



Fergusson College (Autonomous) Pune

Learning Outcomes-Based Curriculum

for

**M. Sc. I - Organic Chemistry**

With effect from June 2019

## Programme Structure

Semester	Course Code	Course Title	Credits
I	CHO4101	Fundamentals of Physical Chemistry	4
	CHO4102	Fundamentals of Inorganic Chemistry	4
	CHO4103	Advanced Organic Chemistry and Spectroscopy	4
	CHO4104	Organic Chemistry Practical - I	4
	CHO4105	Organic Chemistry Practical - II	4
			<b>20</b>
II	CHO4201	Advanced Physical Chemistry	4
	CHO4202	Advanced Inorganic Chemistry	4
	CHO4203	Reaction Mechanism in Organic Chemistry	4
	CHO4204	Organic Chemistry Practical - III	4
	CHO4205	Organic Chemistry Practical - IV	4
			<b>20</b>

**Program Outcomes (POs) for M. Sc. Programme**

<b>PO1</b>	<b>Disciplinary Knowledge:</b> Demonstrate comprehensive knowledge of the discipline that form a part of an postgraduate programme. Execute strong theoretical and practical understanding generated from the specific programme in the area of work.
<b>PO2</b>	<b>Critical Thinking and Problem solving:</b> Exhibit the skill of critical thinking and understand scientific texts and place scientific statements and themes in contexts and also evaluate them in terms of generic conventions. Identify the problem by observing the situation closely, take actions and apply lateral thinking and analytical skills to design the solutions.
<b>PO3</b>	<b>Social competence:</b> Exhibit thoughts and ideas effectively in writing and orally; communicate with others using appropriate media, build effective interactive and presenting skills to meet global competencies. Elicit views of others, present complex information in a clear and concise and help reach conclusion in group settings.
<b>PO4</b>	<b>Research-related skills and Scientific temper:</b> Infer scientific literature, build sense of enquiry and able to formulate, test, analyse, interpret and establish hypothesis and research questions; and to identify and consult relevant sources to find answers. Plan and write a research paper/project while emphasizing on academics and research ethics, scientific conduct and creating awareness about intellectual property rights and issues of plagiarism.
<b>PO5</b>	<b>Trans-disciplinary knowledge:</b> Create new conceptual, theoretical and methodological understanding that integrates and transcends beyond discipline-specific approaches to address a common problem.
<b>PO6</b>	<b>Personal and professional competence:</b> Perform independently and also collaboratively as a part of team to meet defined objectives and carry out work across interdisciplinary fields. Execute interpersonal relationships, self-motivation and adaptability skills and commit to professional ethics.
<b>PO7</b>	<b>Effective Citizenship and Ethics:</b> Demonstrate empathetic social concern and equity centred national development, and ability to act with an informed awareness of moral and ethical issues and commit to professional ethics and responsibility.
<b>PO8</b>	<b>Environment and Sustainability:</b> Understand the impact of the scientific solutions in societal and environmental contexts and demonstrate the knowledge of and need for sustainable development.
<b>PO9</b>	<b>Self-directed and Life-long learning:</b> Acquire the ability to engage in independent and life-long learning in the broadest context of socio-technological changes.

Program Specific Outcomes (PSOs) for M. Sc. Organic Chemistry	
PSO No.	Upon completion of this programme the student will be able to
PSO1	<b>Academic competence</b> (i) Understand fundamental principles and advanced concepts of organic, inorganic and physical chemistry. (ii) Demonstrate understanding of various types of reactions, reaction mechanisms, stereochemistry, photochemistry, rearrangements, heterocyclic and medicinal chemistry, reactions involving use of metals. (iii) Interpret analytical data for structure elucidation obtained using NMR, IR, UV and Mass spectroscopy.
PSO2	<b>Personal and Professional Competence</b> (i) Carry out experiments which include various chemical techniques and also setting of dry reactions, handling of hazardous reagents, assembling of apparatus, isolation of natural products, purification by column chromatography. (ii) Evaluate results obtained, observations and conclusion of experiments. Documentation of results. (iii) Formulate ideas, scientific writing and authentic reporting, effective presentation and communication skills.
PSO3	<b>Research Competence</b> (i) Outline research problem related to research area of interest and planning of methodology for execution. (ii) Review scientific literature and findings in systematic manner and processing of information obtained to understand scope for novelty. (iii) Design novel synthetic routes using a retrosynthetic approach for development of elegant, economic and eco-friendly schemes.
PSO4	<b>Entrepreneurial and Social competence</b> (i) Demonstrate importance of industrial applications of organic chemistry in various fields. (ii) Devise chemical processes with Green approach having advantage in safe operations

<b>F.Y. M.Sc. Semester I</b>		
<b>Title of the Course and Course Code</b>	<b>Fundamentals of Physical Chemistry (CHA4101)</b>	<b>Number of Credits : 04</b>
<b>Course Outcome (COs)</b> <b>On completion of the course, the students will be able to:</b>		
CO1	Recall basic concepts and define different terminologies in thermodynamics, quantum chemistry and chemical kinetics. Differentiate order and molecularity, classical and quantum mechanics.	
CO2	Classify the chemical reactions on the basis of order. Determine the rate equations for the given chemical reaction, Schrödinger equation, wave equation and energy for particle in box	
CO3	Use simple models to predict the physical phenomenon associated with thermodynamics, quantum chemistry and chemical kinetics.	
CO4	Explain and illustrate quantum mechanical models and statistical thermodynamic properties. Relate the role of quantum mechanics in statistical mechanics.	
CO5	Criticize different theories of Reaction rates. Justify activation energy concept and Arrhenius theory for reaction rate.	
CO6	Calculate and integrate the physical parameters for given problems. Formulate and solve scientific problems based on the fundamentals of physical chemistry.	

<b>Unit No.</b>	<b>Title of Unit and Contents</b>
<b>I</b>	<b>Quantum Chemistry</b> Postulates of quantum mechanics, wave functions and probabilities, operators, commutation relationships, Hermitian operators, Commutators. Eigenfunctions and eigenvalues of operators, States as probability distributions and expectation values. Schrodinger equation, particle in a box and degeneracy. Applications- Solution of the Schrodinger equation for the hydrogen atom, radial and angular probability distributions, atomic orbitals, shape of orbitals, radial function, its square and radial distribution curve for atomic orbitals.
<b>II</b>	<b>Statistical thermodynamics:</b> Recapitulation of fundamental concepts of thermodynamics, significance of statistical thermodynamics over classical thermodynamics. Statistical view of entropy, Laws of thermodynamics from statistical considerations, Molecular view of temperature and heat capacity, Maxwell-Boltzmann, Fermi-Dirac and

	Bose-Einstein statistics, Boltzman distribution law, molecular energy levels, Ensembles and canonical ensembles, equilibrium constant in terms of partition functions, residual entropy, translational, rotational and vibrational partition functions, obtaining thermodynamic properties from partition functions.
III	<b>Chemical Kinetics</b> a. Recapitulation: Elementary reaction, half integral order reaction-differential and integral equations, reversible reaction, parallel reaction, consecutive reaction, principle of microscopic reversibility, steady state approximation- elucidating mechanism of a reaction.  b. Theories of Reaction Rates 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 – MichaelisMenton mechanism, Lineweaver and Eadieplot, Linear free energy relationship, potential energy surface.

### Learning Resources

1. Physical Chemistry - P. W. Atkins and De Paule 8<sup>th</sup> 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 5<sup>th</sup> edition, Prentice Hall, 1999
5. Chemical kinetics, Keith J. Laidler, 3<sup>rd</sup> Edition Pearson Education (2003)

Title of the Course and Course Code	Fundamentals of Inorganic Chemistry (CHA4102)	Number of Credits : 04
<b>Course Outcome (COs)</b> <b>On completion of the course, the students will be able to:</b>		
CO1	Outline the concept of symmetry to imagine molecules in three dimensions and identify the symmetry elements and symmetry operations and be able to pass through the molecule. Describe the selection rule and construction of microstate tables for various configurations.	
CO2	Classify the symmetry elements possessed by a molecule and assign it to a point group and determine optical activity and dipole moment. Explain the construction of a matrix representation.	
CO3	Generalise the importance of Orthogonality Theorem and learn the rules for constructing character tables. Outline the fundamental requirement for interpretation of electronic spectra of metal compounds for prediction of their properties.	
CO4	Explain molecular structure by the use of character tables and projection operator techniques. Identify the factors responsible for different magnetic behaviour of materials.	
CO5	Review the concept of SALC, spectrochemical and Nephelauxetic series. Develop the ability to generate a representation of SALC and to reduce it to its irreducible components. Evaluate numerical based on crystal field parameters.	
CO6	Specify and correlate the application of symmetry to spectroscopy to find out which modes are IR and Raman active. Specify the various Quenching of orbital angular momentum.	

Unit No.	Title of Unit and Contents
I	<p><b>Symmetry, Group theory and Spectroscopy</b></p> <p>a. Definitions and Theorems of Group Theory Defining properties of a group, group multiplication table, some examples of group, subgroups, classes</p> <p>b. Molecular Symmetry and Symmetry Groups Symmetry elements and operations, Symmetry planes and reflections, the inversion centre, proper/improper axes and rotation, products of symmetry operations, equivalent symmetry elements and equivalent atoms, symmetry elements and optical isomerism, symmetry point groups, classes of symmetry operations, classification of molecular point groups.</p> <p>c. Representations of Groups, the great orthogonality theorem and its applications, Character tables</p> <p>d. Reducible and irreducible representations, Wave function as a basis for irreducible representations</p> <p>e. Symmetry Adapted Linear Combinations (SALC)- projection operators and their use of constructing SALC</p> <p>f. Molecular Orbital Theory Transformation properties of atomic orbitals, MO's for Sigma bonding AB<sub>n</sub> molecules (tetrahedral AB<sub>4</sub>)</p> <p>g. Application of group theory to infrared spectroscopy Introduction, selection rules, polyatomic molecules, possible vibration in a linear molecule, bending modes, symmetry of vibrations and their IR activity, Group vibration concept and its limitations, IR spectra related to symmetry of some compounds, IR spectra of complex compounds.</p>
II	<p><b>NMR of Inorganic Compounds</b></p> <p>a. Concept of nuclear spin and resonance, fundamentals of coupling and decoupling, coupling constants. Predicting Intensity of NMR lines by binomial, trinomial, tetranomial etc.</p> <p>b. Structure elucidation by <sup>19</sup>F and <sup>31</sup>P NMR spectroscopy. Examples: <sup>19</sup>F NMR spectra of interhalogen compounds, <sup>19</sup>F and <sup>31</sup>P NMR to deduce structures of PF<sub>3</sub>R<sub>2</sub> type compounds, <sup>31</sup>P NMR of Wilkinson catalyst, geometrical isomers of platinum compounds, <i>trans effect</i> and <i>meridional</i>, <i>facial</i> isomers of rhodium compounds.</p> <p>c. General trends in chemical shifts, factors influencing chemical shift-geometry, electronegativity, charge and oxidation state, coordination number, effect of ligands, coordination effect on transition metal. General trends in coupling constant, factors influencing coupling constant-gyromagnetic ratio, periodicity, 's'</p>



	character in the bond, hybridization, coordination number, electronegativity, trans effect, inter bond angles lone pairs and oxidation state.
III	<b>Electron Absorption Spectroscopy</b> <ol style="list-style-type: none"> <li>Concept &amp; Scope of Ligand Fields, Energy levels of transition metal ions, Free ion terms, Spin-orbit coupling.</li> <li>Ligand Field Theory of Coordination Complexes Effect of ligand field on energy levels of transition metal ions, weak cubic ligand field effect on Russell-Saunders terms, strong field effect, Selection rules, Orgel diagram, Correlation diagrams, Tanabe-Sugano Diagrams, Spin-Pairing energies.</li> <li>Electronic spectra of Transition Metal Complexes, Spectra of 1<sup>st</sup> row ions, Spectrochemical &amp; Nephelauxetic series, Charge transfer &amp; luminescence spectra, Calculations of Dq, B, <math>\beta</math> parameters. Magnetic properties of coordination complexes.</li> </ol>

### Learning Resources

1. Chemical Applications of Group Theory, 3<sup>rd</sup> Edn., Author - F. A. Cotton (Wiley, New York)
2. Symmetry and spectroscopy of molecules, 2<sup>nd</sup> Ed. 2009; K. Veera Reddy, (New Age International Publication)
3. Group Theory and its Chemical Applications, P.K. Bhattacharya
4. Inorganic Chemistry: Shriver & Atkins (4<sup>th</sup> 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, 4<sup>th</sup> Edn. (2007).
7. Inorganic Chemistry: Catherine Housecroft
8. Inorganic Chemistry: Messler & Tarr, Pearson Publishers 3<sup>rd</sup> Edition
9. Organometallic Chemistry-A Unified Approach: R. C. Mehrotra & A. Singh
10. Symmetry and group theory-Vijayalaxmi
11. Physical Methods in Chemistry, R. S. Drago, Saunders, Harcourt Brac Javanovich College Publishers, (1992).
12. NMR spectroscopy in Inorganic Chemistry, J. A. Iggo, Oxford University press (2001).
13. Ligand field theory & its applications: B.N. Figgis & M.A. Hitachman (2000) Wiely VCH Publ.

Title of the Course and Course Code	Advanced Organic Chemistry and Spectroscopy (CHA4103)	Number of Credits : 04
<b>Course Outcome (COs)</b>		
<b>On completion of the course, the students will be able to:</b>		
CO1	Recall the concept of aromaticity and its application to identify various organic compounds. Predict and cite examples of aromaticity of heterocyclic and non-heterocyclic compounds.	
CO2	Discuss aromatic substitution reactions and predict the products/intermediates and explain the type of reactions and write their mechanisms	
CO3	Applications of organometallic compounds, ylides and predict products. Determine selectivity and demonstrate their advantages.	
CO4	Identify the products of oxidation-reduction reactions, give examples and determine selectivity of reagents and demonstrate their nature.	
CO5	Review various terms in stereochemistry and explain aspects of configurations in various chiral compounds, prochirality, stereospecific and stereoselective reactions.	
CO6	Revise basic principles of spectroscopy and demonstrate applications of spectroscopic techniques. Propose structures using spectroscopic data.	

Unit No.	Title of Unit and Contents
I.	Aromaticity: Benzenoid, non-benzenoid, antiaromatic, nonaromatic and aromatic compounds
II.	<b>Aromatic Substitution:</b> Recapitulation of Aromatic Nucleophilic and Electrophilic substitution, Benzyne generation under different condition (basic and neutral), orientations and regioselectivity in arynes, and $SN^i$ reactions
III.	<b>Organometallics and Ylides:</b> a. Reactions of organometallic reagents involving Li, Zn, Cu, Mg, Al, Si etc., Hydroboration and synthesis of borane reagents b. Ylides: Phosphorus, Nitrogen and Sulphur ylides in organic synthesis
IV.	a. Oxidation reactions: $CrO_3$ , PDC, PCC, IBX, $KMnO_4$ , $MnO_2$ , Swern, $SeO_2$ , $NaIO_4$ , $Pb(OAc)_4$ , Pd-C, $OsO_4$ , m-CPBA, $H_2O_2$ , Oxone, TEMPO, $O_3$ , etc. b. Reduction reactions: Boranes and hydroboration reactions, MPV

	reduction and reduction with H <sub>2</sub> /Pd-C, Willkinsons catalyst, DIBAL, transfer hydrogenation etc.
V.	<b>Stereochemistry:</b> a. Recapitulation R and S, E and Z, D and L nomenclature of compounds and chirality in allenes, hemisprane, spiranes and biphenyls b. Prochiral relationship, stereospecific and stereoselective reactions,
VI.	<b>Structure determination by spectroscopic techniques</b> a. UV: Factors affecting UV absorption and interpretation of UV spectra b. IR: Basic ideas about IR frequencies, interpretation of IR spectra c. <sup>1</sup> H-NMR: Fundamentals of <sup>1</sup> H-NMR, factors affecting chemical shift, integration coupling (1st order analysis) d. Introduction to CMR and mass spectrometry e. Problems based on UV, IR and <sup>1</sup> H-NMR

## Learning Resources

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
7. Organic Chemistry (5<sup>th</sup> Edn.) Robert. T. Morrison & N. Boyd. Hill edn.
8. Stereochemistry conformations and mechanism by P.S. Kalsi
9. Organic chemistry - by Cram, Hammond, Pine and Handrickson
10. Introduction to spectroscopy - D. I. Pavia, G.M. Lampman, G.S. Kriz, 3rd Edition
11. Spectroscopic methods in organic molecules - D. H. William & I Flemming Mc Graw Hill

Title of the Course and Course Code	Analytical Chemistry Practical – I (CHA4104) (Any 10 Practicals)	Number of Credits : 04
<b>Course Outcome (COs)</b> <b>On completion of the course, the students will be able to:</b>		
CO1	Outline and recall basic knowledge of fundamentals and application of organic and physical chemistry through chemical and scientific theories.	
CO2	Perform the experiment and tabulate the observations.	
CO3	Use of safety responsibilities residing in working with chemicals.	
CO4	Separate components from ternary mixture of organic compounds and determine type of given mixture and physical constants. 4 Demonstrate and employ skills in procedures and instrumental methods applied in organic and physical chemistry practical.	
CO5	Standardize/calibrate the apparatus and instrument. Carry out purification techniques.	
CO6	Write the experimental results and interpret it.	

Unit No.	Contents
I	<b>Organic Practicals</b> a) Separation of three component mixture b) Purification techniques
II	<b>Physical Practicals</b> a) pH metry: To determine dissociation constant and isoelectric point of an amino acid by pH metry b) Conductometry: To determine concentrations of strong acid and weak acid present in the mixture by titration with strong base by conductometric measurements. c) Spectrophotometry: i. To estimate amount of copper by photometric titration with EDTA ii. To determine molecular weight of Cobalt Complex/ amine picrate. d) Potentiometry: To determine stability Constant of a silver ammonium complex. e) Thermodynamics: To determine molar volume and partial molar volume of the components. f) Theoretical experiment: To plots the polar graphs for s and p orbitals using origin software

Title of the Course and Course Code	Analytical Chemistry Practical – II (CHA4105)	Number of Credits : 04
<b>Course Outcome (COs)</b> <b>On completion of the course, the students will be able to:</b>		
CO1	Outline and recall basic knowledge of fundamentals and application of inorganic and physical chemistry through chemical and scientific theories.	
CO2	Perform the experiment and tabulate the observations.	
CO3	Illustrate safety measures related to experiments carried out.	
CO4	Separate components from different analytes using various methods/techniques	
CO5	Standardize/calibrate the apparatus and instrument.	
CO6	Develop skills in procedures and instrumental methods applied in practical tasks. Interpret, conclude and write the experimental results.	

Unit No.	Contents
I	<b>Inorganic Practicals</b> <ol style="list-style-type: none"><li>1. Analysis of silica and manganese from pyrolusite ore.</li><li>2. Determination of tin and lead from solder.</li><li>3. Synthesis and Characterization of Chloro penta-ammine cobalt (III) chloride</li><li>4. Synthesis and Characterization of Nitro penta-amminecobalt (III) chloride</li><li>5. Synthesis and Characterization of Potassium tri-oxalato aluminate</li><li>6. Synthesis and Characterization of Tris acetylacetonato iron (III)</li><li>7. Synthesis and Characterization of Trans-bis glycinate copper (II)</li><li>8. Determination of equilibrium constant of M – L systems Fe(III) - sulphosalicylic acid by Job's continuous variation method spectrometrically.</li><li>9. Verification of Debye Huckle theory of ionic conductance for strong electrolytes KCl, BaCl<sub>2</sub>, K<sub>3</sub>[Fe(CN)<sub>6</sub>] by conductometry.</li><li>10. Analysis of aluminium from alum</li><li>11. Synthesis of MnO<sub>2</sub> / ZnO nanoparticle and its application.</li><li>12. Analysis of Electronic spectra of transition metal complexes at least for one system (d<sup>n</sup> Oh or Td) and calculation of crystal field parameters, inter electronic repulsion parameter and bonding parameter.</li></ol>
II	<b>Physical Practicals</b> <ol style="list-style-type: none"><li>a) Chemical kinetics:<ol style="list-style-type: none"><li>i. To study Kinetic decomposition of diacetone alcohol by dilatometry.</li><li>ii. To determine an order of iodide and persulphate ions by fractional change method.</li><li>iii. To investigate the rate constant of an autocatalytic reaction between potassium permanganate and oxalic acid.</li><li>iv. To investigate effect of Brönsted primary salt on reaction</li><li>v. Chemical Kinetics: To determine temperature coefficient and energy of activation of acid catalyzed ester hydrolysis reaction.</li></ol></li><li>b) Conductometry<ol style="list-style-type: none"><li>i. To study hydrolysis of ethyl acetate by NaOH using conductometric measurements.</li><li>ii. To determine solubility product and thermodynamic properties of sparingly soluble salt by conductometry.</li></ol></li></ol>

## Learning Resources

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.

	<b>F.Y. M.Sc. Semester II</b>	
<b>Title of the Course and Course Code</b>	<b>Advanced Physical Chemistry (CHA4201)</b>	<b>Number of Credits : 04</b>
<b>Course Outcome (COs)</b>		
<b>On completion of the course, the students will be able to:</b>		
CO1	Recall and define basic terminologies in spectroscopy, chemical bonding and nuclear chemistry.	
CO2	Illustrate, classify and compare theoretical and instrumental aspects for various spectroscopic and radio analytical techniques. Summarize different molecular spectroscopic concepts and rules to deduce the molecular structures.	
CO3	Solve and work with numerical based on spectroscopic, radio analytical and chemical bonding concepts. Interpret different types of molecular spectra and structure to evaluate valuable data from it.	
CO4	Explain molecular orbital theory for homonuclear, heteronuclear and polynuclear molecules using quantum rules.	
CO5	Review and relate the concepts involved in different spectroscopic techniques.	
CO6	Formulate and solve scientific problems based on the advanced physical chemistry concepts. Specify the applications of spectroscopy, radio analytical techniques and concepts of chemical bonding in chemistry and interdisciplinary fields.	

Unit No.	Title of Unit and Contents
I	<p>Molecular spectroscopy:</p> <ol style="list-style-type: none"> <li>Electromagnetic spectra, spectral regions, spectral line width, spectral line intensity. Spectrophotometer, resolving power, signal to noise ratio, introduction to Fourier transitions.</li> <li>Visible spectrophotometry and colorimetry: Theory of spectrophotometry and colorimetry, fundamental laws of absorption, Lambert's law, Beer's law, additivity of absorbance, instrumentation, applications.</li> <li>Rotational Spectroscopy: Rotational spectra, classification of molecules, rigid and non rigid rotor, diatomic molecules, effect of temperature and isotope substitution on the rotation spectra, linear and nonlinear polyatomic molecules, relative intensities of spectral lines, Stark effect.</li> <li>Vibrational Spectroscopy: Vibrating diatomic molecule, simple and anharmonic oscillator, diatomic vibrating rotator, vibrational and rotational spectrum of CO, breakdown of the Born Oppenheimer approximation, overtones and combinations, the vibration of polyatomic molecules, instrumentation of IR, principle and application of FTIR.</li> <li>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.</li> <li>Electronic spectroscopy of molecules: Born – Oppenheimer approximation, electronic spectra of diatomic molecules, intensity of vibrational – electronic spectra: The Franck-Condon principle, dissociation energy and dissociation products, rotational fine structure of electronic – vibration transitions, the Fortrat diagram, predissociation</li> <li>Magnetic resonance spectroscopy: <math>^1\text{H}</math> NMR, chemical shift, spin spin coupling, factors affecting chemical shifts. Introduction to <math>^{13}\text{C}</math> NMR, g factor, applications.</li> <li>Mossbauer spectroscopy: Principles and applications of Mossbauer spectroscopy</li> </ol>
II	<p>Chemical bonding:</p> <p>Introduction to electronic structure of molecule, Born Oppenheimer's Approximation, Quantum Theory of molecules, Approximate solution of Schrödinger equation, Approximate method –Variation Method, Valence bond theory (VBT) and Molecular Orbital Theory(MOT), Molecular orbital treatment of hydrogen molecule ion and hydrogen molecule, , Approximations underlying Huckel theory, Applications of Huckel theory to</p>



	ethylene, allyl system, butadiene and benzene, alternate and non-alternate hydrocarbons.
III	Nuclear and radiation Chemistry a. Types and detection of ionizing radiations- $\alpha$ , $\beta$ , $\gamma$ decay and their energies b. Applications of radioisotopes- neutron activation analysis, isotope dilution analysis, radiometric titration and problem solving.

### Learning Resources

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)

Title of the Course and Course Code	Advanced In organic Chemistry (CHA4202)	Number of Credits : 04
<b>Course Outcome (COs)</b> <b>On completion of the course, the students will be able to:</b>		
CO1	Recall the importance of bioinorganic chemistry. Describe the structure and bonding aspects of simple organometallic compounds. Outline basics of substitution reactions of octahedral complexes.	
CO2	Discuss the role of metals in Metalloproteins. Classify the different types of organo-transition metal complexes, catalyzed reactions and factors affecting it.	
CO3	Illustrate the importance and transport of metal ions. Identify back bonding in organometallics and outline the mechanism of hydrolysis in the octahedral system.	
CO4	Explain catalytic reaction involving organometallic compounds. Describe the metal carbonyls, metal clusters, metal nitrosyls and its preparation, structures and properties.	
CO5	Justify the importance and function of metal ions in metalloprotein. Evaluate problems based on electron count in organometallics.	
CO6	Develop basic understandings about redox reaction or electron transfer	

	reactions. Specify the environmental impact of the most inorganic compounds produced on the industrial scale and know different applications of organometallic compounds in medicines.
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Unit No.	Title of Unit and Contents
I	<b>Inorganic reaction mechanism</b> <ol style="list-style-type: none"> <li>Rate of reactions, factors affecting the rate of reactions, techniques for determination of rate of reaction.</li> <li>Ligand substitution reactions of:               <ol style="list-style-type: none"> <li>Octahedral complexes</li> <li>Square planar complexes, trans-effect, its theories and applications. Mechanism and factors affecting these substitution reactions.</li> </ol> </li> <li>Redox reactions: Inner and outer sphere mechanisms, complimentary and non-complimentary reactions.</li> <li>Isomerization reactions and applications</li> </ol>
II	<b>Bioinorganic Chemistry</b> <ol style="list-style-type: none"> <li>Metalloporphyrins with special reference to haemoglobin and myoglobin,</li> <li>Metalloenzymes,</li> <li>Oxygen transport</li> <li>Electron- transfer reactions;</li> <li>Nitrogen fixation,</li> <li>Metal complexes in medicine.</li> <li>Photosystems</li> </ol>
III	<b>Organometallic Chemistry</b> <p>I) Organometallic compounds of transition metals: Synthesis, properties, structure and bonding of the following organometallic compounds:</p> <ol style="list-style-type: none"> <li>Alkyl and Aryl derivatives</li> <li>Carbenes and Carbynes (Fischer and Tropsch)</li> <li>Alkene complexes (Zeise's salt)</li> <li>Alkyne complexes (diphenylacetylene platinum (0))</li> <li>Allyl complexes (diallyl nickel)</li> <li>Cyclopentadiene complexes (ferrocene)</li> </ol> <p>II) Homogenous and Heterogenous Catalysis: Comparison Fundamental reactions steps, turn-over number, turn over frequency catalytic cycle.</p> <p>III) Organometallics as Catalysts in Organic Reaction</p>

	IV) Organometallics in medicine, agriculture, and their biological and environmental aspects
IV	<b>Inorganic cage and cluster compounds</b> <ol style="list-style-type: none"> <li>Bonding in boranes</li> <li>Wade's rule</li> <li>STYX numbers</li> <li>Heteroboranes</li> <li>Carboranes</li> <li>Cluster compounds with ligands and without ligands (Zintl ions)</li> <li>Electron precise compounds and their relation to clusters.</li> <li>Metal-Metal bonding and Metal Clusters</li> <li>Electron Count and Structures of Clusters</li> </ol>

### Learning Resources

1. D. Banerjee, Coordination Chemistry, Tata McGraw Hill, New Delhi, 1993.
2. F. Basalo and R. G. Pearson, Mechanism of Inorganic Reactions, 2nd ed., Wiley, New York, 1967
3. D. Benson, Mechanisms of Inorganic Reactions in solution McGraw – Hill, New York, 1968
4. J. O. Edwards, Inorganic Reaction Mechanisms, Benjamin, New York, 1974
5. Principle of Bioinorganic Chemistry: S.J. Lippard and J, M. Berg
6. Bioinorganic Chemistry: Inorganic Elements in Chemistry of Life: W.Kaim and B. Schwederski
7. Bioinorganic Chemistry: Bertini, Gray, Lippard and Valentine
8. Bioinorganic Chemistry: R.J.P. Williams
9. Bioinorganic Chemistry: Robert Hay
10. Bioinorganic Chemistry: M.N. Hughes
11. James Huheey, F. A. Keiter and R. I. Keiter, Inorganic Chemistry – Principles of Structure and Reactivity, 4th Edition, Harper Collins, 1993
12. Puri, Sharma and Kalia, Principles of Inorganic Chemistry – 31st Edition, Milestone Publishers, 2010
13. R. Sarkar, General and Inorganic Chemistry, Books & Allied (P) Ltd. Calcutta, 2001
14. R. C. Mehrotra, A. Singh, Organometallic Chemistry: A unified approach- 2nd Edition, New Age International Publication, 2006
15. Nanomaterials & Nanochemistry, 2007, Catherine Brechignac, Philippe Houdy, Marcel Lahmani, ISBN 978-3-540-72992-1 Springer Berlin Heidelberg New York.
16. Nanomaterials Chemistry, Recent Developments and New Directions C.N.R. Rao, A. Muller, and A.K. Cheetham, ISBN 978-3-527-31664-9, 2007 WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim.
17. Nano-Surface Chemistry, 2001, Morton Rosoff, ISBN: 0-8247-0254-9, Marcel Dekker Inc. New York.

18. The Chemistry of Nanomaterials, CNR Rao, Muller Cheetham, WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim, 2004.
19. Semiconductor Nanomaterials, Challa S.S.R. Kumar, ISBN: 978-3-527-32166-7, WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim, 2010.

Title of the Course and Course Code	Reaction Mechanism in Organic Chemistry (CHA4203)	Number of Credits : 04
<p align="center"><b>Course Outcome (COs)</b>  <b>On completion of the course, the students will be able to:</b></p>		
CO1	Define and explain recall principles of photochemistry.	
CO2	Explain pericyclic reactions and justify their mechanisms by using correlation diagrams and FMO approach	
CO3	Demonstrate concepts of Carbanions, Enamines and Ynamines and explain their stability, reactivity, selectivity and predict the products.	
CO4	Classify rearrangements. Predict the product and illustrate the reactions involving rearrangements	
CO5	Review carbenes, nitrenes, free radicals and discuss their methods of synthesis and predict products in related reactions.	
CO6	Specify neighbouring group participation (NGP) and predict the products in reactions involving NGP. Explain different mechanisms of ester and amide hydrolysis.	

Unit No.	Title of Unit and Contents
I.	<b>Photochemistry:</b> General basic principles, initiators and sensitizers photochemistry of carbonyl compounds, alkenes, dienes, polyenes and aromatic compounds, photorearrangements and named reactions
II.	<b>Pericyclic reactions:</b> Electrocyclic, Cycloaddition, Sigmatropic and ene reactions. 1,3-dipolar additions, Analysis by correlation diagrams, FMO approach and ATS concept. Application of pericyclic reactions.
III.	Carbanions, Enamines and ynamines - Formation, stability and related name reactions
IV.	Reactions of carbenes and nitrenes: <i>N</i> -heterocyclic carbene and nitrenes-generation, stability and reactivity
V.	Neighbouring group participation: NGP involving Nitrogen, Sulphur and Carbon atoms, C-C and C=C.

VI.	Rearrangements: Anionic, cationic and free radical
VII.	Free radical - Generation, stability, Nucleophilic and electrophilic radicals, characteristics reactions, -free radical substitution, addition to multiple bonds, Radicals in synthesis: Inter and intra molecular C-C bond formation via mercuric hydride, tin hydride, thiol donors, cleavage of C-X, C-Sn, C-Co, C-S, O-O bonds, Oxidative coupling, C-C bond formation in aromatics, S <sub>N</sub> Ar reactions, Mechanisms in biological chemistry
VIII.	Ester and amide hydrolysis (only major acid, base catalyzed and neutral condition mechanisms)

## Learning Resources

Mechanism and structure in Organic Chemistry – E. S. Gould (Holt, Rinehart and Winston)

1. Advanced organic chemistry by J. March, 6<sup>th</sup> Ed.
2. Advanced organic chemistry. F. A. Carey and R. J. Sundberg, 5th Ed. Springer (2007)
3. A guidebook to mechanism in organic chemistry – Peter Sykes 6<sup>th</sup> Ed. Orient Longman
4. Organic Chemistry – J. Clayden, N. Greeves, S. Warren and P. Wothers. Oxford University Press (2001)
5. Radicals in Organic Synthesis B. Giese, Pergamon press (1986)
6. Physical Organic chemistry – J. Hine
7. A guidebook to mechanism in organic chemistry – Peter Sykes 6<sup>th</sup> Ed. Orient Longman
8. Modern Synthetic reactions- H.O. House

<b>Title of the Course and Course Code</b>	<b>Analytical Chemistry Practical – III (CHA4204)</b>	<b>Number of Credits : 04</b>
<b>Course Outcome (COs)</b> <b>On completion of the course, the students will be able to:</b>		
CO1	Describe the theoretical principles and concepts related to experiments.	
CO2	Represent the results of scientific work in oral, written, graphical and electronic formats.	
CO3	Apply laboratory skills in organic and physical chemistry. Carry out single stage preparation along. Demonstrate software related to chemistry.	
CO4	Identify and analyse the product obtained by different techniques. Demonstrate purification technique.	
CO5	Justify the steps to standardize the methods and instruments .	
CO6	Perform experiments, analyze and interpret the experimental results	
<b>Unit No.</b>	<b>Contents</b>	
I	<b>Organic Practicals</b> a. TLC b. Column Chromatography c. Distillation d. Use of chemistry software like ChemDraw, Chems sketch e. Single stage preparations: oxidation, reduction, alkylation, formylation, cycloaddition etc.	

<b>II</b>	<b>Physical Practicals</b> <ol style="list-style-type: none"> <li>a. Radioactivity:               <ol style="list-style-type: none"> <li>1. To determine counting errors of Giger Muller counter.</li> <li>2. To determine <math>E_{\max}</math> of <math>\beta</math> radiation and absorption coefficients in Al by Geiger Muller counter</li> </ol> </li> <li>b. Viscometry To determine radius of glycerol molecule by viscosity.</li> <li>c. Conductometry To study the hydrolysis of <math>\text{NH}_4\text{Cl}</math> by Conductometry.</li> <li>d. Spectrum Analysis To analyze crystal structure from single crystal X-ray pattern.</li> <li>e. Theoretical Experiment To study statistical treatment of experimental data.</li> <li>f. pH metry To determine Hammett constant of ortho, meta, para amino/nitro benzoic acid.</li> </ol>
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<b>Title of the Course and Course Code</b>	<b>Chemistry Practical Course - IV (CHA4205)</b>	<b>Number of Credits : 04</b>
<b>Course Outcome (COs)</b> <b>On completion of the course, the students will be able to:</b>		
CO1	Describe the theoretical principles and concepts related to experiments.	
CO2	Represent the results of scientific work in oral, written, graphical and electronic formats.	
CO3	Execute chemical analysis for different samples. Implement problem solving, critical thinking and analytical reasoning as applied to scientific problems.	
CO4	Analyze data from a range of physical techniques to characterise different compounds.	
CO5	Justify the steps to prepare and standardize different solutions.	
CO6	Design and perform scientific experiments. Interpret and write the experimental results with standards.	

Unit No.	Contents
I	<b>Inorganic Practicals:</b> <ol style="list-style-type: none"> <li>1. Analysis of silica and iron from hematite ore</li> <li>2. Analysis of cupronickel/stainless steel alloy.</li> <li>3. Synthesis and characterization of Tris (ethylene diammine) Ni (II) thiosulphate.</li> <li>4. Synthesis and characterization of Tris triphenylphosphine copper nitrate</li> <li>5. Synthesis and characterization of Cis and Trans dichloro bis(ethylenediamine) Co (III) chloride.</li> <li>6. Synthesis and characterization of Tris acetylacetonato manganese</li> <li>7. Synthesis and characterization of Potassium trioxalato chromate</li> <li>8. Determination of iron by solvent extraction techniques using 8-hydroxyquinoline reagent.</li> <li>9. 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).</li> <li>10. Estimation of phosphate from waste water by calibration curve method.</li> <li>11. Synthesis of Fe<sub>2</sub>O<sub>3</sub>/ZnS nanoparticles.</li> </ol>
II	<b>Physical Practicals</b> <ol style="list-style-type: none"> <li>a. Conductometry               <ol style="list-style-type: none"> <li>1. To determine equivalent conductance at infinite dilution, dissociation constant of Acetic Acid and to study Debye Huckel Limiting law</li> <li>2. To determine critical micellar concentration (CMC) and G of micellization of sodium dodecyl sulphate (SDS).</li> </ol> </li> <li>b. Potentiometry               <p>To determine Solubility and solubility product of a sparingly soluble salt.</p> <p>To determine strength of commercial vinegar by potentiometric titration</p> </li> <li>c. Potentiometry:               <p>To estimate amount of halides, present in the mixture</p> </li> <li>d. pH metry:               <p>To determine dissociation constants of tribasic acid (phosphoric acid)</p> </li> <li>e. Spectrophotometry               <p>To study simultaneous determination of cations from binary mixture</p> </li> </ol>



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**Learning Resources**

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. Ligand Field Theory, B. N. Figgis.