic Chemistry by Eiichiro Ochiai, Elsevier, London, (2008).
6. Bioinorganic Chemistry by Asim K. Das, Books and Allied Pvt. Ltd., Kolkata, (2007).
7. S. J. Lippard and J. M. Berg, Principles of Bioinorganic Chemistry, University Science Books, (1994).
8. I. Bertini, H. B. Grey, S. J. Lippard and J. S. Valentine, Bioinorganic Chemistry, Viva Books Pvt. Ltd., New Delhi (1998).


**BCY 657: Internship**

**L T P C**
**0 0 4 2**

**BCY 661: Minor Project**

**L T P C**
**0 0 4 2**

**BCY 659: Elective-I**

**L T P C**
**3 1 0 4**

A. Supramolecular Chemistry

**L T P C**
**3 1 0 4**

**Unit I**

**Intermolecular interactions:**

Definition of supramolecular chemistry. Nature of binding interactions in supramolecular structures: ion-ion, Ion-dipole, dipole-dipole, H-bonding, cation-p, anion-p, p-p, and van der Waals interactions.

(6-8 lectures)

**Unit II**

**Synthesis of Suparamolecular Structures:**

Synthesis and structure of crown ethers, lariat ethers, podands, cryptands, spherands, calixarenes, cyclodextrins, cyclophanes, cryptophanes, carcerands and hemicarcerands., Host Guest interactions, preorganization and complimentarity, lock and key analogy. Binding of cationic, anionic, ion pair and neutral guest molecules Crystal engineering: role of H-bonding and other weak interactions

(8-10 lectures)

**Unit III**

**Triptycene**

Introduction, synthesis, properties and applications in Environmental and biomedical.

(4-6 lectures)

**Unit IV**

**Supramolecular Polymers:**

Self-assembly molecules: design, synthesis and properties of the molecules, self-assembling by H-bonding, metal-ligand interactions and other weak interactions, metallomacrocycles, catenanes, rotaxanes, helicates and knots. Examples of recent developments in supramolecular chemistry from current literature.

(6-8lectures)

**Unit V**

**Applications and Recent Developments**

Molecular devices: molecular electronic devices, molecular wires, molecular rectifiers, molecular switches, molecular logic. Relevance of supramolecular chemistry to mimic biological systems: cyclodextrins as enzyme mimics, ion channel mimics, supramolecular catalysis etc. Examples of recent developments in supramolecular chemistry from current literature

(8-10 lectures)

**Books Recommended:**


1. Jean-Marie Lehn, Supramolecular Chemistry, VCH, Weinheim (1995).
2. J. L. Serrano, Metallomesogens, VCH, Weinheim (1996).
3. Oliver Kahn, Molecular Magnetism, VCH, Weinheim (1993).
4. F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann, Advanced Inorganic Chemistry, 6th Edn., John Wiley & Sons (Asia), Singapore (2003).


## B. Natural Products and Medicinal Chemistry

**L T P C**

**3 1 0 4**

**Unit I**

**Alkaloids:**

Structure elucidation of alkaloids – a general account; Structure, synthesis, and stereochemistry of Narcotine and Quinine; synthesis and stereochemistry of Morphine, Lysergic acid and Reserpine. Terpenoids: Camphor, Longifolene*, Abietic acid, and Taxol.

(6-8 lectures)

**Unit II**

**Steroids:**

Cholesterol, Cortisone*, and Aldosterone*. Prostaglandins and Thromboxanes : Introduction, nomenclature of prostaglandins and thromboxanes; approaches to prostaglandin synthesis;

cyclohexane precurors (Woodward synthesis of PGF2a), bicycloheptane precursors (Corey's synthesis of prostaglandins E and F). Retrosynthetic Analysis of morphine and reserpine and Longifolene.

(8-10 lectures)

**Unit III**

**Structure and activity:**

Relationship between chemical structure and biological activity (SAR). Receptor Site Theory. Approaches to drug design. Introduction to combinatorial synthesis in drug discovery

**Porphyrins and vitamin $B_{12}$:** Structure elucidation and synthesis of haemin, chlorophyll-a and vitamin-$B_{12}$

(6-8 lectures)

**Unit IV**

**Drugs based on a substituted benzene ring:**

Chloramphenicol, salmeterol, tolazamide, diclophenac, tiapamil, intryptyline. Drugs based on five membered heterocycles : Tolmetin, spiralpril, oxaprozine, sulconazole, nizatidine, imolamine, isobuzole.

(6-8 lectures)

**Unit V**

**(a) Drugs based on six membered heterocycles** : Warfarin, quinine, norfloxacin and ciprofloxacin, methylclothiazide, citrine, terfenadine. Drugs based on seven membered heterocyclic rings fused to benzene: Chlordiazepoxide, diazepam, diltiazem.

**(b) Drugs based on heterocycles fused to two benzene rings:** Quinacrine, tacrine, β-Lactam antibiotics: Penicillin, cephalosporin. Drugs based on five membered heterocycles fused to six membered rings: Acyclovir, methotrexate.

(8-10 lectures)

* Synthesis only.

**Books Recommended:**


1. Nitya Anand, J.S. Bindra and S. Ranganathan, Art in Organic Synthesis, 2nd Edition (1970), Holden Day, San Francisco.
2. S.W. Pelletier, Chemistry of the Alkaloids, Van Nostrand Reinhold Co., New York (1970).
3. K.W. Bentley, The Alkaloids, Vol. I., Interscience Publishers, New York (1957).
4. I. L. Finar, Organic Chemistry, Vol. II, 5th Edition (1975) Reprinted in 1996, ELBS and Longman Ltd, New Delhi
5. J.W. Apsimon, Total Synthesis of Natural Products, Vol. 1-6, Wiley-Interscience Publications, New York.
6. J.S. Bindra and R. Bindra , Creativity in Organic Synthesis.
7. J.S. Bindra and R. Bindra, Prostaglandins Synthesis.
8. K. C. Nicolaou, Classics in Total Synthesis of Natural Products, Vol. I & II.
9. J. Clayden, N. Greeves, S. Warren, and P. Wothers, Organic Chemistry, Chapter 30, Oxford University Press, Oxford (2001).

## C: Materials Chemistry

L T P C
3 1 0 4

**Unit I**

**Synthetic Methods:**

High temperature methods; co-precipitation and precursor method, sol-gel method; combustion synthesis, intercalation/dc-intercalation reactions; High pressure synthesis-hydrothermal and template synthesis; chemical vapour deposition (CVD).

Synthesis of nanoparticle semiconductors, nanowires and nanorods; Synthesis, structures and properties of $C_{60}$ and related compounds; Synthesis, structures and applications of single walled (SWNTs), multi-walled (MWNTs) carbon nanotubes. Other synthetic methods of nanomaterials (micellar and template based methods).

(6-8 lectures)

**Unit II**

**Characterization Techniques:**

**HR-TEM, FE-SEM, Optical spectroscopy: Inductively coupled Plasma- mass spectroscopy (ICP-MS), ICP-AES (Atomic Emission Spectroscopy), ICP-OES (Optical Emission Spectroscopy).**

(6-8 lectures)

**Unit III**

**Electrical, Magnetic and Optical Properties:**

Electrical properties: Band theory of solids-metals and their properties; semiconductors - extrinsic and intrinsic, Hall effect; thermoelectric effects (Thomson, Peltier and Seebeck); insulators-dielectric, ferroelectric, pyroelectric and piezoelectric properties; ionic conductors. Magnetic properties: Cooperative magnetism: Dia-, para-, ferro-, ferri-, and antiferromagnetic types; soft and hard magnetic materials; magnetoresistance.

Optical properties: Construction and application of GaSe and ruby laser.

(6-8 lectures)

**Unit IV**

**Chemistry of Advanced Materials:**

Superconductors: Brief history of superconductors, Properties of superconductors-critical temperature, effect of magnetic field; BCS theory; Superconductivity in 1-2-3 materials. Applications of superconducting materials. Organic superconductors, Fullerenes and doped fullerenes as superconductors.Intercalation compounds of graphite, Polymer-clay nanocomposites, Carbon-Carbon and polymer composite. Surface modification of nanomaterials with specific example to metal and metal oxide nanoparticles and their application in drug delivery, sensors, biosensors, catalysis, and in energy sector.

(8-10 lectures)

**Unit V**

**Chemistry of Porous Materials**: Introduction, Synthesis of porous materials, metal organic frameworks (MOFs), covalent organic frameworks (COFs), porous organic polymers (POPs) and their applications in environmental $CO_2$ capture and conversion, energy and biomedical applications.

(6-8 lectures)



Shaili Pal

Sharma

**Recommended Books:**

1. West, A. R., Solid State Chemistry and its Application, Wiley India, New Delhi (2007).

2. Smart, L. E.; Moore, E. A., Solid State Chemistry: An Introduction, 4th Ed., CRC Press, New Delhi (2017).

2. Kakani, S. L.; Kakani, A., Material Science, 3rd Ed., New Age International Publishers, New Delhi (2016).

4. Skoog, D. A.; Holler, F. J.; Crouch, S. R., Principles of Instrumental Analysis, 6th Ed., Cengage Learning India, New Delhi (2014).

3. Willard, H. H.; Merritt, L. L.; Dean, J. A.; Settle, F. A., Instrumental Methods of Analysis, 7th Ed., CBS Publisher, New Delhi (2007).

6. Drago, R. S., Physical Methods for Chemists, 2nd Ed., Saunders College Publishing, Florida (1999).

4. Poole, C. P. Jr.; Owens, F. J., Introduction to Nanotechnology, Wiley India, New Delhi (2007).

5. Pradeep, T., Nano: The Essentials-Understanding Nanoscience & Nanotechnology, Tata McGraw Hill India, New Delhi (2017).

**Further Reading**

1. Rao, C. N. R.; Gopalakrishnan, J., New Direction in Solid State Chemistry, 2nd Ed., Cambridge University Press, Cambridge (1997).

2. Keer, H. V., Principles of the Solid State, 2nd Ed., New Age International Publishers, New Delhi (2017).

3. Braun, R. D.; Introduction to Instrumental Analysis, 2nd Ed., BSP Books, Hyderabad (2012).

4. Hornyak, G. L.; Tibbals, H. F.; Dutta, J.; Moore, J. J., Introduction to Nanoscience and Nanotechnology, CRC Press, Boca Raton (2008).

5. Viswanathan, B., Nanomaterials, Narosa Publishing House, New Delhi (2014).

# SEMESTER-IV

L T P C
3 0 3 4

**Unit I**

**Acid-Base Equilibria:**

General concept of acid-base equilibria in water and in non-aqueous solvent, Definition of pH and pH scale (Sorenson and operational definitions), and its significance, Hammett acidity function, pH calculation for aqueous solutions of very weak acid and very weak base, salts of weak acid and weak bases, mixture of weak acid and its salts, mixture of weak base and its salts, polybasic acids and their salts, polyamines and amino acid, composition of solution of polybasic acid as a function of pH, protolysis curves. Buffer Solutions: Theory of buffer solution, dilution and salts effects on the pH of a buffer, Buffer index, Criteria and expression of maximum buffer capacity, Application of pH buffers, Preparation of buffer solutions of known ionic strength (Typical examples). Practical limitations in use of buffers, Metal ion buffers and their applications, Biological buffers and their applications.

(8-10 lectures)

**Unit II**

**Photometric Titrations:**

Basic principles, comparison with other titrimetric procedures, types of photometric titration curves, Instrumentation (Titration cell, Detectors, choice of analytical wavelength). Quantitative applications, Typical examples of one component and multicomponent analyses

(6-8 lectures)

**Unit III**

**Chemical Sensors:**

Principles, types of chemical sensors based on the modes of transductions, Types of chemical sensor based on the chemically sensitive materials (solid electrolyte, gas, semiconductor), Humidity sensors, Biosensors, Electrochemical sensors (Potentiometric sensors, Ion-selective electrodes, Membrane electrodes, Amperometric sensors, Clark and Enzyme electrodes).

(6-8 lectures)

**Unit IV**

**(a) Nuclear Magnetic Resonance spectroscopy (NMR): PMR Spectroscopy:** Interpretation of spectra, chemical shift, shielding mechanism and anisotropic effects, chemical exchange and chemical shifts in chiral molecules. Spin-spin interactions, naming spin systems, magnitude of coupling constant: Geminal, vicinal and long range couplings. Second order spectrum and analysis of AB, AMX and ABX systems. Simplification of Complicated Spectra: Aromatic induced shifts spin decoupling, deuterium exchange, spectra at higher fields. Hindered rotation and rate processes. **CMR Spectroscopy:** General considerations, chemical shift, coupling constants. Nuclear Overhauser effect. Spin-spin, spin-lattice relaxations. Off resonance decoupling. DEPT. Interpretation of simple CMR spectra. 2D-NMR: COSY, NOESY and HETCOR

**(b) Electron Spin Resonance Spectroscopy**: Basic principle, Hyperfine Splitting (isotropic systems); the g-value and the factors affecting thereof; interactions affecting electron energies in paramagnetic complexes (Zero-field splitting and Kramer's degeneracy); Electron-electron interactions, Anisotropic effects (the g-value and the hyperfine couplings); Structural applications to transition metal complexes

(12-14 lectures)

**Unit V**

**(a) Mass Spectroscopy:**

Introduction, ion production, fragmentation, factors influencing ion abundance, single and multiple bond cleavage, rearrangements, cleavage associated with common functional groups, molecular ion peak, metastable ion peak, Nitrogen rule and interpretation of mass spectra

**(b) Mössbauer Spectroscopy:** Basic principle, conditions for Mossbauer spectroscopy, Spectral parameters (Isomer shift, electric quadrupole interactions, magnetic interactions), temperature dependent effects, structural deductions for iron and tin complexes, miscellaneous applications.

(6-8 lectures)

**Books Recommended:**


1. D.A. Skoog and D.M. West, Fundamental of Analytical Chemistry, International Edition, 7thEdition (1996), Saunders College Publishing, Philadelphia, Holt, London.
2. R.L. Pecsok, L.D. Shields, T. Cairns and L.C. McWilliam, Modern Methods of Chemical Analysis, 2nd (1976), John Wiley & Sons, New York.
3. D.A. Skoog, Principles of Instrumental Analysis, 5th Edition (1998), Saunders College of Publishing, Philadelphia, London.
4. H.A. Strobel, Chemical Instrumentation: A Schematic Approach, 2nd Edition (1973), Addison Wesley, Reading, Mass.


**List of Experiments:**

1. Synthesis of polyurethane.
2. Applications of NMR spectroscopy ($^{1}H$ & $^{13}C$), UV, IR and Mass Spectroscopy instructure determination of organic and biologically important compounds.
3. Adsorption of acetic acid on charcoal to verify Freundlich adsorption isotherm and Langmuir isotherm.
4. Determination of Biological Oxygen Demand (BOD) and Chemical Oxygen Demand (COD) in a waste water sample.
5. Synthesis and Characterization of nanoparticles (ZnO).

## BCY652: Energy and Environmental Sustainability

**L T P C**
**3 1 0 4**

**Unit I**

**Environmental Pollution:**

Sources, effects and control measures of air pollution, water pollution, soil pollution, marine pollution, noise pollution, thermal pollution and radioactive pollution. Solid waste management- causes, effects and control measures of urban and industrial wastes, E- waste- Sources and management, Biomedical waste-Sources and management. Role of individuals and authorities in pollution control.

(8-10 lectures)

**Unit II**

**Global Environmental Issues:**

Climate change, global warming, acid rain, ozone layer depletion, $CO_2$ capture and conversion

(8-10 lectures)

**Unit III**

**Sustainability and Environment:**

Sustainable development, water conservation, rainwater harvesting, watershed management, waste land reclamation, environmental impact assessment (EIA), Environmental auditing, environment protection acts, Air (Prevention and control of pollution) act and water (Prevention and control of pollution) act, Introduction to ISO 14000, carbon footprint, cleaner development mechanism (CDM), concept of 4R's, Environmental ethics.

(8-10lectures)

**Unit IV**

**Energy Management:**

Earth's global energy balance, energy budget – past and present, energy conservation, energy efficiency and sustainable energy systems.

(4-6 lectures)

**Unit V**

**Energy Technologies and Environment:**

Electrical energy and steam energy; Fossil fuels, hydropower and nuclear energy; Solar energy, wind energy and biofuels; Wave, ocean thermal, tidal energy and ocean currents; Geothermal energy; Future energy sources; Hydrogen fuels; DSSC; Sustainable energy.

(6-8 lectures)

**Books Recommended**


1. Ranjan Rakesh, Kothari D.P, Singal K.C, "Renewable Energy Sources and EmergingTechnologies",2nd Ed. Prentice Hall of India,2011
2. Roger A.Messenger, Jerry Ventre, "Photovoltaic System Engineering", 3rd Ed, 2010 5.James F.Manwell, Jon G.McGowan,
3. Anthony L Rogers, "Wind energy explained: Theory Design and Application", John Wiley and Sons 2nd Ed,2010.


**BCY 654: Elective-II**

**A. Green Chemistry**

**L T P C**
**3 1 0 4**

**Unit I**

**Introduction to Green Chemistry**

What is Green Chemistry? Need for Green Chemistry. Goals of Green Chemistry. Limitations/ Obstacles in the pursuit of the goals of Green Chemistry

(4-6 lectures)

**Unit II**

**Principles of Green Chemistry and Designing a Chemical synthesis:**

Twelve principles of Green Chemistry with Their Explanations; Designing a Green Synthesis using these principles; Prevention of Waste/ byproducts; maximum incorporation of the materials used in the process into the final products, Atom Economy, calculation of atom economy of the rearrangement, addition, substitution and elimination reactions. Prevention/ minimization of hazardous/ toxic products reducing toxicity risk, Green solvents, solventless processes. Energy requirements for reactions – alternative sources of energy; Selection of starting materials; avoidance of unnecessary derivatization; catalysis and green chemistry. Prevention of chemical accidents designing greener processes, minimization, simplification, substitution, moderation and limitation. Strengthening/ development of analytical techniques to prevent and minimize the generation of hazardous substances in chemical processes.

(12-16 lectures)

**Unit III**

**Examples of Green Synthesis/ Reactions and Some Real World Cases:**

(a). Green Synthesis of the following compounds: adipic acid, catechol, disodium iminodiacetate (alternative to Strecker synthesis) (b) Microwave assisted reactions in water (c) Ultrasound assisted reactions (d) Surfactants for Carbon Dioxide (e) Designing of Environmentally safe marine antifoulant. (f). An efficient, green synthesis of a compostable and widely applicable plastic (poly lactic acid) made from corn. (g). Healthier Fats and oil by Green Chemistry (h). Development of Fully Recyclable Carpet.

(8-10 lectures)

**Unit IV**

**Hydrogels:**

Introduction, Preparation and their applications.

(2-4 lectures)

**Unit V**

**Future Trends in Green Chemistry Oxidation Reagents and Catalysts:**

Biomimetic, multifunctional reagents; Combinatorial green chemistry; Proliferation of solventless reactions; co crystal controlled solid state synthesis ($C^2S^3$ ); Green chemistry in sustainable development.

(6-8 lectures)

**Books Recommended:**


1. Ahluwalia, V.K. and Kidwai, M.R. New Trends in Green Chemistry, Anamalaya Publishers, 2005
2. Anastas, P.T. and Warner, J.K. Oxford Green Chemistry -Theory and Practical, University Press, 1998
3. Matlack, A.S. Introduction to Green Chemistry, Marcel Dekker, 2001
4. Cann, M.C. and Connely, M.E. Real-World Cases in Green Chemistry, American Chemical Society, Washington, 2000
5. Ryan, M.A. and Tinnesand, M., Introduction to Green Chemistry, American Chemical Society Washington, 2002 Lancaster, Mike, Green Chemistry an Introductory Text 2nd Ed., RSC Publishing,.




Shaili Pal

## B. Solid State Chemistry

**L T P C**
**3 1 0 4**

**Unit I**

**Solid State Reactions:**

General Principles, Experimental procedure, Co-precipitation as precursor to solid-state reactions, Kinetics of solid-state reactions, Crystallization of solutions, melts, glasses and gels. Growth of single crystals: Czochralski, Bridgman and Stockbarger methods. Zone Melting.

(6-8 lectures)

**Unit II**

**X-ray Diffraction & Crystal Structure:**

Diffraction of X-rays by crystals: The Laue equations and Bragg's law, Definitions related to crystal structure, crystallographic direction and crystallographic phases. X-ray diffraction experiments: The powder method and the single crystal method. Reciprocal lattice. Structure factor and its relation to intensity and Electron density. The phase problem. Description of procedure for an X-ray structure analysis

(8-10 lectures)

**Unit III**

**Phase Transitions:**

Thermodynamic and Burger's classification of phase transition, Kinetics of phase transition-nucleation and growth, T-T-T diagrams, Factors influencing kinetics of phase transition, Martensitic and order-disorder transitions.

(6-8 lectures)

**Unit IV**

**Electronic Properties and Band Theory:**

Electronic structure of solids- band theory, Refinement of simple band theory- k-space and Brillouin Zones, Band structure of metals, insulators and semiconductors, Intrinsic and extrinsic semiconductors, Doped semiconductors, p-n junctions. Superconductors Meissner effects, Basic concepts of BCH theory, Josephson devices.

(8-10 lectures)

**Unit V**

**Magnetic Properties:**

Classification of solid materials: Quantum theory of paramagnetics. Cooperative phenomena. Magnetic domains. Hysteresis.

(4-6 lectures)

**Books Recommended:**


1. A.R. West, Solid State Chemistry and its Applications, John Wiley and Sons, Singapore (1984).
2. L.V. Azaroff, Introduction to Solids, Tata McGraw-Hill, New Delhi (1977).
3. L. Smart and E Moore, Solid State Chemistry, Chapman & Hall, Madras (1992).
4. H. V. Keer, Principles of Solid State, Wiley Eastern (1993)

## C. Nanomaterial chemistry

**L T P C**
**3 1 0 4**

### Unit I

**Classification and nomenclature of nanomaterials:** Nanosized metals and alloys, semiconductors, ceramics–a comparison with respective bulk materials, Organic semiconductors, carbon materials, quantum dots, quantum wells, quantum rods, quantum wires, quantum rings; bulk nanostructured, nanocomposites, nanomachines and Devices.

(6-8 lectures)

### Unit II

**Characteristics of Nanomaterials:** Nucleation and growth of nanosystems, selfassembly, functional nanomaterials and nanostructured thin films. Quantum confinement in semiconductors – particle in a box like model for quantum dots, origin of charge on colloidal sols, zeta potential, basics of thermodynamics and kinetics related to nanoparticles.

(6-8 lectures)

### Unit III

**Structure and Morphology of Nanoparticles:** Crystal structure of materials, packing fraction, basics of solid-state chemistry, specific surface energy and surface stress and effect on the lattice parameter. Nanoparticle morphology and morphology of supported particles. Metal nanocrystals by reduction, Solvothermal synthesis, Photochemical synthesis, Electrochemical synthesis, Nanocrystals of semiconductors and other materials by arrested precipitation, Thermolysis routes, Sonochemical routes, Post-synthetic size-selective processing. Sol-gel, Micelles and microemulsions. Characterization Techniques: X-ray diffraction, Scanning Probe Microscopy, SEM, TEM, Optical microscope and their description, operational principle and application for analysis of nanomaterials, UV-VIS-IR Spectrophotometers.

(10-12 lectures)

### Unit IV

**Novel Properties of Nanomaterials:** Size and shape dependent optical, emission, electronic, transport, photonic, refractive index, dielectric, mechanical, magnetic, non-linear optical properties; transition metal sols, origin of plasmon band, Mie theory, influence of various factors on the plasmon absorption, catalytic properties.

(6-8 lectures)

### Unit V

**Classifications and types of nanomaterials as nano particles and $^{1}D$ $^{2}D$ $^{3}D$ nanomaterials.** Concept of bulk versus nanomaterials and dependence of properties on size. Introduction to 'Top down' vs. 'Bottom up' approach of synthesis with suitable examples. Nano synthesis techniques based on liquid and vapor phase as the starting material. The study of wet chemical method like sol-gel method, hydrothermal, micro emulsion technique, chemical reduction, decomposition of organometallic precursors and chemical vapor deposition, metallo-organic chemical vapor deposition. Cryochemical synthesis, study of rapid solidification route, electro and electroless deposition etc. along with suitable examples

(10-12 lectures)



Shaili Pal

Verma

**Recommended Books**

1. Klabunde, K.J. (Ed.), "Nanoscale Materials in Chemistry", John Wiley & Sons Inc. 2001
2. Nalwa, H.S. (Ed.), "Encyclopedia of Nanoscience and Nanotechnology" 2004
3. Sergeev, G.B. Nanochemistry, Elsevier, B.V. 2010
4. Schmid, G. (Ed.), "Nanoparticles", Wiley-VCH Verlag GmbH & Co. KgaA.2004
5. Rao, C.N.R., Müller, A. and Cheentham, A.K. (Eds.),"Chemistry of Nanomaterials", Wiley – VCH. 2005.
6. Nanostructures and Nanomaterials, synthesis, properties and applications by Guozhong Cao, Imperial College Press, 2004.
7. Nanoscale materials in chemistry by Kenneth J. Klabunde, Wiley Interscience Publications,2001.

## D. Polymer chemistry

**L T P C**
**3 1 0 4**

### UNIT I

**Introduction**

Historical background, types, classification and importance of polymers, chemical and geometrical structure, physical state and thermal transition: crystalline melting temperature, Tm and glass transition temperature, Tg. Properties of polymers: thermal, mechanical, rheological and electrical properties. Applications and future trends of polymers

(6-8 lectures)

### UNIT II

**Polymerization Processes**

Step polymerization, chain polymerization including carbonyl polymerization, ionic polymerization, co-ordination polymerization, atom transfer free radical polymerization, supramolecular polymerization, ring opening polymerization, metathesis polymerization, group transfer polymerization; emulsion polymerization, step-growth copolymerization. Reactivity ratio and control of molecular weight in polymerization.

(8-10 lectures)

### UNIT III

**Polymer Characterization**

Average molecular weight concept, Number average, weight average, viscosity average molecular weights. Polydipersity and molecular weight distribution. The practical significance of molecular weight. Measurement of molecular weights. End group analysis, viscosity, light scattering, osmotic and ultrantracentrifugation methods, fractionation of polymers, Gel permeation chromatography (GPC). Chemical analysis of polymers: Spectroscopic methods, X-ray diffraction study, microscopy, thermal analysis.

(8-10 lectures)

### UNIT IV

**Thermodynamics of Polymer Solutions**

Shaili Pal

Chain conformation, kinetic chain length; molecular dimensions in solution, solubility of polymers, solubility parameters, transfer process, lattice theory, thermodynamics of polymer dissolution; $\Delta H$, $\Delta S$ and $\Delta G$ of mixing; Flory–Huggins theory.

(6-8 lectures)

**Recommended Books**


1. Sun, S. F., Physical Chemistry of Macromolecules: Basic Principles and Issues, 2nd Ed., Wiley-Blackwell, New York (2004).
2. Odian, G., Principle of Polymerization, 4th Ed., Wiley-Blackwell, New York (2004).
3. Flory, P. J., Principles of Polymer Chemistry, Asian Books, New Delhi (2006).
4. Gowariker, V. R.; Viswanathan, N. V.; Sreedhar, J., Polymer Science, New Age International Publishers, New Delhi (2011).


BCY656: Capstone Project

| L | T | P | C |
|---|---|---|---|
| 0 | 0 | 16 | 8 |

## MASTER OF SCIENCE IN CHEMICAL SCIENCES

## SEMESTER WISE COURSE STRUCTURE & EVALUATION SCHEME

### SEMESTER I

| S. No. | Course Type | Subject Code | Course title | Credits | L T P | Sessional Marks | | | | ESM | Total Marks |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | MSE | TA | Lab | Total | | |
| 1 | PCC | BCY 551 | Inorganic Chemistry I | 4 | 3 0 3 | 15 | 20 | 15 | 50 | 50 | 100 |
| 2 | PCC | BCY 553 | Physical Chemistry I | 4 | 3 0 3 | 15 | 20 | 15 | 50 | 50 | 100 |
| 3 | PCC | BCY 555 | Organic Chemistry I | 4 | 3 0 3 | 15 | 20 | 15 | 50 | 50 | 100 |
| 4 | PCC | BCY 557 | Analytical Chemistry I | 4 | 3 0 3 | 15 | 20 | 15 | 50 | 50 | 100 |
| 5 | ESC | BCY 559 | Waste Management Technology | 4 | 3 1 0 | 30 | 20 | | 50 | 50 | 100 |
| Total Credits | | | | | | 20 | | | | | |

### SEMESTER- II

| S. No. | Course Type | Subject Code | Course title | Credits | L T P | Sessional Marks | | | | ESM | Total Marks |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | MSE | TA | Lab | Total | | |
| 1 | PCC | BCY 550 | Inorganic Chemistry II | 4 | 3 0 3 | 15 | 20 | 15 | 50 | 50 | 100 |
| 2 | PCC | BCY 552 | Physical Chemistry II | 4 | 3 0 3 | 15 | 20 | 15 | 50 | 50 | 100 |
| 3 | ESC | BCY 558 | Material Characterization Techniques | 4 | 3 1 0 | 30 | 20 | | 50 | 50 | 100 |
| 4 | PCC | BCY 554 | Organic Chemistry II | 4 | 3 0 3 | 15 | 20 | 15 | 50 | 50 | 100 |
| 5 | PCC | BCY 556 | Analytical Chemistry II | 4 | 3 0 3 | 15 | 20 | 15 | 50 | 50 | 100 |
| Total Credits | | | | | | 20 | | | | | |

## SEMESTER- III

| S. No. | Course Type | Subject Code | Course title | Credits | L T P | Sessional Marks | | | | ESM | Total Marks |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | MSE | TA | Lab | Total | | |
| 1 | PCC | BCY 651 | Physical Chemistry III | 4 | 3 0 3 | 15 | 20 | 15 | 50 | 50 | 100 |
| 2 | PCC | BCY 653 | Organic Chemistry III | 4 | 3 0 3 | 15 | 20 | 15 | 50 | 50 | 100 |
| 3 | ESC | BCY 655 | Bioinorganic Chemistry | 4 | 3 1 0 | 30 | 20 | | 50 | 50 | 100 |
| 4 | ISC | BCY 657 | Internship | 2 | 0 0 4 | | 50 | | 50 | 50 | 100 |
| 5 | PEC | BCY 659 | Elective-1 | 4 | 3 1 0 | 30 | 20 | | 50 | 50 | 100 |
| 6 | PCC | BCY 661 | Minor Project | 2 | 0 0 4 | | 50 | | 50 | 50 | 100 |
| Total Credits | | | | | 20 | | | | | | |

## SEMESTER- IV

| S. No. | Course Type | Subject Code | Course title | Credits | L T P | Sessional Marks | | | | ESM | Total Marks |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | MSE | TA | Lab | Total | | |
| 1 | PCC | BCY 650 | Analytical Chemistry III | 4 | 3 0 3 | 15 | 20 | 15 | 50 | 50 | 100 |
| 2 | ESC | BCY 652 | Energy and Environmental Sustainability | 4 | 3 1 0 | 30 | 20 | | 50 | 50 | 100 |
| 3 | PEC | BCY 654 | Elective-II | 4 | 3 1 0 | 30 | 20 | | 50 | 50 | 100 |
| 4 | PCC | BCY 656 | Capstone Project | 8 | 0 0 16 | | 50 | | 50 | 50 | 100 |
| Total Credits | | | | | 20 | | | | | | |



Shaibi Pal

Verma