# M.Sc. Degree Analytical Chemistry Programme

#### Aim and Objective of the Syllabi

#### Aim

Chemistry is a central subject of science. It is also closely related to daily life. The Master's program not only offers the option of focusing on a specialist area but students will also acquire the necessary skills for this and they will learn to think independently and act responsibly.Graduates will become familiar with the terminologies and special aspects of chemistry, its strengths and limitations and will be able to apply their knowledge to new issues and situations, even in an interdisciplinary context. They will gain knowledge and practical skills relating to the current state of research in selected fields. They will be able to analyze chemical issues and assess them critically, to develop independent solution strategies and to estimate their impacts in a wider context. The broad spectrum of the academic program will ensure that students acquire the skills necessary for demanding fields of activity in industry, economy and administration

#### Objective

The Master's course in chemistry is designed with an objective to teach post graduates with the skills to critically assess and deal with issues requiring the utilization of chemical principles from each subdisciplines such as organic, inorganic, physical, analytical and biochemistry. It is the objective of the chemistry program to teach students the necessary knowledge in a way that enables them to familiarize themselves quickly with new developments, to be introduced to new areas and to make independent contributions to further developments of research and technology in their specialized area once they have finished their program.

## Semester 1 PG1ANL C01 Inorganic Chemistry - I

#### **Aimsand Objectives**

This is a chemistry module designed for chemistry majors and featuresthe principles of coordination chemistry, boron compounds and that of nuclear chemistry. In depth discussion about coordination compounds focusing primarily on their structure and various aspects of bonding will be done. The course covers synthesis, structure and bonding of organometallic compounds. Kinetics of reactions of metal complexes and their mechanism will also be illustrated. The learners should be able to apply these topics in various fields.

- To mould the chemistry majors in coordination chemistry, boron compounds and nuclear chemistry
- To understand the structure and various aspects of bonding in the coordination compounds
- To achieve knowledge about the synthesis, structure and bonding of organometallic compounds
- To illustrate the kinetics of reactions and their mechanism of metal complexes
- To acquire ability to apply the theoretical knowledge in various fields

## PG1 ANL C02 Organic Chemistry - I

#### **Aims and Objectives**

The module deals primarily with the basic principles to understand the structure and reactivity oforganic molecules. Emphasis is on substitution and elimination reactions of aliphatic and aromatic compounds.

Learners will get the essential ideas on how simple molecules can beconstructed. Bonding in conjugated systems, reactions mechanism, organic transformations and stereochemistry will likewise be discussed.

- To understand the structure and reactivity of organic molecules
- To emphasize the substitution and elimination reactions of aliphatic and aromatic compounds
- To get an idea about the construction of simple organic molecules
- To impart knowledge about stereochemistry of organic compounds and basic principles of conformational analysis
- To know the bonding in conjugated systems and various reaction mechanisms

#### PG1 ANL C03 Theoretical Chemistry - I

#### Aims and Objectives

This module looks at quantum chemistry and group theory. A more profound comprehension of quantum chemistry beginning from its postulates and basic systems such as particle-in-a-box to hydrogen like atoms is explored. The second part of the module looks at molecular symmetry and applications in molecular orbitals analysis and vibrational spectroscopy, electronic transitions of carbonyl chromophore and origin of selection rule of electronic transition. Learners will be able to apply these ideas to individual atoms and molecular systems.

- To get a comprehensive idea about quantum chemistry and group theory
- To discuss the emergence of classical mechanics over quantum mechanics
- To get an awareness about the basic postulates of quantum chemistry and its application to hydrogen and hydrogen like atoms
- To acquire knowledge for deriving the wave function, energy, momentum etc. of a particle under different conditions of motions
- To impart knowledge about the molecular symmetry and its applications in molecular orbitals analysis
- To gain information about various spectroscopic techniques, their selection rules and applications based on group theory
- To solve the problems based on the theories

## PG1 ANL C04 Physical Chemistry - I

#### Aims and Objectives

Physical chemistry is the study of phenomena in chemical systems in terms of physical concepts and laws. module, different branches of thermodynamics will In this be explored. In ClassicalThermodynamicskinetic theory of gases, and the energetics of chemical reactions will be explored. Thermodynamics of natural processes and energy transformations in living organisms will be discussed in Irreversible thermodynamics. Statistical Thermodynamics looks at the relationship between molecular and bulk properties of matter, including examples such as the use of partition functions in equilibrium, transition states and heat capacity of chemical systems. Learners will be familiarized with the behavior of matter in bulk.

- To study the different phenomena in chemical systems in terms of physical concepts and laws
- To analyze different branches of thermodynamics like *Classical Thermodynamics, Irreversible thermodynamics* and *Statistical Thermodynamics*

- To explore the kinetic theory of gases and the energetics of chemical reactions
- To discuss thermodynamics of natural processes and energy transformations in living organisms
- To correlate themolecular and bulk properties of matter, including partition functions in equilibrium, transition states and heat capacity of chemical systems
- To familiarise the behaviour of matter in bulk
- To solve the problems based on the theories

## Semester 2

## PG2 ANL C05 Inorganic Chemistry - II

#### Aims and Objectives

This module coversthree parts: non-aqueous solvents, bioinorganic chemistry and organometallic chemistry. Part 1 deals with acid-base concept and reactions in non-aqueous solvents.Part 2 describes basic principles and concepts of bioinorganic chemistry including the mechanisms of reactions catalyzed by metalloproteins, and kinetics of electron transfer in proteins. Part 3 focusses on thespectral and magnetic properties of transition metal complexes. A comprehensive discussion on inorganic cages and metal clusters follows. The learners will understand the different modes of reactions oforganometallic compounds and their applications can be explored.

- To understand the basic concepts and principles of bioinorganic chemistry
- To familiarise the mechanisms and kinetics of different reactions catalysed by metalloenzymes
- To explore the electronic spectra and magnetic properties of transition metal complexes
- To study the stereochemistry of coordination compounds
- To understand the different reactions and catalysis of organometallic compounds

## PG2 ANL C06 Organic Chemistry - II

## Aims and Objectives

This module covers the study of a selected series of organic reactions involving reactive intermediates and/or molecular rearrangements. Emphasis is placed on an understanding of their reaction mechanisms. These will include reactions involving carbocations, carbanions, carbenes, carbenoids, nitrenes and arynes as intermediates. Reactions initiated by radicals will be covered. Comprehensive discussions on organic photochemistry including the rules and stereochemical consequences in pericyclic reactions will be given. The learners should be able to apply these ideas in the field of organic synthesis.

- To understand the basic concepts of selected series of organic reactions involving reactive intermediates and/or molecular rearrangements
- To acquire knowledge about name reactions involving radical intermediates
- To understand the symmetry properties of molecular orbitals of selected compounds
- To develop idea about pericyclic reactions
- To understand the basic principles of photochemistry and to apply these principles in different photochemical reactions

## PG2 ANL C07 Theoretical Chemistry - II

## **Aims and Objectives**

The objective of this model is to familiarize the learner with the approximation methods of quantum mechanics and its applications to the various theories of chemical bonding. Molecular structure evaluation

using group theory will enable the learners to apply it in the field of spectroscopy. To apply the concept of molecular modelling to isolated molecular systems.

- To get idea about various approximation methods to solve many electron systems other than simple systems.
- To discuss the applications of variation method and perturbation method for He atom
- To get an awareness about the SCF, HFSCF methods etc.
- To acquire ability to solve Schrödinger equations for molecules.
- To familiarize with the approximation methods of quantum mechanics and its applications to the various theories of chemical bonding.
- To acquire ability to apply MO treatment to homo and heteronuclear molecules
- To impart knowledge about the HMO theory and its applications to various molecules
- To evaluate molecular structure by using group theory
- To gain information about computational chemistry as a tool and find its applications
- To familiarize different molecular mechanics methods and to understand different force fields
- To achieve knowledge about different methods like HF, Ab initio, molecular mechanics semiempirical, DFT etc.
- To acquire ability to write the Z matrix of different type of molecules
- To familiarize about GAMESS/Firefly and its applications
- To solve the problems based on the theories

## PG2 ANL C08 Physical Chemistry - II

#### Aims and Objectives

In this module, the basic idea of how light interacts with matter, in particular atoms and molecules will be conferred. Microwave, infrared, Raman, electronic and nuclear magnetic resonance spectroscopic techniques will be discussed. Students will be able to apply these principles in the area of molecular spectroscopy.

- To understand the origin of different spectra and characterise the regions of the electromagnetic spectrum.
- To familiarise the microwave spectroscopy and its applications
- To identify Morse potential energy diagram and different types of bands and different types of vibrations and the application of IR spectroscopy
- To get aware about FT spectroscopy and FTIR
- To characterize term symbols and electronic spectra of different molecules
- To identify different types of lasers and realise its applications
- To understand the Mossbauer spectroscopy by learning the principle and recording of spectrum including Doppler effect, chemical shift etc.
- To familiarise the Raman spectroscopy and its applications
- To interpret the complementarities of Raman and IR spectra
- To understand the basic principles of NMR spectroscopy
- To familiarise the second order effects on spectra
- To understand NOE effect, two dimensional NMR, COSY and HETCOR, <sup>13</sup>C NMR,
- To familiarise EPR and NQR spectroscopy

#### PG2 ANL P01 Inorganic Chemistry Practical - I

#### **Aims and Objectives**

This is a module intended for chemistry majors. It deals with qualitative and quantitative inorganic analysis along with preparation and characterization of inorganic complexes. The learners will have the option to apply these ideas in various fields pertaining to inorganic chemistry.

- To familiarise different metal salts including rare earths
- To analyse quantitatively different ions using colorimetry
- To characterize the synthesised inorganic complexes

#### PG2 ANL P02 Organic Chemistry Practical - I

#### **Aims and Objectives**

In this module, students will learn to apply various techniques to separate a mixture into its individual components and identify each component. Guided under the general principles of analytical and physical chemistry, these techniques include solvent extraction, TLC and column chromatography. Students will also acquire the skill to use the computational tools to draw the reaction schemes and mechanisms of various organic reactions.

- To develop skill in separating different organic mixtures and analyse it
- To familiarise various separation techniques such as solvent extraction, TLC and column chromatography
- To acquire skill to draw structure of organic compounds and the reaction schemes and mechanism of organic reactions using Chemsketch

#### PG2 ANL P03 Physical Chemistry Practical - I

#### Aims and Objectives

In this module, students will learn about the practical applications of variousprinciples of physical chemistry like phase rule, adsorption, and surface tension.Learners will be able to use computational software to predict the geometry of a molecule, calculate its energy levels, assess the HOMO and LUMO energy, and predict its spectral behavior.

- To familiarise different isotherms and to determine the concentration of the given acid using the isotherms
- To construct the phase diagrams of simple eutectics and three component systems
- To acquire knowledge about the effect of salts on miscibility temperature
- To calculate distribution coefficient and equilibrium constant based on distribution law
- To determine the surface tension of a liquid by various methods
- To acquire knowledge about computational software likeGAMESS/Firefly
- To predict the geometry of a molecule, calculate its energy levels, assess the HOMO and LUMO energy by using GAMESS/Firefly.

## Semester 3

## PG3ANL C09 Inorganic chemistry-III (Solid State Chemistry)

- To get an understanding about the structure of solids, defects in solids and different solid state reactions
- To discuss the electrical, magnetic and optical properties in the solid state
- To study different types of cage, ring and cluster compounds in inorganic systems
- To acquire some knowledge about different types of organometallic polymers
- To understand the chemistry, properties and applications of different inorganic materials in chemistry

# PG3CHEC10 ORGANIC CHEMISTRY-III(ORGANICSYNTHESES) Aim:

## **Course Outcomes:**

- To identify the basic principles, terminology and important strategies of retro synthesis
- To make awareness about the reagents and basic organic reactions
- To study the influence of light and thermal energy for the formation of cyclic systems
- To aware of basic ideas and applications of supramolecular chemistry
- To understand the structure determination and synthesis of natural products

## PG3 ANL C11 Physical chemistry (Theory) (III Semester)

Aim: This subject is designed to impart fundamental knowledge on topics like kinetics, surfacechemistry, catalysis, colloids,macromolecules and photochemistry etc. **Objectives:** 

- To give an in-depth account of different theories of reaction rates, kinetics of fast reactions, chain reactions, reaction in solution and polymerization.
- To study the chemistry of surfaces and various techniques employed for the characterization of different types of surface phenomena and the importance of adsorption process and catalytic activity at the solid surfaces
- To impart knowledge about acid-base, enzyme and surface catalysis.
- To recognize the general properties of colloids and macromolecules
- To acquire knowledge of photochemistry and photophysical principles, their applications

## **Outcome:**

• The student will acquire knowledge about different theories on reaction rate.

- The student can analyse the mechanistic path and the experimental conditions of different types of reactions.
- The student will acquire knowledge about different chain reactions and polymerization reactions.
- Will able to illustrate the different techniques for analysing fast reactions.
- Will acquire knowledge about the acid base catalysis, enzyme catalysis and their principles.
- Will appreciate the applications of chemical principles in industrial synthesis.
- The student will able to describe characteristics of colloids and compare different molecular weight averages.
- Gains numerical ability and analysing power to solve problems .

# PG3 ANL C12 Spectroscopic Methods in Chemistry Course outcome

- Achieve advanced knowledge about the interactions of electromagnetic radiation and matter and their applications in spectroscopy.
- To understand the selection rules of UV-Visible spectroscopy and learn the various rules to calculate the absorption maxima.
- Study the chirooptical properties and do the problems
- Be able to analyse and interpret IR spectroscopic data based on stereochemistry and various factors influencing the spectra
- Studythe basic principles of NMR and factors influencing spectra and understand the advanced topicslike two dimensional spectroscopy.
- Study mass spectroscopic techniques and problems based on it.
- Be able to solve problems related to the structure and to study molecular interactions by choosing suitable spectroscopic methods and interpreting corresponding data.

## Semester 4

## PG4ANL E01 Analytical Procedures

- Aims and Objectives
- This module is aimed at the principles of different analytical procedures. The student will gain familiarity with the fundamental analytical techniques including statistical awareness about different types of errors, hypothesis testing using statistical analysis. Achieve advanced knowledge about different analytical procedures like gravimetry, and different types of titration. Able to understand sampling and different analysis procedures involved in environmental monitoring, soil, air pollution monitoring sampling, analysis of metals, alloys, minerals, food and drug analysis. Achieve advanced knowledge about nanomaterials and hazards of handling ordinary, corrosive and poisonous chemicals. Able to understand about fire hazards and how to handle carcinogens. The student will gain familiarity with Toxicology and residual analysis.

#### **PG4ANL E02 Instrumental Methods of Analysis**

#### **Aims and Objectives**

This module is aimed at the principles and particularly applications of advanced analytical techniques. The student will gain familiarity with the fundamental principles, instrumentationaspects as well as analytical applications of modern spectrometric techniques as well as advances inmicroscopy and mass spectrometry. After having read this module, students should have gained expertise in advanced analytical techniques to play leadership roles in industrial and academic research laboratories in different fields, including biomedical, environmental, food, forensic, materials, and pharmaceutical analysis.

# PG4ANL E03- MODERN ANALYTICAL TECHNIQUES AND GREEN CHEMISTRY

## Aims and Objectives:

This is a module intended for chemistry majors. It deals with Analytical techniques and Green chemistry. Concentrating on potentiometry, polarography, Voltametric techniques, Amperometry, capillaryelectrophoresis and electro chromatography, Thermal analysis and Radiochemical analysis, Chromatography and their applications in analysis. Automated systems

- To get an awareness about different analytical techniques in chemical analysis
- Came to know about the different type of electrodes, and their application in PH measurement and Potentiometric titrations,
- Understand the TG, DTA, DSC, TMA, DA and their applications and principle and applications of isotopic dilution methods and radiometric titrations.
- To acquire knowledge on Different chromatographic techniques their advantages and applications.
- To understand the automated systems .
- To acquire general awareness on green chemistry, green solvents and green principles of organic synthesis.

## PG4CHE P04– INORGANIC CHEMISTRY PRACTICAL – 2

#### **Aims and Objectives**

This is a module intended for chemistry majors. It deals with quantitative inorganic analysis of simple binary mixtures of metallic ions in solution by volumetric and gravimetric methods. Includes the analysis of the alloys and ores. The learners will have the option to apply these ideas in various fields pertaining to inorganic chemistry.

- To estimate simple binary mixtures of metallic ions in solution by volumetric and gravimetric methods.
- To analyse different alloys and ores

## PG4ANL P05 ORGANIC CHEMISTRY PRACTICAL 2

- To acquire skill in estimation of various organic compounds volumetrically and colorimetrically
- To familiarise two stage preparation of organic compounds
- To develop skill in green methods for preparing organic compounds using green solvents as well as Microwave assisted Organic Synthesis.

• To develop skill for predicting the FTIR, UV-Visible, <sup>1</sup>H and <sup>13</sup>C NMR spectra of the substrates and products at each stage of the synthesis.

#### PG1 ANL P03 Instrumental Analysis Practical

#### **Aims and Objectives**

In this module, students will learn about the practical applications of various principles of physical chemistry like refractometry, polarimetry, potentiometry, conductometry, nephelometry, UV – visible spectrophotometry, polarography and related experiments, electrogravimetric estimation of Cu, Ni, and Pb and flame photometry.

#### **Outcome:**

- To acquire knowledge in quantitative estimation of different salts by using nephelometry.
- To acquire knowledge in various spectrophotometric techniques and to determine various ions quantitatively.
- To acquire knowledge in qualitative and quantitative estimation of pure organic liquids and oils by using refractometry.
- To know how titrations can be done based on conductometric and potentiometric principles.
- To acquire knowledge in the principles regarding various equations and to determine the properties like solubility of sparingly soluble salts, pka values and the degree of ionization etc.,
- Get aware about polarography and related experiments.
- To acquire knowledge in the principles regarding electro gravimetric experiments and flame photometric experiments.