Anekant Education Society's

TULJARAM CHATURCHAND COLLEGE
of Arts, Science and Commerce, BARAMATI
(AUTONOMOUS)

Department of Chemistry

Scheme of Course Structure (F. Y. B. Sc.) 2019-2020

Sr. No	Class	Semester	Code	Paper	Paper Title	Credit	Exam	Marks
1	F Y B Sc	I	CHEM1101	Theory	Physical and Inorganic Chemistry- I	2	I / E	50 + 50
2	F Y B Sc	I	CHEM1102	Theory	Organic and Inorganic Chemistry- I	2	I / E	50 + 50
3	F Y B Sc	II	CHEM1201	Theory	Physical and Inorganic Chemistry- II	2	I / E	50 + 50
4	F Y B Sc	II	CHEM1202	Theory	Organic and Inorganic Chemistry- II	2	I / E	50 + 50
5	F Y B Sc	Annual	CHEM1203	Practical	Chemistry Practical- I	4	I / E	50 + 50

Department of Chemistry

Scheme of Course Structure (M.Sc. I) 2019- 2020

Sr. No	Class	Semester	Code	Paper	Paper Title	Credit	Exam	Marks
1	M.Sc. I	I	CHP-4101	Theory	Fundamentals of Physical Chemistry- I	4	I / E	50 + 50
2	M.Sc. I	I	CHI-4102	Theory	Molecular Symmetry and Chemistry of P- block elements	4	I / E	50 + 50
3	M.Sc. I	I	CHO-4103	Theory	Basic Organic Chemistry	4	I / E	50 + 50
4	M.Sc. I	I	CHA-4104	Theory	Safety in Chemical Laboratory and Good Laboratory Practices	4	I / E	50 + 50
5	M.Sc. I	I	CHP-4105	Practical	Physical Chemistry Practical	4	I / E	50 + 50
6	M.Sc. I	I	CHO-4106	Practical	Organic Chemistry Practical	4	I / E	50 + 50
7	M.Sc. I	I			Skill Development	2		
8	M.Sc. I	I			Certificate Course	2		
9	M.Sc. I	II	CHP-4201	Theory	Fundamentals of Physical Chemistry- II	4	I / E	50 + 50
10	M.Sc. I	II	CHI- 4202	Theory	Coordination and Bioinorganic Chemistry	4	I / E	50 + 50
11	M.Sc. I	II	CHO-4203	Theory	Synthetic organic chemistry and Spectroscopy	4	I / E	50 + 50
12	M.Sc. I	II	CHA-4204	Theory	General Chemistry (any two parts)	4	I / E	50 + 50
13	M.Sc. I	II	CHI-4205	Practical	Inorganic Chemistry Practical	4	I / E	50 + 50
14	M.Sc. I	II	CHA-4206	Practical	Analytical Chemistry Practical	4	I / E	50 + 50
15	M.Sc. I	II			Skill Development	2		
16	M.Sc. I	II			Introduction Cyber Security – I	2		

Department of Chemistry

SYLLABUS FOR CERTIFICATE COURSE (For M. Sc. I):- 2 Credits

TITLE: - INSTRUMENTAL METHODS OF CHEMICAL ANALYSIS

1) Introduction of principle of UV –Visible Spectroscopy, Instrumentation and applications
2) Introduction of principle of FTIR Spectroscopy, Instrumentation and applications.
3) Introduction of principle of HPLC ,Instrumentation and applications
4) Introduction of principle of Atomic Absorption Spectroscopy, Instrumentation and applications

(12 theory lectures and 18 hours practical / hands on instrumental training.)
Evaluation: Online test and practical examination.

Department of Chemistry

SYLLABUS (CBCS) FOR F. Y. B. Sc. CHEMISTRY
SEMESTER- I (2019-2020)

CHEM1101: Physical and Inorganic Chemistry- I (2 Credits, 36 L)

A. Learning Objective:

1. To introduce basic concepts of mathematics useful to solve problems related to chemistry.
2. To adequate students with states of matter and their properties and basic methods of measurements.
3. To learn basic of mole concept, methods for expressing concentration of solution, preparation of standard solution and redox reactions.

B. Learning Outcome:

1. This course makes understanding of use of mathematical concepts in chemistry, correlation in chemical variables graphically.
2. Students should able to know states of matter, properties associated and measurement. Also the concepts like mole, molecular weight, equivalent weight, GMV relationship, standardization of solution and balancing the redox reactions should be understood.

SECTION I: PHYSICAL CHEMISTRY (24 L)

1. Chemical Mathematics (6 L)

Functions and variables: Variables as function, variables used in chemistry
Logarithm - Characteristic and mantissa, Rules of logarithm, Change of sign and base, Problems based on pH and pOH calculations.
Derivative: Rules of differentiation, partial differentiation, problems related to chemistry,
Integration: Rules of integration, definite and indefinite, problems related to chemistry.
Graph of linear function: Equation of straight line, equation from data of graph, plotting the graph from the data of chemical properties, problems.

2. Gaseous and Liquid States (8 L)

Introduction: States of matter and their properties.
Gaseous state : Significance of ideal and kinetic gas equation (no derivation), Real gases- Compressibility factor, van der Waal's equation of state, critical constants, correlation between critical constants and van der Waal's constants.
Liquid state: Properties of liquids, vapor pressure and its measurement by isoteniscopic method, Viscosity and its measurements by Ostwald's viscometers, Liquid crystals: Introduction, their types and applications in various fields.

3. Solid State (10 L)

Definition of space lattice, unit cell;
Laws of crystallography – (i) Law of constancy of interfacial angles, (ii) Law of rationality of indices (iii) Law of symmetry, Symmetry elements in crystals.
Fundamental crystal systems, Characteristic of simple cubic, face-centered cubic and body-centered cubic systems, Interplanar distances in cubic crystals, X-ray diffraction by crystals, Derivation of Bragg equation, Determination of crystal structure of NaCl, Numerical

SECTION II: INORGANIC CHEMISTRY (12 L)

1. Mole concept and Stoichiometry: (5 L)

Mole concept - Determination of molecular weight by gram molecular volume relationship, problems based on mole concept

Methods of expressing concentration -strength, normality, molarity, molality, mole fraction, %w/v, %w/w, % v/v, ppt, ppm, ppb,

Standardization of solutions, primary and secondary substances, preparation of standard solutions of acids and bases, problems based on acid base titrations only

2. Oxidation –Reduction: (7 L)

Definitions to related terms like oxidation, reduction, oxidizing agent, reducing agent oxidation number, valency,

Balancing of redox reactions using oxidation number method and ion electron method,

Problems based on equivalent weight of oxidant and reductant.

References:

1. Physical Chemistry, P. W. Atkins, ELBS, 5th Edition.
2. Principles of Physical Chemistry, Maron and Prutton, 4th Edition.
3. Physical Chemistry, G. M. Barrow 4th Edition.
4. Quantum Chemistry, I. Levine, 5th Edition.
5. Essentials of Physical Chemistry, Bhal and Tuli,
6. Principles of Physical Chemistry, Puri, Sharma and Phathania
7. Mathematical Preparation of Physical Chemistry, F. Daniel, Mc Graw Hill.
8. Concise Inorganic Chemistry, J. D. Lee, 5th Edition
9. Concept and Models of Inorganic Chemistry, Douglus and Daniel, 3rd Edition
10. Inorganic Chemistry, James Hughey

SEMESTER- I

CHEM1102: Organic and Inorganic Chemistry I (2 Credits, 36 L)

A. Learning Objective:

1. To know the fundamental concepts which govern the structure, bonding, properties and reactivity of organic molecules such as covalent character, hybridization, bond angles, bond energies, bond polarities and shapes of molecules.
2. To become familiar with drawing of organic molecules and arrow pushing concept.
3. Students are expected to know common and IUPAC names, methods of preparation and chemical reactions of alkanes, alkenes, alkynes and homocyclic, aromatic hydrocarbons and application of Huckel's rule.
4. The students are expected to know structure, nomenclature, preparation and reactions of organic compounds.
5. To understand the use of possible reagents to bring about the given conversion with possible product and identify the major and minor products.
6. To know silent features of periodic table with reference to S-block elements (symbols electronic configuration, trends and properties). Separation method by using crown ether, compounds and applications of S block elements.

B. Learning Outcome:

1. This course makes understanding of structure, bonding, properties and reactivity of organic molecules.
2. Students are able to draw of organic molecules with arrow pushing concept, IUPAC names, and methods of preparation of organic compounds.
3. Students should know structure, nomenclature, preparation and reactions of organic compounds and use of possible reagents.
4. Students should know details about S block elements.

SECTION I: ORGANIC CHEMISTRY (24 L)

1. **Chemical Bonding, structure of Organic Molecules: (5 L)**

Covalent bond, Hybridization - sp, sp^2 and sp^3 hybridization, Bond length, Bond angle, Bond energy, Inter and Intra molecular forces and their effects

Ref. 2: Pages 9 - 17, 20 – 29

Drawing organic molecules, zigzag structures, Lewis structure and formal charge, Arrow pushing concept

Ref. 1: Pages 31 - 36, 116 – 127

2. **Chemistry of Hydrocarbons: (7 L)**

Alkanes - Introduction, Nomenclature, Physical properties, Preparations, Reactions of alkanes, Analysis of alkanes

Ref. 2: Sec. 2.1 – 2.3, Sec. 3.6 – 3.12, Sec. 3.15 – 3.17, Sec. 3.18, 3.19, 3.30, 3.32, Sec. 3.34

Pages: 39 – 41, 86 – 94, 97 – 106, 118, 120, 122

Alkenes-Introduction, higher alkenes, Nomenclature, Physical properties, Preparations, Reactions of alkenes, Analysis of Alkenes
Ref. 2: Sec. 8.7 to 8.9, 8.11 to 8.13, Sec. 9.1, 9.2, 9.27
Pages: 282 – 285, 287 – 293, 309, 317 – 323, 360 - 362
Dienes - Structure & Properties, Conjugated dienes, Reactions of dienes, Analysis of dienes
Ref. 2: Sec. 11.17, 11.19, 11.21, 11.22, 11.26
Pages: 409 – 417, 421, 422
Alkynes: Introduction, Nomenclature, Physical properties, Preparation, Reactions & analysis of alkynes
Ref. 2: Sec. 12.1 - 12.8, 12.14
Pages: 425 – 434, 440
Introduction to homocyclic aromatic hydrocarbons (benzene), Huckel's rule of aromaticity, Reactions of benzene – Sulphonation, Nitration, Halogenation, Friedel Craft reactions
Ref. 2: Sec. 14.1 - 14.5, 14.10, 14.11, 14.12, Relevant pages from 15.1 – 15.21
Pages: 493 – 499, 504, 508 – 511, Relevant pages from 517 – 546

3. Chemistry of functional groups (12 L)
Alkyl halides: Introduction, Nomenclature, Physical properties, General methods for preparation, Chemical reactions, Analysis of alkyl halides
Ref. 2: 5.3 – 5.7, 5.24
Pages: 167 – 174, 211
Alcohols: Introduction, Nomenclature, Physical properties, General methods for preparation, Chemical reactions, Analysis of alcohols
Ref. 2: 6.1 – 6.5, 6.10, 6.11, 6.22
Pages: 211 – 218, 222 – 226, 243 – 244
Ethers: Introduction, Nomenclature, Physical properties, General methods for preparation, Chemical reactions, Analysis of ethers
Ref. 2: 6.16 – 6.21, 6.23
Pages: 237 – 242, 244 - 245
Carboxylic acids: Introduction, Nomenclature, Physical properties, General methods for preparation, Chemical reactions, Analysis of carboxylic acids
Ref. 2: 19.1 – 19.4, 19.6, 19.9, 19.21
Pages: 713 – 722, 725 – 728, 744 - 745
Amines: Introduction, Nomenclature, Physical properties, General methods for preparation, Chemical reactions, Analysis of amines
Ref. 2: 22.1 – 22.5, 22.8, 23.1 – 23.3, 23.12, 23.19
Pages: 821 – 825, 828 – 830, 845 – 849, 866 – 869, 876 - 877
Phenols: Introduction, Nomenclature, Physical properties, General methods for preparation, Chemical reactions, Analysis of phenols
Ref. 2: 24.1 – 24.3, 24.7, 24.8, 24.16
Pages: 889 – 893, 898 – 902, 912

SECTION II: INORGANIC CHEMISTRY (12 L)

1. Chemistry of S- block elements (12 L)

Recapitulation of periodic table, special position of Hydrogen in the long form of periodic table, properties of S -block elements with reference to electronic configuration, extraction, trends and properties.

Introduction to crown ether and cryptans, separation of S- block elements using crown ethers.

Compounds of S- block elements: oxides, hydroxides, peroxides, superoxide, and halides.

Applications of S-block elements in industrial, biological and agricultural field.

Ref. 6 & 9.

References

1. Organic Chemistry-Clayden, Oxford Uni. Press
2. Organic Chemistry-Morrison and Boyd, 6th Edn.
3. A guide book to Mechanism in Organic Chemistry-Peter Syke, 6th Edn.
4. Stereochemistry of Organic Compounds-Eliel Tata Mc Graw Hill 1989
5. Principles of Physical Chemistry by S.H. Marron & C.F. Pruton, 4th Edn.
6. Concise Inorganic Chemistry-J.D. Lee, 2nd Edition-Relevant pages.
7. Concept & model of Inorganic Chemistry-Douglas Mc Doniels, 3rd Edn.
8. New guide to Modern Valance Theory-G.I. Brown, 3rd Edn.
9. Inorganic Chemistry-James Hughey
10. General Chemistry - Raymand Chang

SEMESTER- II

CHEM1201: Physical and Inorganic Chemistry II (2 Credits, 36 L)

A. Learning Objective:

1. To introduce basic concepts in atomic structure: Bohr model, energy level diagrams, hydrogen spectra, related principles. Schrödinger equation is the basis of quantum chemistry that has been introduced for hydrogen atom.
2. To adequate students with basic concepts in thermodynamics, statements first law of thermodynamics, use of thermodynamic state functions and thermochemical calculations.
3. To learn basic principle and concepts of theories of overlapping of atomic orbitals. Types of hybridizations involving s , p and d orbitals.
4. To understand the basic of VSEPR theory, bonding and shapes of simple molecules.

B. Learning Outcome:

1. This course makes understanding of assumptions of Bohr model, atomic spectra, Schrödinger equation for hydrogen atom and related mathematical calculations.
2. Students should able to know elementary chemical thermodynamics, laws and state functions used in thermo chemical calculations.
3. Student should able to understand basic principle and concepts of overlapping of atomic orbital focusing on VSEPR theory for simple molecules.

SECTION I: PHYSICAL CHEMISTRY (24 L)

1. Atomic Structure: (12 L)

Introduction, atomic spectrum of hydrogen, Bohr model of hydrogen atom-derivation of atomic radius and energy, energy level diagram of hydrogen atom , Failure of Classical mechanics- black body radiation, photoelectric effect, electron diffraction, atomic spectra, quantization of energy, de Broglie's hypothesis, Heisenberg's uncertainty principle (without proof), wave equation, time independent Schrödinger equation, hydrogen atom (expressions only)., wave functions for s and p atomic orbital's,

2. Chemical Thermodynamics: (12 L)

Definitions of thermodynamic terms: System, surroundings etc. Types of systems, intensive and extensive properties, State and path functions, Thermodynamic processes, concept of heat and work

First Law of Thermodynamics: Statement, definition of internal energy and enthalpy, Heat capacity, heat capacities at constant volume and pressure and their relationship, Joule's law – Joule-Thomson coefficient and inversion temperature. Calculation of w, q, dU & dH for the expansion of ideal gases under isotheral and adiabatic conditions for reversible process.

Thermo chemistry: Standard state, standard enthalpy of formation – Hess's Law of heat summation and its applications, Heat of reaction at constant pressure and at constant volume, Enthalpy of neutralization, Bond dissociation energy and its calculation from thermochemical data, temperature dependence of enthalpy, Kirchhoff's equation

SECTION II: INORGANIC CHEMISTRY (12 L)

1. Chemical Bonding and Structure: (3 L)
Recapitulation of bonds: Ionic, covalent, coordinate and metallic.
Types of overlaps: s-s. s-p ,p-p, p-d, d-d with examples, formation of sigma and pi bond.
Theories of bonding: Valence bond theory, Heitler –London theory, Pauling Slater theory.

2. Concept of hybridization: (6 L)
Definition and need of hybridization, steps involved in hybridization ,explanation of covalency of atom in the moles based on hybridization, types of hybridization involving in s, p and d orbital .

3. The VSEPR Theory: (3 L)
Introduction, need and assumptions of VSEPR theory, bonding and shapes of irregular molecules as – ClF_3, BrF_3, Cl_2O, BrF_5, $TeCl_4$, XeO_3, $XeOF_4$, limitations of VSEPR theory.

References:

1. Physical Chemistry, P. W. Atkins, ELBS, 5th Edition.
2. Principles of Physical Chemistry, Maron and Prutton, 4th Edition.
3. Physical Chemistry, G. M. Barrow 4th Edition.
4. Quantum Chemistry, I. Levine, 5th Edition.
5. Essentials of Physical Chemistry, Bhal and Tuli,
6. Principles of Physical Chemistry, Puri, Sharma and Phathania
7. Mathematical Preparation of Physical Chemistry, F. Daniel, Mc Graw Hill.
8. Concise Inorganic Chemistry, J. D. Lee, 5th Edition
9. Concept and Models of Inorganic Chemistry, Douglus and Daniel, 3rd Edition
10. Inorganic Chemistry, James Hughey

SEMESTER- II

CHEM1202: Organic and Inorganic Chemistry II (2 Credits, 36 L)

A. Learning Objective:

1. To understand concept of isomerism, types of isomers and their stereochemistry.
2. To find R/S configuration in compounds containing two Chiral centers.
3. To use different reagents in organic synthesis.
4. To know silent features of periodic table with reference to P-block elements (symbols electronic configuration, trends and properties). Structures of compounds and applications of P block elements and inter halogen compounds.

B. Learning Outcome:

1. This course makes understanding of concept of isomerism, types of isomers and their stereochemistry and R/S configuration in compounds containing two Chiral centers.
2. Students are able to use different reagents in organic synthesis.
3. Students should know details about P- block elements.

SECTION I: ORGANIC CHEMISTRY (24 L)

1. Stereochemistry (12 L)

Concept of isomerism, types of isomers, representation of organic molecules (Projection formulae), conformational isomerism in alkanes (Ethane, propane and n-butane) with energy profile diagrams, Geometrical isomerism - Definition, conditions for geometrical isomers, physical and chemical properties, E/Z nomenclature of geometrical isomers, Optical isomers, chirality, optical isomerism with one asymmetric carbon atom, specific rotation, enantiomerism, R/S nomenclature R/S system nomenclature with wedge and Fischer representation of two chiral centres, erythro, threo, meso-diastereomers with R/S configuration.

Ref. 1, 2, 3,

Ref. 2: Relevant pages from Sec. 3.2 – 3.5, Sec.4.1 – 4.20, Sec. 8.6

Ref. 3: Relevant pages from Sec. 12.1 – 12.2 (Pages 318 – 321)

2. Reagents in Organic Synthesis (12 L)

Catalytic hydrogenation including liquid phase hydrogenation, Birch reduction, NaBH4, $LiAlH_4$, Sn/HCl, Oxidation reagents: $KMnO_4$, $K_2Cr_2O_7$, Jones reagent, PCC, per acids, OsO_4, synthesis and application of EAA and Malonic ester

Ref. 1 & 3

SECTION II: INORGANIC CHEMISTRY (12 L)

1. Chemistry of P-Block Elements (12 L)

Position of elements in the periodic table, electronic configuration of elements, trends in properties like: atomic size, ionization potential, electro negativity, electron affinity, reactivity, oxidation state, anomalous behavior of first member of each group

Structure and Properties of - 1) Borates and Halides of Aluminium 2) Allotropes of Carbon 3) Oxyacids of Phosphorous and Sulphur 4) Interhalogen compounds

References:

1. Organic Chemistry-. Morrison and Boyd, 6th edition, prentice hall, 2001.
2. Stereochemistry of carbon compounds - E. L. Eliel
3. Reactions, rearrangements and reagents – S N Sanyal
4. Inorganic Chemistry-James Hughey
5. General Chemistry - Raymond Chang
6. Concise Inorganic Chemistry-J.D. Lee, 5th Edition-Relevant pages.
7. Concept & model of Inorganic Chemistry-Douglas Mc Daniels, 3rd edition.

CHEM1203: Chemistry Practical Course (4 Credits)

1. Physical Chemistry: 7 Experiments.

2. Inorganic Chemistry: 7 Experiments.

3. Organic Chemistry: 7 Experiments.

1. Physical Chemistry (Minimum 7 experiments)

1. Sketch the polar plot of S and P orbital's.
2. Plot the graph of following functions using excel / graph paper-
   a) Linear function b) Exponential function c) Logarithmic function
3. Assign the lattice structure of NaCl crystal by given data.
4. Determine the ionization potential of hydrogen atom using hydrogen spectrum.
5. Determine the gas constant R in various units by eudiometer method.
6. Determine the relative viscosity of given organic liquids by viscometer.
7. Determine ΔH and ΔS for the following chemical reactions

i) $Zn_{(s)} + CuSO_{4\,(aq)} \rightarrow Cu_{(s)} + ZnSO_{4\,(aq)}$

ii) $3Mg_{(s)} + 2\,FeCl_{3\,(aq)} \rightarrow 2\,Fe_{(s)} + 3\,MgCl_{2\,(aq)}$

8. Determine the heat of solution of KNO_3 / NH_4Cl

2. Inorganic Chemistry (Minimum 7 experiments)

1. Determine the hardness of water from a given water sample by EDTA method.
2. Analysis of mixed alkali by volumetric method.
3. Determine the number of water molecules of $BaCl_2.2H_2O$/ $MgSO_4.7H_2O$.
4. Standardization of NaOH solution and find the strength of given HCl solution.
5. Standardization of $KMnO_4$ solution and find the strength of given solution.
6. Inorganic Qualitative analysis (Four mixtures without phosphate and borate)

3. Organic Chemistry (Minimum 7 experiments)

1. Determine the amount of acetic acid in commercial vinegar volumetrically.
2. Determine amount of aspirin in APC tablet volumetrically.
3. Techniques: (Micro scale)
   i. Crystallization ii. Sublimation iii. Thin layer chromatography
4. Organic Qualitative analysis of single compound (at least one compound in each type):
   Type, Preliminary tests, and Physical constant

References:

1. Senior Practical physical chemistry, Khosala and Garg.
2. Experiments in Chemistry, D.V. Jahagirdar.
3. Textbook of qualitative analysis, A. I. Vogel 4th Edition
4. Textbook of practical organic chemistry, A .I. Vogel.

Department of Chemistry
M. Sc. I Chemistry (2019-2020)
Physical Chemistry Semester – I

CHP-4101: Fundamentals of Physical Chemistry-I (4 Credits, 48 L, 12 T)

SECTION - I

Thermodynamics, Quantum Chemistry and Polymer Chemistry (2 Credits, 24 L, 6T)

(A) Thermodynamics :(16 L)

1. **Recapitulation**: System and types of system, surrounding, state variables, Heat, work & Conservation of energy – The basic concepts, Zeroth law, First law, Work of compression & expansion, free expansion, expansion against constant pressure, reversible expansion. Heat: - heat capacity, enthalpy. State functions & differentials – State functions, changes in internal energy, temperature dependence of the internal energy, temperature dependence of the enthalpy. Work of adiabatic expansion – Irreversible adiabatic expansion, reversible adiabatic expansion.

(2L)

2. **The second law of Thermodynamics**: Measuring the dispersal the entropy. The second law, the definition of entropy, the entropy changes in the system, Entropy changes in the universe – The entropy change when a system is heated. Entropy changes in surroundings, The entropy of phase transition. The entropy of irreversible changes. Concentrating on the system – The Helmholtz and Gibbs function, Significances of Helmholtz function, Maximum work, Significances of Gibbs function. Evaluating the entropy & Gibbs function. The third law of thermodynamics, absolute entropies, standard molar Gibbs function.
(5L)

3. **Combining First & Second law**: Properties of Gibbs energy, The temperature dependence of the Gibbs energy. The pressure dependence of the Gibbs energy. Chemical potential of a perfect gas. The open system & changes of composition.
(3L)

4. **Changes of State I**: Physical Transformation of pure materials, The stabilities of phases, Phase equilibrium & phase diagrams. The solid – liquid boundary. The liquid - vapor boundary. The solid-vapor boundary.
(2L)

5 Changes of State II : Physical transformation of simple mixtures, partial molar quantities – Partial molar volume, Partial molar Gibbs function. The thermodynamics of mixing – the Gibbs function of mixing, thermodynamics mixing functions. The chemical potential of liquid-liquid mixture.
(2L)

6. Colligative properties – The common features, the elevation of boiling point, the depression of freezing point, solubility, osmosis and osmotic pressure. Mixtures of volatile liquids -vapor pressure diagram. Raoult's law, van't Hoffs factor
(2L)

(B) Quantum Chemistry: **(6L)**

Historical development of quantum theory, failure of classical mechanics, black body radiation, photo electric effect, Atomic spectra, wave particle duality, uncertainty principle, Schrodinger equation, particle in one dimensional box, hydrogen like atoms (No derivation), Postulates, HMOT- Ethylene, Propylene, Butadiene, Cyclobutadine .

(C) Polymer Chemistry: **(2L)**

Terms used- monomer, polymer, homopolymer, heteropolymer, processes of polymerization: addition and condensation. Molecular weight of polymer. Some important polymers,

p
r
o
b
l
e
m
s

SECTION-II

Chemical kinetics and reaction dynamics (2 Credits, 24 L, 6 T)

1. Recapitulation: The rate of reaction, rate laws and rate constants, the determination of rate, zero order, first order, second order reactions, half lives, fractional order reactions, order and molecularity, factors affecting the rate of reaction. **(2L)**

2**. Complex and simple reaction**: reactions approaching equilibrium, consecutive reactions, opposing reactions, chain reaction- explosion, photochemical reactions. **(2L)**

3. **Approximate methods to solve complex reactions**: The kinetics of complex reactions, the steady state approximations, pre equilibria approximation, Lindeman mechanism for unimolecular reactions. **(3L)**

4. **Methods of studying fast reactions**: flash photolysis, flow techniques, relaxation methods, pulse radiolysis. **(2L)**

5. Molecular reaction dynamics- collision theory-the basic calculations, the steric requirements, Diffusion control reactions- classes of reactions, diffusion and reactions, details of diffusion, Activated complex theory- the reaction coordinate and the transition state, the formation and decay of the activated complex, how to use the Eyring equation, thermodynamics aspects, reactions between ions in solution state. **(5L)**

6. Enzyme catalysts: Michaelis-Menten mechanism, limiting rate, Lineweaver Burk and Eadie plots, enzyme inhibition, competitive and non-competitive inhibition. **(4L)**

7. Molecular Thermodynamics: Molecular energy levels, Boltzmann distribution law, partition functions and ensembles, translational, rotational and vibrational partition functions of diatomic molecules, Obtaining energy, heat capacity, entropy free energy, equilibrium constants from partition functions, equipartition of energy, Maxwell-Boltzmann, Fermi-Dirac and Bose-Einstein statistics.

(6L)

References

1. Physical Chemistry- P.W.Atkin and De Paule 8th edition (2010)
2. Physical Chemistry-T. Engel and P. Reid, Pearson Education (2006)
3. Physical Chemistry and molecular approach- D. Mcquarie and J. Simon (University Science) (2000)
4. Physical Chemistry for Bilogical Sciences by Raymond Change (Universal books) (2000)
5. Physical Chemistry – Marron and Prouton
6. Physical Chemistry- G.M. Barrow, Tata McGraw Hill 1988
7. Quantum Chemistry- I. Levine 5th edition, Prentice Hall, 1999.
8. Quantum Chemistry- R. K. Prasad.
9. Physical Chemistry- Puri, Sharma, Pathania.
10. Chemical Kinetics- K.J. Laidler.
11. Thermodyanamics for Chemists- S.Glasstone.

Inorganic Chemistry Semester – I

CHI-4102: Molecular Symmetry & Chemistry of P-Block Elements (4 Credits, 48 L, 12 T)

SECTION - I

Molecular Symmetry & Its Application (2 Credits, 24 L, 6T)

A) Definitions & Theorems of Group Theory :
Introduction , defining properties of a group , Group multiplication table, some examples of group ,Subgroups, Classes **(2L)**

B) Molecular Symmetry and Symmetry Groups:
Symmetry elements and operations, Symmetry planes and reflections, the inversion centre, proper axes and proper rotations, improper axes and improper rotation, products of symmetry operations, equivalent symmetry, elements and equivalent atoms, general relations symmetry elements and symmetry operations, symmetry elements and optical isomerism, symmetry point groups, classes of symmetry operations, classification of molecular point groups. **(6L)**

C) Representation of Group :
Matrix representation and matrix notation for geometric transformation. The great Orthogonality theorem and its consequence, character table. (No mathematical part) **(4L)**

D) Group Theory & Quantum Mechanics:
Wave function as the basis for irreducible representation. **(4L)**

E) Symmetry Adapted Linear Combination :-

a) Projection operator & their use of construct SALC (Construction of SALC for sigma bonding for molecules belonging point groups : D_{2h}, D_{3h},D_{4h} ,C_{4v},Td,Oh , normalization of SALC) . **(5L)**

b) Molecular Orbital Theory : Transformation Properties of atomic orbital , MO's for sigma bonding AB_n molecules , Td, AB_4 & Oh AB_6 cases **(3L)**

References:

1. Symmetry in Chemistry: H. Jaffe' and M. Orchin (2002)
2. Group theory and its chemical application: P.K. Bhattacharya 2^{nd} edn. (1989) (Himalaya Publication)
3. Inorganic Chemistry: Shriver and Atkins, 4^{th} edn. (2003) Oxford.
4. Inorganic Chemistry: Verra Ready.
5. Concise inorganic Chemistry: F.A.Cotton.

SECTION-II
Chemistry of Main group elements (2 Credits, 24 L, 6 T)

1. **Hydrogen and its compounds**:
   Hydrides: Classification, electron deficient, electron precise and electron rich hydrides. PH_3 , SbH_3 , AsH_3 , Selenides, Tellurides **(2L)**

2. **Alkali and alkaline earth metals**:
   Solutions in non-aqueous MediaApplication of crown ethers in extraction of alkali and alkaline earth metals ,Cryptans. **(2L)**

3. **Organometallic Compounds of Li, Mg, Be**:
   Classification, Synthesis, Structure, Properties and Uses. **(3L)**

4. **Boron Group**:
   Boron Hydrides (Closo,Nido,Arachno,Hypo) , preparation, structure and Bonding with reference to LUMO,HOMO, interconversion of lower and higher boranes, Metalloboranes, Carboranes, Reactions of organoboranes . **(4L)**

5. **Carbon Group**:
   Allotropes of Carbon, C60 and compounds (fullerenes), Intercalation compounds of Graphite, Carbon nanotubes, synthesis, properties, structure-single walled, multi walled, applications. **(2L)**

6. **Organometallic compounds**
   Organometallic compounds of Si, Sn, Pb, Ga, As, Sb, Bi. Structures, synthesis, Reactions. **(3L)**

7. **Nitrogen Group**:
   Nitrogen activation, Boron nitride, Oxidation states of nitrogen and their interconversion, PN and SN Compounds, NOx and their redox chemistry. **(3L)**

8. **Oxygen Group**:
   Metal Selenides and Tellurides, oxyacids, and oxoanions of sulphur & nitrogen. Ring, Cage and Cluster compounds of p-block elements. Silicates, including Zeolites **(3L)**

9. **Halogen Group**:
   Interhalogens, pseudo-halogen, Synthesis, Properties and applications, Structure, Oxyacids and Oxoanions of Halogens, Bonding **(2L)**

References:

1. Inorganic Chemistry: Shriver & Atkins (4th edition 2003, Oxford)
2. Concise Inorganic Chemistry, J. D. Lee, Fourth Edn.(Chapman and Hall)
3. Inorganic chemistry: Principle of structures & reactivity, Hubeey, Keiter, Medhi, Pearson Education, 4^{th} Edn.(2007).
4. Inorganic Chemistry: Catherine Housecroft
5. Inorganic Chemistry: Messler & Tarr, Pearson Publishers 3rd Edition
6. Organometallic Chemistry-A Unified Approach: R. C. Mehrotra & A. Singh

Organic Chemistry

Semester - I

CHO-4103: Basic organic chemistry (4 Credits, 48L, 12 T)

SECTION -I

Structure, reactivity and Stereochemistry (2 credits, 24 L, 6 T)

1. **Structure and reactivity: (10 L)**
   a) Chemical bonding and basis of reactivity- Chemical bond, delocalization, conjugation, resonance, hyperconjugation, tautomerism, inductive effects.
   b) Acidity and basicity: various structural effects, hard and soft acid and base concept.
   c) Aromaticity: Benzenoid and non-benzenoid compounds, Huckels rule, antiaromaticity, Application to carbocyclic and heterocyclic systems, annulenes, azulenes, current concepts of aromaticity.

2. **Stereochemistry: (14 L)**
   a) Sterochemical principles, enantiomeric relationship, distereomeric relationship, R and S, E and Z nomenclature in C, N, S, P containing compounds, Prochiral relationship, stereospecific and stereoselective reactions, optical activity in biphenyls, spiranes, allenes.
   b) Conformational analysis of six member rings and their stabilities

SECTION-II

Organic reaction mechanism (2 credits, 24 L, 6 T)

1. **Organic reaction intermediates: (4 L)**
   Structure, stability and reactions of reactive intermediates, carbenes, nitrenes, carbocations, carbanions and free radicals.

2. **Substitution reaction:**
   a) Aliphatic nucleophilic substitution **(6 L)**
   SN1, SN2 mechanism, NGP by pi and sigma bonds, classical and non-classical carbocations, phenonium ions, norbornyl system, carbocation rearrangement in NGP, SNi mechanism, nucleophilic substitution in allylic,trigonal and vinylic carbon. Effect of structure, nucleophile, leaving group and solvent on rate of SN1 and SN2 reactions, ambident nucleophile and regioselectivity.

   b) Aromatic electrophilic substitution **(4 L)**
   Arenium ion mechanism, orientation and reactivity, energy profile diagram, ortho, para, ipso attack, orientation in other ring systems, six and five membered heterocycles with one hetero atom. Important reactions like Friedel crafts alkylation and acylation, Nitration, halogenation, formylation, chloromethylation, sulphonation, diazonium coupling.

   c) Aromatic nucleophilic substitution **(2 L)**
   SNAr, SN1, benzyne and SNR1 reactions, reactivity: effect of substrate structure, leaving group and attacking nucleophile, Chichibabin reaction.

   d) Addition reactions **(4 L)**
   Addition to C-C multiple bonds - mechanism and stereochemical aspects of addition reaction involving electrophile, nucleophile and free radicals, regio and chemo selectivity, orientation and reactivity, conjugate addition- Michael addition.

   e) Elimination reactions **(4 L)**
   E1, E2, E1cb mechanisms, orientation and stereochemistry in elimination reaction, reactivity effect of structure, attacking and leaving group, competition between elimination and substitution, syn eliminations.

References:

1. Organic Chemistry–by J. Clayden, N. Greeves, S. Warren and P. Wothers (Oxford)
2. Advanced Organic Chemistry –by J. March 6th Edition
3. Advanced Organic Chemistry (part A) –by A. Carey and R.J. Sundberg
4. Stereochemistry of carbon compound-by E.L. Eliel
5. Stereochemistry of organic compound-by Nasipuri
6. Guide book to Reaction Mechanism –Peter Sykes

Analytical Chemistry

Semester – I

CHA-4104: Safety in Chemical Laboratory and Good Laboratory Practices

(4 Credits, 48 L, 12 T)

SECTION -I

1. **History and importance of safety and health in Laboratory**
   Importance of Safety and security, responsibility and accounting for safety, types of hazards and risk in chemical laboratory, Moral legal and financial reasons. Introduction to different types of Hazards **(4L)**
   Ref. 1 Page 1-11

2. **Establishing Effective chemical safety and security management**
   Introduction, responsibility of laboratory safety and security, ten step to creating an effective laboratory chemical safety and security management safety **(2L)**
   Ref.1 Page 15-19

3. **Personnel protective and other safety equipments**
   Personnel clothing, foot protection, eye and face protection, safety shield, fire safety equipments, heat and smoke detector, respirators, safety showers, eye wash unit **(3L)**

   Ref. 1 Page 215-220

4. **Assessing routes of exposure for toxic chemicals**
   Inhalation, contact with skin and eye, ingestion, assessing risk with acute toxicology, specific chemical hazard, First aid for contact of different chemicals on skin, eyes, and inhalation ingestion. **(4L)**
   Ref. 1 Page 201-210.
5. **Assessing hazards and risk in the laboratory**
   Introduction, consulting source of information, evaluating the toxic risk of laboratory chemicals, assessing flammable, reactive and explosive hazards, Assessing physical hazards, assessing bio hazards **(7L)**
   Ref. 1 Page 73-90
6. **Managing Chemicals**
   Introduction, green chemistry for every laboratory, purchasing chemicals, inventory and tracking of chemicals, storage of chemicals, transfer, transport, shipment of chemicals. **(4L)**
   Ref. 1 Page 92-104

SECTION-II

1. **Working with Chemicals**

   Introduction, careful planning , general procedure for working with hazardous chemicals, working with substance of high toxicity, working with bio hazards material, working with flammable chemicals, working with highly reactive or explosive chemicals **(8L)**

   Ref. 1 Page 107-125

2. **Working with laboratory equipments**

   Introduction, working with electrically powered equipment, working with compressed gases, working with high and low pressure and temperatures. **(3L)**

   Ref. 1 Page 137-143

3. **Managing chemical waste**

   Introduction, identifying waste and its hazards, collecting and storing waste, treatment and hazard reduction, disposal options. **(5L)**

   Ref. 1 Page 152-161.

4. **Introduction to Good Laboratory Practices and its applications**

   General introduction, Drug development process and non-regulated vs. regulated area, GMP, Introduction to GLP and its applications, GLP Training, introduction, Fundamental points of GLP **(4L)**

   Ref. 2 Page 9-18

5. **Rules for conduct of studies**

   General aspects, Study plan of protocol, Content of the protocol, Identification, Approval of protocol, protocol amendment, Standard operating procedures, SOP system overview **(4L)**

   Ref. 2 Page 27-36

References:

1) Chemical Laboratory Safety and Security, A Guide Prudent Chemical Management Edited by Lisa Moran and Tina Masciangioli Available Online www.nap.edu (Free)

2) Hand Book, Good Laboratory Practice (GLP) Available Online (Free)

Physical Chemistry Practical

CHP-4105: - Physical Chemistry Practical (4 Credits,)

A) Conductometry: (Any Three)

1. Study the Hydrolysis of NH_4Cl or CH_3COONa or aniline hydrochloride.

2. Determination of equivalent conductance at infinite dilution and dissociation constant of acetic acid.
3. Study the second order velocity constant of the hydrolysis of ethyl acetate by sodium hydroxide.

4. Determination of ΔG, ΔH, and ΔS of silver benzoate by conductometry.

B) Potentiomerty: (Any Two)

1. Determination of stability Constant of a complex ion.

2. Determination of Solubility and solubility product of a sparingly soluble salt.

3. Estimation of amount of halides present in the mixture.

C) pH metry: (Any Two)

1. Determination of the acid and base dissociation constant of an amino acid and hence the isoelectric point of the acid.
2. Determination of dissociation constants of tribasic acid (phosphoric acid)

3. Determination of Hammett constant of o-, m-, p- amino/nitro benzoic acid.

D) Polarography: (Any One)

1. Determination of half wave potential (E1/2) and unknown concentration of an ion.

2. Amperometric titration of $Pb(NO_3)_2$ with $K_2Cr_2O_7$.

E) Colorimetry/Spectrophotometry: (Any Three)

1. Simultaneous determination of cations from the mixture.

2. Determination of amount of copper by photometric titration with EDTA.

3. Study the kinetics of iodination of acetone spectrophtometrically.

4. Determination of indicator constant of given indicator by spectrometric scanning and recording the absorbance in UV-Visible region.

F) Radioactivity: (Any One)

1. Determination of plateu voltage, dead time and counting errors of G.M. Counter.

2. Determination of E_{max} of the β radiation and absorption coefficients in Al.

G) Chemical Kinetics: (Any Three)

1. Study of Kinetic decomposition of diacetone alcohol by dilatometry.
2. Determination of individual orders of iodide and persulphate ions and overall order of oxidation reaction of iodide ion by persulphate ion.
3. Investigation of influence of ionic strength on rate constant (Brönsted primary salt effect).
4. Determination of temperature coefficient and energy of activation of acid catalyzed ester hydrolysis reaction.

H) Non-Instrumental: (Any Three)

1. Determination of glycerol radius by viscosity.
2. Determination of partial Molar Volume and the densities of a series of solutions and to calculate the molar volumes of the components.
3. Determination of molecular weight by steam distillation.
4. Determination of freezing point curve and composition of mixture of naphthalene and biphenyl.
5. Investigation of stability of three component system and hence draw a tie line on bimodal curve.

References:

1. Practical physical chemistry, A. Findlay, T.A. Kitchner (Longmans, Green and Co.)
2. Experiments in Physical Chemistry, Wilson, Newcombe, Denko. Richett (Pergamon Press)
3. Senior Practical Physical Chemistry, B.D. Khosla and V.S. Garg (R. Chand and Co., Delhi.).
4. Experimental Physical Chemistry by D. P. Shoemaker, Mc. Growhill, 7th Edition, 2003.
5. Physical chemistry by Wien (2001)
6. Practical physical chemistry, B. Vishwanathan and P.S. Raghavan, 2nd edition, (2012)
7. Practical Physical Chemistry, J.B. Yadav
8. Essentials of practical Physical Chemistry, Rajboj and Chandhekar
9. Practical Physical Chemistry, Athawale and Mathur.

Organic Chemistry Practical

CHO-4106: Organic Chemistry Practical (4 Credits)

A) Three component mixture separation and analysis using ether.
(Minimum 8 mixtures including amino acid)

B) Synthesis, Purification and Characterization (minimum 8 preparations)

1) 2-Methoxy naphthalene to 1-formyl-2- methoxy naphthalene
2) *o*-Phenylene diamine to Benzimidazole
3) Anthranilic acid to 2-iodo /2-choro benzoic acid
4) Vanillin to vanillyl Alcohol
5) Benzil to benzilic Acid
6) Benzyl cyanide to phenyl acetic acid
7) Benzaldehyde to chalcones using green method
8) Glycine to benzoylglycine
9) Nitrobenzene to m-di-nitrobenzene
10) m-di-nitrobenzene to m-nitroaniline
11) Benzoic acid to ethylbenzoate
12) Diel's Alder reaction of anthracene and maleic anhydride
13) 4-nitrotoulene to 4-nitrobenzoic acid

Reference:

1. Textbook of practical organic chemistry – A.I. Vogel

Physical Chemistry Semester – II

CHP-4201: Fundamentals of Physical Chemistry-II (4 Credits, 48 L, 12 T)

SECTION - I

Molecular Spectroscopy (2 Credits, 24 L, 6 T)

1. **Recapitulation**: Fourier transforms, Regions of spectrum, factors affecting the width and intensity of spectral lines. **(1L)**

2. **Microwave spectroscopy**: rotation spectra of di and poly atomic molecules- rigid and non-rigid rotor, effect of isotopic substitution, Problems **(3L)**

3. **Infra red spectroscopy** : Harmonic and anharmonic oscillator, vibrational spectra of di and poly- atomic molecules, coarse and fine structure, Nuclear spin effect, applications. **(5L)**

4. **Raman Spectroscopy**: Introduction, Rotational Raman- spectra, Vibrational Raman Spectra, polarization of light and Raman effect, structure elucidation from combined Raman and IR spectroscopy, application. **(5L)**

5. **Electronic spectroscopy of molecules**: Born – Oppenheimer approximation, electronic spectra of diatomic molecules, vibrational coarse structure, rotational fine structure, dissociation energy and dissociation products, electronic structure of diatomic molecules, molecular photoelectron spectroscopy, frank condom principle, application. **(6L)**

6) **ESR and Mossbauer spectroscopy**: Principle and applications. **(2L)**

7) **NMR** – Principle and Chemical applications of ^{1}HNMR in structure elucidation. **(2L)**

References:

1. Fundamentals of molecular spectroscopy: C.N. Banewell and E.Mc. Cash (Fourth edition).

2. Molecular Spectroscopy: P.S. Sindhu, New Age international Publication.(Second edition)

3. Molecular Spectroscopy: Suresh Chandra, Narosa Publication House (2009)

SECTION-II

Nuclear and Radiation Chemistry (2 Credits, 24 L, 6 T**)**

1. **Radioactivity**: recapitulation – type of radioactive decay, Decay Kinetics, Detection and measurement of nuclear radiation (G. M. & Scintillation counter) Problems **(3L)**

2. **Elements of radiation chemistry** – Radiation chemistry, interaction of radiation with matter, passage of neutrons through matter, interaction of γ radiation with matter, Units for measuring radiation absorption, Radiation dosimetry, Radiolysis of water, free radicals in water radiolysis, Radiolysis of some aqueous solution. Problems
(6L)

3. **Nuclear Reactor**: - The fission energy, The Natural uranium reactor, the four factor formula- The reproduction factor K, the classification of reactor. Reactor power, Critical size of thermal reactor, excess reactivity & control, the Breeder reactor, The Indians nuclear energy programme, Reprocessing of spent fuel, Recovery of Uranium & Plutonium, Nuclear waste management, Natural nuclear reactor.
(6L)

4. **Isotopes for nuclear reactors.** Isotope separation, Enrichment factor, various methods for separation of selected isotopes, **(3L)**

5. **Applications of radioactivity**: Typical reaction involved in preparation of radio isotopes: ^{3}H, ^{14}C, ^{22}Na, ^{32}P, ^{35}S and ^{127}I. General Principles of using radioisotopes as a tracers. Physico-chemical applications: Determination of diffusion coefficient, surface area and solubility. Analytical applications: Neutron activation analysis (NAA), Isotope dilution analysis (IDA), radiometric titration (RT). Industrial applications: radiation gauging, friction and wear out, gamma radiography. Problems
(6L)

References:

1. Elements of Nuclear chemistry – H.J. Arnikar, fourth edition wiley Estern Ltd.

2. Source book of atomic energy – S. Glasston, D. Van Norton Company

3. Chemical applications of radioisotopes – H.J. M. Brown Buffer & Jammer Ltd.

Inorganic Chemistry Semester – II

CHI- 4202: Coordination and Bioinorganic Chemistry (4 Credits, 48 L, 12 T)

SECTION - I

Coordination Chemistry (2 Credits, 24 lectures, 6 T)

1. **Concept & Scope of Ligand Fields:**
   Recapitulation of CFT, Free ion Configuration, Terms and States, Energy level of transition metal ions, free ion terms, term wave functions, spin-orbits coupling. **(4L)**
2. **Ligand field theory of coordination complexes:**
   Effect of ligand field on energy level of transition metal ions,weak cuabic ligand field effect on Russell-Saunders terms, strong field effect, correlation diagrams, Tanabe Sugano diagrams, spin pairing energies**.** **(7L)**
3. **Electronic spectra of Transition Metal Complexes:**
   Introduction, Band intensities, band energies, band width and shapes, spectra of 1^{st}, 2^{nd} and 3^{rd} row ions and rare earth ion complexes, spectrochemical and Nephlauxetic series, charge transfer and luminescence, spectra, calculations of Dq, B, β parameters. **(7L)**
4. **Magneto Chemistry**
   Origin magnetism, types of magnetism, Curie law, Curie-Weiss Law, Magnetic properties of complexes-paramagnetism 1st & 2nd Ordered Zeeman effect, quenching of orbital angular momentum by Ligand fields, Magnetic properties of A, E & T ground terms in complexes, spin free spin paired equilibria**.**
   (6L)

References:

1. Ligand field theory & its applications: B.N. Figgis & M.A. Hitachman (2000) Wiely VCH Publ.
2. Symmetry and spectroscopy of molecules, Second Ed^{n}, by K. Veera Reddy, New Age International Publication, 2009.
3. Elements of magnetochemistry, R. L. Datta and Syamal, Second Ed^{n}, Afiliated East West Press Pvt. Ltd. 2007.

SECTION-II

Bioinorganic Chemistry (2 Credits, 24 Lectures, 6 T)

1. Introductions of Bioinorganic chemistry **(1L)**
2. Principles of coordination chemistry related to Bioinorganic chemistry research and protein, Nuclic acid and other metal bonding biomolecules. **(7L)**
3. Biochemistry of Na, K and Ca with respect to Na/K pumps, Calmodulin and blood coagulation. **(8L)**
4. Biochemistry of following elements:
   a) Iorn: Ferritin, Transferrin, Ferredoxin, Rubreddoxin, Porphyrin based system **(6L)**
   b) Manganese: Photosynthesis **(2L)**

References:

1. Principle of Bioinorganic chemistry: S. J. Lippard and J.M. Berg
2. Bioinorganic chemistry: Inorganic elements in chemistry of life W. Kain and B. Schwederski
3. Bioinorganic chemistry: Bertini, Grey, Lippard and Valentine
4. Bioinorganic chemistry: R. J. P, Willams
5. Bioinorganic chemistry: Robert Hay
6. Bioinorganic chemistry: M. N. Hughes

Semester – II

CHO-4203: Synthetic organic chemistry and spectroscopy (4 Credits, 48 L, 12T)

SECTION – I

A) Synthetic Organic Chemistry (2 Credits, 24 L, 6 T)

1. **Oxidation reactions: (6 L)**
   CrO_3, PDC, PCC, $KMnO_4$, MnO_2, Swern, SeO_2, $Pb(OAc)_4$, Pd-C, OsO_4, m-CPBA, O_3, $NaIO_4$, HIO_4, DDQ, Oppenauer oxidation.
2. **Reduction reactions: (4 L)**
   Boranes and hydroboration reactions, MPV reduction, reduction with H_2/Pd-C, Willkinsons catalyst, DIBAL, Wolff Kishner reduction, Birch reduction, $NaCNBH_3$
3. **Molecular Rearrangements: (6 L)**
   Beckmann, Schmith, Wolff, Lossen, Bayer-villiger, Sommelet, Favorskii, Benzil-benzilic acid, Fries, Claisen, Cope, Brook, Benzidine, Pummener rearrangement
4. **Ylides: (4 L)**
   Phosphorus, Nitrogen and Sulphur ylides- synthesis and their reactions.
5. **Addition to carbonyl group: (4 L)**
   Grignard, organo zinc, organo copper, organo lithium, reagents to carbonyl and unsaturated carbonyl compounds.

SECTION-II:

B) Spectroscopy (2 Credits 24 Lectures, 6T)

1. **UV:**
   Factors affecting UV absorption and interpretation of UV spectra of aromatic compounds **(4 L)**
2. **IR:**
   Principal, Basic Important functional group frequencies, factors affecting IR frequencies, interpretation of IR spectra **(4 L)**
3. **^{1}H NMR: (8 L)**
   Fundamentals of ^{1}H NMR, factors affecting chemical shift, integration, coupling (1st order analysis)
4. **Introduction to CMR: (4 L)**
   Natural abundance, chemical shift values, proton coupled and proton decoupled spectra, DEPT
5. **Mass spectrometry: (4 L)**
   Principal, Instrumentation, Terminologies, Rules of fragmentation, McLafferty rearrangement, Rule of 13, fragmentation pattern of some important functional groups.

References:

1. Organic Chemistry – J. Clayden, N. Greeves, S. Warren and P. Wothers (Oxford)
2. Modern Synthetic reactions- H.O. House
3. Organic Synthesis – M.B. Smith
4. Advanced Organic Chemistry (part A & B)– A. Carey and R.J. Sundberg
5. Stereochemistry conformations and mechanism by P.S. Kalsi
6. Organic chemistry –by Cram, Hammond, Pine and Handrickson
7. Introduction to spectroscopy – D.l. Pavia, G.M. Lampman, G.S. Kriz, 3rd Edition
8. Spectroscopic methods in organic melecules – D.H. William & I Flemming Mc Graw Hill
9. Mechanism and Structure in Organic Chemistry - E.S. Gould

Analytical Chemistry
Semester II
CHA-4204: General Chemistry (Any two parts) (4 Credits, 48 L, 12 T)

Part A-Modern Separation Methods and Hyphenated Techniques (2 Credits, 24 L, 6 T)

1. **Mass Spectrometry**

Principle, Instrumentation, Ionization methods- Electron bombardment ionization, Arc and spark ionization , Photo-ionization, Thermal ionization, Chemical ionization, Mass Analyzer-Magnetic, Double focusing, Time of flight, Quadrupolar, Ion cyclotron resonance analyzer, Correlation of mass spectra with molecular structure and molecular weight, Isotopic Abundances, Fragmentation patterns, Quantitative analysis, Applications and Problems, Fourier transform mass spectrometry, Tandem mass spectrometry, Inductively coupled plasma-mass spectrometry. **(8 L)**

Ref. 1, Pages 647-696; Ref.2 Pages 465-506

2. **Gas Chromatography**

Theory and Instrumentation of GC, Sample injection –Split and split less injection, Column types, Solid/Liquid Stationary phases, Column switching techniques, Basic and specialized detectors, elemental detection , Chiral separations, Gas chromatographs and chemical analysis, Interfacing of gas chromatography with mass spectrometry, Application of GLC, Use of GC-MS, High speed chromatography, Gas solid chromatography and Problems. **(8 L)**

Ref.2, Pages 540-569; Ref.3 Pages 125-143, Ref.4 Pages 947-970

3. **High Performance Liquid Chromatography (HPLC)**

Theory and instrumentation of HPLC, Optimization of column performance, Gradient elution and related procedure, Derivatization, Mobile phase Delivery System, Sample injection, Separation column, Detector, Interfacing HPLC With Mass spectrometry, Structure types of column packing, Adsorption Chromatography, Bonded phase chromatography, Reversed phase chromatography, Ion Pair Chromatography, Ion exchange Chromatography, Size Exclusion Chromatography, GC-MS and LC – MS, Applications and problem. **(8 L)**

Ref.2 Pages 580-650, Ref.4 Pages 974-992

References:

1. Introduction to Instrumental Analysis, R.D. Braun, Mc Graw-Hill. Inc.1987
2. Instrumental Methods of chemical Analysis, H.H. Willard, L.L. Merrite Jr.,J.A.Dean & F.A. Settle Jr.,6th Edition, Wadsworth Publishing Company, USA ,1986
3. Handbook of Instrumental Techniques for Analytical Chemistry, F.A. Settle editor, Prentice Hall Inc. A Simon and Schuster Company , New Jersey, 1997
4. Fundamentals of Analytical Chemistry , D.A. Skoog, D.M. west, F.J. Holler, S.R. Crouch,7th Edition , Thomson Asia Pte. Ltd, Singapore, 2004

Part-B: Basic Biochemistry (2 Credits, 24 L, 6 T)

1. **Introduction to Biochemistry**: Scope of the subject in pharmaceutical sciences, Biochemical reactions, Highlights of prokaryotic and Eukaryotic cell metabolism.

2. **Biochemical Morphology**: Prokaryotes and Eukaryotes, Cell structure, sub-cellular components: Nucleus, plasma membranes, endoplasmic reticulum, Lysosome, Peroxisomes, Golgi apparatus, and Mitochondria.

3. **Biomembrane**: Structure, functions and composition, Model proposed , Function and properties of membrane, Transport hypothesis, Active and passive facilitated transport, Na+, K+, H+, pumps, glucose transport, Excitable membrane, drug transport.

4. **Biomolecules:** Proteins*:* Introduction, functional, classification of amino acids, classification, physicochemical properties, Optical activity, Reaction with ninhydrin, Formaldehyde, Amino acids, Essential and non essential amino acids, efficacy, structure, peptide bond, end group analysis, Helix, B-sheet structure, tertiary, quaternary structure, globular protein, fibrous protein, amino acid therapy, Protein engineering Carbohydrates: complex carbohydrate, structure of Chitin, Starch, Glycogen +Metabolism
   Lipids: definition, classification, functions, types of fatty acids, and its biological role and metabolism.

5. **Enzymes**: Introduction, classification according to the reaction catalysis and source) structure of enzyme, co factures, active sites, Binding sites, Km, Vmax, Enzyme kinetics, Double reciprocal plot, effect of substrate, pH ionic strength, Concentration, Temperature on the rate of enzyme reactions, Enzyme inhibition(competitive, uncompetitive, noncompetitive and irreversible), Enzyme biotechnology. Manufacturing of medicinal compounds by enzymatic reactions, Penicillin acylase for the production 6-APA, Therapeutical uses of enzymes.

References:

1. Principals of biochemistry, Albert Lehninger (CBS Publisher and Distributers Pvt. Delhi.
2. Biochemistry Lubert Stryer, W. H. (Freeman and company New York)
3. Harper's Biochemistry by R.K. Murray, D. I. Granner, P. A. Mayes, (Prentice Hall International Inc.)
4. Practical Clinical Biochemistry, Harold Varley, (CBS Publisher and Distributers Pvt. Delhi.
5. Molecular Biology, J.D. Watson (The Benjamin/ Cumming Company, Inc.)

Part C- Concepts of Analytical Chemistry (2 credits, 24L, 6T)

1. **Data handling and spreadsheets in analytical chemistry**
   Accuracy and precision, Classification of error, Significant figures, Rounding off, Ways of expressing accuracy, mean, deviation, average deviation, Relative mean deviation, average deviation, confidence limit, test of significance, rejection of results and problems. **(8L)**
   Ref. 2:65-99
2. **Sampling , standardization and calibration**
   Analytical samples and methods of sampling, sample handling, Gross sample, preparation of laboratory samples, automated sample handling comparison with standard and problems. **(8L)**
   Ref. 1:175-200
3. **Introduction to analytical separations**
   Separation by precipitation, Separation of species by distillation, Separation by extraction, Separation by ion exchange chromatography, problems. **(8L)**
   Ref. 1:906-946

References

1) Fundamentals of analytical chemistry D.A.Skoog, D.M.West, F.J.Holler, S.R.Crouch, 5th edition , Thomas Asia Pvt. Ltd ,Singapore 2004.
2) Analytical chemistry, G.D. Christian, 6th edition

Part- D: Industrial Methods of Analysis (2 Credits, 24 L, 6 T)

1. **Chemometrics:**
   Concentration of solution based on volume and mass unit, calculations of ppm , ppb and dilution of the solutions , Concept of mole, Stoichiometry of chemical reactions, Concept of gram mole, Limiting reactants, theoretical and practical yield, solubility and solubility equilibria. Concept of formation constant, Stability and instability constants, stepwise formation constants and Numerical problems. **(10 L)**

2. **Quality in Analytical Chemistry**
   Quality systems in chemical laboratories, cost and benefits of quality system, types of quality standards for laboratories, total quality management, quality audits, and qualities reviews , responsibility of laboratory staff for quality and problems. **(6 L)**

3. **Process Instruments and Automated Analysis**
   Introduction, industrial process analyzer, methods based on bulk properties, continuous online process control, automatic chemical analyzers, automatic elemental analyzers, Numerical problems. **(8 L)**

R**ef 3: Pages: 786-828.**

References:

1. Vogel's Text book of Quantitative Analysis.
2. Analytical Chemistry, G.D. Christian, 6 th Edition.
3. Instrumental Methods of Chemical analysis, H. H. Willard, L. L. Merritt Jr., J. A. Dean & F. A. Settle Jr., 6th Edition, Wadsworth Publishing Company, USA,1986

Inorganic Chemistry Practical

CHI-4205: INORGANIC CHEMISTRY PRACTICALS. (4 credits)

1. **Ore Analysis:-(Any 2)**
   a) Determination of Silica & Manganese from Pyrolusite ore.
   b) Determination of Silica & Iron from Hematite ore.
   c) Determination of Copper & Iron from Chalcopyrite ore.

2. **Alloy Analysis :- (Any 2)**
   a) Determination of Tin & lead from Solder alloy
   b) Determination of Iron & Chromium from Stainless steel alloy.
   c) Determination of Copper & Nickel from Cupronickel alloy.

3. **Inorganic synthesis & purity .(Any 6)**
   a) Chloro penta- amine cobalt (III) chloride.
   b) Nitro penta -ammine cobalt (III) chloride.
   c) Nitrito penta- ammine cobalt (III) chloride.
   d) Cis Potassium diaquo dioxalato Chromate (III).
   e) Trans Potassium diaquo dioxalato Chromate (III) .
   f) Potassium tri-oxalato Aluminate .
   g) Tris (acetylacetanato) Mangnese (III).
   h) Bis (acetylacetanato) Copper (II)
   i) Tris (Ethylenediamine) Nickel (II) thiosulphate.

4. **Inorganic Chracterization Techniques :- (Any 1)**
   a) Solution state preparation of $[Ni(en)_3]S_2O_3$, $[Ni(H_2O)_6]Cl_2$, $[Ni(NH_3)_6]Cl_2$. Record absorption spectra in solution of three complexes & analyze it . Arrange three ligands according to their increasing strength depending on observation.
   b) Determination of Magnetic Susceptibility of Mercury tetracynato Cobalt or $[Fe(acac)_3]$ or Ferrous ammonium sulphate by Faraday or Gouy method .

5. **Synthesis of Nanomaterials :-(Any 2)**
   a) Synthesis of nanosize ZnO ,its characterization by UV-Visible Spectroscopy & Removal of dye by ZnO – Photocatalysis.
   b) Synthesis of nanosized α -Fe_2O_3 & Study of adsoption of Phosphate on it.
   c) Synthesis of CdS nanoparticles.
6. **Synthesis & Chracterization :- (Any 1)**
   a) Synthesis & Photochemistry of $K_3[Fe(C_2O_4)_3]3H_2O$
   b) Kinetics of substitution reaction of $[Fe(Phen)_3]^{2+}$

References:

1) Text book of Quantitative Analysis, A.I. Vogel 4^{th} edn (1992)
2) Electronic Spectroscopy by A.B. P. Lever.
3) Inorganic Synthesis (Vol. Series).
4) Practical Manual made by Department of Chemistry, University of Pune.

CHA-4206: -Analytical Chemistry Practical (4 Credits,)

A. Table work: (Any Three)

1. Statistical treatment of experimental data.
2. Analysis of crystal structure from single crystal X-ray pattern.
3. Data analysis, error analysis, least square method.
4. Analysis of given spectra.

B. Use of Chemistry Software: (Any Two)

1. Chem Office: Draw the Structures of simple organic compounds and find out IUPAC name,

   Convert structure to name and predict ^{1}HNMR and ^{13}CMR.

2. ACD/ NMR processor: Convert FID file in spectrum, how to integrate, how to find J value.
3. Endnote: How to add references to word file.

C. Volumetric Analysis: (Any Two)

1. Determination of ibuprofen using acid-base titration.
2. Determination of percentage purity of indomethacin by acid – base titration.
3. Analysis of Vitamin C in juices and squashes.

D. Conductometry: (Any Four)

1. Determination of concentrations of strong acid and weak acid present in the mixture by titration with strong base.
2. Determination of critical micelle concentration (CMC) and ΔG of micellzation of sodium dodecyl sulphate (SDS).
3. Verification of Debye Huckel theory of ionic conductance for strong electrolytes KCl, $BaCl_2$,

   K_2SO_4, $K_3[Fe(CN)_6]$

4. Structural determination of metal complexes by conductometric measurements.
5. To study complex formation between Fe(III) with sulphosalicylic acid by conductometry.
6. Determination of the strength of commercial phosphoric acid / vinegar by conductometric titration.

E. Potentiomerty: (Any Two)

1. Determination of concentrations of strong acid and weak acid present in the mixture by titrating with strong base.
2. Determination of concentrations of reductant or oxidant by redox titration.
3. Complexometric determination using disodium EDTA of Co^{2+}, Al^{3+} and Cu^{2+}

F. Colorimetry/Spectrophotometry: (Any Four)

1. Estimation of phosphate from waste water by calibration curve method.
2. Determination of equilibrium constant of M-L system such as Fe(III) – Sulphosalicylic acid by

   Job´s continuous variation method.

3. Determination of equilibrium constant of M-L system such as Fe(III) – resorcilic acid by Mole ratio method.
4. Determination of iron by solvent extraction technique in a mixture of Fe(III) + Al(III) or Fe(III) + Ni(III) using 8- hydroxyquinoline reagent.

5. Determination of Cu(II) by solvent extraction as Dithiocarbamate / 8- hydroxyquinoline complex.

6. Study of kinetics of iodination of acetone spectrophotometrically.

G. Ion Exchange Chromatography: (Any two)

1. Separation of mixture of Zn (II) and Cd (II) using Amberlite IRA 400 anion exchanger and quantitative estimation of separated ions Zn(II) and Cd (II).

2. Separation of mixture of Zn (II) and Mg (II) using Amberlite IRA 400 anion exchanger and quantitative estimation of separated ions Zn(II) and Mg (II).

3. Separation and estimation of Fe and Al on cation exchanger.

H. Flame photometry: (Any One)

1. Estimation of Ca in milk powder sample by flame photometry.

2. Determination of concentration of Na^+ and K^+ in oral rehydration sachet by flame photometry.

References:

1. Lab Manual: Selected experiments of Pharmaceutical Analysis, Aness A Siddiqui.

2. Experimental physical chemistry, Athawale, Mathur, New age Int. Publishers.

3. Textbook of quantitative analysis A.I. Vogel 4^{th} Edition.

4. Experiments in Chemistry, D.V. Jahagirdar .

5. General Chemistry Experiments,Anil J. Elias University Press.

6. Ligand Field Theory, B.N. Figgis

7. Practical physical chemistry, A. Findlay, T.A. Kitchner (Longmans, Green and Co.)

8. Senior Practical Physical Chemistry, B.D. Khosla and V.S. Garg (R. Chand and Co., Delhi.)

9. Practical physical chemistry, B. Vishwanathan and P.S. Raghavan, 2nd edition, (2012)