Deccan Education Society's

FERGUSSON COLLEGE, PUNE

AUTONOMOUS COLLEGE

SYLLABUS
First Year M. Sc.
[Analytical Chemistry]

Semester - I

[Academic year 2016-2017]

Deccan Education Society's

FERGUSSON COLLEGE, PUNE – 411004

Department of Chemistry

[Autonomous College]

Two Years M. Sc. Degree Course in Chemistry

[Implemented from Academic Year 2016-2017]

M. Sc. Part I Analytical Chemistry Course Structure under CBCS (Autonomy)

Course Structure:

Semester	Course Code	Title of Paper	Theory Credits	No. of Lectures / Practicals
Semester I	CHA4101	Fundamentals of Physical Chemistry	4	60
	CHA4102	Molecular Symmetry and Chemistry of Main Group Elements	4	60
	CHA4103	Fundamentals of Organic Chemistry	4	60
	CHA4104	Safety in Chemical Laboratory and Good Laboratory Practices	4	60
	CHA4105	Analytical Chemistry - Practical Course - I	4	15 Practicals
	CHA4106	Analytical Chemistry - Practical Course - II	4	15 Practicals
	CHA4107	Self-Learning Course - I Chemistry of Life -Biomolecules	1	15
Semester I : Credits			**25**	

Term / Semester	Name of the Paper	Title of Paper	Theory Credits	No. of Lectures / Practicals
Semester II	CHA4201	Advanced Physical Chemistry	4	60
	CHA4202	Coordination and Bioinorganic Chemistry	4	60
	CHA4203	Synthetic Organic Chemistry and Spectroscopy	4	60
	CHA4204	Modern Separation Methods and Chemometrics	4	60
	CHA4205	Analytical Chemistry - Practical Course - III	4	15 Practicals
	CHA4206	Analytical Chemistry - Practical Course - IV	4	15 Practicals
	CHA4207	Self-Learning Course - II Environmental Toxicology and Chemistry	1	15
Semester II : Credits			**25**	

M. Sc. Course in Analytical Chemistry:

Semester	Course Code	Title of the Course	No. of Credits
I	XHR0001	Human Rights - I	1
	XCS0002	Introduction to Cyber Security - I / Information Security - I	1
	XSD0003	Skill Development - I	1
II	XHR0004	Human Rights - II	1
	XCS0005	Introduction to Cyber Security - II / Information Security - II	1
	XSD0006	Skill Development - II	1

Semester I
CHA4101: Fundamentals of Physical Chemistry
SECTION I (2 Credits, 30 L)

1. **Thermodynamics** **(17 L)**
   (a) Fundamental concepts of thermodynamics: Heat, work, internal energy and first law of thermodynamics

   (b) Entropy, Change in entropy, the entropy changes in the system, natural events. Enthalpy, the enthalpy changes in system and surroundings. The Helmholtz & Gibbs function, maximum work. The third law of Thermodynamics, Third law entropies standard molar Gibbs function

   (c) Chemical equilibrium: The temperature dependence of the Gibbs functions. The pressure dependence of the Gibbs functions. Calculating Gibbs energy of mixing, expressing Chemical equilibrium in an ideal gas mixture in terms of μ_i

   (d) Changes of State: Physical Transformation of pure materials. The stabilities of phases, Phase equilibrium & phase diagrams. The solid – liquid boundary. The liquid - vapor boundary. The solid-liquid-vapor boundary. Physical transformation of simple mixtures, partial molar quantities, the thermodynamics of mixing, the chemical potential of liquid-liquid mixture.

Objectives:
1. To state different Laws of Thermodynamics and describe its significance.
2. To calculate the standard entropy change (ΔS_o) for a physical or chemical process given standard entropy values, S_o for reactants and products.
3. To predict the spontaneity of physical and chemical changes using the Second Law of Thermodynamics.
4. To describe the change in free energy of the system for a physical or chemical process in terms of the changes in enthalpy and entropy of the system.
5. To describe the meaning of a positive value, a negative value, and a value of zero, for ΔG (ΔGo).
6. To use the equation, $\Delta G_o = -RT\ln K$, calculate equilibrium constants or standard free energy changes
7. Understand and apply the principles of gas behavior in ideal situations.
   Understand and apply the principles of chemical equilibrium

2. **Molecular thermodynamics:** **(6 L)**

   (a) Molecular energy levels, Boltzmann distribution law, partition functions
   (b) Maxwell-Boltzmann, Fermi-Dirac and Bose-Einstein statistics.

Objectives:
1. Explain statistical physics and thermodynamics as logical consequences of the postulates of statistical mechanics;
2. Apply the principles of statistical mechanics to selected problems
3. Apply the relevant equilibrium ensemble in a given situation
4. Derive partition functions for the various ensembles
5. Obtain ideal gas and chemical equilibrium properties from partition functions

3. Quantum Chemistry (7 L)

(a) Historical development of quantum theory failure of classical mechanics, black body radiation, photo electric effect, specific heats of solids, Atomic spectra, wave particle duality, uncertainty principles,

(b) Schrodinger equation, free particle, particle in one dimensional box,

(c) Hydrogen like atoms (No derivation), atomic orbitals.

Objectives:

1. The differences between classical and quantum mechanics
2. The connection of quantum mechanical operators to observables
3. To study Probabilities, averages, expectation values, and observables of quantum mechanics
4. The connection between common approximation methods and standard chemical frameworks (Born-Oppenheimer approximation, molecular orbitals, for example)
5. Gain an understanding of the historical importance of Bohr's model of the hydrogen atom, its strengths and weaknesses, and how it differs from the Schrödinger equation description of the hydrogen atom.
6. Be able to discuss and interpret experiments displaying wavelike behavior of matter, and how this motivates the need to replace classical mechanics by a wave equation of motion for matter (the Schrödinger equation).
7. Understand the central concepts and principles of quantum mechanics: the Schrödinger equation, the wave function and its physical interpretation, stationary and non-stationary states, time evolution and expectation values.
8. Interpret and discuss physical phenomena in light of the uncertainty relation.

SECTION II (2 Credits, 30 L)

1. Elementary Chemical kinetics and reaction dynamics (22 L)

(a) Introduction to kinetics: The rates of reaction, reaction rate, rate laws & rate constants, the determination of the rate law, first order, second order reactions, half lives, fractional order reactions

(b) Accounting for rate laws, simple reactions, the temperature dependence of reaction rates, reactions approaching equilibrium, consecutive reactions, the steady state approximations, preequilibria, unimolecular reactions.

(c) Reaction dynamics: chain reaction- explosion, photochemical reactions, fast reactions-flash photolysis, flow techniques, relaxation methods.

(d) Molecular reaction dynamics- collision theory-the basic calculations

(e) Theories of reaction rates- 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 (Bronsted primary salt effect).

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

Objectives:

1. To describe how rate laws are determined
2. To describe the relationship between the order of a reactant and the stoichiometric coefficient for the reactant in the overall balanced chemical equation.
3. To state the basis for the "Collision Model of Chemical Kinetics".
4. To describe the relationship between the rate of a chemical reaction and the frequency with which reactant molecules collide.
5. To describe why reactant molecules must have a certain minimum amount of kinetic energy when they collide in order for a chemical reaction to occur.
6. To describe how the collision frequency, kinetic energy and orientation of colliding reactant molecules affect the rate of a chemical reaction.
7. To describe "activation energy".
8. To use the Collision Model of Chemical Kinetics to describe how changes in concentration or temperature affect rates of chemical reactions.
9. To describe how a catalyst increases the rate of a chemical reaction.
10. The application of mathematical tools to calculate thermodynamic and kinetic properties
11. The relationship between microscopic properties of molecules with macroscopic thermodynamic observables
12. The derivation of rate equations from mechanistic data
13. The use of simple models for predictive understanding of physical phenomena associated to chemical thermodynamics and kinetics
14. The limitations and uses of models for the solution of applied problems involving chemical thermodynamic and kinetics

2. Physico-Chemical Techniques **(8 L)**

(a) Introduction to physic-chemical techniques
(b) Conductometry: principle and applications
(c) Potentiometry: principle and applications
(d) pH-metry: principle and applications

Objectives:

1. To understand basic principle and working of pH meter, potentiometer, conductometer.

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. Quantum Chemistry- I. Levine 5th edition, Prentice Hall, 1999.
5. Principles of Instrumental Analysis Skoog, Holler, Niemen 6th edition

CHA4102: Molecular Symmetry and Chemistry of Main Group Elements
SECTION I (2 Credits, 30 L)

1. **Definitions and Theorems of Group Theory: (2 L)**
   Defining properties of a group, group multiplication table, some examples of group, subgroups, classes

2. **Molecular Symmetry and Symmetry Groups: (10 L)**
   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.

3. **Representations of Groups: (5 L)**
   Matrix representation and matrix notation for geometric transformation, The Great Orthogonality Theorem and its consequence, character tables (No mathematical part)

4. **Group theory and quantum mechanics: (4 L)**
   Wave function as basis for irreducible representations

5. **Symmetry Adapted Linear Combinations: (5 L)**
   Projection operators and their use of construct SALC (Construction of SALC for sigma bonding for molecules belonging point groups: D2h, D3h, D4h, C4v, Td, Oh, normalization of SALC.

6. **Molecular Orbital Theory: (4 L)**
   Transformation properties of atomic orbital, MO's for Sigma bonding ABn molecules, tetrahedral AB4 and Oh AB6 cases.

Objectives:

1. Demonstrate understanding of core concepts, methods and limits of scientific investigation to effectively solve problems in inorganic chemistry.
2. Illustrate symmetry concepts and to demonstrate the scope of the symmetry and group theory to inorganic chemistry
3. To recognize the molecular geometries (regular & irregular).
4. To clarify the types of elements and symmetry operations for different molecules.
5. To clarify the principles of the group theory.
6. To understand the relationship between group theory and molecular symmetry
7. To recognize that the optical activity phenomenon through symmetry.
8. To show how to build the character table.

SECTION II (2 Credits, 30 L):

1. **Periodicity in Properties:** **(4 L)**
   Atomic and ionic radii, Ionization energy, electron affinity, ionic radii and electronegativity and trends in periodic table

2. **S block elements:** **(4 L)**
   Comparative study, diagonal relationship, silent features of hydrides, salvation and complexation tendencies including their function in biosystem.

3. **P block elements:** **(18 L)**
   Comparative study including diagonal relationship of group 13 to 17 elements. Compounds like hydrides, oxides, oxyacids and halides of group 13 to 16 elements. Boron Hydrides, preparation and structure, interconversion of lower and higher boranes, Metalloboranes, Carboranes, borazene, Reactions of Organoboranes, silicates, sulphur-nitrogen compounds, interhalogens, pseudohalogens, carbon allotropes.

4. **Organometallic Compounds:** **(4 L)**
   Introduction, Nomenclature and Classification, Synthesis, Properties, bonding and applications

Objectives:

1. To develop an understanding of the range and chemistry of elements in the periodic table and their compounds
2. To provide an understanding of chemical methods employed for problem solving involving inorganic systems
3. Understand the structure of atoms and will apply the periodic laws to predict chemical and physical properties of the elements.
4. Comprehend the nature of compounds, their formation, composition, and nomenclature.
5. Comprehend chemical equations and utilize them in stoichiometric calculations.
6. learn about Periodic law
7. analyze the difference between Groups and Periods
8. predict atomic mass with their atomic number
9. explain critical vocabulary like electronegativity, ionization energy, atomic size and ionic radius
10. analyze periodic trends in properties of elements in periodic table
11. Learn about how to count the oxidation state, and bonding nature of the metal complexes, and through such information.
12. Understand or predict the structures, properties, and reactions of organometallic compounds.

References:

1. Chemical Applications of Group Theory, 3rd Edn., Author - F. A. Cotton (Wiley, New York)
2. Symmetry and spectroscopy of molecules, 2nd Ed. 2009; K. Veera Reddy, (New Age International Publication)
3. Group Theory and its Chemical Applications, P.K. Bhattarchrya
4. Inorganic Chemistry : Shriver & Atkins (4th edition 2003, Oxford)
5. Concise Inorganic Chemistry, J. D. Lee, Fourth Edn.(Chapman and Hall)
6. Inorganic chemistry: principle of structures and reactivity, Huheey, Keiter, Keiter, Medhi, Pearson Education, 4th Edn. (2007).
7. Inorganic Chemistry: Catherine Housecroft
8. Inorganic Chemistry: Messler & Tarr, Pearson Publishers 3rd Edition
9. Organometallic Chemistry-A Unified Approach: R. C. Mehrotra & A. Singh

CHA4103: Fundamentals of Organic Chemistry
SECTION I (2 Credits, 30 L)

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.

d) Structure and stability of reactive intermediates, carbenes, nitrenes, carbocations, carbanions and free radicals.

2. Stereochemistry: **(20 L)**

a) Sterochemical principles, enantiomeric relationship, distereomeric relationship, R and S, E and Z, D and L nomenclature in C, N, S, P containing compounds, Prochiral relationship, stereospecific and stereoselective reactions, optical activity in biphenyls, spiranes, allenes.

b) Conformational analysis of cyclic and acyclic compounds.

Objectives:
1. Appreciation for the nature and scope of organic chemistry.
2. Application of key concepts from organic chemistry including chemical bonding and basis of reactivity
3. Apply acid-base concepts to organic systems: predict ordering of acid or base strength, hard and soft acid and base concept.
4. Learn concept of aromaticity of benzenoid and non-benzenoid system.
5. Recognize and understand stereochemistry and be able to apply E/Z, D/L configuration, stereospecific and stereoselective reactions, optical activity in different types of molecules.
6. Detail study of conformations of cyclic and non cyclic system

SECTION II (2 Credits, 30 L)

1. **Substitution reaction**: **(6 L)**
   i) Aliphatic nucleophilic substitution-SN^1, SN^2 mechanism, NGP by pi and sigma bonds, classical and non-classical carbocations, phenonium ions, norbornyl system, carbocation rearrangement in NGP, SN^i mechanism, nucleophilic substitution in allylic, trigonal and vinylic carbon.
   ii) Effect of structure, nucleophile, leaving group and solvent on rate of SN^1 and SN^2 reactions, ambident nucleophile and regioselectivity.

2. **Aromatic Electrophilic substitution** **(4 L)**
   i) 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.
   ii) Important reactions like Friedel crafts alkylation and acylation, Nitration, halogenation, formylation, chloromethylation, sulphonation, diazonium coupling.

3. Aromatic nucleophilic substitution **(2 L)**

SNAr, SN^1, Benzyne and SNR1 reactions, reactivity: effect of substrate structure, leaving group and attacking nucleophile.

4. Addition reactions **(12 L)**

i) **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.

ii) **Addition to carbonyl group:**
Grignard, organo zinc, organo copper, organo lithium, reagents to carbonyl and unsaturated carbonyl compounds

iii) **Ylides:**
Phosphorus, Nitrogen and Sulphur ylides

5. Elimination reactions: **(6 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.

Objectives:

1. Understand the features of substitution reaction: SN^1, SN^2 reaction, NGP concept, factors affecting on SN^1 and SN^2 reaction.
2. Learn in detail reactions, mechanisms and stereochemistry of different reactions in organic chemistry: aromatic nucleophilic reaction, aromatic Electrophilic reaction, addition to C-C multiple bond, addition to carbonyl group reaction, ylides and elimination reaction.

References:

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

CHA4104: Safety in Chemical Laboratory and Good Laboratory Practices
SECTION I (2 Credits, 30 L)

1. History and importance of safety and health in Laboratory: **(4 L)**
Moral, legal and financial reasons.

2. Different types of Hazards at workplace handling chemicals: **(5 L)**
- Physical, chemical, biological, allergens
- Effect of hazards on health
- Where to find Hazard information-Reading Labels

3. Personal Protective and other safety equipments and their uses: (**12 L)**

Various safety goggles, types of gloves, apron, masks, different filters for masks, face shield, full body suit, safety shoes, helmet, breathing apparatus suit, safety belt, and earmuffs along with inspection methods. Emergency exit, its location and approach path, fire extinguishers, and their periodic inspection, first aid kit, its contents and need for monitoring. Eye wash fountains and safety showers, fire drill, and chemical accident drills, accident free days and incentives to follow safety rules, accident recording and investigation for future controls

4. Material Safety Data Sheets, Globally Harmonised System (GHS) Signs (hhttp://www.calstatela.ed/univ/ehs/msds.php) **(5 L)**
Importance and use of current 16 point format, Labels and pictograms and some of their discrepancies, Globally Harmonized System for SDS, label changes (2014)

5. Inventory Management, Storage and Disposal: **(4 L)**
Inventory Management, Storage, waste Classification, Hazardous waste, Non-Hazardous waste, mixed waste, waste Disposal.

Objectives:

1. Demonstrate safe laboratory skills (including proper handling of materials and chemical waste) for particular laboratory experiments.
2. To understand importance of safety and health in laboratory.
3. Learn and observe the safety and laboratory rules
4. To study safety management guidelines.
5. To describe hazard information: material safety data sheets (MSDSS), understand and communicate about laboratory hazards
6. To study Chemical Management: Inspections, Storage, Waste and Security.

SECTION II (2 Credits, 30 L)

1. Dos and Don'ts: Safe clothing, hair, dangling jewellery responsible attitude, good House Keeping, use proper PPE, No food in Labs. **(2 L)**

2. What to do when things go wrong: **(6 L)**
Spills, mercury spills, Injuries, Fires, building Evacuations, Emergencies

3. OSHA laboratory Standards. **(2 L)**

4. Case studies: Reason for fire or accident, affixing responsibility and proposing action for prevention or minimizing possibility or severity: **(5 L)**
Losses in an accident, Financial and non-financial, Importance of system based solutions over manual action, Economical solutions, Compromise between accident costs and prevention costs.

5. Good Laboratory Practices (GLP): **(15 L)**
Introduction and principles of GLP, performance of Lab studies and calibration using Standard Operating Procedures (SOPs), Instrument validation, reagent certification, Lab notebook maintenance to contemporary standards, maintenance of lab records based on instrument and reagent certification. Introduction to ISO and NABL accreditation.

Objectives:

1. To describe what is GLP. And what are the OECD Principles of Good Laboratory Practice (GLP)
2. To understand types of chemicals / chemical products are covered under the OECD Principles of GLP.

3. To study importunes and benefits standard operating procedures (SOPs).
4. To learn what does NABL stand for. What's its use? What is the difference between ISO certification and NABL accreditation.
5. To identify does NABL follow any ISO guidelines.

References:

1. Chemical Laboratory Safety and Security: A Guide to Prudent Chemical Management, Lisa Moran and Tina Masciangioli, Editors, THE NATIONAL ACADEMIES PRESS Washington, DCwww.nap.edu.
2. Safety in Academic Chemical Laboratory, Vol. II, ACS Publication, 7th Edition (2003).
3. OECD Series on Principles of Good Laboratory Practices and Compliance Monitoring, 1997.
4. Handbook of Good Laboratory Practices, TDR, WHO, UNICEF, UNDP (2009).
5. A Primer for Good Laboratory Practices and Good Manufacturing Practices, L. Huber, Agilent Technologies, 2002.
6. What went wrong By Trevor Kletz, Gulf professional Pubisher.

CHA4105: Analytical Chemistry - Practical Course - I (4 Credits)

1. Organic Practicals:

a) Three component mixture separation and analysis using ether. (8 mixtures minimum)

b) Laboratory Techniques:

i) Recrystallization

ii) Sublimation

2. Physical Practicals:

1. Determination of the acid and base dissociation constant of an amino acid and hence the isoelectric point of the acid.
2. Determination of concentrations of strong acid and weak acid present in the mixture by titration with strong base by conductometric measurements.
3. Determination of partial Molar Volume and the densities of a series of solutions and to calculate the molar volumes of the components.
4. To plots the polar graphs for s and p originals.
5. Determination of amount of copper by photometric titration with EDTA.

CHA4106: Analytical Chemistry - Practical Course - II (4 Credits)

1. Inorganic Practicals:

a) Ore analysis:

i) Analysis of Silica and Manganese from Pyrolusite ore.

ii) Analysis of Silica and Iron from hematite ore.

iii) Analysis of Copper and Iron Chalcopyrite ore.

b) Inorganic Synthesis:

i) Chloro penta-ammine cobalt (III) chloride

ii) Nitro penta-amminecobalt (III) chloride

iii) Potassium tri-oxalato aluminate

c) Spectrophotometry:

Determination of equilibrium constant of M – L systems Fe(III)–Sulphosalicylic acid by Job's continuous variation method.

d) **Conductometry:**
Verification of Debye Huckle theory of ionic conductance for strong electrolytes KCl, $BaCl_2$, $K_3[Fe(CN)_6]$

e) Photochemical study of ferrioxalate:
Synthesis and photochemistry of $K_3[Fe(C_2O_4)_3].3H_2O$

f) Consumer products:
Analysis of aluminum from alum

2. Physical Practicals:

1. Kinetic decomposition of diacetone alcohol by dilatometry.
2. Determination of an order of a reaction by fractional change method.
3. To investigate effect of Brönsted primary salt on reaction.
4. Hydrolysis of ethyl acetate by NaOH.
5. Determination of ΔG, ΔH, and ΔS of $BaSO_4$ by conductometry.

CHA4107: SELF LEARNING COURSE - I
Chemistry of Life - Biomolecules (1 Credit, 15 L)

1. Introduction to Biomolecules **(1 L)**

2. Carbohydrates: Introduction, Classification, structures,.Derivatives of monosaccarides and their functions. **(4 L)**

3. Proteins: Introduction, biological Significance, Amino acids, classification with examples based on R group, essential & nonessential amino acids. zwitter ions and isoelctric pH, titration curve of amino acids. Introduction to peptides and peptide bond formation. **(4 L)**

4. Lipids: Classification, functions. **(2 L)**

5. Nucleic acids: DNA & RNA types, structure and function. **(2 L)**

6. Vitamins: Structure, biochemical functions& deficiency disorders. **(2 L)**

Objectives:

1. To learn the elements present in biomolecules, their basic classification, significance and functions.

References:

1. Organic Chemistry (5th Edn.) Robert. T.Morrison & N. Boyd. Hill edn.
2. Lehninger's Principles of Biochemistry, (4th edn.), David L. Nelson, Michael M.Cox.

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FERGUSSON COLLEGE, PUNE

AUTONOMOUS COLLEGE

SYLLABUS

First Year M. Sc.

[Analytical Chemistry]

Semester - II

[Academic year 2016-2017]

Semester II
CHA4201: Advanced Physical Chemistry
SECTION I (2 Credits, 30 L)

1. **Molecular Spectroscopy**
   a) Introduction to Molecular Spectroscopy **(2 L)**

   b) Microwave spectroscopy, rotation spectra of di and ply atomic molecules, Stark Infra red spectroscopy : Harmonic and an harmonic oscillator, vibrational spectra of di – and poly-atomic molecules, coarse and fine structure, Nuclear spin effect, application **(8 L)**

   c) Raman Spectroscopy: Introduction, Rotational Raman- spectra, Vibrational Raman, Spectra, polarization of light and Raman effect, structure elucidation from combined Raman and IR spectroscopy, applications in structure elucidation. **(8 L)**

   d) Electronic spectroscopy of molecules: Born – Oppenheimer approximation, electronic spectra of diatomic molecules, vibration, al coarse structure, rotational fine structure dissociation energy and dissociation products, electronic structure of diatomic molecules, molecular photoelectron spectroscopy, and application. **(6 L)**

   e) ESR and Mossbauer spectroscopy applications. **(4 L)**

   f) Principles of NMR: Chemical applications of PMR in structure elucidation. **(2 L)**

Objectives:
1. Compare and contrast atomic and molecular spectra.
2. Justify the difference in molecular spectra at room temperature and 10K.
3. Explain basic principles of IR spectroscopy
4. Explain working principles and taking spectrum of IR spectroscopy device
5. Know how nuclear spins are affected by a magnetic field, and be able to explain what happens when radiofrequency radiation is absorbed. 2. Be able to predict the number of proton and carbon NMR signals expected from a compound given its structure. 3. Be able to predict the splitting pattern in the proton NMR spectrum of a compound given its structure.

SECTION II (2 Credits, 30 L)
1. **Radio Chemistry and applications**: **(10 L)**
   a) Recapitulation – type of radioactive decay, Decay Kinetics, Detection & measurement of radiation

   b) Applications of radioactivity: Typical reaction involved in preparation of radio isotopes: 3H, 14 C, 22Na 32P 35S, and I127 General Principles of using radioisotopes. Physical constants – Diffusion coefficients, surface area, solubility. Analytical applications neutron activation analysis, dilution analysis, radiometric titration.

Objectives:
1. Understand and apply the principles of radioactivity and nuclear chemistry.
2. To understand concepts like radioactive decay, Decay Kinetics, Detection & measurement of radiation
3. To study typical reaction involved in preparation of radio isotopes
4. To understand physico-chemical applications of radioactivity

2. Crystallography: **(6 L)**

a) Unit Cell, types of crystals, Miller Indices, Bragg Equation
b) Crystal structure determination from X-ray data, Bravais Lattices.

Objectives:

1. To learn concept of unit Cell, types of crystals, Miller Indices.
2. To derive Bragg Equation and its significance for spectral analysis

3. Chemical Bonding: **(14 L)**

a) Valence Bond theory, hybrid orbitals, geometry and hybridization,
b) Molecular Orbital, Theory of di- and tri- atomic molecules, linear variation method,
c) Approximations underlying Huckel theory, charge density, pi-(mobile) bond order, Aromaticity,
d) Applications of Huckel theory.

Objectives:

1. To understand concepts of Valence Bond theory and Molecular Orbital Theory
2. To understand applications of Huckel theory.

References:

1. Fundamentals of molecular spectroscopy: C.N. Banewell and E.Mc. Cash (Fourth edition).
2. Elements of Nuclear Chemistry, H.J. Arnikar, 4 th edition, New Age Publishers (2008).
3. Physical Chemistry, T. Engel and P. Reid, Pearson Education (2006).
4. Atkins Physical Chemistry, P. W. Atkins and DePaula (Oxford, Eighth Edition)

CHA4202: Coordination and Bioinorganic Chemistry
SECTION I (2 Credits, 30 L)

1. Concept & Scope of Ligand Fields, Free ion Configuration, Terms and States, Energy levels of transition metal ions, free ion terms, term wave functions, spin-orbits coupling. **(4 L)**

2. Ligand Field Theory of Coordination Complexes **(6 L)**
Effect of ligand field on energy levels of transition metal ions, weak cubic ligand field effect on Russell-Saunders terms, strong field effect, correlation diagrams, Tanabe-Sugano Diagrams, Spin-Pairing energies.

3. Electronic spectra of Transition Metal Complexes **(10 L)**
Introduction, Band intensities, band energies, band width & shapes, spectra of 1^{st}, 2^{nd} & 3^{rd} row ions and rare earth ion complexes, spectrochemical & nephlauxetic series, charge transfer & luminescence, spectra, calculations of Dq, B, β parameters.

4. Magnetic Properties of Coordination Complexes **(10 L)**
Origin magnetism, types of magnetism, Curie law, Curie-Weiss Law, Magnetic properties of complexes-paramagnetism 1^{st} & 2^{nd} 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.

Objectives:

1. To understand the key features of coordination compounds, including:
   - The variety of structures
   - Oxidation numbers and electronic configurations
   - Coordination numbers
   - Ligands, chelates
   - Bonding, stability of complexes

2. To be able to use Crystal Field Theory to understand the magnetic properties of coordination compounds.
3. To be able to describe the shapes and structures of coordination complexes with coordination numbers ranging from 4 to 12.
4. To be able to describe the stability of metal complexes by the use of formation constants and to calculate thermodynamic parameters from them. Calculate the spin-only magnetic moment of first row transition metal complexes.
5. To be able to recognize the types of isomers in coordination compounds.
6. To be able to name coordination compounds and to be able to draw the structure based on it's name.
7. To become familiar with some applications of coordination compounds.

SECTION II (2 Credits, 30 L)

1. Overviews of Bioniorganic Chemistry, essential and trace elements in biological processes, classification of biomolecules. **(3 L)**

2. Principles of Coordination Chemistry related to Bioinorganic Research and Protein, Nucleic acids and other metal binding biomolecules. **(10 L)**

3. Biochemistry of following elements: **(10 L)**

a) Metaolporphyrins with special reference to hemoglobin and myoglobin
b) Iron: Ferritin, Transferrin, Fe-S clusters, siderophores, cytochrome P-450
c) Manganese in Photosynthesis, Nitrogen fixation

4. Metals in medicine- Metal deficiency and disease, toxic effects of metals, metals used for diagnosis and chemotherapy with reference to anticancer drugs. **(7 L)**

Objectives:

1. Understand the vital importance of biological chemical trace elements for all life.
2. Identify the fundamental chemical properties of biological trace elements, particularly biological metals.
3. Understand the vital interaction between biological trace elements, particularly transition metals and biological macromolecules such as proteins and DNA.
4. Describe the structure and function of specific metalloproteins engaged in biological dioxygen transport and metalloenzyme function.
5. Understand and apply simple theoretical concepts in the electron transport chains of metalloproteins in photosynthesis and respiration
6. Understand metal-based diseases, toxic metals, and metal-based chemotherapy.
7. Assess biological materials technology, as in biominerals, biological nanoparticles etc
8. Appreciate biotechnology and nanotechnology based on metalloproteins and metal complexes with DNA

References:

1. Ligand field theory & its applications: B.N. Figgis & M.A. Hitachman (2000) Wiely VCH Publ.
2. Symmetry and spectroscopy of molecules, Second Edn, by K. Veera Reddy, New Age International Publication, 2009.
3. Elements of magnetochemistry, R. L. Datta and Syamal, Second Edn, Afiliated East West Press Pvt. Ltd. 2007.
4. Principle of Bioinorganic Chemistry: S.J. Lippard and J,M. Berg
5. Bioinorganic Chemistry: Inroganic Elements in Chemistry of Life: W.Kaim and B. Schwederski

6. Bioinorganic Chemistry: Bertini, Gray, Lippard and Valentine
7. Bioinorganic Chemistry: R.J.P. Willams
8. Bioinorganic Chemistry: Robert Hay
9. Bioinorganic Chemistry: M.N. Hughes

CHA4203: Synthetic Organic Chemistry and Spectroscopy
SECTION I (2 Credits, 30 L)

1. **Oxidation reactions:** **(7 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 etc.

2. **Reduction reactions:** **(6 L)**
   Boranes and hydroboration reactions, MPV reduction and reduction with H_2/Pd-C, Willkinsons catalyst, DIBAL and Wolff Kishner reduction, etc.

3. **Rearrangements:** **(7 L)**
   Beckmann, Hofmann,, Curtius, Smith, Wolff, Lossen, Bayer-villiger, Sommelet, Favorskii, Pinacol-pinacolone, Benzil-benzilic acid, Fries, etc.

4. **Photochemistry:** **(10 L)**
   General basic principles, photochemistry of carbonyl compounds, alkenes, dienes, polyenes and aromatic compounds, photorearrangements, Barton reaction.

Objectives:
1. Apply knowledge of oxidizing reagent in different organic reaction conversions
2. Learn to use of reducing agent: strong, mild reducing agents
3. Applications of variety of rearrangement in organic transformation reactions
4. Explore to the basic concept and principle of photochemistry

SECTION II (2 Credits, 30 L)

1. UV: Factors affecting UV absorption and interpretation of UV spectra **(3 L)**

2. IR: Basic ideas about IR frequencies, interpretation of IR spectra **(5 L)**

3. PMR: Fundamentals of PMR, factors affecting chemical shift, integration coupling (1st order analysis) **(8 L)**

4. Introduction to CMR and mass spectrometry **(4 L)**

5. Problems based on UV, IR and PMR **(10 L)**

Objectives:
1. Study different spectroscopic method to determine the structre of organic compounds Ultraviolet spectroscopy- Infrared spectroscopy - Nuclear Magnetic Resonance spectroscopy
2. Introducing Carbon magnetic Resonance and mass spectrometry
3. Be able to solve problems employing spectroscopic methods including UV spectroscopy, infrared and NMR spectroscopy.

References:

1. Advanced Organic Chemistry, Part A – F. A. Carey and R. J. Sundberg, 5th Ed. Springer (2007)

2. Excited states in Organic Chemistry- J.A. Barltrop and J.D.Coyle, John Wiley & sons
3. Photochemistry and Pericyclic reactions-Jagdamba Singh, Jaya Singh 3rd Ed.
4. Organic photochemistry: A visual approach-Jan Kopecky, VCH publishers (1992).
5. Organic Chemistry – J. Clayden, N. Greeves, S. Warren and P. Wothers (Oxford)
6. Modern Synthetic reactions- H.O. House
7. Organic Synthesis – M.B. Smith
8. Advanced Organic Chemistry (part A & B)– A. Carey and R.J. Sundberg
9. Stereochemistry conformations and mechanism by P.S. Kalsi
10. Organic chemistry –by Cram, Hammond, Pine and Handrickson
11. Introduction to spectroscopy – D.l. Pavia, G.M. Lampman, G.S. Kriz, 3rd Edition
12. Spectroscopic methods in organic melecules – D.H. William & I Flemming Mc Graw Hill
13. Mechanism and Structure in Organic Chemistry - E.S. Gould

CHA4204: Modern Separation Methods and Chemometrics
SECTION I (2 Credits, 30 L)

1. Modern Separation Methods and Hyphenated Techniques

a) Mass Spectrometry **(10 L)**

Principle, Instrumentation, Ionization methods- Electron bombardment ionization, Arc and spark ionization, Photo-ionization, Thermal ionization, Chemical ionization, Mass analyzers- 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,

b) Gas Chromatography **(10 L)**

Theory and Instrumentation of GC, Sample injection- Split and splitless 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, Applications of GLC, Use of GC-MS ,High Speed gas chromatography, Gas- solid chromatography and problems.

c) High Performance Liquid Chromatography (HPLC) **(10 L)**

Theory and instrumentation of HPLC, Optimization of column performance, Gradient elution and related procedures, derivatization, Mobile phase delivery system, sample injection, separation column, detectors, Interfacing HPLC with mass spectrometry, Structure types of column packing, adsorption chromatography, Bonded phase chromatography, reverse phase chromatography, ion–pair chromatography, ion exchange chromatography, size exclusion chromatography, GC-MS and LC-MS, Applications and Problems.

Objectives:

1. To acquire knowledge of Modern Separation Methods and Hyphenated Techniques
    a. Theory and Instrumentation Mass Spectrometry
    b. Theory and Instrumentation Gas Chromatography
    c. Theory and instrumentation High Performance Liquid Chromatography (HPLC)

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. Merritt 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.

SECTION II (2 Credits, 30 L)

1. **Data Handing and Spreadsheets in Analytical Chemistry: (10 L)**
   Accuracy and Precision, classification of errors, Significant figures, rounding off, ways of expressing accuracy, Mean Deviation, Average Deviation, RMD, Standard Deviation, Propagation of errors, Confidence limits, Tests of Significance, Rejection of results, standard addition method, internal standard addition methods and Problems.

2. **Chemometrics: (10 L)**
   Concentration of solution based on volume and mass unit, calculations of ppm , ppb and dilution of the solutions , concept of mmole, stoichiometry of chemical reactions, concept of gmole, limiting reactants, theoretical and practical yield, solubility and solubility equilibria. Concept of formation constant, stability, instability constants, stepwise formation constants and numerical problems.

3. **Quality in Analytical Chemistry: (10 L)**
   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.

Objectives:
1. To learn Data Handing and Spreadsheets in Analytical Chemistry
2. To learn concentration of solution based on volume and mass unit
3. To understand concept of formation constant, Stability, instability constants, stepwise formation constants
4. To learn quality systems in chemical laboratories
5. To be trained in quality standards for laboratories
6. To identify responsibility of laboratory staff for quality

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 &
4. F. A. Settle Jr., 6th Edition, Wadsworth Publishing Company, USA, 1986.

CHA4205: Analytical Chemistry - Practical Course - III (4 Credits)

1. **Organic Practicals:**
   a) **Laboratory Techniques:**
      1. TLC
      2. Column Chromatography
      3. Distillation
      4. Use of chemistry software like ChemDraw, Chemsketch

   b) **Single stage preparations (any 6 preparations)**
      1. 2-Methoxy naphthalene to 1-Formyl-2-methoxy naphthalene
      2. Toluene to 4-Methyl acetophenone
      3. P-aminonitrobenzene to 2-Iodo/2-Choro benzoic acid
      4. Cyclohexanol to Cyclohexanone
      5. Benzaldehyde to Chalcone

6. m-dinitrobenzene to m-Nitroaniline
7. Glycine to benzoyl glycine
8. Diel's alder reaction
9. 2-Naphthol to 2-Methoxy Naphthalene

2. Physical Practicals:

1. Determination of counting errors of counter.
2. Determination of E_{max} of β radiation and absorption coefficients in Al.
3. Determination of glycerol radius by viscosity.
4. Analysis of crystal structure from single crystal X-ray pattern.
5. Statistical treatment of experimental data.

CHA4206: Analytical Chemistry - Practical Course - IV (4 Credits)

1. Inorganic Practicals:

a) Alloy Analysis:

1. Determination of tin and lead from solder.
2. Determination of iron and chromium from stainless steel.
3. Determination of copper and nickel from cupronickel.

b) Inorganic Synthesis:

1. Tris(ethylene di ammine)Ni(II) thiosulphate.
2. Bis[TrisCu(I)thiourea]

c) Solvent Extraction:

Determination of iron by solvent extraction techniques using 8-hydroxyquinoline reagent.

d) Ion-exchange Chromatography:

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)

e) Spectrophotometry:

Estimation of phosphate from waste water by calibration curve method

f) Inorganic Characterization Techniques:

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 all three complexes and analyze it. Arrange three ligands according to their increasing strength depending on your observations.

g) Synthesis of Nanomaterials:

Synthesis of nano size α-Fe_2O_3

2. Physical Practicals:

1. Determination of equivalent conductance at infinite dilution, dissociation constant of Acetic Acid and to study Debey Huckel Limiting law
2. Determination of critical micellar concentration (CMC) and G of micellization of sodium dodecyl sulphate (SDS).
3. Determination of Solubility and solubility product of a sparingly soluble salt.
4. Estimation of amount of halides present in the mixture
5. Determination of dissociation constants of tribasic acid (phosphoric acid)

Reference Books:
1. Text book of Quantitative Analysis, A.I. Vogel 4th Edn. (1992).
2. Experimental Inorganic Chemistry, Mounir A. Malati, Horwood Series in Chemical Science (Horwood publishing, Chichester) 1999.
3. Experiments in Chemistry, D. V. Jahagirdar, Himalaya Publishing House
4. General Chemistry Experiments, Anil. J Elias, University press (2002)
5. Ligand Field Theory, B. N. Figgis.

CHA4207: SELF LEARNING COURSE - II
Environmental Toxicology and Chemistry (1 Credit, 15 L)

1. Introduction - Concept and scope of Environmental toxicology in chemistry **(2 L)**

2. Toxic chemicals in environment **(3 L)**

3. Biochemical effects of
   - i. Trace metal like - lead, Mercury, Arsenic, Cadmium, Chromium **(3 L)**
   - ii. Ozone and PAN **(2 L)**
   - iii. Pesticides **(2 L)**
   - iv. Organic compounds like aromatic hydrocarbon, organic halogen compounds **(3 L)**

Objectives:

To understand the concept of environmental and biochemical effect of various toxic elements, compounds.

References:
1. Environmental Chemistry: B.K. Sharma, and H. Kaur.
2. Elements of Environmental Chemistry: H.V. Jadhav.
3. Environmental Chemistry: S. K. Banerjee.
4. Environmental Chemistry: J. W. Moore and E. A. Moore.