Department of Chemistry

Course Structure

M.Sc. Chemistry (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 659/663/665	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	Molecular Spectroscopy	BCY650	3 0 3	4
2	ESC	Energy and Environmental Sustainability	BCY652	3 1 0	4
3	PEC	Elective II	BCY 654/658/660/662	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**

List of Elective Papers

Elective –I

S. No.	Name of Elective Paper	Elective Paper Code	Credits (L T P C)
1.	Materials Chemistry	BCY-659	3 1 0 4
2.	Supramolecular Chemistry	BCY-663	3 1 0 4
3.	Natural Product and Medicinal Chemistry	BCY-665	3 1 0 4

Elective –II

S. No.	Name of Elective Paper	Elective Paper Code	Credits (L T P C)
1.	Polymer Chemistry	BCY-654	3 1 0 4
2.	Green Chemistry	BCY-658	3 1 0 4
3.	Solid State Chemistry	BCY-660	3 1 0 4
4.	Nanomaterial Chemistry	BCY-662	3 1 0 4

SEMESTER-I

BCY551: Inorganic Chemistry-I

L T P C
3 0 3 4

Unit I- Metal-Ligand Bonding in Transition Metal Complexes:
VSEPR theory & drawbacks; Crystal field Theory; Spectrochemical series; Structural effects: ionic radii and Jahn-Teller effect and it's application; ligand field theory, molecular orbital theory as applied to metal complexes; nephelauxetic effect; experimental evidence for metal-ligand orbital overlap; site selection in spinels.

(6-8 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; Term symbols for metal ions; Orgel energy level and Tanabe-Sugano diagrams for complexes; Charge transfer spectra; electronic spectra of octahedral and tetrahedral complexes; and calculation of ligand-field parameters (Dq, B and β values).

(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.

(6-8 lectures)

Unit V- Cluster Compounds:
Introduction, clusters in elemental states, cluster classification, higher boron hydrides-structures and reactions, Lipscomb topological diagrams and STYX rules, Wade's rule, carboranes, metalloboranes and heteroboranes, metallocarboranes, zintl ions, chevral compounds.

(4-6 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.
5. K. Veera Reddy, *Symmetry and Spectroscopy of Molecules*, New Age International Pvt. Ltd., New Delhi (1999).
6. B.N. Figgis, *Introduction to Ligand Fields,* Wiley Eastern Ltd. New Delhi (1976).
7. M. N. Hughes, Inorganic Chemistry of Biological Processes, 2nd Ed.(1981), John-Wiley & Sons, New York.
8. W. Kaim and B. Schwederski, Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life, an introduction and Guide, Wiley, New York (1995).

9. S. J. Lippard and J. M. Berg, Principles of Bioinorganic Chemistry, University Science Books, (1994).
10. I. Bertini, H. B. Grey, S. J. Lippard and J. S. Valentine, Bioinorganic Chemistry, Viva Books Pvt. Ltd., New Delhi (1998).

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(II) sulfate.
6. Preparation of Mohr's salt.
7. Preparation of chrome alum, $K_2SO_4.Cr_2(SO_4)_3.24H_2O$.

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, 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.

(4-6 lectures)

Unit IV

Quantum Chemistry:

Review of essential mathematical concepts, 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.

(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. Study of kinetics of decomposition of sodium thiosulphate by mineral acids.
2. 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 equivalent conductance of a strong electrolyte at several concentrations at a given temperature.

NCY555: Organic Chemistry-I

L T P C
3 0 3 4

Unit I

Aromaticity:

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

(5-6 lectures)

Unit II

Stereochemistry:

Elements of symmetry, chirality, molecules with more than one chiral center, 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 centers and chiral molecules.

(8-10 lectures)

Unit III

Reaction Intermediates:

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

(6-8 lectures)

Unit IV

Nucleophilic Substitution at Saturated Carbon:

Mechanism and Stereochemistry of S_N1, S_N2, and S_Ni reactions. The reactivity effects of substrate structure, solvent effects.

Nucleophilic Aromatic substitution: The Aromatic S_N1 and S_N2, benzyne mechanisms. Reactivity–effect of substrate structure, leaving group, and attacking nucleophile. Von-Richter reaction, Sommelet Hauser rearrangement, Smiles rearrangement etc.

(8-10 lectures)

Unit V

Neighbouring Group Participation:

Evidences of Neighbouring Group Participation; the phenonium ion, participation by π and σ bonds, Anchimeric assistance. Classical versus non-classical carbonium ions–the present status.

(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
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 organization, 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 equipment.

(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

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. To determine the strength of given alkali mixture (NaOH & Na_2CO_3) by titrating it against standard HCl solution using phenolphthalein and methyl orange as an indicator.
3. To determine the strength of given alkali mixture ($NaHCO_3$ & Na_2CO_3) by titrating it against standard HCl solution using phenolphthalein and methyl orange as an indicator.
4. Determination of hardness of water using EDTA.
5. Determination of % of Chlorine in Bleaching powder.
6. Determination of FAS potentiometrically with standard ceric sulphate solution (Direct and black titration).
7. 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.

SEMESTER-II

BCY550: Inorganic Chemistry-II

L T P C
3 0 3 4

Unit I

Reaction Mechanism in Transition Metal Complexes:

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

(8-10 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 carbonyls, nitrosyls and related pi-acids, alkyl, alkene, alkyne, π-allyl, polyene and cyclopolyene compounds; isolobal analogy, Dewar-Chatt model, oxophilicity,

(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, activation of C-H bond. Metal hydrides (Classical and Non-classical). Agostic interaction. Application of NMR in studying hydrido complexes.

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, Universities Press (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).

List of Experiments:

1. Qualitative Mixture analysis of inorganic mixture. Containing one or two the less common metals: Tl, Mo, W, Zr, Th, V and 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 (III) tihydrate $K_3[Cr(C_2O_4)_3].3H_2O$.
6. Preparation of copper thiourea complex.
7. Preparation of teraammine copper (II)sulphate hydrate.

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, Photoluminescence and Photostationary state, Photosensitization, Rice-Herzfeld mechanisms, photochemical chain reactions (hydrogen and chlorine, hydrogen and bromine).

(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.

(8-10 lectures)

Unit III

Polymer:

Step polymerization, Kinetics of Step-Polymerization, Molecular mass – number and mass average molecular mass, determination of molecular mass by Osmometric, viscosity, light scattering.

(4-6 lectures)

Unit IV

Solid State

Crystal structures, Symmetry, Bonding in solids, Miller indices, Bragg's equation, X-ray analysis of NaCl, Defects in crystal system.

(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 non-ideal 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 dissociation constant k for a weak acid using conductometry.
5. Determination of viscosity average molecular weight of given polymer.

BCY 558: Material Characterization Techniques

L T P C
3 1 0 4

Unit I

Introduction: Need of materials characterization and available techniques.

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

(4-6 Lectures)

Unit II

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

(4-6 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 Tunnelling Microscopy (STM) & Atom Force Microscopy (AFM). Applications, EDAX.

(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.

(8-10 Lectures)

Unit V

X-ray Diffraction: X-ray diffraction techniques, Theory, Instrumentation and applications of X-rays, factors affecting diffracted intensity, application of X-ray diffraction to phase identification, order-disorder transformation, phase diagram evaluation and dislocation density. Comparison of X-ray and neutron diffraction.

(8-10 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.

NCY554 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, [4n], [4n+2] systems, [2+2] addition of ketenes, 1,3-dipolar cycloadditions and cheleotropic reactions. Sigmatropic rearrangement.

Conservation of Orbital Symmetry in Pericyclic Reactions

Woodward-Hoffmann rules; cycloaddition [2+2] and [4+2] and electrocylic reactions. Ene reactions and Cheletropic reactions;

(12-14 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. Vilsmeier-Haak reaction, Bischler-Napierski reaction, Fries rearrangement, photo fries rearrangement, Hoesch reaction.

(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.
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 polarography, principle, Half wave potential and its significance, 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

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, 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, Practical limitations in use of buffers, Biological buffers and their applications.

(6-8 lectures)

Unit III

Photometric Titrations:

Basic principles, comparison with other titrimetric procedures, types of photometric titration curves, instrumentation (Titration cell, Detectors, choice of analytical wavelength). Quantitative applications.

(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

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.

(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.
6. Paper and column chromatography of plant pigments.
7. Conductometric titrations and determination of dissociation constant.

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, stoichiometric 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.

(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:

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 (PbSO4, BaSO4) conductometrically, Potentiometry, pHmetry.

3. Kinetics analysis of Ru(III) catalyzed 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.

NCY653: Organic Chemistry-III

L T P C
3 0 3 4

Unit I

Photochemistry:

Photophysical processes: Jablonskii diagram, photosensitization, quantum yield etc. Photochemistry of alkenes: cis-trans isomerization, 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; 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

Heterocyclic compounds

Introduction, Synthesis and reactivity of common heterocyclic compounds containing one or two heteroatoms (O, N and S).

(6-8 lectures)

Unit V

Reagents and Organic Synthesis:

(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 λ_{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. Transition elements in Biology – their occurrence and function, active site structure and function of metalloproteins. 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 Iron- Sulphur proteins and copper containing proteins. Vitamin B_{12} and cytochromes and their mechanism of actions.

(6-8 lectures)

Unit III

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

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

(6-8 Lectures)

Unit IV

(a) Iron- Containing Enzymes: Cytochrome-c-oxidase, catalases, peroxidases, cytochrome P_{450}.

(b) Iron storage and transport proteins: Ferritin and Transferritin.

(6-8 Lectures)

Unit V

Metals in medicine-therapeutic applications of cis-platin, radio-isotopes and MRI agents. Toxicity of metals, Cd, Hg, Pb and As toxic effects with specific examples. Na^+/ K^+ pump and Deficiency symptoms of some trace metals (Zn, Cu, Co and Fe).

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).
4. Bioinorganic Chemistry by Asim K. Das, Books and Allied Pvt. Ltd., Kolkata, (2007).
5. S. J. Lippard and J. M. Berg, Principles of Bioinorganic Chemistry, University Science Books, (1994).
6. I. Bertini, H. B. Grey, S. J. Lippard and J. S. Valentine, Bioinorganic Chemistry, Viva Books Pvt. Ltd., New Delhi (1998).

NCY 657: Internship

L T P C
0 0 4 2

NCY 661: Minor Project

L T P C
0 0 4 2

ELECTIVE-I

BCY659: Materials Chemistry

L T P C
3 1 0 4

Unit I: Introduction and Synthetic Methods:

Historical Perspective; Importance of Materials, Materials for Future; Classification of Materials; Structures of Materials.

Methods: Co-precipitation Method; Precursor Method; Reduction Method; Spray Drying Method; Sol-gel Method; Hydrothermal Method; Chemical vapour deposition (CVD).

(6-8 lectures)

Unit II: Nanomaterials

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.

(6-8 lectures)

Unit III: Material Characterization Techniques

Crystallinity analysis by Powder X-ray Diffraction (PXRD). Thermal Analysis, Surface morphology analyzed by TEM, SEM and AFM; Qualitative and quantitative analysis by Energy Dispersive Analysis of X-rays (EDAX).

Material properties analyzed by inductively coupled Plasma - mass spectrometry (ICP-MS), ICP-AES (Atomic Emission Spectroscopy) and ICP-OES (Optical Emission Spectroscopy),

(6-8 lectures)

Unit IV: Material 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. Types of Magnetic Properties; soft and hard magnetic materials; magnetoresistance. Instrumentation, working and applications of laser.

(6-8 lectures)

Unit V: 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, Fullerenes and doped fullerenes as superconductors. Intercalation compounds of graphite, Polymer-clay nanocomposites, Carbon and polymer composite, Application of advanced materials in drug delivery and sensors.

(6-8 lectures)

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).
3. 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).
5. 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).
7. Poole, C. P. Jr.; Owens, F. J., *Introduction to Nanotechnology*, Wiley India, New Delhi (2007).
8. Pradeep, T., *Nano: The Essentials-Understanding Nanoscience & Nanotechnology*, Tata McGraw Hill India, New Delhi (2017).

BCY663: 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 Supramolecular Structures:

Synthesis and structure of crown ethers, lariat ethers, podands, cryptands, spherands, calixarenes, cyclodextrins, cyclophanes, cryptophanes, carcerands and hemicarcerands., Host Guest interactions,

preorganization and complementarity, 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 environment 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).

BCY665: 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 precursors (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).

SEMESTER-IV

BCY650: Molecular Spectroscopy

L T P C
3 0 3 4

Unit I

FT-IR and Raman Spectroscopy: Principle, Zero Point Energy, force constant, Selection rules, Modes of vibrations, Hot Bands, Fundamental Bands, Overtones, Factors influencing the band position and intensities, Characteristic vibrational frequencies of different compounds, effect of Hydrogen Bonding on vibrational frequencies.

Introduction theory of Raman spectroscopy, mechanism of Raman and Rayleigh scattering. Rule of Mutual Exclusion, correlation with the molecular structure, Resonance Raman effect, Application of Raman Spectroscopy.

(8-10 lectures)

Unit II

Electronic and Atomic Spectroscopy: UV-visible, Molecular luminescence spectroscopy (fluorescence, phosphorescence, chemiluminescence), X-ray PES. Atomic Absorption Spectroscopy, Atomic Fluorescence Spectroscopy, Atomic Emission Spectroscopy

(6-8 lectures)

Unit III

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

(6-8 lectures)

Unit IV

Nuclear Magnetic Resonance spectroscopy (NMR): **PMR Spectroscopy:** Introduction, basic principles, chemical shift, band multiplets, spin-spin splitting, Factor affecting chemical shift, shielding and deshielding effect, magnitude of coupling constant (J): Geminal, vicinal and long range couplings, Application in elucidation of molecular structure, deuterium exchange, Nuclear Overhauser effect.

CMR Spectroscopy: Basic Principle, chemical shift, coupling constants. Type of ^{13}C, Off resonance decoupling. DEPT, Interpretation of simple CMR spectra. 2D-NMR: COSY, NOESY and HETCOR, Elementary idea of ^{19}F NMR, ^{31}P NMR Spectroscopy.

(10-12 lectures)

Unit V

(a) **Mass Spectrometry**:

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, McLafferty rearrangement 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. Modern Spectroscopy, J. M. Hollas, 4th edition (2004), John Wiley & Sons, Ltd., Chichester.
2. Principle of Fluorescence Spectroscopy, L. R. Lakowicz, 3rd Edition, Springer.
3. Introduction to Molecular Spectroscopy, G. M. Barrow, (1962) McGraw-Hill.

4. Fundamentals of Molecular Spectroscopy, C. N. Banwell and E.M. Mc Cash, 4th edition, (1994), Tata McGraw Hill, New Delhi.
5. Nuclear Magnetic Resonance Spectroscopy, R. K. Harris, (1986), Addison Wesley, Longman Ltd, London
6. Introduction to Magnetic Resonance A. Carrington and A. D. Mc Lachlan, (1979), Chapman and Hall, London.

List of Experiments:

1. Synthesis of polyurethane.
2. Synthesis of Water Soluble Polymer.
3. Calculate the concentration of a dilute aqueous solute using absorbance spectroscopy.
4. Create a standard Beer's Law plot and use it to calculate the concentration of an unknown.
5. Structure determination of organic compound by FTIR analysis.

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. Industrial waste water, its contamination and treatment, 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

Environment protection Law:

Environment protection acts 1986, Aims and objectives of environmental impact assessment (EIA), Environmental auditing, Air and water act (Prevention and control of pollution), Introduction to ISO 14000, carbon footprint, Kyoto Protocol, National Environmental Policy 2006.

(8-10 lectures)

Unit IV

Environmental Sustainability and Energy Management:

Sustainable development, water conservation, rainwater harvesting, watershed management, waste land reclamation, concept of 4R's, Environmental ethics.

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; Sustainable energy; Solar energy, wind energy and biofuels; Ocean energy and current; Geothermal energy; Future energy sources; Hydrogen fuels; DSSC.

(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.

Elective-II

BCY654: 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.

(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.

(6-8 lectures)

UNIT III

Determination of molar masses of polymers

Average molecular weight concept, Number average, weight average, viscosity average molecular weights. Polydispersity and molecular weight distribution. The practical significance of molecular weight. Application of polymers in pharmaceutical, industrial and biomedical field.

(6-8 lectures)

UNIT IV

Polymer Characterization

Measurement of molecular weights. End group analysis, viscosity, light scattering, osmotic and ultracentrifugation methods, fractionation of polymers, Gel permeation chromatography (GPC). Chemical analysis of polymers: Spectroscopic methods, X-ray diffraction study, microscopy, thermal analysis etc.

(6-8 lectures)

UNIT V

Thermodynamics of Polymer Solutions

Chain conformation, kinetic chain length; molecular dimensions in solution, solubility of polymers, solubility parameters, transfer process, lattice theory, thermodynamics of polymer dissolution; ΔH, ΔS and ΔG 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).

BCY658: 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.

BCY660: 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 paramagnetic. 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).

BCY662: 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, self-assembly, 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)

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.

BCY656: Capstone Project

L	T	P	C
0	0	16	8

MASTER OF SCIENCE IN Chemistry (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 659/663/665	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	Molecular Spectroscopy	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 654/658/660/662	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**						

*****