VANITA VISHRAM WOMEN'S UNIVERSITY
SCHOOL SCIENCE AND TECHNOLOGY
DEPARTMENT OF CHEMISTRY

MASTER OF SCIENCE (M.Sc.) CHEMISTRY/ORGANIC CHEMISTRY PROGRAMME
under Learning Outcomes-based Curriculum Framework (LOCF) for Post Graduate (PG) Education

SEMESTER 2
Core Courses (CC), Ability Enhancement Compulsory Courses (AECC), Generic Elective Courses (GE)

Syllabus applicable to the students seeking admission in the following programmes
M.Sc Chemistry/Organic Chemistry under LOCF w.e.f. the Academic Year 2021-2022

1. Preamble – VVWU

Vanita Vishram Women's University (VVWU) is the First-ever Women's University of Gujarat approved by the Government of Gujarat under the provisions of the Gujarat Private Universities Act, 2009. It is a university committed to achieve Women's Empowerment through Quality Education, Skill Development, and by providing employment opportunities to its girl students through its model curriculum, integration of technology in pedagogy and best-in-class infrastructure. The focus is on prioritizing practical component and experiential learning supported through academia-industry linkages, functional MoUs, skill development training, internships etc. It aims at providing opportunities to the girl students for holistic development and self-reliance.

VISION

Empowerment of women through quality education and skill development, so as to make them strong pillars of stability in the society.

MISSION

To provide Education & Professional Training to all women for their all-round development, so as to enable them to become economically independent and socially empowered citizens.

Master of Science (M.Sc.) Chemistry/Organic Chemistry

Semester-2

Core Course

CH21070

Inorganic Chemistry (Credit 4+1)

Course objectives:

- Study of magnetic nature, their types, determination of magnetic susceptibilities
- Gaining of idea based on Coordination of metal complex, Metal carbonyls: Classification, Bonding in metal carbonyls
- Detail study based on organometallic compounds, its rule and types.
- Quantum Study of the particles in different dimensions, and their operators.

Prerequisites:

- Magnetic properties, and its method.
- Different carbonyls compounds, calculation based on CFSE
- Organometallic study of complex
- Quantum nature identification of electrons in space.

Unit-I Magnetic properties and electronic spectra of transition metal complex

Definition of magnetic properties, Types of magnetic bodies, The source of paramagnetism, Diamagnetism and Pascal's constant, example of Pascal's constant, Curie and Curie-Weiss law, Magnetic properties of transition elements, Determination of magnetic susceptibility by Gouy method, Faraday method and Null deflection method, Application of magnetic susceptibility measurements, Temperature-independent Para magnetism, Orbital contribution to magnetic moment, Calculation of spin magnetic moment, Anomalous magnetic moment, Magnetic exchange coupling and Spin Crossover. Magnetic properties of inner transition metal complexes and their spin & orbital moments. Electronic spectra of metal complexes: La Porte rule, Tanabe-Sugano diagram and Orgel diagram for transition metal complex, Charge transfer spectra, Spectroscopic ground state.

Unit–II Coordination Chemistry of Metal Complexes

Crystal field theory: Crystal field effects in octahedral, tetrahedral, square planar, square pyramidal and trigonal bipyramidal complexes, Crystal Field Stabilization Energy (CFSE), Calculation of Crystal Field Stabilization Energies, Factors affecting crystal field splitting energies, Spectrochemical series: Jahn-Teller effect, Nephelauxetic effect, Ligand Field Theory, Term Symbols, Russell-Saunders coupling. Metal carbonyls: Classification, Bonding in metal carbonyls, Effective Atomic Number rule, Vibrational spectra of metal carbonyls for bonding and structural elucidation, Structure of mononuclear metal carbonyls

like Ni(CO)4 and Cr(CO)6, Structure of polynuclear metal carbonyls like Mn2(CO)10 and Fe3(CO)12.

Unit-III Organometallic Chemistry

Classification, Unique reactions in organometallic chemistry like oxidative addition, migratory insertion and reductive elimination, Synthesis of organometallic compounds, Calculation of 18 electron rule and metal-metal bond, Fluxionality of complexes, Metal olefins: Zeiss's salt, Metallocene: Synthesis and electrophilic substitution reactions, Application of organometallic compound in homogeneous catalysis like Monsanto acetic acid synthesis, Cativa process, Hydroformylation reaction, Catalytic deuteration of benzene, Catalytic hydrogenation and Catalytic hydrocyanation of alkene, Wacker(Smith) process and in heterogeneous catalysis like Ziegler-Natta polymerization, Application of organometallic compounds in the production of speciality chemicals.

Unit-IV Quantum Mechanics

Postulates, Schrodinger wave equation, I-D, 2-D, 3-D box, Simple Harmonic oscillator, Polar Coordinates of H-atom, separation of variables, Eigenvalue and eigen equation, expectation value, probability density, Ladders operator, ZPE, Slaters- Codon rule, Rigid rotator, ordinary angular Momentum, generalized angular momentum. Starks effect, Zeeman splitting

Reference Books

- Introduction to magnetochemistry by A. Earnshaw, Elsevier, 2013.
- Elements of Magnetochemistry by R. L. Dutta, A. Syamal, Affiliated East-West Press, 1993.
- Inorganic Chemistry, J.E. Huheey, K.A.Keiter and R.L.Keiter, Harper Cotton College Publications, 1993.
- Concise Inorganic Chemistry by J.D. Lee, Chapman & Hall, 1996.
- Principles of inorganic chemistry by B.R. Puri, L.R. Sharma & K.C. Kalia, Milestone Publishers, 2017.
- Introduction to Coordination Chemistry by G. A. Lawrance, John Wiley & Sons, 2013.
- Text Book of Coordination Chemistry by R. K. Sharma, Discovery Publishing House, 2007.
- Essentials of Coordination Chemistry: A Simplified Approach with 3D Visuals by Vasishta Bhatt, Academic Press, 2015.
- Inorganic Chemistry by J. E .House, Academic Press, 2010.
- Inorganic Chemistry by G. L. Miessler, P. J. Fischer, D. A. Tarr, Pearson, 2014.
- Shriver and Atkins' Inorganic Chemistry by P. Atkins, T. Overton, OUP Oxford, 2010.
- Concise coordination chemistry by M. J. Xavier, R. Gopalan, V. Ramalingam, Sangam Books Limited, 2001.
- Organometallic Chemistry by R. C. Mehrotra, New Age International, 2007.

- Basic Organometallic Chemistry: Concepts, Syntheses and Applications by B. D. Gupta, Universities Press, 2011.
- The Organometallic Chemistry of the Transition Metals, R. H. Crabtree, John Wiley & Sons, 2014.
- Organometallic Chemistry and Catalysis by D. SeeAstruc, Springer Science & Business Media, 2007.
- Quantum Chemistry, N. Levine, Prentice Hall, New York

Courses Outcome:

Will provide idea for the determining the magnetic nature of the complex, also in knowing the nature of splitting of complex and its energies, formation of organometallic compound, and way of learning quantum chemistry of different molecules

Core Course

CH21080

Organic Reaction-I (Credit 4+1)

Course objective:

- Understanding the mechanism of organic reactions and its applications.
- Basic oxidative addition, transmetallation, isomerization and reductive elimination used in organic reaction mechanism
- Detailed concept of pericyclic reactions. (cycloaddition. electrocyclic, sigmatropic and group transfer reactions)
- Chemistry of selected reagents and its usefulness in organic transformations.
- Organic transformations using photochemistry (rearrangement, addition, cleavage, isomerization, dimerization reactions)

Prerequisite:

- Basic concept of intermediates and its preparations.
- Molecular Orbital theory and its application.
- Basic concepts of HOMO and LUMO of organic molecules.
- General aspects of oxidation and reduction reactions.
- Basic concept of cleavage reaction.

Unit-I: Organic Name Reactions

General nature, method, mechanism and synthetic applications of the following reactions: (i) Johnson–Corey–Chaykovsky reaction (ii) Dakin reaction, (iii) Darzens glycidic ester synthesis, (iv) Wittig reaction (v) Willgerodt reaction, (vi) Peterson olefination (vii) H. V. Z. reaction, (viii) McMurry reaction (ix) Corey-Fuchs reaction (x) Michael addition (xi) Ugi reaction (xii) Mannich reaction

Unit-II: Pericyclic Reaction

Introduction - Definition, Characteristics and Classification Molecular orbitals and symmetry properties of ethylene, 1,3- butadiene, 1,3,5- hexatriene and allyl systems. Electrocyclic Reactions: Woodward-Hoffmann Correlation diagram and derivation of selection rules, Conrotatory and disrotatory motions, FMO and PMO approach for 4n and (4n+2) Pi electron system and allyl systems. Cycloaddition Reactions: Antarafacial and suprafacial additions. FMO and PMO approach for 4n and (4n+2) Pi electron Systems (No correlation diagram), Diels-Alder reaction, stereoselectivity, Effect of substituents. Sigmatropic rearrangements: Suprafacial and antarafacial shifts involving H & C moieties, retention and inversion of configurations. The Cope and Claisen rearrangements, Ene reaction, 1, 3- dipolar cycloadditions. Examples of electrocyclic, cycloaddition and sigmatropic rearrangements.

Unit-III: Organic Transformation and Reagents

I. Sharpless epoxidation II. Umpolung reagent (1,3-dithiane) III. Dess martin periodinane IV. DDQ V. Tri-n-butyltin hydride $(C_4H_9)_3SnH$ VI. Diisobutyl aluminum hydride (DIDAL-H) VII. Lithium diisopropylamide (LDA) VIII. OZONE IX. Crown ethers X. Wilkinson's Catalyst

Unit-IV: Photochemistry

A. Energy of molecules, photochemical energy, electronic excitation, Jablonski diagram, laws of photochemistry, quantum efficiency.

B. Photochemistry of carbonyl compounds- α- cleavage of acyclic, cyclicand α-β unsaturated cleavage of carbonyl compounds, β- cleavage of, inter and intramolecular hydrogen abstraction, addition to carbon- carbon double bond, photo reduction of carbonyl compounds.

C. Photo induce rearrangement of enones, dienones and alkenes. Photochemistry of alkenes and aromatic compounds- isomerization, dimerization and addition reactions.

Reference book:

- Reaction Mechanism in Organic Chemistry by S. M. Mukherji and S. P. Singh (McMillan India Ltd., 1976).
- Organic Chemistry (5/e) by Morrison & Boyd (Prentice Hall).
- Advanced Organic Chemistry by Carey & Sundberg (3rd edition).
- A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, Longman.
- Name Reactions by A. R. Parikh & H.A. Parikh
- Reaction Mechanism and Reagents in Organic Chemistry by C.R. Chatwal (Himalaya Publishing House, Bombay, 1987).
- Organic Chemistry-Reactions and Mechanism by P S Kalsi
- Advanced Organic Chemistry: Reactions and Mechanisms by M.S. Singh
- Photochemistry and Pericyclic Reactions by Jagdamba Singh
- Pericyclic reactions: A text book by S. Sankararaman
- Excited states in Organic Chemistry by J. D. Coyle and J. A. Barltrop
- March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure by Michael B. Smith
- Advanced Organic Chemistry: Part B: Reaction and Synthesis by Carey & Francis
- Organic Chemistry by Jonathan Clayden.

Courses Outcome:

- A familiarity with, and application carbon-carbon bond forming reaction,
- Ability transformed organic molecules through pericyclic reactions and selected reagents.
- Application of photochemistry to organic molecules.

Core Course

CH21090

Physical Chemistry (Credit 4+1)

Course objective:

- To understand the Debye Huckel Theory of ion-ion interactions.
- To understand the concept of Nuclear Magnetic Resonance (NMR) Spectroscopy
- To study Isotopes Separation Methods, Particle Accelerators and Nuclear Projectiles.
- Brief understanding of Surfactants.

Prerequisites:

Lerner should have:

- Basic understanding of electrochemistry
- Brief understanding of molecular spectroscopy
- Knowledge of isotopes and nuclear reactions.
- Basic of Surfactants.

Unit-I: Electrochemistry

Debye-Huckel theory of interionic attraction (qualitative account only), relaxation effect and electrophoretic effect. Ionic strength, Activity coefficient and its determination by solubility and EMF method. Dissociation constant, relation between thermodynamic dissociation constant and dissociation function. Determination of dissociation constant of monobasic acid by conductance method and approximate EMF method, Numericals.

Unit-II: Molecular Spectroscopy-II

Nuclear Magnetic Resonance (NMR) Spectroscopy: Introduction, Principle, Instrumentation, Position of Signals, Chemical Shifts, Delta and Tau Scales, Spin-spin coupling, Peak Area ; Integration and Splitting Pattern, examples of NMR spectra, Magnetic Resonance Imaging (MRI)

Unit-III: Nuclear Chemistry-II

(A) Isotopes Separation Methods: Stable and unstable isotopes, separation of isotopes by different methods, gaseous diffusion, thermal diffusion, distillation, chemical exchange methods, Bainbridge velocity focusing mass spectrograph, Dempsters direction focusing mass spectrograph

(B) Particle Accelerators: Linear accelerator, Cyclotron, Numerical problems on Cyclotron

(C) Nuclear Projectiles: particles used as projectiles, Merits and demerits of different projectiles

Unit-IV: Surfactants

Surface active agents, classification of Surface active agents, micellization, hydrophobic interaction, critical micellar concentration (CMC), factors affecting the CMC of surfactants, Krafft point and cloud point, counter ion binding to micelles, thermodynamics of micellization-mass action and phase separation model, solubilization, microemulsion, reverse micelles.

Reference Books:

- Physical Chemistry, P. W. Atkins, 6th Edition, ELBS.
- Physical Chemistry by Protuon and Marron
- A Textbook of Physical Chemistry, Vol. 4, K. L. Kapoor, McMillan, 1985
- Essentials of physical chemistry by A. S. Bhal and G. D. Tuli, Pub : S. Chand
- Modern Electrochemistry, Vol. 1 & 2, J.O.M. Bookris and A. K. N. Reddy.
- Introduction to Electrochemistry by Glasstone.
- Introduction to Molecular Spectroscopy, G. M. Barrow , McGraw – Hill.
- R.M. Silverstein, G.C. Bassler & T.C. Morrill: Spectroscopic Identification of Organic Compounds, John Wiley & Sons.
- John R. Dyer, Applications of absorption spectroscopy of organic compounds, Prentice Hall India (2012).
- Basic Principles of Spectroscopy, R. Chang, McGraw-Hill
- Essentials of Nuclear Chemistry by H. J. Arnikar (Wiley Eastern Ltd., 1981).
- Introduction to Colloid and Surface Chemistry by Shaw.
- Micelles, Theoretical and Applied Aspects, V. Morol, Plenum.

Learning outcomes

After completion the course, the learner shall be able to:

- Explain qualitative interaction of ionic systems based on Debye-Huckel theory.
- Knowledge for the separation of isotopes by different methods.
- Solve some simple NMR spectra.
- Study of Surfactants and their micellization process.

Core Course

CH21100

Inorganic Chemistry Practical (Credit 2)

1. Inorganic gravimetric estimation:

   a. Estimation of Cu^{+2} as CuSCN
   b. Estimation of Ca^{+2} as $CaC_2O_4.H_2O$
   c. Estimation of Ba^{+2} as $BaSO_4$

2. Inorganic volumetric estimation (Any six)

   a. Estimation of % Purity of Manganese Salt.
   b. Estimation of Aluminium by back titration.
   c. Estimation of Ca^{+2} and Pb^{+2} in the admixture.
   d. Estimation of Carbonate-Bicarbonate in mixture using pH-meter.
   e. Estimation of available chlorine (ClO^-) in bleaching powder.
   f. Estimation of Iron in Iron Ore.
   g. Estimation of Fe^{+2} and Cr^{+3} in the given admixture.
   h. Analysis of Solder and Type metal (Alloy Analysis).

Reference books:

- Quantitative Chemical Analysis, R.B. Fischer and D.G. Peters, 3rd Edition, D.B. Saunders Company, 1968 or latest edition.
- Laboratory directions for analytical separation and determinations, C.T. Kenner, MacMillan Company, New York, 1971.
- Inorganic Qualitative analysis, A.I. Vogel, 5th Edition, ELBS/ Longman, 1989.
- Vogel's text books of Quantitative Chemical Analysis, Revised by G.H. Jeffery, J. Bassett, J. Mendham and R.C. Danney, Fifth Edition, ELBS/ Longman, 1989.
- Spot tests in inorganic analysis, F. Feigel, 5th Edition, Elsevier (1958).
- Colorimetric methods of analysis, Snell and Snell, D. Van Nostrand, latest edition.E.D.T.A. titrations, latest edition, Fleshka, Pergamon process.

Core Course

CH21100

Organic Chemistry Practical (Credit 2)

Course objective:

- Preparation and use of reagents in various organic transformation reactions.
- Understand the techniques to monitor the reaction.
- To understand estimations of various compounds.

Prerequisite:

- Students should be aware about name reactions.
- Basic idea about Unit process and unit operation.
- Basic idea about molecular rearrangement.
- Basic idea about process of estimations.
- MSDS of chemicals.

I. Preparation of organic compounds (Simple one or two step preparations involving different techniques) (Minimum six)

(i) Diazotization reaction: Orange-I
(ii) Friedl-Craft's reaction: Resacetophenone from Resorcinol.
(iii) Cannizzaro reaction: Benzoic acid from Benzaldehyde via KOH
(iv) P-bromoaniline from Acetanilide via p-bromoacetanilide.
(v) m-phenylenediamine from Nitrobenzene via m-dinitrobenzene
(vi) β- Resorcilic acid from resorcinol
(vii) P-chloro benzoic acid from p-toluidine via p-chloro toluene
(viii) Aldol condensation: Chalcone from Benzaldehyde + Acetophenone (Claisen Schmidt reaction)
(ix) Gabriel phthalimide synthesis.
(x) Preparation of Congo red dye from naphthionic acid via hydrozobenzene

II. Quantitative Estimations: (Minimum three)

a. Estimation of ester + acid

b. Estimation of formaldehyde

c. Estimation of amide + acid

d. Determination of aromatic primary amines by either diazotization or indirect diazotization.

e. To determine the amount of acetamide in the given solution hydrolysis by NaOH.

Reference Books:

- A text book of practical organic chemistry – A. I. Vogel
- Practical organic Chemistry – Mann and Saunders
- A handbook of quantitative and qualitative analysis – H. T. Clarke
- Comprehensive Practical Organic Chemistry: Qualitative Analysis V K Ahluwalia& S. Dhingra.
- Comprehensive Practical Organic Chemistry: Preparations and Quantitative Analysis V K Ahluwalia & R. Aggarwal Universities Press.
- An Advance Course in Practical Chemistry, A K. Nad, B. Mahapatra and A. Ghoshal.

Core Course

CH21110

Physical Chemistry Practical (Credit 2)

Course objective:

- Use of pH metry dissociation constant of a given dibasic acid.
- To study hydrolysis of ester by conductometry.
- To study solubility of sparingly soluble salt by potentiometrically.
- Determination of equilibrium constant and formula of a complex.
- To find concentration of supplied unknown solution colorimetrically.
- Determine the molecular weight of a given polymer.
- Determination of energy of activation for the given reaction.

Prerequisites:

- Theoretical understanding and operational knowledge of pH meter and potentiometer.
- Theoretical understanding hydrolysis of ester and operational knowledge of conductometry.
- Operational knowledge of Colorimeter.
- Theoretical understanding of phase diagrams.
- Brief knowledge of energy of activation.

Experiments:

1. Determine the dissociation constant of a given dibasic acid pH-metrically.
2. Determine the velocity constant of the hydrolysis of ethyl acetate with sodium hydroxide at room temperature by conductance measurements.
3. Determine the solubility of silver chloride in water potentiometrically.
4. To determine the concentration of given components in a mixture colorimetrically.
5. Determine the equilibrium constant of the reaction $I^- + I_2 = I^{3-}$ by distribution method.
6. Investigation the reaction between H_2O_2 and HI at two different temperatures and calculate the energy of activation for the reaction.

7. Determine the formula of a complex between Cu^{2+} and NH_3 by distribution method. $Cu^{2+} + nNH_3 = [Cu(NH_3)_n]^{2+}$
8. Determine the molecular weight of a given polymer from viscosity measurement.

Learning outcomes

After completion the course, the learner shall be able to:

- Find dissociation constant of a given acid and solubility of sparingly soluble salt.
- Calculate the energy of activation for the given reaction.
- Find equilibrium constant and determine the formula of a complex.
- Study and analyse the phase diagram of a three-component system.
- Find molecular weight of a given polymer from viscosity measurement.

Core Course

CH21110

Analytical Chemistry Practical (Credit 2)

Course objectives:

- Ion exchange separation and quantification
- Flame emission quantitative analysis
- Alloy analysis
- Water analysis
- IR Spectral analysis

Prerequisites:

- Basic of ion exchange chromatography
- Flame emission spectroscopy
- Water pollutants analysis parameter
- Functional group frequency

Experiments: Practicals to be performed: (Any Six)

- Ion exchange separation of (Fe+3 & Co+2) and determination of Fe+3 colorimetric.
- Determination of total salt content by ion exchange chromatography.
- Determination of Na & Ca in cola drinks and fruit juices using flame photometric techniques.
- Analysis of brass alloys for Copper and Zinc Content.
- Conductometric determination of vanillin in Vanilla.
- Determination of dissolved oxygen in water.
- Determination of chemical oxygen demand (COD).
- Structural characterization of compounds by infrared spectroscopy.

- Determination of sulphate (SO_4^{-2}) in a given water sample using complexometric titration.
- Determination of Cu^{+2} and Ca^{+2} in a mixture using EDTA by spectrophotometric method.
- Determination of phosphate (PO_4^{-3}) in a given mixture so spectrophotometrically.
- Analysis of basic parameters of different water samples. (TDS. Alkalinity, Hardness, Chloride measurement).

Course outcomes:

- Able to apply the knowledge of taught concepts during practicals performance.