Deccan Education Society's

FERGUSSON COLLEGE (Autonomous), PUNE - 411004

Two Years
M. Sc. Degree Course in Chemistry
(Organic Chemistry)

REVISED SYLLABUS
Semester I and II

First Year M. Sc.
[Organic Chemistry]

[Academic year 2017-2018]

Deccan Education Society's

FERGUSSON COLLEGE (Autonomous), PUNE – 411004

Department of Chemistry

[Autonomous College]

Two Years M. Sc. Degree Course in Chemistry

[Implemented from Academic Year 2017-2018]

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

Course Structure:

Term / Semester	Name of the Paper	Title of Paper	Theory Credits	No. of Lectures / Practicals
First Term / Semester I	CHO4101	Fundamentals of Physical Chemistry	4	60
	CHO4102	Molecular Symmetry and Chemistry of Main Group Elements	4	60
	CHO4103	Fundamentals of Organic Chemistry	4	60
	CHO4104	Good Laboratory Practices and Biomolecules	4	60
	CHO4105	Chemistry Practical Course - I	4	15 Practicals
	CHO4106	Chemistry Practical Course - II	4	15 Practicals
	CHO4107	Self-Learning Course – I Chemistry - Review writing	1	15
Semester I : Credits			**25**	

Term / Semester	Name of the Paper	Title of Paper	Theory Credits	No. of Lectures / Practicals
Second Term / Semester II	CHO4201	Advanced Physical Chemistry	4	60
	CHO4202	Coordination and Bioinorganic Chemistry	4	60
	CHO4203	Synthetic Organic Chemistry and Spectroscopy	4	60
	CHO4204	Modern Separation Methods and Chemometrics	4	60
	CHO4205	Chemistry Practical Course - III	4	15 Practicals
	CHO4206	Chemistry Practical Course - IV	4	15 Practicals
	CHO4207	Self-Learning Course - II Environmental Toxicology and Chemistry	1	15
Semester II : Credits			**25**	

Faculty of Science
Extra Credits for Post Graduate Courses

M. Sc. Part I Course in Organic 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

First Term : Semester I
CHA4101: Fundamentals of Physical Chemistry
(4 Credits, 60 L + T)

1. Thermodynamics

a. Chemical Thermodynamics (8 L)

Recapitulation- First law, second law and third law of thermodynamics – dependence of enthalpy, entropy and free energies on pressure and temperature, partial molar quantities, enthalpy and entropy of mixing.

b. Molecular Thermodynamics (10L)

Maxwell-Boltzmann, Fermi-Dirac and Bose-Einstein statistics Molecular energy levels, Boltzman distribution law, residual entropy, partition functions and ensembles, translational, rotational and vibrational partition functions, Obtaining thermodynamic properties from partition functions.

Objectives:

1. To know significance of laws of thermodynamics
2. To understand concept of spontaneity of the reaction.
3. To know non zero entropy near 0K
4. To interpret partition functions.

2. Quantum Chemistry (12L)

Failures of classical mechanics- Atomic spectra, wave particle duality, uncertainty principle, wave function and its interpretation, operators, eigen value equation, expectation value, Schrodinger equation, particle in a box, particle in 2D box, particle in box 3D, degeneracy. Applications- Hydrogen-like atoms- R, Θ and φ equation (no derivation), atomic orbitals, shape of orbitals, radial function, its square and radial distribution curve for atomic orbitals.

Objective:

1. To know concept of quantization.
2. To understand equivalence of quantum mechanics and classical mechanics.
3. To envisaging Bhor correspondence principle.
4. To understand free electron approximation and electronic spectra.
5. To represent atomic orbitals.

3. Chemical Kinetics

a. Recapitulation (10L)

Elementary reaction, half integral order reaction- differential and integral equations, reversible reaction, parallel reaction, consecutive recation, principle of microscopic reversibility, steady state approximation- elucidating mechanism of a reaction.

b. Theories of Reaction Rates (20L)

i. Arrhenius theory, collision theory and transition state theory, enthalpy, free energy and entropy of activation, correlation of steric factor in collision theory and entropy of activation, rationalizing steric factor.

ii. Unimolecular reactions, dependence of rate constant on pressure, dielectric constant and ionic strength (primary and secondary salt effect). Enzyme catalysis – Michaelis Menton mechanism, Lineweaver and Eadie plot,Linear free energy relationship, potential energy surface.

Objective:

1. To describe the relationship between the order of a reactant and the stoichiometric coefficient for the reactant in the overall balanced chemical equation.
2. To state the basis for the "Collision Model of Chemical Kinetics".
3. To describe the relationship between the rate of a chemical reaction and the frequency with which reactant molecules collide.
4. To describe "activation energy".

5. To use the Collision Model of Chemical Kinetics to describe how changes in concentration or temperature affect rates of chemical reactions.
6. To know the application of mathematical tools to calculate thermodynamic and kinetic properties
7. To derivation of rate equations from mechanistic data
8. To use of simple models for predictive understanding of physical phenomena associated to chemical thermodynamics and kinetics

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

CHO4102: Molecular Symmetry and Chemistry of Main Group Elements
(4 Credits, 60 L + T)

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 applications, character tables

4. **Group Theory and Quantum Mechanics (4 L)**
   Reducible and irreducible representations, Wave function as a basis for irreducible representations

5. **Symmetry Adapted Linear Combinations (6 L)**
   Projection operators and their use of constructing 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, Applications to spectra.

6. **Molecular Orbital Theory (3 L)**
   Transformation properties of atomic orbitals, MO's for Sigma bonding ABn molecules, tetrahedral AB_4 and Oh AB_6 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 of 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.

7. Periodicity in Properties (4 L)

Atomic and ionic radii, Ionization energy, electron affinity, ionic radii and electronegativity and trends in periodic table, Slater rules for EAN-rationalizing periodic properties

8. S Block Elements (4 L)

Comparative study, diagonal relationship, silent features of hydrides, salvation and complexation tendencies including their function in biosystem.

9. 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 –Fullerene.

10. 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
10. Symmetry and group theory-Vijayalaxmi

CHO4103 : Fundamentals of Organic Chemistry
(4 Credits, 60 L + 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.
   d. Structure and stability of reactive intermediates, carbenes, nitrenes, carbocations, carbanions and free radicals.

2. **Stereochemistry** **(20 L)**
   Origin of Chirality factors related to chirality 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, skew compounds.
   Conformational analysis of cyclic and acyclic compounds, thilodimide.
   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

3. **Substitution Reaction** **(6 L)**
   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, Effect of structure, nucleophile, leaving group and solvent on rate of SN^1 and SN^2 reactions, ambident nucleophile and regioselectivity.

4. **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.

5. **Aromatic Nucleophilic Substitution** **(2 L)**
   SNAr, SN^1, Benzyne genrationunder different condition (basic and neutral), orientations and regioselectivity in arynes, quantitative and qualitative estimations of arynes and SNR1 reactions, reactivity: effect of substrate structure, leaving group and attacking nucleophile.

6. **Addition Reactions** **(12 L)**
   Addition to C-C multiple bonds
   Mechanism and stereochemical aspects of addition reaction involving electrophile, nucleophile and free radicals, Regioselectivity and chemoselectivity, orientation and reactivity, conjugate addition, Michael addition and retro Michael reaction .

Addition to carbonyl group

Introduction of Organometalic compounds, Grignard, organo zinc, organo copper, organo lithium, reagents to carbonyl and unsaturated carbonyl compounds

Ylides

Phosphorus, Nitrogen and Sulphur ylides.

7. **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 bonds, 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

CHO4104: Good Laboratory Practices and Biomolecules
(4 Credits, 60 L + T)

1. **Good Laboratory Practices**

a) Different types of Hazards at workplace handling chemicals: **(1 L)**
Physical, chemical, biological, allergens, Effect of hazards on health, Where to find Hazard information-Reading Labels

b) Personal Protective and other safety equipments and their uses: **(4 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

c) Material Safety Data Sheets, Globally Harmonised System (GHS) Signs (hhtp://www.calstatela.ed/univ/ehs/msds.php) **(2 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)

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

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

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

g) 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. 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.
7. To describe what is GLP. And what are the OECD Principles of Good Laboratory Practice (GLP)
8. To understand types of chemicals / chemical products are covered under the OECD Principles of GLP.
9. To study importunes and benefits standard operating procedures (SOPs).
10. To learn what does NABL stand for. What's its use? What is the difference between ISO certification and NABL accreditation.
11. To identify does NABL follow any ISO guidelines.

2. Biomolecules

a) Cell Structure and function Prokaryotes & Eukaryotes membrance & cell structure, subcellular components; nucleus, Mitochondria, Endoplasmic reticulum, Golgi apparatus, Lysosomes, peroxisomes. **(4 L)**

b) Water **(2 L)**

c) Proteins Introduction, Amino acids, Classification of amino acids, physicochemical properties, reactions with different reagents, Essential & nonessential amino acids. Peptides, end terminal analysis, Primary secondary, tertiary and quaternay structures of Priteins Helix, sheets, super secondary structure, triple helix structures,globular and fibrous proteins **(8 L)**

d) Carbohydrates: Introduction, Classification, structures, stereo chemical properties and functions. Derivatives of monosaccarides and their functions. **(5 L)**

e) Lipids:Classification, functions. Membrane structure, its organization & functions **(4 L)**

f) Nucleic acids: DNA & RNA types, structure and function. Super coiling of DNA Central dogma, physicochemical properties. **(3 L)**

g) Vitamins: Structure, biochemical functions & deficiency disorders. **(4 L)**

Objectives:

1. To understand the concept of biomolecules.
2. To study function and importance of biomolecules.
3. To understand Cell Structure and function.
4. To learn role of vitamins.

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

CHO4105: Chemistry Practical Course I
(4 Credits : 10 Organic & 5 Physical Experiments)

1. **Organic Practicals**
   1. Three component mixture separation and analysis using ether **(10 mixtures minimum)**
   2. Laboratory Techniques
      i) Recrystallization
      ii) Sublimation

2. **Physical Practicals (Any Five)**
   a) pH metry
      1. Determination of the acid and base dissociation constant of an amino acid and hence the isoelectric point of the acid by pH metry.
   b) Conductometry
      2. Determination of concentrations of strong acid and weak acid present in the mixture by titration with strong base by coductometric measurements.
   c) Spectrophotometry
      3. Determination of amount of copper by photometric titration with EDTA.
   d) Potentiomerty
      4. Determination of stability Constant of a silver ammonium complex.
   e) Chemical Kinetics
      5. Determination of temperature coefficient and energy of activation of acid catalyzed ester hydrolysis reaction.
   f) Thermodynamics
      6. Determination of partial molar volume and the densities of a series of solutions and to calculate the molar volumes of the components.
   g) Theoretical experiment:
      7. To plots the polar graphs for s and p originals.

Scheme of Practical Examination
CHO4105: Chemistry Practical Course I

Note:
1. The practical examination in the subject will be conducted for SIX HOURS duration.
2. The practical examination in the subject will be conducted for 50 marks.
3. Certified Laboratory Journal is compulsory for the examination.
4. Oral/viva examination is compulsory
5. Book/s printed material, cyclostyled or typed material will be allowed during the practical examination.
6. Examiner/s will arrange Q1 and Q2 experiments for conducting practical examination.
7. Lucky draw system will be followed for the students for practical examination by the examiners.
8. Log table and calculators are allowed during the practical examination.
9. Mobile/s is/are strictly not allowed during the practical examination in laboratory.

The candidate has to perform the following question/s for practical examination.

Q 1A:	Organic Experiment	15 Marks
Q I B:	Laboratory Technique	5 Marks
Q 2	Physical Experiment	20 Marks
Q 3	Viva/Oral	5 Marks
Q 4	Journal	5 Marks

CHO4106: Chemistry Practical Course II
(4 Credits : 10 Inorganic & 5 Physical Experiments)

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 (Any Five)**
   - **h) Chemical kinetics**:
     1. Kinetic decomposition of diacetone alcohol by dilatometry.
     2. Determination of an order of iodide and persulphate ions by fractional change method.
     3. To investigate the rate constant of an autocatalytic reaction between potassium permanganate and oxalic acid.
     4. To investigate effect of Brönsted primary salt on reaction
   - **i) Conductometry**
     5. Hydrolysis of ethyl acetate by NaOH using conductometric measurements.
     6. Determination of ΔG, ΔH, and ΔS of $BaSO_4$ by conductometry.
   - **j) Spectrophotometry**
     7. Study the kinetics of iodination of acetone spectrophotometrically.

Scheme of Practical Examination
CHO4106: Chemistry Practical Course II

Note:
1. The practical examination in the subject will be conducted for SIX HOURS duration.
2. The practical examination in the subject will be conducted for 50 marks.
3. Certified Laboratory Journal is compulsory for the examination.

4. Oral/viva examination is compulsory
5. Book/s printed material, cyclostyled or typed material will be allowed during the practical examination.
6. Examiner/s will arrange Q1 and Q2 experiments for conducting practical examination.
7. Lucky draw system will be followed for the students for practical examination by the examiners.
8. Log table and calculators are allowed during the practical examination.
9. Mobile/s is/are strictly not allowed during the practical examination in laboratory.

The candidate has to perform the following question/s for practical examination.

Q1	Inorganic Experiment	20 Marks
Q 2	Physical Experiment	20 Marks
Q 3	Viva/Oral	5 Marks
Q 4	Journal	5 Marks

CHO4107: SELF-LEARNING COURSE – I (1 Credit, 15 L)

Chemistry - Review Writing

Students are expected to write one review in their interested chemistry current research area.

Objectives:

1. To learn the concept of literature survey.
2. To understand the concept from national and international publications and journals.
3. Students should able to write the understood concept in their own words.

Second Term : Semester II

CHA4201: Advanced Physical Chemistry

(4 Credits, 60 L + T)

1. **Molecular spectroscopy:**
   - **a.** Electromagnetic spectra, spectral regions, spectral line width, spectral line intensity. Spectrophotometer, resolving power, signal to noise ration, introduction to Fourier transitions. **(2L)**
   - **b.** Rotational spectra, classification of molecules, rigid rotor, diatomic molecules, most intense line in the rotational spectra, effect of temperature and isotope substitution on the rotation spectra, linear tri atomic molecules, stark effect. **(5L)**
   - **c.** Vibrational spectra, harmonic oscillator, diatomic molecule, fundamental frequency, origin of overtones and combination bands, morse potential, dissociation energy, normal vibrations, assigning normal vibrations of ClO_3 and BF_3. **(5L)**
   - **d.** 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. **(4L)**
   - **e.** Electronic spectroscopy of molecules: Born – Oppenheimer approximation, electronic spectra of diatomic molecules, vibration, al coarse structure, rotational fine structure dissociation energy and dissociation products, Brige Sponer method, fortrat parabola, solvent effect, oscillator strength. **(6L)**
   - **f.** Magnetic resonance spectroscopy, ^{1}H NMR, chemical shift, spin spin coupling, factors affecting chemical shifts. Introduction to ^{13}C NMR, g factor, applications. Mossbauer spectroscopy. **(8L)**

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

2. **Chemical bonding** **(22L)**

   Recapitulation of quantum concepts, Approximate solution of Schordinger equation, linear variation method, H_2 molecule, Heitler London theory, valance bond theory, sp, sp^2, sp^3 hybridization, hybrid orbitals, molecular orbital theory, theory of di- and tri- atomic molecules, Approximations underlying Huckel theory, charge density, pi-(mobile) bond order, free valence index, Applications of Huckel theoryto ethylene, allyl system, butadiene and benzene, alternate and non-alternate hydrocarbons.

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

3. **Nuclear and radiation Chemistry** **(8L)**
   - **a. Types and detection of ionizing radiations-** α, β, γ decay and their energies
   - **b. Applications of radioisotopes-** neutron activation analysis, isotope dilution analysis, radiometric titration and problem solving.

   Objectives:
   1. To understand concepts like radioactive decay
   2. To understand applications of radioactivity

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)

5. Physical Chemistry and molecular approach - D. Mcquarie and J. Simon (University Science) (2000)

CHO4202: Coordination and Bioinorganic Chemistry
(4 Credits, 60 L + T)

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:
   a. The variety of structures
   b. Oxidation numbers and electronic configurations
   c. Coordination numbers
   d. Ligands, chelates
   e. 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.

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

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

7. 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

8. Metals in medicine - Metal deficiency and disease, toxic effects of metals, metals used for 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

CHO4203: Synthetic Organic Chemistry and Spectroscopy
(4 Credits, 60 L + T)

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, air oxidationetc.

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, reduction under acidic, basic and neutral conditionetc.

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

4. **Photochemistry** **(13 L)**
   General basic principles, initiators and sensitizers 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

5. UV: Factors affecting UV absorption and interpretation of UV spectra

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

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

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

8. 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

CHO4204: Modern Separation Methods and Chemometrics
(4 Credits, 60 L + T)

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
2. Theory and Instrumentation Mass Spectrometry
3. Theory and Instrumentation Gas Chromatography
4. 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.

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. 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.

4. 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.

CHO4205: Chemistry Practical Course III
(4 Credits : 10 Organic & 5 Physical Experiments)

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-amino benzoic acid to p-Iodo 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 (Any Five)**
   a) **Radioactivity:**
      1. Determination of counting errors of Giger Muller counter.
      2. Determination of E_{max} of β radiation and absorption coefficients in Al by Geiger Muller counter
   b) **Viscometry**
      3. Determination of glycerol radius by viscosity.
   c) **Conductometry**
      4. Study the Hydrolysis of NH4Cl by Conductometry.
   d) **Spectrum Analysis**
   5. Analysis of crystal structure from single crystal X-ray pattern.
   e) **Theoretical Experiment**
      6. Statistical treatment of experimental data.
   f) **pH metry**
      7. Determination of Hammett constant of ortho, meta, para amino/nitro benzoic acid.

Scheme of Practical Examination
CHO4205: Chemistry Practical Course III

Note:

1. The practical examination in the subject will be conducted for SIX HOURS duration.
2. The practical examination in the subject will be conducted for 50 marks.
3. Certified Laboratory Journal is compulsory for the examination.
4. Oral/viva examination is compulsory
5. Book/s printed material, cyclostyled or typed material will be allowed during the practical examination.
6. Examiner/s will arrange Q1 and Q2 experiments for conducting practical examination.
7. Lucky draw system will be followed for the students for practical examination by the examiners.
8. Log table and calculators are allowed during the practical examination.
9. Mobile/s is/are strictly not allowed during the practical examination in laboratory.

The candidate has to perform the following question/s for practical examination.

Q 1	Organic Experiment	20 Marks
Q 2	Physical Experiment	20 Marks
Q 3	Viva/Oral	5 Marks
Q 4	Journal	5 Marks

CHO4206: Chemistry Practical Course IV
(4 Credits : 10 Inorganic & 5 Physical Experiments)

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 diammine)Ni(II) thiosulphate.
      2. Tris Cu(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 (Any Five)**
   a) **Conductometry**
      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).

   b) **Potentiometry**
      3. Determination of Solubility and solubility product of a sparingly soluble salt.
      4. Determination of strength of commercial vinegar by potentiometric titration

   c) **Potentiometry**:
      5. Estimation of amount of halides present in the mixture

   d) **pH metry:**
      6. Determination of dissociation constants of tribasic acid (phosphoric acid)

   e) **Spectrophometry**
      7. Simultaneous determination of cations from the mixture

References:

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.

Scheme of Practical Examination

CHO4206: Chemistry Practical Course IV

Note:

1. The practical examination in the subject will be conducted for SIX HOURS duration.
2. The practical examination in the subject will be conducted for 50 marks.
3. Certified Laboratory Journal is compulsory for the examination.
4. Oral/viva examination is compulsory
5. Book/s printed material, cyclostyled or typed material will be allowed during the practical examination.
6. Examiner/s will arrange Q1 and Q2 experiments for conducting practical examination.
7. Lucky draw system will be followed for the students for practical examination by the examiners.
8. Log table and calculators are allowed during the practical examination.
9. Mobile/s is/are strictly not allowed during the practical examination in laboratory.

The candidate has to perform the following question/s for practical examination.

Q 1	Inorganic Experiment	20 Marks
Q 2	Physical Experiment	20 Marks
Q 3	Viva/Oral	5 Marks
Q 4	Journal	5 Marks

CHO4207: 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
   a. Trace metal like - lead, Mercury, Arsenic, Cadmium, Chromium **(3 L)**
   b. Ozone and PAN **(2 L)**
   c. Pesticides **(2 L)**
   d. Organic compounds like aromatic hydrocarbon, organic halogen compounds **(3 L)**

Objective:

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