NEHRU GRAM BHARATI VISHWAVIDYALAYA

KOTWA- JAMUNIPUR- DUBAWAL
ALLAHABAD (UTTAR PRADESH)

[w.e.f. Academic Session 2017-18 onwards]

SYLLABUS

For the

M.Sc. – Chemistry

(A Four Semester Course)

Based on

Choice Based Credit System (CBCS)

M.Sc. (Chemistry)
Course Structure (CBCS Pattern)

Department of Chemistry
NGB Vishwavidyalaya
Allahabad-221505

M.Sc. (Semester I and Semester II)
(Effective from 2017 onwards)

Semester I — Number of Credits = 18

Paper	Code	Type	Title	Credit	Marks
Paper I	MCH-401	Core 1	Inorganic Chemistry I	3	100 [80+20*]
Paper II	MCH-402	Core 2	Organic Chemistry I	3	100 [80+20*]
Paper III	MCH-403	Core 3	Physical Chemistry I	3	100 [80+20*]
Paper IV	MCH-404	Core 4	Quantum Chemistry	3	100 [80+20*]
Practical I	MCH-4L1	Lab 1	Inorganic Chemistry Laboratory	3 (6)	50**
Practical II	MCH-4L2	Lab 2	Organic Chemistry Laboratory	3	50**
			Total	18	500

* Sessional Exam
** Experimental = 30; Laboratory Record = 10; Viva-voce = 10
The experimental part shall contain any two exercise from the given list.

Semester II Number of Credits = 18

Paper	Code	Type	Title	Credit	Marks
Paper V	MCH-405	Core 5	Inorganic Chemistry II	3	100 [80+20*]
Paper VI	MCH-406	Core 6	Organic Chemistry II	3	100 [80+20*]
Paper VII	MCH-407	Core 7	Physical Chemistry II	3	100 [80+20*]
Paper VIII	MCH-408	Core 8	Introduction to Analytical Chemistry	3	100 [80+20*]
Practical III	MCH-4L3	Lab 3	Physical Chemistry Laboratory	3 (6)	50**
Practical IV	MCH-4L4	Lab 4	Analytical and Computational Chemistry Laboratory	3	50**
			Total	18	500

* Sessional Exam
** Experimental = 30; Laboratory Record = 10; Viva-voce = 10
The experimental part shall contain any two exercise from the given list.

M.Sc. (Semester III and Semester VI)
(Effective from 2017 onwards)

Semester III Number of Credits = 18

Paper	Code	Type	Title	Credit	Marks
Paper I	MCH-501	Core 9	Group theory and Molecular Spectroscopy	3	100 [80+20*]
Paper II	MCH-502	Core 10	Statistical Thermodynamics	3	100 [80+20*]
Paper III	MCH-503	Core 11	Spectroscopic Identification of Organic Compounds	3	100 [80+20*]
Paper IV	MCH-504	Core 12	Organic Reactions Mechanisms.	3	100 [80+20*]
Practical I	MCH-5L1	Lab 5	Synthetic Chemistry Laboratory	3	50**
Practical II	MCH-5L2	Lab 6	Spectroscopic Methods	3	50**
			Total	18	500

* Sessional Exam
** Experimental = 30; Laboratory Record = 10; Viva-voce = 10
The experimental part shall contain any two exercise from the given list.

Semester IV Number of Credits = 18

Paper	Code	Type	Title	Credit	Marks
Paper V	MCH-505	Elective 1		3	100 [80+20*]
Paper VI	MCH-506	Elective 2		3	100 [80+20*]
Paper VII	MCH-507	Elective 3		3	100 [80+20*]
Paper VIII	MCH-508	Core 13	Organic Photochemistry and Pericyclic Reactions	3	100 [80+20*]
Practical III	MCH-5L3	Lab 7	Extraction and Chromatography	3	50**
Practical IV	MCH-5L4	Lab 8	Project/Dissertation/ Seminar	3 (6)	50
			Total	18	500

* Sessional Exam
** Experimental = 30; Laboratory Record = 10; Viva-voce = 10
The experimental part shall contain any two exercise from the given list.

List of elective Papers:

1. Catalysis and Green Chemistry
2. Concepts in Organic Synthesis.
3. Electrochemistry.
4. Organometallic Chemistry of Transition Metals
5. Bioinorganic Chemistry.
6. Bioorganic and Medicinal Chemistry.
7. Nanochemistry.
8. Cheminformatics.
9. Analytical Chemistry.

Syllabus

M.Sc (Chemistry)

Semester I

Inorganic Chemistry I (MCH-401)

Unit I

Review of Bohr's theory, its limitations and atomic spectrum of hydrogen atom.

Wave mechanics: de Broglie equation, Heisenberg's Uncertainty Principle and its significance. Schrödinger's wave equation, significance of ψ and ψ^2. Quantum numbers and their significance. Normalized and orthogonal wave functions. Sign of wave functions. Radial and angular wave functions for hydrogen atom. Radial and angular distribution curves. Shapes of s, p, d and f orbitals. Pauli's Exclusion Principle, Hund's rule of maximum multiplicity, aufbau principle and its limitations.

Unit II

Bonding and structure: Types of bonds, orbital symmetry and overlaps, concept of MO and VB theory, concept of hybridization, bond energy and covalent radii, conceptof resonance, molecular dipole moment; polarizing power and polarizability,Fajan's rules.

Unit III

Inorganic Spectroscopy I: Number of microstates and term symbols for gaseous free atoms and ions. Spin-orbit coupling in free ion terms. Hunds rules. Splitting of spectroscopic terms of p^2 and d^2configurations.

Unit IV

Inorganic Spectroscopy II: Principles of Electronic Spectroscopy-Franck-Condon principle, selection rules, band intensities and vibronic coupling Band width. Different types of electronic transitions and molar absorption coefficient.

Unit V

Introduction to transition metal complexes: Brief review ofthe general characteristics of transition elements, types of ligands, nomenclatureof coordination complexes, chelates, chelate effect, geometry and isomerism, formation of complexes, stability constants, Werner, Sidzwickand VSEPR theory.

Books Suggested (Names of Publishers may vary as per copyright status):

1. Principles of Inorganic Chemistry, B.R.Puri, L.R. Sharma, K.C. Kalia, Milestone Publishers and Distributors/ Vishal Publishing Co.
2. Advanced Inorganic Chemistry, F.A. Cotton and Wilkinson, John Wiley.
3. Concise Inorganic Chemistry, J.D. Lee,Wiley.
4. Inorganic Chemistry, J.E. Huhey, Harpes& Row.
5. Chemistry of the Elements. N.N. Greenwood, A. Earnshow, Pergamon.
6. Inorganic Electronic Spectroscopy, A.B.P. Lever, Elsevier.
7. Comprehensive Coordination Chemistry eds., G. Wilkinson, R.D. Gillars and J.A. Mc Cleverty,Pergamon.

Organic Chemistry I(MCH-402)

Unit I

Principles of stereochemistry: Configurational and conformational isomerism in acyclic and cyclic compounds; stereogenicity, stereoselectivity, enantioselectivity, diastereoselectivity and asymmetric induction.

Unit II

Aromaticity: Benzenoid and non-benzenoid compounds – generation and reactions.

Unit III

Organic reactive intermediates; Generation, stability and reactivity of carbocations, carbanions, free radicals, carbenes, benzynes and nitrenes.

Unit IV

Aliphatic Nueleophilic Substitution:
The S_N2, S_N1, mixed S_N1 and S_N2 and SET mechanisms.
The neighboring group mechanism, neighboring group participation by p and s bonds, anchimeric assistance. Classical and nonclassicalcarbocations, phenonium ions, norbornyl system, common carbocation rearrangement. The S_Ni mechanism. Nucleophilic substitution at an allylic, aliphatic trigonal and vinylic carbon. Reactivity effects of substrate structure, attacking nucleophile, leaving group and reaction medium, phase transfer catalysis, ambident nucleophile and regioselectivity.

Unit V

Aliphatic Electrophilic Substitution
Bimolecular mechanisms, - S_E2 and S_E1. The S_E1 mechanism, electrophilic substitution accompanied by double bond shifts. Effect of substrates, leaving group and the solvent polarity on the reactivity.

Books Suggested(Names of Publishers may vary as per copyright status):

1. Advanced Organic Chemistry, Jagdamba Singh, PragatiPrakashan.
2. Organic Chemistry: Concepts and Applications, Jagdamba Singh, PragatiPrakashan.
3. Advanced Organic Chemistry-Reactions, Mechanism and Structure, Jerry March,John Wiley.
4. Advanced Organic Chemistry Part A: Structure and Mechanisms, Francis A.Carey,RichardJ.Sundberg, Springer.
5. A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, Longman.
6. Structure and Mechanism in Organic Chemistry, C.K. Ingold, Cornell UniversityPress.
7. Organic Chemistry, R.T. Morrison, R.N. Boyd, Prentice-Hall.
8. Reaction Mechanism in Organic Chemistry, S.M. Mukherji, S.P. Singh,Macmillan.
9. Stereochemistry of Organic Compounds, D.Nasipuri, New Age International.
10. Stereochemistry of Organic Compounds, P.S. Kalsi, New Age International.

Physical Chemistry I(MCH-403)

Unit I

Molecular Spectra: Basic concepts of molecular spectroscopy Classification of spectra. Characterization of electromagnetic radiations. Regions of the Spectrum.

Rotation Spectra: Rigid and non-rigid rotation spectra-selection rule Centrifugal distortion. Isotopic Shift. Spectra of polyatomic molecules. Rotational function. Experimental techniques. Vibration Rotation Spectra: Simple harmonic oscillator. Vibrational energy. Anharmonicity. Principle of vibration-rotation spectra. Selection rule. PQR branches. Vibration in polyatomic molecules. Effect of nuclear spin. Isotopic shift. Group frequency. Experimental techniques.

Unit II

Thermodynamics:

Brief resume of concepts of laws of thermodynamics, free energy, chemical potential and entropies. Partial molar free energy, partial molar volume and partial molar heat content and their significance. Determinations of these quantities. Concept of fugacity and determination of fugacity.

Unit III

Non-ideal systems: Excess functions for non-ideal solutions. Activity, activity coefficient, Debye Huckel theory for activity coefficient of electrolytic solutions; determination of activity and activity coefficients; ionic strength. Application of phase rule to three component systems; second order phase transitions.

Nernst heat theorem and its application to non-condensed systems. Statements of the third law of thermodynamics. Derivation of unattainability of absolute zero. The relationship between entropy constant and Nernst chemical constant. Applications of the third law.

Unit IV

Adsorption:

Surface tension, capillary action, pressure difference across curved surface (Laplace equation), vapour pressure of droplets (Kelvin equation), Gibbs adsorption isotherm, estimation of surface area (BET equation), Surface films on liquids (Electro-kinetic phenomenon).

Unit V

Micelles:

Surface active agents, classification of surface active agents, micellization, hydrophobic interaction, critical micellar concentration (CMC), factors affecting the CMC of surfactants, counter ion binding to micelles, thermodynamics of micellization-phase separation and mass action models, solublization, micro emulsion, reverse micelles.

Books Suggested(Names of Publishers may vary as per copyright status):

1. Physical Chemistry, P.W. Atkins, ELBS.
2. Physical Chemistry, Levine
3. Fundamental of Molecular Spectroscopy, C.N. Banwell.
4. Thermodynamics, Gurdeep Raj
5. Chemical Kinetics. K.J. Laidler, McGraw-Hill.
6. Physical Chemistry, G. W.Castellan.
7. Theory of Adsorption and Catalysis, A. Clark.
8. Micelles, Theoretical and Applied Aspects, V. MOraoi, Plenum.
9. Introduction to Polymer Science, V.R. Gowarikar, N.V. Vishwanathan, J.Sridhar, Wiley Eastern.

Quantum Chemistry(MCH-404)

Unit I

Origin of quantum theory. Black body radiation. Wien and Rayleigh Jeans laws. Planck's law and energy of harmonic oscillator.

Unit II

Concept of operators in quantum mechanics- operators for velocity, kinetic energy, momentum and angular momentum. Laplacian and Hamiltonian operator, Schrödinger's equationand its solution for Hydrogen atoms. Derivation of Heisenberg's uncertainty principle.

Unit III

Quantum mechanical approaches to molecular Bonding, Born-Oppenheimer approximation. Valence bond theory and molecular orbital theories. Valence bond theory and its application to homonuclear (Hydrogen) and heteronuclear (HCI) diatomics.

Unit IV

LCAO-MO treatment of hydrogen molecule ion. Comparative study of MO and VB theory.The variation theorem, linear variation principle. Perturbation theory (First order and nondegenerate). Applications of variation method and perturbation theory to the Helium atom.

Unit V

Huckel molecular orbital theory and its application to hybridization systems (ethylene, butadiene, allyls and benzene). Calculation of delocalization energy. Physical significance of charge density and bond order. Calculation of bond length.Perturbation methods in LCAO-MO theory. Extended Huckel molecular orbital theory and SCF-MO method.

Books Suggested(Names of Publishers may vary as per copyright status):

1. Introduction to Quantum Chemistyry, A.K. Chandra, Tata Mc Graw Hill.
2. Quantum Chemistry, Ira N. Levine, Prentice Hall.
3. Introduction to Quantum Chemistry-R.K. Prasad, New Age Publication.

Inorganic Chemistry Laboratory (MCH-4L1)

1. Qualitative analysis of inorganic mixture for seven radicals only (including interfering radicals, insolubles, and two rare elements.

2. Quantitative separation and estimation of individual metal component from binary mixture solution (either both component gravimetrically or one component gravimetrically and other one volumetrically).

Organic Chemistry Laboratory (MCH-4L2)

Organic synthesis: Any two from

Acylation: Acetylation of cholesterol and separation of cholesteryl acetate by column chromatography.

Oxidation: Adipic acid by chromic acid oxidation of cyclohexanol.

Aldol condensation: Dibenzalacetone from benzaldehyde.

Sandmeyer reaction: p-Chlorotoluenefrom p-toluidine.

Cannizzaro reaction: p-Chlorobenzaldehyde as substrate.

Friedel Crafts reaction: Benzoyl propionic acid from succinic anhydride and benzene.

Aromatic electrophilic substitutions: Synihesis of p-bromoanline.

Rearrangement: Synthesis of benzilic acid by benzil-benzilic acid rearrangement. Pinacol-pinacolonerearrangement in Benzpinacol.

Semester II

Inorganic Chemistry II(MCH-405)

Unit I

Theories of the co-ordinate linkage: Valence bond, crystal field, ligand field and molecular orbital theories. Crystal field splittings of d-orbitals in octahedral, trigonal bipyramidal, square pyramidal, tetragonal and square planar fields. Crystal field stabilization energy (CFSE). M.O. energy level diagram for octabedral and tetrahedral complexes (with s bonding only). Spectrochmical series.

Unit II

Electronic absorption spectra of transition metal complexes. Orgel diagrams for d^1, d^4, d^6 and d^9configurations with D ground state. Jahn-Teller effect. Stabilization of less familiar oxidation states of transition metals via coordination.

Unit III

Metal Carbonyls and Nitrosyls: Mononuclear and polynuclearcorbonyls and their structures. Nature of M-C-O bonding. Preparation of metal corbonyls and their reactions. Metal nitrosyls-bonding and structure. Metal carbonyl-nitrosyl complexes.

Unit IV

Chemistry of f-Block Elements: Comparative study of lanthanides and actinides with special reference to electronic structure. Oxidation state, coordination number, structure, stereochemistry and magnetic and spectral properties.

Unit V

General chemistry of actinides including E.M.F. diagrams. Extraction and metallurgy of thorium and uranium. Technicalproduction of plutonium. Separation of transamericiumelements.

Books Suggested(Names of Publishers may vary as per copyright status):

1. Advanced Inorganic Chemistry, F.A. Cotton, Wilkinson, John Wiley.
2. Inorganic Chemistry: Principles of Structure and Reactivity, Huheey, Medhi, Pearson Education India.
3. Physical Methods in Inorganic Chemistry, R S.Drago, Affiliated East-West Press Pvt. Ltd.

4. Chemistry of the Elements. N.N. Greenwood, A. Earnshow, Pergamon.
5. Inorganic Electronic Spectroscopy, A.B.P. Lever, Elsevier.
6. Comprehensive Coordiantion Chemistry eds., G. Wilkinson, R.D. Gillars, J.A. Mc Cleverty,Pergamon.

Organic Chemistry II(MCH-406)

Unit I

Aromatic Electrophilic Substitution:

The arenium ion mechanism, orientation and reactivity, energy profile diagrams. The ortho/para ratio, ipso attack. Diazonium coupling Vilsmeier reaction, Gatterman-Koch reaction.

Unit II

Aromatic Nucleophilic Substitution:

The S_NAr, $S_N1$benzyne and $S_{RN}1$ mechanisms. Reactivity-effect of substrate structure, leaving group and attacking nucleophile. The von Richter, Sommelet-Hauser and Smiles rearrangements.

Unit III

Free Radical Reactions:

Types of free radical reactions, free radical substitution mechanism, mechanism at an aromatic substrate, neighboring group assistance, reactivity for aliphatic and aromatic substrates at a bridgehead, Reactivity in the attacking radicals. The effect of solvent on reactivity. Allylic halogenation (NBS), oxidation of aldehydes to carboxylic acids, auto oxidation, coupling of alkynes and arylation on aromatic compounds by diazonium salts. Sandmeyerreation. Free radical rearrangement. Hunsdiecker reaction.

Unit IV

Addition to Carbon-Hetero Multiple Bonds:

Mechanism of metal hydride reduction of saturated and unasaturated carbonyl compounds, acids, esters and nitriles. Addition of Grignard reagents, organozinc and organolithium reagents to carbonyl and unsaturated carbonyl compounds, Witting reaction.

Mechanism of condensation reactions involving enolates-Aldol, Knoevenagel, Claisen, Mannich, Benzoin, Perkin and Stobbe reactions. Hydrolysis of esters and amides, ammonolysis of esters.

Unit V

Elimination Reactions:

The E_2, E_1 and E_1cB mechanisms, orientation of the double bond. Reactivity-effects of substrate structures, attacking base, the leaving group and the medium. Mechanism and orientation in pyrolytic elimination.

Books Suggested(Names of Publishers may vary as per copyright status):

1. Advanced Organic Chemistry, Jagdamba Singh, PragatiPrakashan.
2. Organic Chemistry: Concepts and Applications, Jagdamba Singh, PragatiPrakashan.
3. Advanced Organic Chemistry Part A: Structure and Mechanisms, Francis A. Carey,Richard J.Sundberg, Springer.
4. A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, Longman.
5. Structure and Mechanism in Organic Chemistry, C.K. Ingold, Cornell UniversityPress.
6. Organic Chemistry, R.T. Morrison, R.N. Boyd, Prentice-Hall.
7. Reaction Mechanism in Organic Chemistry, S.M. Mukherji, S.P. Singh,Macmillan.

Physical Chemistry II (MCH-407)

Unit I

Chemical Kinetics:

Basic Chemical Kinetics, molecularity, order and rate of reactions, collision theory of reaction rates, steric factor, activated complex theory, Arrhenius equation and the activated complex theory; ionic reactions, kinetic salt effects, steady state kinetics, kinetic and thermodynamic control of reactions, treatment of unimolecular reactions.

Unit II

Dynamic chain (hydrogen-bromine reaction, pyrolysis of acetaldehyde, decomposition of ethane), photochemical (hydrogenbromine and hydrogen-chlorine reactions) and homogenous catalysis,kinetics of enzyme reactions, general features of fast reactions, study of fast reactions by flow method, relaxation method, flash photolysis ad the nuclear magnetic resonance method.

Unit III

Dynamics of unimolecular reactions (Lindemann Hinshelwood and Rice-Ramsperger-Kassel-Marcus (RRKM) theories for unimolecular reactions).

Unit IV

Chemistry of Macromolecules:

Introduction to type of polymers. Step polymerization. Kinetics of step polymerization. Statistical approach to Gelation. Molecular weight distribution in linear polycondenstion (Derivation of size distribution). Molecular weight averages. Methods of determining the molecular weight by osmotic pressure, light scattering, sedimentation and viscosity methods.

Unit V

Non Equilibrium Thermodynamics:

Thermodynamic criteria for non-equilibrium states, entropy production and entropy flow, entropy balance equations for different irreversible processes (e.g., heat flow, chemical reaction etc.) transformations of the generalized fluxes and forces, non equilibriumstationary states, phenomenological equations, microscopic reversibility and Onsager's reciprocity relations, electrokinetic phenomena, diffusion, electric conduction.

Books Suggested(Names of Publishers may vary as per copyright status):

1. Physical Chemistry, P.W. Atkins, ELBS.
2. Physical Chemistry, Levine
3. Thermodynamics, Gurdeep Raj
4. Chemical Kinetics. K.J. Laidler, McGraw-Hill.
5. Physical Chemistry, G. W.Castellan.
6. Kinetics and Mechanism of Chemical Transformation J.Rajaraman, J.Kuriacose, Mc Millan.
7. Introduction to Polymer Science, V.R. Gowarikar, N.V. Vishwanathan, J.Sridhar, Wiley Eastern.
8. Polymer Chemistry, B. K. Sharma.

Introduction to Analytical Chemistry(MCH-408)

Unit I

Errors analysis: Accuracy and precision, absolute, relative, determinate and indeterminate errors, statistical treatment of random errors, computation rules for significant figures, method of least squares, mean deviations, and standard deviation.

Unit II

Tests of significance, the't' test, the 'F' test, the χ^2 (chi-squares) test, distribution normalcy test.

Regression analysis; methods of least squares the correlation coefficient, Rejection of observations; the 'Q' test.

Unit III

Titrations: Acid-base, complexometric, conductometric and potentiometric titration- theory of acid base indicators, Mohr, Volhard and Fajan's methods, EDTA based titration, Redox indicators, and their use in volumetric analysis.

Unit IV

Methodology and instrumentation of spectrophotometry in visible, ultraviolet and infra-red regions, spectrometric error, deviation from Beer's law, analysis of mixtures.

Spectrophotometric methods for investigations of composition and stability of metal complexes in solutions.

Unit V

Separation Techniques: Solvent extraction, thin-layer chromatography, gas chromatography (GC), liquid chromatography (LC), high performance liquid chromatography (HPLC), ion exchange chromatography, gel permeation chromatography. Chromatography coupled instrumentation.

Books Suggested(Names of Publishers may vary as per copyright status):

1. Analytical Chemistry, G.D. Christian, J.Wiley.
2. Fundamentals of analytical Chemistry, D.A. Skoog. D.M. West, F.J. Hooler, W.B.Saunders.
3. Principles of Instrumental analysis, D.A. Skoog, J.L. Loary, W.B. Saunders.
4. Principles of Instrumental Analysis, D.A. Skoog, W.B. Saunders.
5. Quantitative Analysis, R.A. Day, Jr., A.L. Underwood, Prentice Hall.
6. Environmental Solution, S.M. Khopkar, Wiley Eastern.
7. Basic Concepts of Analysis Chemistry, S.M. Khopkar, Wiley Eastern.
8. Handbook of Instrumental Techniques for Analytical Chemistry, F. Settle,Prentice Hall.

Physical Chemistry Laboratory (MCH-4L3) (Any two exercise):

(i) Determination of the velocity constant of the reaction between acetone and iodine catalysed byHCI/H_2SO_4.
(ii) Determination of velocity constant of saponification of ethyl acetate with sodium hydroxide.
(iii) Kinetics of reaction between copper sulphate and sugars in alkaline medium.
(iv) Titration of acid versus base using pH meter and calculation of pKa value of an acid.
(v) Elevation of boiling point using Landberger's apparatus.
(vi) To study the adsorption of oxalic acid on activated charcoal and test the validity of Freundilich's adsorption isotherm.
(vii) Rast method for determining molar mass.

Analytical and Computational Chemistry Laboratory (MCH-4L4) (Any two exercise):

1. Separation techniques: Ion-exchange and solvent extraction.

2. Chromatography: Paper, TLC, Electrophoresis.

3. Spectrophotometry.

4. Electrometric techniques: pH, Conductometry, Potentiometry (Ag, Sb, Pt electrodes).

5. Role of computer software and program in solving chemistry problems

6. Introduction to different structure, object drawing & solving software's, structural elucidation and reaction pathway prediction using analytical tools, different mathematical and analytical tools (Gaussian, MATLAB and Mathematica) will be introduced.

Semester III

Group theory and Molecular Spectroscopy(MCH-501)

Unit I

Group Theory: Introduction, Molecular symmetry and point groups, symmetry elements and operators, classes of symmetry operation, symmetry classification ofmolecules.Matrixrepresentation of symmetry operations, representation of groups, character, reducible and irreducible representations, great orthogonality theorem, character tables, symmetry properties of Hamiltonian operator, mutual exclusion principle.

Unit II

Rotational, Vibrational and Electronic spectroscopy:Electromagnetic radiation, interaction of electromagnetic radiation with matter, quantum mechanical approach - transition probabilities: Einstein coefficients, pure vibrational and rotational spectra, selection rules, vibrational and rotational spectra of polyatomic molecules, normal modes, anharmonicity, selection rules.

Unit III

Raman Effect: classical and quantum theory of Raman effect, rotational and vibrational Raman spectra. Franck-Condon principle, transition moments, assignment of electronic transitions of N_2, H_2O and formaldehyde using group theory.

Unit IV

Introduction to NMR: Origin of magnetic moments in matter, electronic and nuclear moments, interaction with magnetic field,Larmor equation - conditions for magnetic resonance absorption, relaxation times, line widths and line shapes, ring currents, diamagnetic anisotropy, spin-spin splitting, high resolution NMR spectra of simple molecules.

Unit V

Other Resonance Spectroscopy Methods:-EPR, NQR and Mossbauer spectroscopic techniques - Electron spin resonance: g value, hyperfine structure, ESR of organic free radicals, ESR of inorganic ions, ESR of simple free radicals in solutions – NQR. The principles of Mossbauer spectroscopy. Origin of isomer shifts, quadrupole splitting and h. f. s.

Books Suggested(Names of Publishers may vary as per copyright status):

1. Physical Methods in Chemistry, R.S. Drago, Saunders College.
2. Symmetry and Groups Theory in Chemistry, S.K.Dogra, H.S.Randhawa, New Age International
3. Chemical Applications of Group Theory, F.A. Cotton, Wiley.
4. Inorganic Spectroscopic Methods, Alan K. Brisdon, Oxford University Press.

Statistical Thermodynamics(MCH-502)

Unit I

Quantum states and complexions. The combinatory rule. System with definite total energy. Degeneracy of energy levels Probability and most probable distribution. Indistinguishability. Maxwell-Boltzmann statistics, partition function. Translational, rotational, vibrational and electronic partition functions. Internal energy and heat capacity in terms of partition function.

Unit II

Indistinguishability of gas molecules. Maxwell-Boltzmann law for gaseous system. Thermodynamic functions for gaseous systems. Molar heat capacity of gases. Heat capacity of hydrogen at low temperatures. Heat capacities of monatomic crystals. The Einstein model. Debye's theory of solid. Heat capacities of crystals at very low temperatures. Calorimetric entropy. Spectroscopic entropy, Comparison of calorimetric and spectroscopic entropies.

Unit III

Third Law of thermodynamics (i) Nernst heat theorem, (ii) Entropy of chemical reactions (iii) statements of third law of thermodynamics and (iv) Conventional entropies.

Unit IV

Expression for equilibrium constant in terms of partition functions. Equilibrium constants of simple systems - (i) Ionization of metal atoms, (ii) Dissociation of diatomic molecules and (iii) Isotopic exchange equilibria. Calculation of thermodynamic properties from spectroscopic data.

Unit V

Bose- Einstein statistics, Fermi-Dirac Statistics, Comparison of M-B, B-E and F-D statistics. Fermi-Dirac gas (electron gas in metals), Bose-Einstein gas (liquid Helium).

Books Suggested(Names of Publishers may vary as per copyright status):

1. Statistical Mechanics, B.K. Agarwal, M. Eisner, Wiley Eastern, New Delhi
2. Statistical Mechanics, D.A. Mcquarrie, California University Science Books
3. Statistical Mechanics, R. K. Pathria, Butterworth-Heinemann.

4. Statistical Mechanics, R. K. Pathria, Paul D. Beale, Elsevier.
5. Statistical Mechanics, N. Davidson, Mc Graw Hill Book Co. New York

Spectroscopic Identification of Organic Compounds(MCH-503)

Unit I

Introduction to spectroscopic techniques: Electromagnetic spectrum, absorption of energy by organic compounds. Types of spectroscopic methods for organic structure elucidation.Applications of UV – Visible and IR spectroscopies in organic structure elucidation.Various electronic transitions (200-800 nm), Beer-Lambert law. Characteristic vibrational frequencies of alkanes, alkenes, alkynes, aromatic compounds, alcohols, ether's, phenols and amines. Detailed study of vibrational frequencies of carbonyl compounds. Effect of hydrogen bonding on vibrational frequencies.

Unit II

Nuclear Magnetic Resonance Spectroscopy:

Basic principles. Introduction to NMR techniques. CW and FT NMR techniques. ^{1}H NMR Spectral parameters – intensity, chemical shift, multiplicity, coupling constant. Analysis of first order and second - order spectra. Structure determination of organic compounds by ^{1}H NMR spectra.

Unit III

Carbon-13 NMR Spectroscopy:

General considerations, chemical shift (aliphatic olefinic , alkyne, aromatic,heteroaromatic and carboynl carbon), coupling constants. Two dimension NMRspectroscopy-COSY, NOESY, DEPT, HMBC and HMQC techniques.

Unit IV

Introduction ion production. Factors affecting fragmentation, ion analysis, ion abundance Mass spectral fragmentation of organic compounds, common functional groups, molecular ion peak, metastable peak. Mc Lafferty rearrangement. Nitrogen rule. High resolution mass spectrometry.

Unit V

Solution of Structural problems by joint application of UV, IR, NMR ^{1}H and^{13}C) and mass spectroscopy.

Books Suggested(Names of Publishers may vary as per copyright status):

1. Organic Spectroscopy, L.D.S.Yadav, Springer.
2. Elementary Organic Spectroscopy, Y R Sharma, S Chand.
3. Spectroscopy of Organic Compounds, P.S.Kalsi, New Age International.
4. Application of Absorption Spectroscopy of Organic Compounds,J. R. Dyer, Prentice Hall,
   New Delhi.
5. Spectroscopic Identification of Organic Compounds, R.M. Silverstein, F.X. Webster, John Wiley, New York.
6. Spectroscopic Methods in Organic Chemistry, D.H. Williams, I.F. Fleming, Tata-McGraw Hill, New Delhi.
7. Organic Spectroscopy, William Kemp, Palgrave Macmillan.

Organic Reactions Mechanisms(MCH-504)

Unit I

Molecular Rearrangements I:

1. Migration to electron deficient carbon atom - Pinacole-Pinacolone rearrangement, Wagner-Meerweian rearrangement, Tiffenev-Demjanov ring expansion, Dienone-Phenol rearrangement, Benzil-Benzilic acid rearrangement, Favorski rearrangement.

Unit II

Molecular Rearrangements II:

1. Migration to electron deficient nitrogen atom - Wolf, Hofmann, Curtius, Losen, Schmidt, Beckmann rearrangement.

2. Migration to electron deficient oxygen atom - Baeyer-Villiger rearrangement.

3. Stevens, Witting, Neber rearrangements and rearrangement of amino ketones.

Unit III

Oxidation:

Introduction, Different oxidative processes. Hydrocarbons-alkenes, aromatic rings, saturated C-H groups (activated and unactivated) Alcohols, diols, aldehydes, ketones, ketals and carboxylic acids, amines, hydrazines, and sulphides. Oxidations with ruthenium tetraoxide, iodobenzene diacetate and thallium. (III) Nitrate.

Unit IV

Reduction:

Introduction, Different reductive processes. Alkanes, alkenes, alkynes, and aromatic rings. Carbonyl compounds-aldehydes, ketones, acids and their derivatives. Epoxides - Hydrogenolysis.

Unit V

Organometallic Reagents:

Principle, preparations, properties and applications of the following in organic synthesis with mechanistic details. Group I and II metal organic compounds: Li, Mg, Hg, Cd, Zn and Ce Compounds.

Books Suggested(Names of Publishers may vary as per copyright status):

1. Advanced Organic Chemistry, Jagdamba Singh, PragatiPrakashan.
2. Reactions, Rearrangements and Reagents, S.N. Sanyal, BharatiBhawan Publishers & Distributors.
3. Advanced Organic Chemistry-Reactions, Mechanism and Structure, Jerry March, John Wiley.
4. Advanced Organic Chemistry Part A: Structure and Mechanisms, Francis A. Carey,Richard J.Sundberg, Springer.
5. A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, Longman.
6. Structure and Mechanism in Organic Chemistry, C.K. Ingold, Comell University Press.
7. Organic Chemistry, R.T. Morrison, R.N. Boyd, Prentice-Hall.
8. Modern Organic Reactions, H.O. House, Benjamin.
9. Organic Reactions and Their Mechanisms, P.S.Kalsi, New Age International,
10. Reaction Mechanism in Organic Chemistry, S.M. Mukherji, S.P. Singh, Macmillan.

Synthetic Chemistry Laboratory (MCH-5L1) (Any two exercise):

[A] Multi-step synthesis of Organic Compounds: (any two from the list given below)

The exercises should illustrate the use of organic reagents and may involve purification of the products by chromatographic techniques.

Photochemical reaction: Benzophenone→Benzpinacol→Benzpinacolone
Beckmann rearrangement: Benzanilide from benzene, Benzene→Benzophenone→Benzphenone oxime→ Benzanilide.

Benzilic acid rearrangement: Benzilic acid from benzoin, Benzoin→Benzil→Benzilic acid

Synthesis of heterocyclic compounds:

Skraup synthesis: Preparation of quinoline from aniline.

Fischer-Indole synthesis: Preparation of 2-phenylindole from phenylhydrazine

Enzymatic synthesis:

Enzymatic reduction: Reduction of ethylacetoacetate using Baker's yeast to yield enantiomeric excess of S (+) ethytl-3-hydroxybutanoate and determine its optical purity.

Biosynthesis of ethanol from sucrose.

Synthesis using microwaves: Alkylation of diethyl malonate with benzyl chloride.

Synthesis using phase transfer catalyst: Alkylation of diethyl malonate or ethyl acetoacctate with an alkyl halide.

[B] Preparations (Complex compounds); (any two from the list given below):

(a) Ferric alum (ferric ammonium sulphate)

(b) Tetraammine copper (II) sulphate

(c) Potassium trioxalatochromate (III)/aluminate (III)/ferrate (III)

(d) Silver/copper tetraiodomercurate (II)

(e) Sodium hexanitritocobaltate (III)

(f) Prussian blue

(g) Ammonium diamminetetrathiocyanato-chromate (III)

(h) Pentamminechloro-nitritocobalt (III) chloride

(i) Hexaureachromium (III) chloride trihydrate

Spectroscopic Methods (MCH-5L2) (Any two exercise):

1. Identification of organic compound by the analysis of their spectral data (UV, IR, PMR, CMR and MS).

2. Spectrophotometric (UV/VIS) Estimations:

i. Amino acids ii. Proteins iii. Carbohydrates iv. Cholesterol v. Ascorbic acid vi. Aspirin vii. Caffeine.

3. Colorimetric determination of copper, iron and phosphate.

4. Spectrophotometric methods for investigations of composition and stability of metal complexes in solutions.

Semester IV

Elective 1 (MCH-505): Choose from the list of elective papers.

Elective 2 (MCH-506): Choose from the list of elective papers.

Elective 3 (MCH-507): Choose from the list of elective papers.

Organic Photochemistry and Pericyclic Reactions(MCH-508)

Unit I

Organic Photochemistry I:

Photochemistry of Carbonyl Compounds:Photochemistry of enones, hydrogen abstraction, rearrangements of α, β unsaturated ketones and cyclohexadienones, photochemistry of p-benzoquniones.

Unit II

Organic Photochemistry II

Photochemistry of unsaturated system: Olefins, cis-trans isomerization, dimerization, hydrogen abstraction and additions. Acetylenes-dimerization, Dienes-photochemistry of 1, 3-butadiene,(2+2) additions leading to cage structures, photochemistry of cyclohexadienes.

Unit III

Organic Photochemistry III

Photochemistry of aromatic compounds-exited state of benzene and its 1, 2 and 1, 3-shifts, Photo-Fries rearrangement, Photo-Fries reaction of anilides, photosubstitution reaction of benzene derivatives. Photolysis of nitride esters and Barton reaction.

Unit IV

Pericyclic Reactions:

Molecular orbital symmetry, Frontier orbitals of ethylene, 1, 3-butadiene, 1, 3, 5-hexatriene and allylsystem. Classification of pericyclic reactions, Woodward-Hoffmann correlation diagrams. FMO and PMO approach. Electrocyclic reactions-conrotatory and disrotatory motions, 4n, 4n+2 and allyl systems. Cycloadditions-antrafacial and suprafacial additions. 4n and 4n+2 systems, 2+2 addition of ketenes, 1, 3 dipolor cycloadditions and cheleotropic reactions.

Unit V

Sigmatropic rearrangements:

Suprafacial and antarafacial shifts of H, sigmatropic shifts involving carbon moieties, retention and inversion of configuration, (3,3) and (5,5) sigmatropicrearrangements. detailed treatment of Claisen, Cope and aza-Cope rearrangements. Fluxional tautomerism. Ene reaction.

Books Suggested(Names of Publishers may vary as per copyright status):

1. Photochemistry and Pericyclic Reactions, JagdambaSingh,Jaya Singh, New Age International
2. Reaction Mechanism in Organic Chemistry, S. M. Mukherjee, S.P. Singh, Macmillan India Ltd., New Delhi.
3. Pericyclic Reactions, S.M. Mukherjee, S.P. Singh, MacMillan India, New Delhi.
4. Advanced Organic Chemistry / Organic Synthesis,Jagdamba Singh, L D S Yadav, PragatiPrakashan,
5. Pericyclic Reactions, I. Fleming, Oxford University Press, Oxford.
6. Molecular Orbitals and OrganicChemical Reactions, Ian Fleming, Wiley.

Extraction and Chromatography (MCL- 5L3) (Any two exercise):

[A] Extraction of Organic Compounds from Natural Sources:

1. Isolation of caffeine from tea leaves. 2. Isolation of nicotine dipcirate from tobacco.

3. Isolation of lycopene from tomatoes. 4. Isolation of b-carotene from carrots.

5. Isolation of eugenol from cloves. 6. Isolation of (+) limonine from citrus rinds.

[B] Separation offollowing cations by Paper Chromatography:

(i) Ag(I), Pb(II) and Hg(II)

(ii) Hg(II), Cu(II) and Pb(II)

(iii) Ni(II), Co(II) and Zn(II)

(iv) Ni(II), Co(II) and Cu(II)

[C] Separation and identification of the components present in the given organic mixture by chromatographic methods.

Project/Dissertation/Seminar (MCH-5L4)

Individual faculty members will float stipulated number of projects. Students have to consult respective faculty members and select projects. More than one student can work under a single project based on nature of the project. Guide allotment for MSc project will be based on choice cum merit.

Once guide allotment (either single or more than one guide) is declared, student has to submit research proposal and give a presentation, either individually or one member from the group. Research proposal andpresentation carries 20 marks. Students will be periodically assessed for their project work by individual faculty member or group of faculty members. The final submission of the research project, i.e., small thesis, presentation and comprehensive viva carries 40 marks.

Note:

1. Student should submit 3 copies of the final research project copy in hard binding format with all declarations and signatures.

2. For referencing any ACS journal pattern should be followed.

Seminar:

Student should approach faculty members for seminar presentation on recent literature on particular topic. The remaining 20 marks will be credited for this assessment.

Elective Papers (MCH-50X)

Electives will be covered according to availability of expert faculty members in the Department. Students will be given choice to select and as per majority students choice elective will be

conducted. In total, students have to take three discipline specific electives for completing M.Sc. Course.

1. **Catalysis and Green Chemistry**

Unit I

Basic Principles of Green Chemistry:Prevention of waste by products, maximum incorporation of the reactants into the final product, prevention or minimization of hazardous products, designing safer chemicals, energy requirements for synthesis, selection of appropriate solvent, selection of starting materials, use of protecting groups.

Unit II

Green Reagent:Dimethylcarbonate, polymer supported reagent, polymer supported peracids, Poly-N-bromosuccinimide (PNBS), sulfonazide polymer, polystyrene Wittig reagent and polymer supported peptide coupling agent, miscellaneous reagents.

Unit III

Introduction and Basic concept of green catalysis, Application of catalyst functionality, concepts for control of reaction, selectivity and kinetic models.Steps in catalytic reaction (Adsorption and Kinetic models).Selection and design and Preparation of catalysts.

Unit IV

Green Catalyst:Acid catalyst, oxidation catalyst, basic catalyst, polymer supported catalyst, polystyrene – aluminium chloride, polymer supported photosensitizers, miscellaneous illustration and solid support reagents.

Unit V

Aqueous Phase Reactions:Diels-Alder reaction, Claisen rearrangement, Wittig-Horner reaction, Michael reaction, Aldol condensation, Knoevenagel reaction, Pinacol coupling, Benzoin condensation, Claisen- Schmidt condensation. Strecker synthesis, Wurtz reaction, Oxidations, Reductions, Polymerization reactions, photochemical reactions, electrochemical synthesis & miscellaneous reactions in Aqueous Phase.

Books Suggested(Names of Publishers may vary as per copyright status):

1. New Trends in Green Chemistry,V.K. Ahluwalia, M.Kidwai, Anamaya publishers, New Delhi.
2. Introduction to Green Chemistry, V.Kumar.

3. Green Chemistry: Theory and Practice, Paul T. Anasta,John C. Warner, Oxford University Press.
4. Catalysis: Concepts and Green Applications, Gadi Rothenberg, Wiley.

2. Concepts in Organic Synthesis

Unit I

Disconnection Approach: General introduction to synthons and Synthetic equivalents, Disconnections, (C-C, C-S, C-O, bonds), Functional group interconversion, chemoselectivity, cyclisation reaction, choosing synthetic route for small and large scale synthesis.

Unit II

Synthetic Strategies: (a) For formation of carbon-carbon bond (b) For formation of carbon-nitrogen bond (c) Formation of carbon-halogen bond (d) Ring Synthesis and (e) Multistep Synthesis.

Unit III

(i) Protecting Groups: Principle of protection of alcoholic, amino, carbonyl and carboxylic groups.
(ii) Stereochemistry in organic synthesis: Stereoselectivity and stereospecificity. Regioselectivity and regiospecificity: Assymmetric synthesis-Sharpless asymmetric epoxidation.An introduction to computer aided designing of organic synthesis.

Unit IV

Reagents in Organic Synthesis:
(i) Complex metal hydrides. (ii) Gilman's reagent. (iii) Lithium disopropyl amide (LDA). (iv) Dicyclohexylcarbodimide (DCC).(v) 1,3-Dithiane (Reactivity Umpolung). (vi) Trimethylsily iodide.(vii) Tri n-butyltin hydride. (viii) Crown ethers. (ix) Merrifield resin. (x) Wilkinson's Reagent.(xi) Peterson's Synthesis (xii) Organic per acids.(xiii) Baker's yeast.

Unit V

Selective organic name reaction and their synthetic application: (i) Stork Enamine reaction. (ii) Favorskii reaction. (iii) Ene Reaction. (iv) Barton Reaction.(v) Hofmann-Loffler-Freytag Reaction. (vi) Shapiro Reaction.(vii) Chichibabin Reaction. (viii) Robinson annulation.
Nitrogen, Sulphur and Phosphorus Ylides: Preparation and their synthetic applications.

Books Suggested(Names of Publishers may vary as per copyright status):

1. Organic Synthesis, Jagdamba Singh, L.D.S. Yadav, PragatiPrakashan
2. Advanced Organic Chemistry, Jagdamba Singh, PragatiPrakashan.
3. Organic Chemistry: Concepts and Applications, Jagdamba Singh, PragatiPrakashan.
4. Advanced Organic Chemistry Part B: Reaction and Synthesis, Francis A. Carey,Richard J.Sundberg, Springer.
5. A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, Longman.
6. Advanced Organic Chemistry, ArunBahl, B S Bahl, S Chand.

3. Electrochemistry

Unit I

Equilibrium electrochemistry: Activities in electrolytic solutions, mean activity coefficient, Debye-Huckel treatment of dilute electrolyte solutions, origin of electrode potential, half-cellpotential, electrochemical cell, Nernst equation, thermodynamics of electrochemical cell.

Unit II

Dynamicelectrochemistry: Electrical double layer - electrode kinetics, rate of charge transfer, current density, Butler- Volmer equation,

Unit III

Introduction to polarography, cyclic voltammetry, theory of corrosion and inhibition of corrosion.

Unit IV

Bioelectrochemistry: bioelectrodics, membrane potentials, simplistic theory, modern theory, electrical conductance in biological organism: electronic, protonic electrochemical mechanism of nervous systems, enzymes as electrodes.

Unit V

Electrochemical sensors: Potentiometric sensors, Ion-selective electrodes, Membrane electrodes, Amperometric sensors, Clark and Enzyme electrodes).

Books Suggested(Names of Publishers may vary as per copyright status):

1. Modern Electrochemistry, Vol. 1, Vol. 2A and Vol. 2 B, J.O'M. Bockris, A.K.N. Reddy,Plenum Press, New York.
2. Electrochemical Methods: Fundamentals and Applications, A.J. Bard, L.R. Faulkner, John Wiley and Sons, New York.

4. Organometallic Chemistry of Transition Metals

Unit 1

Inorganic π Acid Ligands: Dioxygen and dinitrogen, nitrosyl, tertiary phosphines and arsines as ligands.Complexes of σ donor ligands: Transition metal alkenyls, alkynyls, carbenes and carbines.

Unit II

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

Unit III

Transition organometalic compounds:
Transition metal compounds with bonds to hydrogen, boron, silicon

Unit IV

Transition metal compounds in catalysis: Hydrogenation, hydroformylation and polymerization; Wacker Process.

Unit V

Transition metal Compounds with M-H bonds: Metal hydrides (classical and non classical). Agosticinteraction. Application of NMR in studying hydrido complexes.

Books Suggested(Names of Publishers may vary as per copyright status):

1. Advanced Inorganic Chemistry, F.A. Cotton, G. Wilkinson, John Wiley and Sons, NY.
2. The Organometallic Chemistry of Transition Metals, R. H. Crabtree, John Wiley.
3. Principles and Applications ofOrganotransition Metal Chemistry,J.P. Collman, L.S. Hegedus, J.R. Norton, R.G. Finke, Univ. Sci. Books, Mill Valley. California.

5. Bioinorganic Chemistry

Unit I

Complexes of Biological Significance: Metal complexes of amino acids and peptides. Metal complexes of nucleic acid bases, nucleosides and nucleotides. Metal complexes of porphyrins and pthalocyanins.

Unit II

Synthetic model oxygen carrier complexes and model dinitrogen complexes. Phosphates and bioenergetics. Phosphorylation and phosphorolysis. Adenine nucleotides in metabolic energy transfer. Oxidation of glucose and the role of phosphate.

Unit III

Role of Metal Ions in Biological Systems: Essential and trace metal ions. Metal ions storage and transport (Na, K, Ca, Mg, Fe, Cu and Zn)-Ferritin and Transferrin. Metal ion toxicity and its cure by chelating agents. Pharmacological activity and metal chelates. Carcinogenic metals, carcinogenic and carcinostatic ligands.

Unit IV

Metallo Proteins and Metallo Enzymes: Function, electronic structure, bonding and stereochemistry of the active site. Natural Oxygen Carrying Proteins-Haemoglobin, Myoglobin, Hemerythrins and Hemocyanin,

Unit V

Electron Transport Proteins (a) Iron-Sulfur Proteins-Rubredoxin and Ferredoxins, (b) Cytochromes (types a, b and c).

Books Suggested(Names of Publishers may vary as per copyright status):

1. Bioinorganic Chemistry: Inorganic Elements in theChemistry of Life, An Introduction and Guide, W. Kaim, B. Schwederski, Wiley, New York.
2. Inorganic Chemistry of Biological Processes, M. N. Hughes , John-Wiley and Sons, New York.
3. Principles of Bioinorganic Chemistry, S. J. Lippard, J. M. Berg, University Science Books.
4. Bioinorganic Chemistry, I. Bertini, H. B. Grey, S. J. Lippard, J. S. Valentine, Viva Books Pvt. Ltd., New Delhi.

6. Bioorganic and Medicinal Chemistry

Unit I

Enzymes: Introduction and historical perspective, chemical and biological catalysis, remarkable properties of enzymes like catalytic power, specificity and regulation. Nomenclature and classification, extraction and purification. Fisher's lock and key and Koshland's induced fit hypothesis, concept and identification of active site by the use of inhibitors, affinity labeling and enzyme modification by site-directed mutagenesis. Enzyme kinetics, Michaelis-Menten and Lineweaver-Burk plots, reversible and irreversible inhibition.

Unit II

Mechanism of Enzyme Action: Transition-State theory, orientation and steric effect, acid-base catalysis, covalent catalysis, strain or distortion. Examples of some typical enzyme mechanisms for chymotrypsin, ribonuclease, lysozyme and carboxypeptidase A.

Unit III

Relationship of chemical structure and biological activities and theories of drug action. Detailed study of following classes:
(i) Antineoplastic Agents: Introduction, cancer chemotherapy, role of alkylating agents and antimetabolites in treatment of cancer.Mention of carcinolytic antibiotics and mitoptic inhibitors. Synthesis of mechlorethamine, cyclophosphamide, melphalan, uracil, amustards, and 6-mercaptopurine products.
(ii) Cardiovascular Drugs: Cardiovascular diseases, drug inhibitionof peripheral sympathetic function. Direct acting arteriolar dilators. Synthesis of amyl nitrate, hydralaxine, verapamil, methyldopa and diazoxide propanol.

Unit IV

(i) Local Anti-infective Drugs: Antitubercular drugs and Antimalerial drugs: Introduction and general mode of action. Study of sulphonamides, ciprofloxacin, norfloxacin,, amino salicylic acid.
(ii) Psychoactive Drugs: CNS depressants general anaesthetics, hypnotics, sedatives, anti-anxiety drugs, benzodiazepines. Antipsychotic drugs: diazepam, alprazolam, trimethadione, barbiturates and glutethimide.
(iii) Antibiotics: Penicillin G, chloramphenicol, cephalosporin, tetracycline and streptomycin.

Unit V

Vitamins and Hormones: Detailed study of chemistry of Vit. B_1, Vit. $C_{1,}$ Pantothenic acid, Biotin (Vitamin H) and α-tocopherol (Vitamin E). Biological action of vitamins.
Insect hormones : Pheromones and Juvenile hormones; Plant hormones: Gibberellins.

Books Suggested(Names of Publishers may vary as per copyright status):

1. Introduction to Bioorganic Chemistry and Chemical Biology,David Van Vranken, Gregory A, Garland Science (Taylor & Francis).
2. Natural Products Chemistry, Jagdamba Singh, PragatiPrakashan.
3. Chemistry of Natural Products,R.H. Thomson,Wiley, New York.
4. Organic Chemistry, Volume 2: Stereochemistry and the Chemistry Natural Products, I.L.Finar, Pearson Education India.

7. Nanochemistry

Unit I

Introduction: History scope and perspectives of nanochemistry. Synthesis and Stabilization of Nanoparticles, Chemical Reduction; Reactions in Micelles, Emulsions, and Dendrimers; Photochemical and Radiation Chemical Reduction.

Unit II

Experimental Techniques: Transmission and scanning electron microscopy, Probe Microscopy, X-ray diffraction, Neutron diffraction, Miscellaneous Techniques, Comparison of Spectral Techniques used for Elemental Analysis.

Unit III

Size Effects in Nanochemistry: Models of Reactions of Metal Atoms in Matrices; Properties; Kinetic Peculiarities of Chemical Processes on the surface of Nanoparticles; Thermodynamic Features of Nanoparticles.

Unit IV

Applications of Nanoparticle in various fundamental research, industries, medical field.

Unit V

Environmental issue; toxicity, biosafety and ethical issue in applications of Nanoparticle.

Books Suggested(Names of Publishers may vary as per copyright status):

1. Nanomaterials and Nanochemistry, edited by C. Brechignac, P. Houdy, M. Lahmani, Springer-Verlag, Berlin.
2. Nanoparticle Technology Handbook. M. Hosokawa, K. Nogi, M. Naito, T.Yokoyama (Eds.), Elsevier.
3. Nanotechnology Basic Calculations for Engineers and Scientists, Louis Theodore, John Wiley and Sons.

4. Nanochemistry: A Chemical Approach to Nanomaterials, Geoffrey A Ozin, André Arsenault, Ludovico Cademartiri, RSC Publishing.

8. Cheminformatics

Unit I

Introduction to cheminformatics, History and Evolution of cheminformatics, Use of cheminformatics, Prospects of cheminformatics, Molecular Modeling and Structure Elucidation.

Unit II

Role of computers in chemical research, Introduction to Chemoinformatics, Representation and manipulation of 2D and 3D molecular structures, Chemical Databases- Design, Storage and Retrieval methods.

Unit III

Reaction databases, Representation of chemical reactions, Search techniques (Full, Sub and Super structure), Similarity searches, modelling of small molecules.

Unit IV

Prediction of Properties of Compounds, Linear Free Energy Relations, Quantitative Structure-Property Relations, Descriptor Analysis; Model Building, Modeling Toxicity, Structure-Spectra correlations, Prediction of NMR, IR and Mass spectra.

Unit V

Combinatorial chemistry and Library design –Introduction, Data visualization, Data mining methods, Prediction of ADMET properties, Chemoinformatics tools for drug discovery.

Books Suggested(Names of Publishers may vary as per copyright status):

1. An Introduction to Chemoinformatics, Andrew R. Leach, V.J. Gillet, Springer.
2. Chemoinformatics: A Textbook, Johann Gasteiger, Thomas Engel, Wiley-VCH.
3. Chemoinformatics: Theory, Practice, & Products, Barry A. Bunin, Brian Siesel, Guillermo Morales, Jürgen Bajorath, Springer.

9. Analytical Chemistry

Unit I

Introduction to Analytical Chemistry- Methods of qualitative and quantitative analysis.

Unit II

Thermal Analysis: Introduction, types and applications of thermoanalytical methods, thermogravimetry etc.

Unit III

Electro Analytical Techniques: Voltametry, Amperometry, Coulometry, Conductometry, Potentiometry.

Unit IV

Diffraction Techniques: Introduction, types and applications with special reference to x-ray diffraction technique.

Unit V

Electrochemical Techniques:Introduction and applications of Electrolysis, Electrophoresis.

Books Suggested(Names of Publishers may vary as per copyright status):

1. Analytical Chemistry, G.D. Christian, J.Wiley.
2. Fundamentals of analytical Chemistry, D.A. Skoog. D.M. West, F.J. Hooler, W.B.
3. Saunders.
4. Analytical Chemistry-Principles, J.H. Kennedy, W.B. Saunders.
5. Analytical Chemistry-Principles and Techniques, LG. Hargis, Prentice Hall.
6. Principles of Instrumental analysis, D.A. Skoog, J.L. Loary, W.B. Saunders.
7. Principles of Instrumental Analysis, D.A. Skoog, W.B. Saunders.
8. Quantitative Analysis, R.A. Day, Jr., A.L. Underwood, Prentice Hall.
9. Environmental Solution, S.M. Khopkar, Wiley Eastern.
10. Basic Concepts of Analysis Chemistry, S.M. Khopkar, Wiley Eastern.
11. Handbook of Instrumental Techniques for Analytical Chemistry, F. Settle, Prentice Hall.