Maharaja's College Ernakulam

A GOVERNMENT AUTONOMOUS COLLEGE

Re-Accredited by NAAC with 'A Grade'
Affiliated to Mahatma Gandhi University
Centre of Excellence under Govt. of Kerala
Identified by UGC as College with Potential for Excellence

POST GRADUATE & RESEARCH DEPARTMENT
OF
CHEMISTRY

Post Graduate Curriculum and Syllabus

(All Branches)

For 2019 Admission Onwards

M.Sc. ANALYTICAL CHEMISTRY

FOREWORD

The Board of Studies in Chemistry take this opportunity to express our deep appreciation to all academicians and professionals who participated in the series of workshops organized by the Board for restructuring curriculum and syllabi of the PG courses in Chemistry - M.Sc Chemistry, M.Sc Analytical Chemistry, M.Sc Pharmaceutical Chemistry and M.Sc Applied Chemistry. We express our profound gratitude to the Honourable Vice-Chancellor, Pro-Vice Chancellor, Members of the Syndicate and Members of the Academic Council, Mahatma Gandhi University, for their sincere co-operation and guidance for completion of this work. Our special thanks are due to Chairman and members of the Governing Council, Chairman and members of the Academic Council, Maharaja's College, Ernakulam.

We also extend our gratitude to Prof. (Dr). K. K. Mohammed Yusuff, Professor (Retd.), Department of Applied Chemistry, Cochin University of Science and Technology, Prof. (Dr). S. Sugunan, Professor (Retd.), Department of Applied Chemistry, Cochin University of Science and Technology, Prof. (Dr). K. Girish Kumar, Professor, Department of Applied Chemistry, Cochin University of Science and Technology, Prof. (Dr). K. Sreekumar, Professor, Department of Applied Chemistry, Cochin University of Science and Technology, Dr. E. Prasad, Associate Professor, Department of Chemistry, IIT, Madras, Dr. Kochubaby Manjooran, Dy.Manager (Energy and Envt), BPCL, Kochi Refinery, Sri. M. G. Rajagopalan, Associate Professor (Retd.) Maharaja's College, Ernakulam, Smt. K. T. Geethabali, Associate Professor (Retd.), Maharaja's College, Ernakulam, Dr. T. Narayanan, Associate Professor (Retd.), Maharaja's College, Ernakulam, Dr. Lissamma Koshy, Associate Professor (Retd.), Maharaja's College, Ernakulam and Dr. Anitha I, Principal, KKTM College, Pullut who were entrusted with the responsibility as experts for the revision of the syllabus of different subjects. The Board of Studies in Chemistry expresses the whole hearted gratitude to all those who have helped in this endeavour.

The task of preparing the curricula and syllabi and bringing it out in the present form for all the four M.Sc courses was not simple but it was possible with dedicated efforts and wholehearted support and involvement of all the members of the BOS and the faculty members of the Department of Chemistry. I would like to express my sincere thanks to all my fellow members of BOS and the faculty members of the Department of Chemistry for all their help, cooperation, encouragement, active participation and useful suggestions for the completion of syllabus.

Chairman

Board of Studies

BOARD OF STUDIES MEMBERS

External Experts

- **Prof. (Dr). K. Girish Kumar**
  Professor and Head, Department of Applied Chemistry,
  Cochin University of Science and Technology, Kochi
- **Dr. M.R Prathapachandra Kurup**
  Professor and Head
  Department of Chemistry
  Central University of Kerala, Padannakkad-671314
- **Shri .Benny Antony**
  Arjuna Extracts, Aluva
- **Dr. T. Narayanan**
  Associate Professor (Retd.),
  Maharaja's College, Ernakulam

Internal Board of Studies -1

- **Sri. K. P. Ashokan** *(Chairman)*
- **Dr. Bindu Sharmila T K**
  Assistant Professor
- **Dr. Sreesha Sasi**
  Assistant Professor
- **Dr. Suja N R**
  Assistant Professor
- **Dr. Meera Gopal**
- **Dr. Amrutha S Rajan**
  Assistant Professor
- **Dr. Jolly V Antony**
  Assistant Professor

LIST OF FACULTY MEMBERS

- **Sri. Ashokan K P**
  Associate Professor
- **Smt. Femina K S**
  Assistant Professor
- **Dr. Amrutha S Rajan**
  Assistant Professor
- **Sri Jolly V Antony**
  Assistant Professor
- **Dr. Vidya Raman**
  Assistant Professor
- **Dr. Zeena P Hamza**
  Assistant Professor
- **Dr. Rejimon P K**
  Assistant Professor
- **Dr.Neena George**
  Assistant Professor
- **Dr. Julie Chandra C.S**
  Assistant Professor
- **Shri. Deepak. J. Prabhu**
  Assistant Professor
- **Dr. Meera Gopal**
  Assistant Professor
- **Dr. Bindu Sharmila T K**
  Assistant Professor
- **Dr. Sreesha Sasi**
  Assistant Professor
- **Dr. Suja N R**
  Assistant Professor
- **Dr. Prasanthkumar. K. P**
  Assistant Professor
- **Dr. Sobhi Daniel**
  Assistant Professor
- **Dr.Seena E.B**
  Assistant Professor
- **Dr. Sajith Menon**
  Assistant Professor
- **Dr. Alson Mart**
  Assistant Professor
- **Dr. Sreejesh P.R**
  Assistant Professor

PROGRAMME STRUCTURE

Examination

- There shall be end semester examination at the end of each semester.
- The answers must be written in English except for those coming under Faculty of Languages.
- Practical examinations shall be conducted by the college at the end of even semesters only.
- Project evaluation and Viva -Voce shall be conducted at the end of the programme only.
- Practical examination, Project evaluation and Viva-Voce shall be conducted by two external examiners.

END-Semester Examination

- The examinations shall normally at the end of each semester. There shall be one end-semester examination of 3 hours duration in each lecture based course and practical course.
- A question paper may contain short answer type/annotation, short essay type questions/problems and long essay type questions.

Evaluation and Grading

Evaluation

The evaluation scheme for each course shall contain two parts; (a) in-semester evaluation and (b) end-semester evaluation. 20 marks shall be given to in-semester evaluation and the remaining 80 marks to end-semester evaluation. Both in-semester and end semester evaluation shall be carried out by using in mark system. Both internal and external marks are to be mathematically rounded to the nearest integer.

Internal evaluation

The internal evaluation shall be based on predetermined transparent system involving periodic written tests, assignments, seminars and attendance in respect of theory courses and based on written tests, lab skill/records/viva and attendance in respect of practical courses. The marks assigned to various components for in-semester evaluation is as follows.

Components of In-semester Evaluation (For theory)

Components	Component Marks
Assignment	4
Seminar	4
Two Test papers*	8
Attendance	4
Total	20

*Marks of Test Papers shall be the average

Components of In-semester Evaluation (For Practical)

Components	Component Marks
Attendance	4
Laboratory Involvement	4
Written/Lab Test	4
Record*	4
Viva	4
Total	20

*Marks awarded to Record should be related to number of experiments recorded

Components of In-semester Evaluation (For Project)

Components	Marks
Topic/Area selected	2
Experimentation/Data collection	4
Punctuality	2
Compilation	4
Content	4
Presentation	4
Total	**20**

a) Evaluation of Attendance

% of attendance	Mark
95 and above	4
85 to 94	3
80 to 84	2
75 to 79	1
< 75	0

(Decimals are to be rounded to the next higher whole number)

a) Evaluation of Assignment

Components	Marks
Punctuality	1
Content	1
Conclusion	1
Reference/Review	1
Total	**4**

b) Evaluation of Seminar

Components	Marks
Content	1
Presentation	2
Reference/Review	1
Total	**4**

To ensure transparency of the evaluation process, the in-semester marks awarded to the students in each course in a semester shall be published on the notice board at least one week before the commencement of external examination. There shall not be any chance for improvement for in semester marks. The course teacher and the faculty advisor shall maintain the academic record of each student registered for the course and a copy should be kept in the college for at least one year for verification.

End-Semester Evaluation:

The end-semester evaluation in theory courses is to be conducted by the college with question papers set by external experts. The answers must be written in English except those for the Faculty of Languages. The evaluation of the answer scripts shall be done by examiners based on a well-defined scheme of valuation. The end-semester evaluation shall be done immediately after the examination preferably through Centralized Valuation.

Photocopies of the answer scripts of the external examination shall be made available to the students for scrutiny on request and revaluation/scrutiny of answer scripts shall be done as per the request of the candidate by paying fees.

The question paper should be strictly on the basis of model question paper set by BOS and there shall be a combined meeting of the question paper setters for scrutiny and finalization of question paper. Each set of question should be accompanied by its answer scheme for valuation.

Pattern of Questions

The question setter shall ensure that questions to course should satisfy weightage to objectives and weightage to difficulty levels.

Weightage to Objectives	
Objectives	**%**
Understanding	25
Critical Evaluation	50
Application	25

Weightage to difficulty levels	
Level of difficulty	**%**
Easy	20
Average	60
Difficult	20

Question paper setters shall also submit a detailed scheme of evaluation along with the question paper. A question paper shall be a judicious mix of objective type, short answer type, short essay type /problem solving type and long essay type questions.

Pattern of questions for end semester examination

	Total no. of questions	**Number of questions to be answered**	**Marks of each question**	**Total marks**
	12	10	2	20
	10	6	5	30
	4	2	15	30
TOTAL	**26**	**18**	x	**80**

Grades for Courses

For all courses (theory & practical), grades are given on a 10-point scale based on the total percentage of marks ***(ISA+ESA)*** as given below

Percentage of Marks	**Grade**	**Grade Point (GP)**
95 and above	S Outstanding	10
85 to below 95	A^+ Excellent	9
75 to below 85	A Very Good	8
65 to below 75	A- Good	7
55 to below 65	B^+ Above Average	6
50 to below 55	B Average	5
40 to below 50	C Pass	4
Below 40	F Fail	0
	Ab Absent	0

Credit Point and Credit Point Average:

Credit Point (CP) of a course is calculated using the formula

CP = C × GP, where C = Credit; GP = Grade point

Semester Grade Point Average (SGPA) of a Semester is calculated using the formula

SGPA= TCP/TC, where TCP = Total Credit Point of that Semester TC = Total Credit of that Semester

Cumulative Grade Point Average (CGPA) of a Programme is calculated using the formula

CGPA = ∑(TCP ×TC)÷∑TC

CGPA shall be rounded off to two decimal places.

Grades for the different semesters and overall programme are given based on the corresponding CPA as shown below:

GPA	Grade
Equal to 9.5 and above	***S Outstanding***
Equal to 8.5 and below 9.5	***A+ Excellent***
Equal to 7.5 and below 8.5	***A Very Good***
Equal to 6.5 and below 7.5	***A- Good***
Equal to 5.5 and below 6.5	***B+ Above Average***
Equal to 5.0 and below 5.5	***B Average***
Equal to 4.0 and below 5.0	***C Pass***
Below 4.0	***F Failure***

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 sub-disciplines 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 comprehensionof 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 conceptsand laws. In this module,different branches of thermodynamics will be explored. In *ClassicalThermodynamics*kinetic 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, ^{13}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) <u>(III Semester)</u>

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**

1. 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, capillary-electrophoresis 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, ^{1}H and ^{13}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.

M.Sc. ANALYTICAL CHEMISTRY

<table>
<tr><th rowspan="2"></th><th rowspan="2">Code</th><th rowspan="2">Course</th><th rowspan="2">Hours/ week</th><th rowspan="2">Total Hours</th><th rowspan="2">Credit</th><th colspan="3">Marks</th></tr>
<tr><th>Internal</th><th>External</th><th>Total</th></tr>
<tr><td rowspan="7">Semester 1</td><td>PG1ANL C01</td><td>Inorganic Chemistry-I (Coordination & Nuclear Chemistry)</td><td>4</td><td>72</td><td>4</td><td>20</td><td>80</td><td>100</td></tr>
<tr><td>PG1ANL C02</td><td>Organic Chemistry-I (Structure, Reactivity & Stereochemistry)</td><td>4</td><td>72</td><td>4</td><td>20</td><td>80</td><td>100</td></tr>
<tr><td>PG1ANL C03</td><td>Theoretical Chemistry-I (Quantum Chemistry and Group Theory)</td><td>4</td><td>72</td><td>4</td><td>20</td><td>80</td><td>100</td></tr>
<tr><td>PG1ANL C04</td><td>Physical chemistry- I (Kinetic Theory, Thermodynamics and Statistical Thermodynamics)</td><td>3</td><td>54</td><td>3</td><td>20</td><td>80</td><td>100</td></tr>
<tr><td>PG2ANL P01</td><td>Inorganic Chemistry Practical–1</td><td>3</td><td>54</td><td colspan="4" rowspan="3">Evaluation at the end of second semester</td></tr>
<tr><td>PG2ANL P02</td><td>Organic Chemistry Practical-1</td><td>3</td><td>54</td></tr>
<tr><td>PG2ANL P03</td><td>Physical Chemistry Practical -1</td><td>4</td><td>72</td></tr>
<tr><td></td><td></td><td>Total</td><td>25</td><td>450</td><td>15</td><td></td><td></td><td></td></tr>
<tr><td rowspan="7">Semester 2</td><td>PG2ANL C05</td><td>Inorganic Chemistry-II (Bioinorganic & Organometallic Chemistry)</td><td>4</td><td>72</td><td>4</td><td>20</td><td>80</td><td>100</td></tr>
<tr><td>PG2ANL C06</td><td>Organic Chemistry- II (Reaction Mechanism)</td><td>4</td><td>72</td><td>4</td><td>20</td><td>80</td><td>100</td></tr>
<tr><td>PG2ANL C07</td><td>Theoretical Chemistry – II (Chemical Bonding and Computational Chemistry)</td><td>4</td><td>72</td><td>4</td><td>20</td><td>80</td><td>100</td></tr>
<tr><td>PG2ANL C08</td><td>Physical chemistry- II (Molecular Spectroscopy)</td><td>3</td><td>54</td><td>3</td><td>20</td><td>80</td><td>100</td></tr>
<tr><td>PG2ANL P01</td><td>Inorganic Chemistry Practical–1</td><td>3</td><td>54</td><td>3</td><td>20</td><td>80</td><td>100</td></tr>
<tr><td>PG2ANL P02</td><td>Organic Chemistry Practical-1</td><td>3</td><td>54</td><td>3</td><td>20</td><td>80</td><td>100</td></tr>
<tr><td>PG2ANL P03</td><td>Physical Chemistry Practical -1</td><td>4</td><td>72</td><td>3</td><td>20</td><td>80</td><td>100</td></tr>
<tr><td></td><td></td><td>Total</td><td>25</td><td>450</td><td>24</td><td></td><td></td><td></td></tr>
</table>

Semester 3	PG3ANL C09	Inorganic chemistry-III (Solid State Chemistry)	4	72	4	20	80	100
	PG3ANL C10	Organic chemistry- III (Organic Syntheses)	4	72	4	20	80	100
	PG3ANL C11	Physical chemistry- III (Chemical Kinetics, Surface Chemistry and Photochemistry)	4	72	4	20	80	100
	PG3ANL C12	Spectroscopic Methods in Chemistry	3	54	3	20	80	100
	PG4ANL P04	Inorganic Chemistry Practical–2	3	54	Evaluation at the end of fourth semester			
	PG4ANL P05	Organic Chemistry Practical-2	3	54				
	PG4ANL P06	Instrumental Analysis Practical	4	72				
		Total	**25**	**450**	**15**			
Semester 4	PG4ANL E01	Elective –I Analytical Procedures	5	90	4	20	80	100
	PG4ANL E02	Elective –II Instrumental Methods of Analysis	5	90	4	20	80	100
	PG4ANL E03	Elective –III Modern Analytical Techniques And Green chemistry	5	90	4	20	80	100
	PG4ANL E04	Elective –IV Polymer Chemistry	5	90	4	20	80	100
	PG4ANL E05	Elective –V Applied Analysis and Aquatic Resources	5	90	4	20	80	100
	PG4ANL P04	Inorganic Chemistry Practical–2	3	54	3	20	80	100
	PG4ANL P05	Organic Chemistry Practical-2	3	54	3	20	80	100
	PG4ANL P06	Instrumental Analysis Practical	4	72	3	20	80	100
	PG4ANL D01	Project			2		100	100
	PG4ANL V01	Viva			2	20	80	100
		Total	**25**	**450**	**25**			
Grand Total					**80**			

SEMESTER 1

PG1ANL C01 INORGANIC CHEMISTRY – I

(COORDINATION & NUCLEAR CHEMISTRY)

Credit: 4 **Contact Lecture Hours: 72**

Module 1: Coordination Chemistry- Structural Aspects and Bonding (18 Hrs)

1.1 Classification of complexes based on coordination numbers and possible geometries. σ and π bonding ligands such as CO, NO, CN^-, R_3P and Ar_3P.

1.2 Splitting of *d* orbitals in octahedral, tetrahedral, square planar, square pyramidal and trigonal bipyramidal fields, LFSE, *Dq* values, Jahn Teller (JT) effect, theoretical failure of crystal field theory, evidence of covalency in the metal ligand bond, nephelauxetic effect, ligand field theory, molecular orbital theory- M.O energy level diagrams for octahedral and tetrahedral complexes with and without π-bonding, experimental evidences for π-bonding

Module 2: Kinetics and Mechanism of Reactions in Metal Complexes (18 Hrs)

2.1 Thermodynamic and kinetic stability, kinetics and mechanism of nucleophilic substitution reactions in square planar complexes, *trans* effect-theory and applications.

2.2 Kinetics and mechanism of octahedral substitution- water exchange, dissociative and associative mechanisms, base hydrolysis, racemization reactions, solvolytic reactions (acidic and basic).

2.3 Electron transfer reactions: outer sphere mechanism- Marcus theory, inner sphere mechanism-Taube mechanism.

Module 3: Organometallic Compounds- Synthesis, Structure and Bonding (18 Hrs)

3.1 Organometallic compounds with linear π- donor ligands- olefins, acetylenes, dienes and allyl complexes-synthesis, structure and bonding.

3.2 Complexes with cyclic π-donors- metallocenes and cyclic arene complexes structure and bonding. Hapto nomenclature. Carbene and carbyne complexes.

3.3 Preparation, properties, structure and bonding of simple mono and binuclear metal carbonyls, metal nitrosyls, metal cyanides and dinitrogen complexes. Polynuclear metal carbonyls with and without bridging. Carbonyl clusters- LNCCS and HNCCS, Isoelectronic and isolobal analogy, Wade Mingos rules, cluster valence electrons.

Module 4: Electron deficient compounds (9 Hrs)

4.1. Electron deficient compounds – synthesis, reactions, structure and bonding. Boron hydrides, styx numbers, Boron cluster compounds. Wade's rule, Hydroborate anions, Organoboranes and hydroboration, Polyhedral anions, Carboranes, Metalloboranes, Borazines – Structure and bonding of borazines and Borides.

Module 5: Nuclear Chemistry (9 Hrs)

5.1 Fission products and fission yield. Neutron capture cross section and critical size. Nuclear fusion reactions and their applications. Chemical effects of nuclear transformations. Positron annihilation. Principles of counting technique such as G.M. counter, proportional, ionization and scintillation counters. Cloud chamber.

5.2 Synthesis of transuranic elements such as Neptunium, Plutonium, Curium, Berkelium, Einsteinium, Mendelevium, Nobelium, Lawrencium and elements with atomic numbers 104 to 109.

5.3 Analytical applications of radioisotopes- radiometric titrations, kinetics of exchange reactions, measurement of physical constants including diffusion constants, neutron activation analysis, prompt gamma neutron activation analysis and neutron absorptiometry.

5.4 Applications of radio isotopes in industry, medicine, autoradiography, radiopharmacology, radiation safety precaution, nuclear waste disposal.

5.5 Radiation chemistry of water and aqueous solutions- Fricke solution, Ceric ammonium solution. Measurement of radiation doses. Relevance of radiation chemistry in biology.

References

[1] J.E. Huheey, E.A. Keiter, R.L. Keiter, Inorganic Chemistry Principles of Structure and Reactivity, 4th Edn., Harper Collins College Publishers,1993.

[2] F.A. Cotton, G Wilkinson, C.A. Murillo, M. Bochmann, Advanced Inorganic Chemistry, 6th Edn., Wiley-Interscience, 1999.

[3] K.F. Purcell, J.C. Kotz, Inorganic Chemistry, Holt-Saunders, 1977.

[4] P. Powell, Principles of Organometallic Chemistry, 2nd Edn., Chapman and Hall,1988.

[5] F. Basolo, R.G. Pearson, Mechanisms of Inorganic Reaction, John Wiley & Sons, 2006.

[6] B.E. Douglas, D.H. McDaniel, J. J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd Edn., Wiley-India, 2007.

[7] B.D. Guptha, A.J Elias, Basic Organometallic Chemistry, Universities Press, 2010.

[8] H.J. Arnikar, Essentials of Nuclear Chemistry, Wiley Eastern, 1982.

[9] S.N. Goshal, Nuclear Physics, S. Chand and Company, 2006.

PG1ANL C02 ORGANIC CHEMISTRY - I

(STRUCTURE, REACTIVITY & STEREOCHEMISTRY)

Credit: 4 **Contact Lecture Hours: 72**

Module 1: MO Theory and Aromaticity (9 Hrs)

1.1 Review of basic concepts in organic chemistry: bonding, hybridization, MO picture (allyl system, 1,3-butadiene and benzene), inductive effect, electromeric effect, resonance effect, hyperconjugation, steric effect. Bonding weaker than covalent bonds.

1.2 The formalism of curved arrow mechanisms. Practicing of line diagram drawing.

1.3 Concept of aromaticity: delocalization of electrons - Hückel's rule, criteria for aromaticity, examples of neutral and charged aromatic systems, azulenes, annulenes, mesoionic compounds. NMR as a tool for aromaticity. Antiaromatic and homoaromatic systems. Fullerenes, Carbon nanotubes and Graphene.

Module 2: Investigation of Organic Reaction Mechanisms (9 Hrs)

Energy profiles, Methods of determining reaction mechanisms, Kinetic and thermodynamic control of reactions. The Hammond postulate. Principle of microscopic reversibility. Marcus theory. The Hammett equation and its applications. Taft equation. Linear free energy relationships. Solvent polarity and parameters. Y, Z and E parameters and their applications. Primary and secondary kinetic isotope effects. Salt effects and special salt effects in SN reactions. Solvent effect. Bulk and specific solvent effects. Introduction to carbon acids - pKa of weak acids, kinetic and thermodynamic acidity. Phase transfer catalysis and its applications. Steric effects. HSAB principle and its applications in organic reactions.

Module 3: Review of Organic Reaction Mechanisms (18 Hrs)

3.1 Review of organic reaction mechanisms with special reference to nucleophilic and electrophilic substitution at aliphatic carbon (S_N1, S_N2, S_Ni, S_E1, S_E2), elimination (E1 and E2). Elimination vs substitution.

3.2 A comprehensive study on the effect of substrate, reagent, leaving group, solvent and neighbouring group on nucleophilic substitution (S_N2 and S_N1) and elimination (E1 and E2) reactions.

3.3 Addition reactions (regioselectivity- Markovnikov's addition- carbocation mechanism, anti-Markovnikov's addition- radical mechanism).

3.4 Mechanism of electrophilic and nucleophilic aromatic substitution reactions with examples. Arenium ion intermediates. S_N1, S_NAr, $S_{RN}1$ and Benzyne mechanisms.

3.5 Catalysis by acids, bases and nucleophiles with examples from acetal, cyanohydrin and ester formation and hydrolysis reactions- $A_{AC}2$, $A_{AC}1$, $A_{AL}1$, $B_{AC}2$ and $B_{AL}1$ mechanisms.

Module 4: Stereochemistry of Organic Compounds (18 Hrs)

4.1 Stereoisomerism: Definition based on symmetry and energy criteria. Projection formulae. Configurational isomerism. Geometrical isomerism- nomenclature, methods of determination of geometrical isomers based on physical properties, NMR spectroscopy and chemical methods. Optical isomerism, nomenclature.

4.2 Introduction to molecular symmetry and chirality: Examples from common objects to molecules. Axis, plane, center and alternating axis of symmetry.

4.3 Center of chirality: Molecules with C, N, S based chiral centers, absolute configuration, enantiomers, racemic modifications, R and S nomenclature using Cahn-Ingold-Prelog rules, molecules with a chiral center and C_n, molecules with more than one center of chirality, definition of diastereoisomers, constitutionally symmetrical and unsymmetrical chiral molecules, erythro and threo nomenclature.

4.4 Axial, planar and helical chirality with examples, stereochemistry and absolute configuration of allenes, biphenyls, binaphthyls, ansa and cyclophanic compounds, spiranes, exocyclic alkylidene cycloalkanes.

4.5 Topicity and prostereoisomerism, topicity of ligands and faces as well as their nomenclature. NMR distinction of enantiotopic/diastereotopic ligands.

4.6 Chiral drugs.

Module 5: Conformational Analysis (18 Hrs)

5.1 Conformational descriptors- factors affecting conformational stability of molecules. Conformational analysis of acyclic and cyclic systems: substituted ethanes, cyclohexane and its derivatives, decalins, adamantane, congressane, sucrose and lactose. Bridged bicyclic systems- norbornane, camphor, bicyclo[2.2.2]octane.

5.2. Conformation and reactivity of elimination (dehalogenation, dehydrohalogenation, semipinacolic deamination and pyrolytic elimination- Saytzeff and Hofmann eliminations), substitution and oxidation of 2° alcohols. Chemical consequence of conformational equilibrium - Curtin Hammett principle.

References

[1] R. Bruckner, Advanced Organic Chemistry: Reaction Mechanisms, Academic Press, 2002.

[2] I. Fleming, Frontier Orbitals and Organic Chemical Reactions, Wiley, 1976. [3

[3] I. Fleming, Molecular Orbitals and Organic Chemical Reactions, Wiley, 2009.

[4] H.O. House, Modern Synthetic Reactions, Organic Chemistry Monograph Series, Benjamin, 1965.

[5] F.A. Carey, R.A. Sundberg, Advanced Organic Chemistry, Part A: Structure and Mechanisms, 5th Edn., Springer Science & Business Media, 2007.

[6] F.A. Carey, R.A. Sundberg, Advanced Organic Chemistry, Part B: Reaction and Synthesis, 5th Edn., Springer Science & Business Media, 2007.

[7] J. Clayden, N. Greeves, S. Warren, P. Wothers, Organic Chemistry, Oxford University Press, 2004.

[8] M.B. Smith, J. March, March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure, 6th Edn., John Wiley & Sons, 2007.

[9] M.B. Smith, March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure, 6th Edn., John Wiley & Sons, 2013.

[10] T.H. Lowry, K.S. Richardson, Mechanism and Theory in Organic Chemistry, 2nd Edn., Harper & Row, 1981.

[11] P. Sykes, A Guide Book to Mechanism in Organic Chemistry, 6th Edn., Pearson

Education India, 1986.

[12] N.S. Isaacs, Physical Organic Chemistry, ELBS/Longman, 1987.

[13] D. Nasipuri, Stereochemistry of Organic Compounds: Principles and Applications, 3rd Edn., New Age Pub. Ltd., 2010.

[14] D.G. Morris, Stereochemistry, RSC, 2001.

[15] E.L. Eliel, S.H. Wilen, Stereochemistry of Organic Compounds, John Wiley & Sons, 2008.

[16] P.S. Kalsi, Stereochemistry, Conformation and Mechanism, 5th Edn., New Age International Pub. Ltd., 2004.

PG1ANL C03 THEORETICAL CHEMISTRY – I

(QUANTUM CHEMISTRY AND GROUP THEORY)

Credit: 4 **Contact Lecture Hours: 72**

Module 1: Formulation of Quantum Chemistry (18 Hrs)

1.1 Mathematical Concepts (5 Hrs)

Co-ordinate systems: Cartesian, Cylindrical polar and Spherical polar coordinates and their relationships. Complex numbers: definition, Complex conjugate, absolute value of a complex number, complex functions. Operator algebra: linear and nonlinear operators, Hermitian operators, del and del-squared operators. Eigen function and eigen values of an operator, Eigen value equation, Eigen functions of Commuting operators. Well behaved functions, Normalized and Orthogonal functions.

1.2 Evolution of Quantum Mechanics (5 Hrs)

Failure of classical mechanics: The black body radiation, Compton effect, photoelectric effect, atomic spectra. Need of quantum mechanics. Concept of matter wave, de Broglie relation and its experimental proof, Uncertainty principle and its consequences. Wave function and Born interpretation, Schrödinger's wave mechanics, Deduction of Schrodinger equation from classical wave equation.

1.3 Postulates of Quantum Mechanics (4 Hrs)

Detailed discussion of postulates: State function postulate. Operator postulate. Eigen value postulate. Expectation value postulate. Postulate of time dependent Schrodinger equation of motion, Conservative system and time-independent Schrodinger equation.

1.4 Quantum Mechanics of Translational Motion (4 Hrs)

Particle in one-dimension with infinite potential walls, particle in a three dimensional box-separation of variables- rectangular box and cubic box, degeneracy. Introduction to tunnelling with experimental evidence.

Module 2: Applications of Quantum Chemistry (18 Hrs)

2.1 Quantum Mechanics of Hydrogen-like Atoms (5 Hrs)

Potential energy of hydrogen-like systems. The wave equation in spherical polar coordinates: separation of variables- R, Θ and Φ equations and their solutions, wave functions and energies of hydrogen-like atoms. Orbitals- radial functions, radial distribution functions, angular functions and their plots.

2.2 Quantum Mechanics of Vibrational Motion (5 Hrs)

One-dimensional harmonic oscillator (complete treatment), Hermite equation (solving by method of power series), Hermite polynomials, recursion relation, wave functions and energies-important features, Harmonic oscillator model and molecular vibrations. Rodrigue's formula, Three dimensional harmonic oscillator.

2.3 Quantum Mechanics of Rotational Motion (5 Hrs)

Rotational motion: co-ordinate systems, Cartesian, Cylindrical polar and Spherical polar coordinates and their relationships. The wave equation in Spherical polar coordinates-particle on a ring, the Φ equation and its solution, wave functions in the real form. Non-planar rigid rotor (or particle on a sphere)-separation of variables, the Φ and the Θ equations and their solutions, Legendre and associated Legendre equations, Legendre and associated Legendre polynomials. Spherical harmonics (imaginary and real forms)- polar diagrams of spherical harmonics.

2.4 Orbital and Spin angular momentum (3 Hrs)

Quantisation of angular momentum, quantum mechanical operators corresponding to angular momenta, (L_x, L_y, L_z and L^2). Commutation relations between these operators. Spherical harmonics as eigen functions of angular momentum operators L_z and L^2. Space quantization. The postulate of spin by Uhlenbeck and Goudsmith, discovery of spin- Stern Gerlach experiment. Spin orbitals- construction of spin orbitals from orbital and spin functions.

Module 3: Molecular Symmetry and Mathematical group (18 Hrs)

3.1 Symmetry elements and symmetry operations. Conditions for a set of elements to form a group, sub groups, abelian and cyclic groups, Point groups. Multiplication of operations. Group multiplication table of C_{2v}, C_{2h} and C_{3v} groups (H_2O, Trans N_2F_2 and NH_3 as examples). Similarity transformation and classes in a group.

3.2 Matrices: addition and multiplication of matrices, inverse and orthogonal matrices, character of a matrix, block diagonalisation, matrix representation of symmetry operations, representation of groups by matrices, construction of representation using vectors and atomic orbitals as basis, representation generated by Cartesian coordinates positioned on the atoms of a molecule (H_2O as example).

3.3 Reducible and Irreducible representations (IR). Reduction formula, reduction of reducible representation to IRs.

Module 4: Applications of Group Theory **(18 Hrs)**

4.1 The Great Orthogonality theorem. Rules derived from GOT (proof not required). Setting up of character table of C_{2v}, C_{3v}, C_{2h}, C_{4v} and C_3 groups. Direct product representations.

4.2 Applications in quantum mechanics, transition moment integral, vanishing of integrals. Jahn – Teller effect, Woodward – Hoffmann rules.

4.3 Applications in vibrational spectra: symmetry aspects of molecular vibrations, vibrations of polyatomic molecules-selection rules for vibrational absorption. Determination of the symmetry of normal modes of H_2O, Trans-N_2F_2 and NH_3 using Cartesian coordinates and internal coordinates. Complementary character of IR and Raman spectra- determination of the number of active IR and Raman lines.

4.4 Application in electronic spectra: selection rules for electronic transition, electronic transitions due to the carbonyl chromophore in formaldehyde.

References

[1] I.N. Levine, Quantum Chemistry, 6th Edn., Pearson Education Inc., 2009.

[2] P.W. Atkins, R.S. Friedman, Molecular Quantum Mechanics, 4th Edn., Oxford University Press, 2005.

[3] D.A. McQuarrie, Quantum Chemistry, University Science Books, 2008.

[4] J.P. Lowe, K. Peterson, Quantum Chemistry, 3rd Edn., Academic Press, 2006.

[5] R. Anatharaman, Fundamentals of Quantum Chemistry, Macmillan India, 2001.

[6] R.K. Prasad, Quantum Chemistry, 3rd Edn., New Age International, 2006.

[7] T. Engel, Quantum Chemistry and Spectroscopy, Pearson Education, 2006.

[8] H. Metiu, Physical Chemistry: Quantum Mechanics, Taylor & Francis, 2006.

[9] L. Pauling, E.B. Wilson, Introduction to Quantum Mechanics, McGraw-Hill, 1935.

[10] M.S. Pathania, Quantum Chemistry and Spectroscopy (Problems & Solutions), Vishal Publications, 1984.

[11] F.A. Cotton, Chemical Applications of Group Theory, 3rd Edn., Wiley Eastern, 1990.

[12] L. H. Hall, Group Theory and Symmetry in Chemistry, McGraw Hill,1969.

[13] V. Ramakrishnan, M.S. Gopinathan, Group Theory in Chemistry, Vishal Publications, 1992.

[14] S. Swarnalakshmi, T. Saroja, R.M. Ezhilarasi, A Simple Approach to Group Theory in Chemistry, Universities Press, 2008.

[15] S.F.A. Kettle, Symmetry and Structure: Readable Group Theory for Chemists, 3rd Edn., Wiley, 2007.

[16] A. Vincent, Molecular Symmetry and Group Theory: A Programmed Introduction to Chemical Applications, 2nd Edn., Wiley, 2000.

[17] A.S. Kunju, G. Krishnan, Group Theory and its Applications in Chemistry, PHI Learning, 2010.

PG1ANL C04 - PHYSICAL CHEMISTRY - I

(KINETIC THEORY, THERMODYNAMICS AND STATISTICAL THERMODYNAMICS)

Credit: 3 **Contact Lecture Hours: 54**

Module 1: Kinetic theory **(9 Hrs)**

Kinetic theory of gases, derivation of Maxwell's law of distribution of velocities, graphical representation, experimental verification of the law, most probable velocity, derivation of average, RMS and most probable velocities, collision diameter, collision frequency in a single gas and in a mixture of two gases, mean free path, frequency of collision, effusion, the rate of effusion, time dependence of pressure of an effusing gas, transport properties of gases. Viscosity, thermal conductivity and diffusion. Determination of viscosity of gases. Influence of temperature and pressure on transport properties.

Module 2: Classical Thermodynamics **(18 Hrs)**

2.1 Entropy, dependence of entropy on variables of a system (S, T and V; S, T and P). Thermodynamic equations of state. Irreversible processes - Clausius inequality.

2.2 Free energy, Maxwell relations and significance, temperature dependence of free energy, Gibbs-Helmholtz equation, applications of Gibbs-Helmholtz equation.

2.3 Partial molar quantities, chemical potential and Gibbs-Duhem equations, determination of partial molar volume and enthalpy.

2.4 Fugacity, relation between fugacity and pressure, determination of fugacity of a real gas, variation of fugacity with temperature and pressure. Activity, dependence of activity on temperature and pressure.

2.5 Thermodynamics of mixing, Gibbs-Duhem-Margules equation, Konowaloff's rule, Henry's law, excess thermodynamic functions- free energy, enthalpy, entropy andvolume. Determination of excess enthalpy and volume.

2.6 Chemical affinity and thermodynamic functions, effect of temperature and pressure on chemical equilibrium- van't Hoff reaction isochore and isotherm.

2.7 Third law of thermodynamics, Nernst heat theorem, determination of absolute entropies using third law, entropy changes in chemical reactions.

2.8 Three component systems- graphical representation. solid-liquid equilibria- ternary solutions with common ions, hydrate formation, compound formation. Liquid-liquid equilibria- one pair of partially miscible liquids, two pairs of partially miscible liquids, and three pairs of partially miscible liquids.

Module 3: Irreversible Thermodynamics and Bioenergetics (9 Hrs)

3.1 Thermodynamics of irreversible processes with simple examples. Uncompensated heat and its physical significance. Entropy production- rate of entropy production, entropy production in chemical reactions, the phenomenological relations, the principle of microscopic reversibility, the Onsager reciprocal relations thermal osmosis, thermoelectric phenomena.

3. 2 Bioenergetics: Coupled reactions, ATP and its role in bioenergetics, high energy bond, free energy and entropy change in ATP hydrolysis, thermodynamic aspects of metabolism and respiration, glycolysis, biological redox reactions.

Module 4: Statistical Thermodynamics (18 Hrs)

4.1 Permutation, probability, apriori and thermodynamic probability, Stirling's approximation, macrostates and microstates, Boltzmann distribution law, partition function and its physical significance, phase space, different ensembles, canonical partition function, distinguishable and indistinguishable molecules, partition function and thermodynamic functions, separation of partition function- translational, rotational, vibrational and electronic partition functions. Thermal de-Broglie wavelength.

4.2 Calculation of thermodynamic functions and equilibrium constants, statistical interpretation of work and heat, Sakur-Tetrode equation, statistical formulation of third law of thermodynamics, thermodynamic probability and entropy, residual entropy, heat capacity of gases - classical and quantum theories, heat capacity of hydrogen.

References

[1] P.W. Atkins, Physical Chemistry, ELBS, 1994.

[2] K.J. Laidler, J.H. Meiser, B.C. Sanctuary, Physical Chemistry, 4th Edn., Houghton Mifflin, 2003.

[3] G.W. Castellan, Physical Chemistry, Addison-Wesley, 1983.

[4] R.P. Rastogi, R.R. Misra, An introduction to Chemical Thermodynamics, Vikas Publishing House, 1996.

[5] J. Rajaram, J.C. Kuriakose, Thermodynamics, S Chand and Co., 1999.

[6] M.C. Gupta, Statistical Thermodynamics, New Age International, 2007.

[7] M.W. Zemansky, R.H. Dittman, Heat and Thermodynamics, Tata McGraw Hill, 1981.

[8] I. Tinoco, K. Sauer, J.C. Wang, J.D. Puglis, Physical Chemistry: Principles and Applications in Biological Science, Prentice Hall, 2002.

[9] L.K. Nash, Elements of Classical and Statistical Mechanics, 2nd Edn., Addison-Wesley, 1972.

[10] D.A. McQuarrie, J.D. Simon, Physical Chemistry: A Molecular Approach, University Science Books, 1997.

[11] F.W. Sears and G.L. Salinger, An Introduction to Thermodynamics, Kinetic Theory of Gases and Statistical Mechanics, Addison-Wesley.

[12] C. Kalidas, M.V. Sangaranarayanan, Non-equilibrium Thermodynamics, Macmillan India, 2002.

[13] R.K. Murray, D.K. Granner, P. A. Mayes, V.W. Rodwell, Harper's Biochemistry, Tata McGraw Hill, 1999.

SEMESTER 2

PG2ANL C05 INORGANIC CHEMISTRY- II

(BIOINORGANIC & ORGANOMETALLIC CHEMISTRY)

Credits: 4 **Contact Lecture Hours: 72**

Module 1: Bioinorganic Compounds (18 Hrs)

1.1 Essential and trace elements in biological systems, structure and functions of biological membranes, mechanism of ion transport across membranes, sodium pump, ionophores, valinomycin and crown ether complexes of Na^+ and K^+, ATP and ADP. Photosynthesis- chlorophyll a, PS I and PS II. Role of calcium in muscle contraction, blood clotting mechanism and biological calcification.

1.2 Oxygen carriers and oxygen transport proteins- haemoglobins, myoglobins and haemocyanin, haemerythrins and haemevanadins, cooperativity in haemoglobin. Iron storage and transport in biological systems- ferritin and transferrin. Redox metalloenzymes-cytochromes, peroxidases and superoxide dismutase and catalases. Nonredox metalloenzymes- Carboxypeptidase A- structure and functions. Nitrogen fixation- nitrogenase, vitamin B_{12} and vitamin B_{12} coenzymes.

1.3 Metals in medicine- therapeutic applications of *cis*-platin, radio-isotopes and MRI agents. Toxic effects of metals (Cd, Hg, Cr and Pb).

Module 2: Inorganic Chains (9 Hrs)

2.1 Chains - catenation, homo and heterocatenation. Silicate minerals. Structure of silicates common silicates, silicates containing discrete anions, silicates containing infinite chains, silicates containing sheets, framework silicates. Silicones. Zeolites synthesis, structure and applications. Isopoly acids of vanadium, molybdenum and tungsten. Heteropoly acids of Mo and W. Condensed phosphates-preparation, structure and applications. Phosphate esters in biological systems. Polythiazil- one dimensional conductors.

Module 3: Spectral and Magnetic Properties of Metal Complexes (18 Hrs)

3.1 Electronic Spectra of complexes- Term symbols of d^n system, Racah parameters, splitting of terms in weak and strong octahedral and tetrahedral fields. Correlation diagrams for d^n and d^{10-n} ions in octahedral and tetrahedral fields (qualitative approach), *d-d* transition, selection rules for electronic transition- effect of spin orbit coupling and vibronic coupling.

3.2 Interpretation of electronic spectra of complexes- Orgel diagrams, demerits of Orgel diagrams, Tanabe-Sugano diagrams, calculation of Dq, B and β (Nephelauxetic ratio) values, spectra of complexes with lower symmetries, charge transfer spectra, luminescence spectra.

3.3 Magnetic properties of complexes- paramagnetic and diamagnetic complexes, molar susceptibility, Gouy method for the determination of magnetic moment of complexes, spin only magnetic moment. Temperature dependence of magnetism- Curie's law, Curie-Weiss law. Temperature Independent Paramagnetism (TIP), Spin state cross over, Antiferromagnetism- inter and intra molecular interaction. Anomalous magnetic moments.

3.4 Elucidating the structure of metal complexes (cobalt and nickel complexes) using electronic spectra, IR spectra and magnetic moments.

Module 4: Stereochemistry of Coordination Compounds (9 Hrs)

4.1 Geometrical and optical isomerism in octahedral complexes, resolution of optically active complexes, determination of absolute configuration of complexes by ORD and circular dichroism, stereoselectivity and conformation of chelate rings, asymmetric synthesis catalyzed by coordination compounds.

4.2 Linkage isomerism- electronic and steric factors affecting linkage isomerism. Symbiosis- hard and soft ligands, Prussian blue and related structures, Macrocycles- crown ethers.

Module 5: Reactions of Organometallic Compounds (9 Hrs)

5.1 Substitution reactions- nucleophilic ligand substitution, nucleophilic and electrophilic attack on coordinated ligands.

5.2 Addition and elimination reactions- 1,2 additions to double bonds, carbonylation and decarbonylation, oxidative addition and reductive elimination, insertion (migration) and elimination reactions.

5.3 Rearrangement reactions, redistribution reactions, fluxional isomerism.

Module 6: Catalysis of Organometallic Compounds (9 Hrs)

6.1 Alkene hydrogenation, Tolman catalytic loop, Synthesis gas, Hydroformylation, Monsanto Acetic acid process, Wacker process, Zeigler Natta catalysis.

References

[1] F.A. Cotton, G. Wilkinson, Advanced Inorganic Chemistry: A Comprehensive Text, 3rd Edn., Interscience,1972.

[2] J.E. Huheey, E.A. Keiter, R.A. Keiter, Inorganic Chemistry Principles of Structure and Reactivity, 4th Edn., Pearson Education India, 2006.

[3] K.F. Purcell, J.C. Kotz, Inorganic Chemistry, Holt-Saunders, 1977.

[4] R.W. Hay, Bio Inorganic Chemistry, Ellis Horwood, 1984.

[5] B.E. Douglas, D.H. McDaniel, J.J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd Edn., Wiley-India, 2007.

[6] B.D. Guptha, A.J Elias, Basic Organometallic Chemistry, Universities Press, 2010.

[7] R.S. Drago, Physical Methods in Chemistry, Saunders College, 1992.

[8] B.N. Figgis, M.A. Hitchman, Ligand Field Theory and its Applications, Wiley-India, 2010.

[9] J.D. Lee, Concise Inorganic Chemistry, 4th Edn., Wiley-India, 2008, 17.

[10] A.B.P. Lever, Inorganic Electronic Spectroscopy, 2nd Edn., Elsevier, 1984.

PG2ANL C06 ORGANIC CHEMISTRY - II

(REACTION MECHANISM)

Credit: 4 **Contact Lecture Hours: 72**

Module 1: Chemistry of Carbocations (9 Hrs)

1.1 Formation, structure and stability of carbocations. Classical and non-classical carbocations.

1.2 C-X bond (X = C, O, N) formations through the intermediary of carbocations. Molecular rearrangements including Wagner-Meerwein, Pinacol-pinacolone, semi-pinacol, Dienone-phenol and Benzilic acid rearrangements, Prins reaction, Demjanov rearrangement. Oxymercuration, halolactonisation.

Module 2: Chemistry of Carbanions (18 Hrs)

2.1 Formation, structure and stability of carbanions. Reactions of carbanions: C-X bond (X = C, O, N) formations through the intermediary of carbanions. Chemistry of enolates, Kinetic and thermodynamic enolates- Lithium and boron enolates in Michael and aldol reactions, alkylation and acylation of enolates. Chemistry of enamines, Stork-Enamine reaction.

2.2 Nucleophilic additions to carbonyls groups. Reactions involving carbanions- mechanisms of Claisen, Dieckmann, Knoevenagel, Stobbe, Darzen and acyloin condensations, Shapiro reaction and Julia elimination. Favorskii rearrangement.

2.3 Reactions of carbonyl compounds: oxidation, reduction (Clemmensen and Wolff-Kishner), addition reactions (addition of cyanide, ammonia, alcohol), Aldol condensation, Cannizzaro reaction, addition of Grignard reagent.

2.4 Structure and reactions of α, β- unsaturated carbonyl compounds involving electrophilic and nucleophilic addition- Michael addition, Mannich reaction, Robinson annulation.

2.5 Ylids: chemistry of phosphorous and sulphur ylids - Wittig and related reactions, Peterson olefination.

Module 3: Carbenes, Carbenoids, Nitrenes and Arynes (9 Hrs)

3.1 Generation, structure and reactions of carbenes. Rearrangement reactions of carbenes: Wolff rearrangement, generation and reactions of ylids by carbenoid decomposition.

3.2 Structure, generation and reactions of nitrenes. Hoffmann, Curtius, Lossen, Schmidt and Beckmann rearrangement reactions.

3.3 Arynes: generation, structure, stability and reactions. Orientation effect, amination of haloarenes.

Module 4: Radical Reactions (9 Hrs)

4.1 Generation and detection of radical intermediates and its (a) addition to alkenes, alkynes (inter and intramolecular) for C-C bond formation - Baldwin's rules (b) fragmentation and rearrangements. Hydroperoxide: formation, rearrangement and reactions. Autoxidation.

4.2 Name reactions involving radical intermediates: Barton deoxygenation and decarboxylation, McMurry coupling.

Module 5: Concerted reactions (18 Hrs)

5.1 Symmetry properties of molecular orbitals of ethylene and conjugated systems with three or more atoms, Woodward – Hoffmann rule, Conservation of orbital symmetry and stereo chemical courses.

5.2 Pericyclic reactions like Electrocyclic (butadiene-cyclobutene and hexatriene-cyclohexadiene interconversions), Cycloadditions (2+2) & (4+2), Sigmatropic (1,3), (1,5) and (3,3), Cheletropic including Cheletropic eliminations and Ene reaction with stereo chemical aspects.

5.3 Diels- Alder reactions with stereochemical aspects.

5.4 Analysis of Pericyclic Reactions. (i) FMO method (ii) Orbital- correlation method and (iii) PMO method.

5.2 Highlighting pericyclic reactions in organic synthesis such as Claisen, Cope, Mislow-Evans, Wittig and Sommelet-Hauser rearrangements. dipolar cycloaddition (introductory). Unimolecular pyrolytic elimination reactions, decomposition of cyclic azo compounds, β-eliminations involving cyclic transition states such as N-oxides, acetates and xanthates.

Module 6: Organic Photochemistry (9 Hrs)

6.1 Photochemical processes. Energy transfer. Jablonski diagram, sensitization and quenching. Singlet and triplet states and their reactivity.

6.2 Photoreactions of carbonyl compounds, enes, dienes and arenes. Norrish reactions of acyclic ketones. Patterno-Buchi, Barton, Photo-Fries and Di-л methane rearrangements. Photoreactions of Vitamin D. Photosynthesis and photochemistry of vision. Singlet oxygen generation and their reactions**.**

References

[1] R. Bruckner, Advanced Organic Chemistry: Reaction Mechanism, Academic Press, 2002.

[2] F.A. Carey, R.A. Sundberg, Advanced Organic Chemistry, Part A: Structure and Mechanisms, 5th Edn., Springer Science & Business Media, 2007.

[3] F.A. Carey, R.A. Sundberg, Advanced Organic Chemistry, Part B: Reactions and Synthesis, 5th Edn., Springer Science & Business Media, 2007.

[4] W. Carruthers, I. Coldham, Modern Methods of Organic Synthesis, Cambridge University Press, 2005.

[5] J. March, M.B. Smith, March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 6th Edn., Wiley, 2007.

[6] T.H. Lowry, K.H. Richardson, Mechanism and Theory in Organic Chemistry, Harper & Row, Publishers, Inc., New York, 1976.

[7] I. Fleming, Frontier Orbitals and Organic Chemical Reactions, Wiley, 1976.

[8] S. Sankararaman, Pericyclic Reactions-A Text Book, Wiley VCH, 2005.

[9] R.T. Morrison, R.N. Boyd, S.K. Bhatacharjee, Organic Chemistry, 7th Edn., Pearson, 2011.

[10] J. Clayden, N. Greeves, S. Warren, P. Wothers, Organic Chemistry, Oxford University Press, 2004.

[11] N.J. Turro, V. Ramamurthy, J.C. Scaiano, Principles of Molecular Photochemistry: An Introduction, University Science books, 2009.

[12] N.J. Turro, Modern Molecular Photochemistry, Benjamin Cummings, 1978.

[13] K.K.R. Mukherjee, Fundamentals of Photochemistry, New Age Pub. Ltd, 1978.

[14] Jagadamba Singh, Jaya Singh, Photochemistry and Pericyclic Reactions, 3rd Edn., New Age International Publ. Ltd.

PG2ANL C07 THEORETICAL CHEMISTRY - II

(CHEMICAL BONDING AND COMPUTATIONAL CHEMISTRY)

Credit: 4 **Contact Lecture Hours: 72**

Module 1: Approximate Methods in Quantum Mechanics (18 Hrs)

1.1 Many-body problem and the need of approximation methods, independent particle model. Variation method, variation theorem with proof, illustration of variation theorem using the trial function x(a-x) for particle in a 1D – box and using the trial function e^{-ar} for the hydrogen atom, variation treatment for the ground state of helium atom.

1.2 Perturbation method, time-independent perturbation method (non-degenerate case only), first order correction to energy and wave function, illustration by application to particle in a 1D-box with slanted bottom, perturbation treatment of the ground state of the helium atom. Qualitative idea of Hellmann-Feynman theorem.

1.3 Hartree Self-Consistent Field method. Spin orbitals for many electron atoms- symmetric and antisymmetric wave functions. Pauli's exclusion principle. Slater determinants. Qualitative treatment of Hartree-Fock Self-Consistent Field (HFSCF) method. Roothan's concept of basis functions, Slater type orbitals (STO) and Gaussian type orbitals (GTO), sketches of STO and GTO.

Module 2: Chemical Bonding (18 Hrs)

2.1 Schrödinger equation for molecules. Born-Oppenheimer approximation. Valence Bond (VB) theory, VB theory of H_2 molecule, singlet and triplet state functions (spin orbitals) of H_2.

2.2 Molecular Orbital (MO) theory, MO theory of H_2^+ ion, MO theory of H_2 molecule, MO treatment of homonuclear diatomic molecules Li_2, Be_2, N_2, O_2 and F_2 and hetero nuclear diatomic molecules LiH, CO, NO and HF. Bond order. Spectroscopic term symbols for diatomic molecules. Comparison of MO and VB theories.

2.3 Hybridization, quantum mechanical treatment of sp, sp^2 and sp^3 hybridisation. Semiempirical MO treatment of planar conjugated molecules, Hückel Molecular Orbital (HMO) theory of ethene, allyl systems, butadiene and benzene. Calculation of charge distributions, bond order and free valency.

Module 3: Applications of Group Theory in Chemical Bonding (9 Hrs)

3.1 Applications in chemical bonding, construction of hybrid orbitals with BF_3, CH_4, and PCl_5 as examples. Transformation properties of atomic orbitals. Symmetry adapted linear combinations (SALC) of C_{2v}, C_{3v}, C_{2h}, C_3 and D_{3h} groups. MO diagram for water and ammonia.

Module 4: Computational Chemistry (18 Hrs)

4.1 Introduction: computational chemistry as a tool and its scope.

4.2 Potential energy surface: stationary point, transition state or saddle point, local and global minima.

4.3 Molecular mechanics methods: force fields-bond stretching, angle bending, torsional terms, non-bonded interactions, electrostatic interactions. Mathematical expressions. Parameterisation from experiments of quantum chemistry. Important features of commonly used force fields like MM3, MMFF, AMBER and CHARMM.

4.4 Ab initio methods: A review of Hartee-Fock method. Basis set approximation. Slater and Gaussian functions. Classification of basis sets - minimal, double zeta, triple zeta, split valence, polarization and diffuse basis sets, contracted basis sets, Pople style basis sets and their nomenclature, correlation consistent basis sets.

4.5 Hartree-Fock limit. Electron correlation. Qualitative ideas on post Hartree-Fock methods-variational method, basic principles of Configuration Interaction (CI). Perturbational methods-basic principles of Møller Plesset Perturbation Theory.

4.6 General introduction to semiempirical methods: basic principles and terminology.

4.7 Introduction to Density Functional Theory (DFT) methods: Hohenberg-Kohn theorems. Kohn-Sham orbitals. Exchange correlation functional. Local density approximation. Generalized gradient approximation. Hybrid functionals (only the basic principles and terms need to be introduced).

4.8 Model Chemistry-notation, effect on calculation time (cost).

4.9 Comparison of molecular mechanics, ab initio, semiempirical and DFT methods

Module 5: Computational Chemistry Calculations (9 Hrs)

5.1 Molecular geometry input- Cartesian coordinates and internal coordinates, Z-matrix. Z-matrix of: single atom, diatomic molecule, non-linear triatomic molecule, linear triatomic molecule, polyatomic molecules like ammonia, methane, ethane and butane. General format of GAMESS/Firefly input file. GAMESS/Firefly key word for: basis set selection, method selection, charge, multiplicity, single point energy calculation, geometry optimization, constrained optimization and frequency calculation.

5.2 Identifying a successful GAMESS/Firefly calculation-locating local minima and saddle points, characterizing transition states, calculation of ionization energies, Koopmans' theorem, electron affinities and atomic charges.

5.3 Identifying HOMO and LUMO-visualization of molecular orbitals and normal modes of vibrations using suitable graphics packages.

References

[1] I.N. Levine, Quantum Chemistry, 6th Edn., Pearson Education, 2009.

[2] D.A. McQuarrie, Quantum Chemistry, University Science Books, 2008.

[3] R.K. Prasad, Quantum Chemistry, 3rd Edn., New Age International, 2006.

[4] F.A. Cotton, Chemical Applications of Group Theory, 3rd Edn., Wiley Eastern,1990.

[5] V. Ramakrishnan, M.S. Gopinathan, Group Theory in Chemistry, Vishal Publications, 1992.

[6] A.S. Kunju, G. Krishnan, Group Theory and its Applications in Chemistry, PHI Learning, 2010.

[7] E.G. Lewars, Computational Chemistry: Introduction to the Theory and Applications of Molecular and Quantum Mechanics, 2nd Edn., Springer, 2011.

[8] J.H. Jensen, Molecular Modeling Basics, CRC Press, 2010.

[9] F. Jensen, Introduction to computational chemistry, 2nd Edn., John Wiley & Sons, 2007.

[10] A. Leach, Molecular Modeling: Principles and Applications, 2nd Edn., Longman, 2001.

[11] J.P. Fackler Jr., L.R. Falvello (Eds.), Techniques in Inorganic Chemistry: Chapter 4, CRC Press, 2011.

[12] K.I. Ramachandran, G. Deepa, K. Namboori, Computational Chemistry and Molecular Modeling: Principles and Applications, Springer, 2008.

[13] A. Hinchliffe, Molecular Modelling for Beginners, 2nd Edn., John Wiley & Sons,2008.

[14] C.J. Cramer, Essentials of Computational Chemistry: Theories and Models, 2nd Edn., John Wiley & Sons, 2004.

[15] D.C. Young, Computational Chemistry: A Practical Guide for Applying Techniques to Real-World Problems, John Wiley & Sons, 2001.

Softwares

Molecular Mechanics:

01. **Arguslab** available from www.arguslab.com/
02. **Tinker** available from www.dasher.wustl.edu/ffe/

Ab initio, semiempirical and dft:

01. **Firefly / PC GAMESS** available from http://classic.chem.msu.su/gran/gamess/
02. **WINGAMESS** available from http://www.msg.ameslab.gov/gamess/

Graphical User Interface (GUI):

01. **Gabedit** available from http://gabedit.sourceforge.net/
02. **wxMacMolPlt** available from http://www.scl.ameslab.gov/MacMolPlt/
03. **Avogadro** from http://avogadro.openmolecules.net/wiki/Get_Avogadro

PG2ANL C08 PHYSICAL CHEMISTRY - II

(MOLECULAR SPECTROSCOPY)

Credit: 3 **Contact Lecture Hours: 54**

Module 1: Microwave and Infrared Spectroscopy (18 Hrs)

1.1 Origin of spectra: origin of different spectra and the regions of the electromagnetic spectrum, intensity of absorption, influencing factors, signal to noise ratio, natural line width-contributing factors, Lamb dip spectrum, Born Oppenheimer approximation, energy dissipation from excited states (radiative and non-radiative processes), relaxation time.

1.2 Microwave spectroscopy: principal moments of inertia and classification of molecules (linear, symmetric tops, spherical tops and asymmetric tops), selection rules, intensity of rotational lines, relative population of energy levels, derivation of J_{max}, effect of isotopic substitution, calculation of intermolecular distance, spectrum of non rigid rotors, rotational spectra of polyatomic molecules, linear and symmetric top molecules, Stark effect and its application, nuclear spin and electron spin interaction, chemical analysis by microwave spectroscopy.

1.3 Infrared spectroscopy: Morse potential energy diagram, fundamentals, overtones and hot bands, determination of force constants, diatomic vibrating rotator, break down of the Born-Oppenheimer approximation, effect of nuclear spin, vibrational spectra of polyatomic molecules, normal modes of vibrations, combination and difference bands, Fermi resonance, finger print region and group vibrations, effect of H-bonding on group frequency, disadvantages of dispersive IR, introduction to FT spectroscopy, FTIR.

Module 2: Electronic, Mossbauer and Raman spectroscopy (18 Hrs)

2.1 Electronic spectroscopy: Term symbols of diatomic molecules, electronic spectra of diatomic molecules, selection rules, vibrational coarse structure and rotational fine structure of electronic spectrum, Franck-Condon principle, predissociation, calculation of heat of dissociation, Birge and Sponer method, electronic spectra of polyatomic molecules, spectra of transitions localized in a bond or group, free electron model.

Different types of lasers- solid state lasers, continuous wave lasers, gas lasers and chemical laser, frequency doubling, applications of lasers, introduction to UV and X-ray photoelectron spectroscopy.

2.2 Mossbauer spectroscopy: principle, Doppler effect, recording of spectrum, chemical shift, factors determining chemical shift, application to metal complexes, MB spectra of Fe(II) and Fe(III) cyanides.

2.3 Raman spectroscopy: scattering of light, polarizability and classical theory of Raman spectrum, rotational and vibrational Raman spectrum, complementarities of Raman and IR spectra, mutual exclusion principle, polarized and depolarized Raman lines, resonance Raman scattering and resonance fluorescence.

Module 3: Resonance Spectroscopy (18 Hrs)

3.1 NMR spectroscopy : Interaction between nuclear spin and applied magnetic field, nuclear energy levels, population of energy levels, Larmor precession, relaxation methods, chemical shift, representation, examples of AB, AX and AMX types, exchange phenomenon, factors influencing coupling, Karplus relationship.

3.2 FTNMR, second order effects on spectra, spin systems (AB, AB_2), simplification of second order spectra, chemical shift reagents, high field NMR, double irradiation, selective decoupling, double resonance, NOE effect, two dimensional NMR, COSY and HETCOR, ^{13}C NMR, natural abundance, sensitivity, ^{13}C chemical shift and structure correlation, introduction to solid state NMR, magic angle spinning.

3.3 EPR spectroscopy: electron spin in molecules, interaction with magnetic field, g factor, factors affecting g values, determination of g values ($g_{\parallel}$ and $g_{\perp}$), fine structure and hyperfine structure, Kramers' degeneracy, McConnell equation.

3.4 An elementary study of NQR spectroscopy.

References

[1] C.N. Banwell, E.M. McCash, Fundamentals of Molecular Spectroscopy, 4th Edn., Tata McGraw Hill, 1994.

[2] G. Aruldhas, Molecular Structure and Spectroscopy, Prentice Hall of India, 2001.

[3] P.W. Atkins, Physical Chemistry, ELBS, 1994.

[4] R.S. Drago, Physical Methods in Inorganic Chemistry, Van Nonstrand Reinhold, 1965.

[5] R.S. Drago, Physical Methods in Chemistry, Saunders College, 1992.

[6] K.J. Laidler, J.H. Meiser, Physical Chemistry, 2nd Edn., CBS, 1999.

[7] W. Kemp, NMR in chemistry-A Multinuclear Introduction, McMillan, 1986.

[8] H. Kaur, Spectroscopy, 6th Edn., Pragati Prakashan, 2011.

[9] H. Gunther, NMR Spectroscopy, Wiley, 1995.

[10] D.A. McQuarrie, J.D. Simon, Physical Chemistry: A Molecular Approach, University Science Books, 1997.

[11] D.N. Sathyanarayana, Electronic Absorption Spectroscopy and Related Techniques, Universities Press, 2001.

[12] D.N. Sathyanarayana, Vibrational Spectroscopy: Theory and Applications, New Age International, 2007.

[13] D.N. Sathyanarayana, Introduction to Magnetic Resonance Spectroscopy ESR, NMR, EQR, I.K. International Publishing House Pvt. Limited, 2009.

SEMESTERS 1 AND 2

PG2ANL P01 INORGANIC CHEMISTRY PRACTICAL – 1

Credit: 3 **Contact Lab Hours: 54 + 54 = 108**

PART I

Separation and identification of four metal ions of which two are rare/ less familiar such as Tl, W, V, Se, Te, Ti, Ce, Th, Zr, U, Mo and Li and common cations - Ag^{+}, Hg^{2+}, Pb^{2+}, Cu^{2+}, Bi^{2+}, Cd^{2+}, As^{3+}, Sn^{2+}, Sb^{3+}, Fe^{2+}, Fe^{3+}, Al^{3+}, Cr^{3+}, Zn^{2+}, Mn^{2+}, Co^{2+}, Ni^{2+}, Ca^{2+}, Sr^{2+}, Ba^{2+}, Mg^{2+}, Li^{+}, Na^{+}, K^{+}, NH_4^{+} (interfering acid radicals are not present). Confirmation by spot test (Minimum **8** mixtures are to be recorded).

PART II

1. Argentometric estimation of chlorides
2. Cerimetry – Fe(II) and nitrate
3. Potassium iodate – iodide estimation of Sn(II)

PART III

Colorimetric estimation of Cr, Fe, Ni, Mn, Cu, NH_4^{+}, nitrate and phosphate ions.

PART IV

Preparation and characterization of complexes using IR, NMR and electronic spectra.

1. Tris (thiourea) copper (I) complex
2. Potassium tris (oxalate) aluminate (III)
3. Tetrammine copper (II) sulphate
4. Mercury tetra thiocyanato cobaltate (III)

References

[1] A.I. Vogel, A Text Book of Qualitative Inorganic Analysis Including Elementary Instrumental Analysis, 3rd Edn., ELBS.
[2] G. Svelha, Text Book of Vogel's Macro and Semi-micro Inorganic Analysis, revised, Orient Longman.
[3] V.V. Ramanujam, Inorganic Semi micro Qualitative Analysis, The National Publishing Co., Chennai.
[4] I. M. Koltoff, E.B. Sandell, Text Book of Quantitative Inorganic Analysis, 3rd Edn, McMillian, 1968.

PG2ANL P02 ORGANIC CHEMISTRY PRACTICAL - 1

Credit: 3 **Contact Lab Hours: 54+54=108**

PART I

General methods of separation and purification of organic compounds such as:

1. Solvent extraction
2. Soxhlet extraction
3. Fractional crystallization
4. TLC and Paper Chromatography
5. Column Chromatography
6. Membrane Dialysis

PART II

A. Separation of organic binary mixtures:- 1. Quantitative separation of a mixture of two components by solvent extraction 2. Purification of the separated samples by distilling and crystallization. 3. Determination of physical constants of separated and purified samples (No need of bifunctional compounds).

B. Separation of organic mixtures by TLC and calculation of R_f values.

C. Separation/purification of organic mixtures by column chromatography.

PART III

Drawing the structures of organic molecules and reaction schemes and mechanisms by ChemDraw, SymyxDraw and Chemsketch.

1. Cycloaddition of diene and dienophile (Diels-Alder reaction).
2. Oxidation of primary alcohol to aldehyde and then to acid.
3. Benzoin condensation.
4. Esterification of simple carboxylic acids.
5. Aldol condensation.

PART IV- Viva voce

References

[1] A.I. Vogel, A Textbook of Practical Organic Chemistry, Longman, 1974.

[2] A.I. Vogel, Elementary Practical Organic Chemistry, Longman, 1958.

[3] F.G. Mann, B.C Saunders, Practical Organic Chemistry, 4th Edn., Pearson Education India, 2009.

[4] R. Adams, J.R. Johnson, J.F. Wilcox, Laboratory Experiments in Organic Chemistry, Macmillan, 1979.

[5] A.I. Vogel, A.R. Tatchell, B.S. Furnis, A.J. Hannaford, P.W.G. Smith, Vogels Text Book of Practical Organic Chemistry, 5th Edn., Prentice Hall, 1989.

[6] R.K Bansal, Laboratory Manual of Organic Chemistry, 5th Edn., New Age Publishers, 2013.

[7] N.K.Vishnoi, Advanced Practical Organic Chemistry, 3rd Edn., Vikas Publishing House, 2009.

[8] J.B. Cohen, Practical Organic Chemistry, Mc Graw Hill.

[9] C.E Bella and DF Taber, Organic Chemistry Laboratory, Thomson.

[10] P.D.L Lampman and Chriz, Introduction to Organic Laboratory Techniques, College publishing.

[11] Monograph on green laboratory experiments, DST, Govt of India.

[12] http://sdbs.riodb.aist.go.jp/sdbs/cgi-bin/direct_frame_top.cgi.

PG2ANL P03 PHYSICAL CHEMISTRY PRACTICAL - 1

Credit: 3 **Contact Lab Hours: 72+72 =144**

(One question each from both parts A and B will be asked for the examination)

Part A

I. Adsorption

1. Verification of Freundlich and Langmuir adsorption isotherm: charcoal-acetic acid or charcoal-oxalic acid system.
2. Determination of the concentration of the given acid using the isotherms.

II. Phase diagrams

1. Construction of phase diagrams of simple eutectics.
2. Construction of phase diagram of compounds with congruent melting point: diphenyl amine-benzophenone system.
3. Effect of (KCl/succinic acid) on miscibility temperature.
4. Construction of phase diagrams of three component systems with one pair of partially miscible liquids.

III. Distribution law

1. Distribution coefficient of iodine between an organic solvent and water.
2. Distribution coefficient of benzoic acid between benzene and water.
3. Determination of the equilibrium constant of the reaction $KI + I_2 \leftrightarrow KI_3$

IV. Surface tension

1. Determination of the surface tension of a liquid by
   a) Capillary rise method
   b) Drop number method
   c) Drop weight method
2. Determination of parachor values.

3. Determination of the composition of two liquids by surface tension measurements.

Part B

Computational Chemistry Experiments

V. Experiments illustrating the capabilities of modern open source/free computational chemistry packages in computing single point energy, geometry optimization, vibrational frequencies, population analysis, conformational studies, IR and Raman spectra, transition state search, molecular orbitals, dipole moments etc.

Geometry input using Z-matrix for simple systems, obtaining Cartesian coordinates from structure drawing programs like Chemsketch.

References

[1] J.B. Yadav, Advanced Practical Physical Chemistry, Goel Publishing House, 2001.

[2] G.W. Garland, J.W. Nibler, D.P. Shoemaker, Experiments in Physical Chemistry, 8th Edn., McGraw Hill, 2009.

[3] J.H. Jensen, Molecular Modeling Basics, CRC Press, 2010.

[4] GAMESS documentation available from: http://www.msg.ameslab.gov/gamess/documentation.html.

SEMESTER 3

PG3ANL C09 INORGANIC CHEMISTRY- III

(SOLID STATE CHEMISTRY)

Credits: 4 **Contact Lecture Hours: 72**

Module 1: Solid State Chemistry **(18 Hrs)**

1.1 Structure of solids: Imperfections in solids-point defects, line defects and plane defects. Structure of compounds of AX (Zinc blende, Wurtzite), AX_2 (Rutile, fluorite, antifluorite), A_mX_2 (Nickel Arsenide), ABX_3 (Perovskite, Ilmenite). Spinels. Inverse spinel structures.

1.2 Solid state reactions-diffusion coefficient, mechanisms, vacancy diffusion, thermal decomposition of solid- Type I reactions, Type II reactions.

1.3 Phase transition in solids: classification of phase transitions-first and second order phase transitions, Martensitic transformations, order-disorder transitions and spinodal decomposition. Kinetics of phase transitions, sintering. Growing single crystals-crystal growth from solution, growth from melt and vapour deposition technique.

Module 2: Electrical, Magnetic and Optical Properties **(18 Hrs)**

2.1 Free electron theory and MO theory of solids. Energy bands-conductors and non-conductors, intrinsic and extrinsic semiconductors. Electrons and holes. Mobility of charge carriers. Hall Effect. Pyroelectricity, piezo electricity and ferro electricity. Conductivity of pure metals.

2.2 Magnetic properties of transition metal oxides, garnets, spinels, ilmenites and perovskites, magnetoplumbites.

2.3 Optical properties-photoconductivity, photovoltaic effects, luminescence. Applications of optical properties

2.4 Super conductivity- Type I and Type II superconductors, Frolich diagram, Cooper pairs, theory of low temperature super conductors, junctions using superconductors, BCS theory of superconductivity (derivation not required). Super conducting cuprates - YBaCu oxide system, Meisner effect, conventional superconductors, organic superconductors, fullerenes, carbon nanotubes, high temperature superconductors.

Module 3: Inorganic Rings, Cages and Clusters (18 Hrs)

3.1 Ring silicates and silicones, phosphorous-nitrogen compounds, phosphazenes. Heterocyclic inorganic ring systems-structure and bonding in phosphorous-sulphur and sulphur-nitrogen compounds. Homocyclic inorganic ring systems-structure and bonding in sulphur, selenium and phosphorous compounds. Polythiazil-one dimensional conductors

3.2 Cages: synthesis, structure and bonding of cage like structures of phosphorous. Boron cage compounds- Wade Mingos Lauher rules, MNO rule, boranes, carboranes, metallacarboranes

3.3. Metal clusters: dinuclear compounds of Re, Cu and Cr, metal-metal multiple bonding in $(Re_2X_8)^{2-}$, trinuclear clusters, tetranuclear clusters, hexanuclear clusters. Polyatomic zintl anion and cations. Infinite metal chains.

Module 4: Organometallic Polymers (9 Hrs)

Polymers with organometallic moieties as pendant groups, polymers with organometallic moieties in the main chain, condensation polymers based on ferrocene and on rigid rod polyynes, polymers prepared by ring opening polymerization, organometallic dendrimers.

Module 5: Chemistry of Materials (9 Hrs)

Glasses, ceramics, composites, nanomaterials-preparative procedures. Sol-gel synthesis, glassy state-glass formers and glass modifiers, ceramic structures - mechanical properties, clay products, refractories- characterizations, properties and applications.

References

[1] L.V. Azaroff, Introduction to Solids, Mc Graw Hill, 1984.

[2] A.R. West, Solid State Chemistry and its Applications, Wiley-India, 2007.

[3] D.K. Chakrabarty, Solid State Chemistry, New Age Pub., 2010.

[4] D.M. Adams, Inorganic Solids: An Introduction to Concepts in Solid State Structural Chemistry, Wiley, 1974.

[5] C.N.R. Rao, K.J. Rao, Phase Transitions in Solids, McGraw Hill, 2010.

[6] B.E. Douglas, D.H. McDaniel, J.J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd Edn., John Wiley & sons, 2006.

[7] A. Earnshaw, Introduction to Magnetochemistry, Academic Press, 1968.

[8] J.E. Huheey, E.A. Keiter, R.L. Keiter, Inorganic Chemistry Principles of Structure and Reactivity, 4th Edn., Harper Collins College Pub.,1993, 33.

[9] F.A. Cotton, G. Wilkinson, C.A. Murillo, M. Bochmann, Advanced Inorganic Chemistry, 6th Edn., Wiley-Interscience,1999.

[10] K.F. Purcell, J.C. Kotz, Inorganic Chemistry, Holt-Saunders, 1977.

[11] P.C. Jain, M. Jain, Engineering Chemistry, 12th Edn., Dhanpat Rai Pub., 2006.

[12] C.V. Agarwal, Chemistry of Engineering Materials, 9th Edn., B.S. Pub., 2006.

[13] B.D. Guptha, A.J Elias, Basic Organometallic Chemistry, Universities Press, 2010.

PG3ANL C10 ORGANIC CHEMISTRY - III

(ORGANIC SYNTHESES)

Credit: 4 **Contact Lecture Hours: 72**

Module 1: Retrosynthetic Analysis (9 Hrs)

1.1 Basic principles and terminology of retrosynthesis. Important strategies of retrosynthesis. Functional group interconversion. Umpolung. Synthesis of aromatic compounds. One group C-X disconnections of carbonyl derivatives and alkyl halides. Two group C-X disconnections- 1,1-, 1,2- and 1,3-difunctionalised compounds. One group C-C disconnections of alcohols and carbonyl compounds. Two group C-C disconnections- 1,2- and 1,3-difunctionalised compounds.

1.2 Amine synthesis: Primary amine, other routes to amines using reduction, reagents for the synthon NH_2^-. Alkene synthesis- from alcohols and derivatives, Wittig reaction.

Module 2: Organometallics (9 Hrs)

Preparation and applications in organic synthesis of (i) Organo lithium compounds and addition to −C=O, −COOH and –$CONR_2$ (ii) Lithium dialkylcuprates (Gilman reagent) and reaction with alkyl halides, aryl halides and enones (iii) Alkynyl Cu(I) reagents and Glaser coupling (iv) Dialkyl cadmium compounds and (v) Benzenetricarbonyl chromium and reaction with carbanions.

Module 3: **Organic Synthesis via Oxidation and Reduction (18 Hrs)**

3.1 Survey of organic reagents and reactions in organic chemistry with special reference to oxidation and reduction. Metal based and non-metal based oxidations of (a) alcohols to carbonyls (Chromium, Manganese, Aluminium and Silver based reagents) (b) alkenes to epoxides (peroxides/per acids based)- Sharpless asymmetric epoxidation, Jacobsen epoxidation, Shi epoxidation (c) alkenes to diols (Manganese and Osmium based)- Prevost reaction and Woodward modification (d) alkenes to carbonyls with bond cleavage (Manganese and Lead based, ozonolysis) (e) alkenes to alcohols/carbonyls without bond cleavage hydroboration-oxidation, Wacker oxidation, Selenium/Chromium based allylic oxidation (f) ketones to ester/lactones- Baeyer-Villiger oxidation.

3.2 (a) Catalytic hydrogenation (Heterogeneous: Palladium/Platinum/Rhodium and Nickel, Homogeneous: Wilkinson) (b) Metal based reductions- Birch reduction, Pinacol formation, acyloin formation (c) Hydride transfer reagents from Group III and Group IV in reductions - $LiAlH_4$, DIBAL-H, Red-Al, $NaBH_4$ and $NaCNBH_3$, selectrides, trialkylsilanes and trialkylstannane. Meerwein-Pondorff-Verley reduction. Baker's yeast.

Module 4: Modern Synthetic Methods and Reagents (18 Hrs)

4.1 Baylis-Hillman reaction, Henry reaction, Nef reaction, Kulinkovich reaction, Ritter reaction, Sakurai reaction, Tishchenko reaction, Noyori reaction. Brook rearrangement. Tebbe olefination. Metal mediated C-C and C-X coupling reactions: Heck, Stille, Suzuki, Negishi, Sonogashira, Nozaki-Hiyama, Buchwald- Hartwig, Ullmann reactions, Wohl-Ziegler reaction. Reagents such as NBS, DDQ, DCC, Gilmann reagent.

4.2 Introduction to multicomponent reactions- Three component reactions (Mannich reaction, Passerini reaction, Biginelli reaction), Four component reactions (Ugi reaction). Click reactions (elementary idea only).

Module 5: Construction of Carbocyclic and Heterocyclic Ring System (9 Hrs)

5.1 Different approaches towards the synthesis of three, four, five and six-membered rings. Photochemical approaches for the synthesis of four membered rings, oxetanes and cyclobutanes, ketene cycloaddition (inter and intra molecular), Pauson-Khand reaction, Volhardt reaction, Bergman cyclization, Nazarov cyclization, Mitsunobu reaction, cation-olefin cyclization and radical-olefin cyclization. Construction of macrocyclic rings-ring closing metathesis.

5.2 Formation of heterocyclic rings: 5- and 6-membered and condensed ring heterocyclic compounds with one or more than one hetero atom like N, S or O - pyrrole, furan, thiophene, pyridine, imidazole, thiazole, oxazole, pyrimidines, purines, quinoline and isoquinoline.

Module 6: Protecting Group Chemistry (9 Hrs)

6.1 Protection and deprotection of hydroxy, carboxyl, carbonyl, and amino groups. Chemo and regio selective protection and deprotection. Illustration of protection and deprotection in synthesis.

6.2 Protection and deprotection in peptide synthesis: common protecting groups used in peptide synthesis, protecting groups used in solution phase and solid phase peptide synthesis (SPPS).

6.3 Role of trimethyl silyl group in organic synthesis.

References

[1] M.B. Smith, Organic Synthesis, 3rd Edn., Wavefunction Inc., 2010.

[2] F.A. Carey, R. I. Sundberg, Advanced Organic Chemistry, Part A and B, 5th Edn., Springer, 2007.

[3] S. Warren, P. Wyatt, Organic Synthesis: The Disconnection Approach, 2nd Edn., Wiley, 2008.

[4] V.K. Ahluwalia, Oxidation in Organic Synthesis, CRC Press, 2012.

[5] I. Ojima, Catalytic Asymmetric Synthesis, 3rd Edn., John Wiley & Sons, 2010.

[6] W. Carruthers, I. Coldham, Modern Methods of Organic Synthesis, 4th Edn., Cambridge University Press, 2004.

[7] J. Clayden, N. Greeves, S. Warren, P. Wothers, Organic Chemistry, Oxford University Press, 2004.

[8] R. Noyori, Asymmetric Catalysis in Organic Synthesis, John Wiley & Sons, 1994.

[9] L. Kuerti, B. Czako, Strategic Applications of Named Reactions in Organic Synthesis, Elsevier Academic Press, 2005.

[10] R.O.C. Norman, J.M. Coxon, Principles of Organic Synthesis, 3rd Edn., Chapmann and Hall, 1993.

[11] E. J. Corey, Xue-Min Cheng, The Logic of Chemical Synthesis, Wiley, 1995.

[12] J. Zhu, Q. Wang, M. Wang (Eds), Multicomponent Reactions in Organic Synthesis, Wiley VCH, 2015.

[13] F. Rutjes, V.V. Fokin, K.B. Sharpless, Click Chemistry: In Chemistry, Biology and Macromolecular Science, Wiley, 2012.

PG3ANL C11- PHYSICAL CHEMISTRY- III

(CHEMICAL KINETICS, SURFACE CHEMISTRY AND PHOTOCHEMISTRY)

Credit: 4 **Contact Lecture Hours: 72**

Module 1: Chemical Kinetics **(18 Hrs)**

1.1 Theories of reaction rates: Collision theory- steric factor, potential energy surfaces. Conventional transition state theory- Eyring equation. Comparison of the two theories. Thermodynamic formulation of the two theories. Thermodynamic formulation of the reaction rates. Significance of $\Delta G^{\#}$, $\Delta H^{\#}$ and $\Delta S^{\#}$. Volume of activation. Effect of pressure and volume on velocity of gas reactions.

1.2 Lindemann-Hinshelwood mechanism, qualitative idea of RRKM theory, chain reactions: free radical and chain reactions, steady state treatment, Kinetics of H_2-Cl_2 and H_2-Br_2 reactions, Rice-Herzfeld mechanism, branching chains H_2-O_2, Semonov-Hinshelwood mechanism of explosive reactions, mechanisms of step- growth, ionic and addition polymerization, kinetics of anionic and cationic polymerization.

1.3 Fast reactions: relaxation, flow and shock methods, flash photolysis, NMR and ESR methods of studying fast reactions.

1.4 Reactions in solution: factors determining reaction rates in solutions, effect of dielectric constant and ionic strength, cage effect, Bronsted-Bjerrum equation, primary and secondary kinetic salt effect, influence of solvent on reaction rates, significance of volume of activation, linear free energy relationship, kinetic isotope effect.

Module 2: Surface Chemistry **(18 Hrs)**

2.1 Surface: Different types of surfaces, thermodynamics of surfaces, Gibbs adsorption equation and its verification, surface excess, surface tension and surface concentration, surfactants and micelles, general properties of emulsions, foam structure, aerosols, surface films, surface pressure and surface potential and their measurements and interpretation. Application of low energy electron diffraction and photoelectron spectroscopy, ESCA and Auger electron spectroscopy, scanning probe microscopy, ion scattering, SEM and TEM in the study of surfaces.

2.2 Adsorption: The Langmuir theory, kinetic and statistical derivation, multilayer adsorption-BET theory and derivation of isotherm, Use of Langmuir and BET isotherms for surface area determination. Application of Langmuir adsorption isotherm in surface catalysed reactions, the Eley-Rideal mechanism and the Langmuir-Hinshelwood mechanism, flash desorption.

2.3 Surface Enhanced Raman Scattering, surfaces for SERS studies, chemical enhancement mechanism, surface selection rules, spectrum of 2-aminophenol, applications of SERS.

Module 3: Catalysis (9 Hrs)

3.1 Acid-base catalysis: specific and general catalysis, Skrabal diagram, Bronsted catalysis law, prototropic and protolytic mechanism with examples, acidity function.

3.2 Enzyme catalysis and its mechanism, Michaelis-Menton equation, effect of pH and temperature on enzyme catalysis.

3.3 Mechanisms of heterogeneous catalysis: unimolecular and bimolecular surface reactions, mechanisms of catalyzed reactions like ammonia synthesis, Fischer- Tropsch reactions, hydrogenation of ethylene and catalytic cracking of hydrocarbons and related reactions.

Module 4: Colloids and Macromolecules (9 Hrs)

4.1 Colloids: Zeta potential, electrokinetic phenomena, sedimentation potential and streaming potential, Donnan membrane equilibrium.

4.2 Macromolecules: Molecular mass- different averages, relation between different averages, calculation of different averages, methods of molecular mass determination- osmotic pressure, viscosity, sedimentation and light scattering methods.

Module 5: Photochemistry (18 Hrs)

5.1 Quantum yield, chemical actinometry, excimers and exciplexes, photosensitization, chemiluminescence, bioluminescence, thermoluminescence, pulse radiolysis, hydrated electrons, photostationary state, dimerization of anthracene, ozone layer in the atmosphere.

5.2 Principle of utilization of solar energy, solar cells and their working.

5.3 Quenching of fluorescence and its kinetics, Stern-Volmer equation, concentration quenching, fluorescence and structure, delayed fluorescence, E-type and P-type, effect of temperature on emissions, photochemistry of environment, green house effect, two photon absorption spectroscopy, lasers in photochemical kinetics.

References

[1] J. Rajaram, J.C. Kuriakose, Kinetics and Mechanisms of Chemical Transformations, Macmillan India, 2000.

[2] K.J. Laidler, Chemical kinetics, 3rd Edn., Harper & Row, 1987.

[3] C. Kalidas, Chemical Kinetic Methods: Principles of Fast Reaction Techniques and Applications, New Age International, 2005.

[4] J.W. Moore, R.G. Pearson, Kinetics and Mechanisms, John Wiley & Sons, 1981.

[5] P.W. Atkins, Physical Chemistry, ELBS, 1994.

[6] D.A. McQuarrie, J.D. Simon, Physical chemistry: A Molecular Approach, University Science Books,1997

[7] A.W. Adamson, A.P. Gast, Physical Chemistry of Surfaces, 6th Edn., John Wiley & sons, 1997.

[8] K.K. Rohatgi-Mukherjee, Fundamentals of Photochemistry, 2nd Edn., New Age International,1986.

[9] G. Aruldhas, Molecular structure and Spectroscopy, PHI Learning, 2007.

PG3A C12 SPECTROSCOPIC METHODS IN CHEMISTRY

Credit: 3 **Contact Lecture Hours: 54**

Module 1: Ultraviolet-Visible and Chirooptical Spectroscopy (9 Hrs)

1.1 Energy levels and selection rules, Woodward-Fieser and Fieser-Kuhn rules.

1.2 Influence of substituent, ring size and strain on spectral characteristics. Solvent effect, Stereochemical effect, non-conjugated interactions.

1.3 Problems based on the above topics.

1.4 Chirooptical properties- ORD, CD, octant rule, axial haloketone rule, Cotton effect.

Module 2: Infrared Spectroscopy (9 Hrs)

2.1 Fundamental vibrations, characteristic regions of the spectrum (fingerprint and functional group regions), influence of substituent, ring size, hydrogen bonding, vibrational coupling and field effect on frequency, determination of stereochemistry by IR technique.

2.2 IR spectra of C=C bonds (olefins and arenes) and C=O bonds.

2.3 Problems on spectral interpretation with examples.

Module 3: Nuclear Magnetic Resonance Spectroscopy (18 Hrs)

3.1 Magnetic nuclei with special reference to ^{1}H and ^{13}C nuclei. Chemical shift and shielding/deshielding, factors affecting chemical shift, relaxation processes, chemical and magnetic non-equivalence, local diamagnetic shielding and magnetic anisotropy. ^{1}H and ^{13}C NMR scales.

3.2 Spin-spin splitting: AX, AX_2, AX_3, A_2X_3, AB, ABC, AMX type coupling, first order and non-first order spectra, Pascal's triangle, coupling constant, mechanism of coupling, Karplus curve, quadrupole broadening and decoupling, diastereomeric protons, virtual coupling, long range coupling. NOE and cross polarization.

3.3 Simplification of non-first order spectra to first order spectra: shift reagents, spin decoupling and double resonance, off resonance decoupling. Chemical shifts and homonuclear/heteronuclear couplings. Basis of heteronuclear decoupling, ^{19}F and ^{31}P NMR.

3.4 2D NMR and COSY, HOMOCOSY and HETEROCOSY

3.5 Polarization transfer. Selective Population Inversion. DEPT. Sensitivity enhancement and spectral editing, MRI.

3.6 Problems on spectral interpretation with examples.

Module 4: Mass Spectrometry (9 Hrs)

4.1 Molecular ion: ion production methods (EI). Soft ionization methods: SIMS, FAB, CA, MALDI, Field Desorption and Electrospray Ionization. Magnetic, TOF, quadrupole and ion cyclotron mass analysers. MS^n technique. Fragmentation patterns-nitrogen and ring rules. McLafferty rearrangement and its applications. HRMS, MS-MS, LC-MS, GC-MS.

4.2 Problems on spectral interpretation with examples.

Module 5: Structure Elucidation Using Spectroscopic Techniques (9 Hrs)

5.1 Identification of structures of unknown organic compounds based on the data from UV-Vis, IR, ^1H NMR and ^{13}C NMR spectroscopy (HRMS data or Molar mass or molecular formula may be given).

5.2 Interpretation of the given UV-Vis, IR and NMR spectra.

References

[1] D.L. Pavia, G.M. Lampman, G.S. Kriz, Introduction to Spectroscopy, 3rd Edn., Brooks Cole, 2000.

[2] A.U. Rahman, M.I. Choudhary, Solving Problems with NMR Spectroscopy, Academic Press, 1996.

[3] L. D. Field, S. Sternhell, J. R. Kalman, Organic Structures from Spectra, 4th Edn., John Wiley & sons, 2007.

[4] C.N. Banwell, E.M. McCash, Fundamentals of Molecular Spectroscopy, 4th Edn., Tata McGraw Hill, 1994.

[5] D.F. Taber, Organic Spectroscopic Structure Determination: A Problem Based Learning Approach, Oxford University Press, 2007.

[6] H. Gunther, NMR Spectroscopy, 2nd Edn., Wiley, 1995.

[7] R. M. Silverstein, F. X. Webster, D. J. Kiemle, D. L. Bryce, Spectroscopic Identification of Organic Compounds, 8th Edn., Wiley, 2015.

[8] D.H. Williams, I. Fleming, Spectroscopic Methods in Organic Chemistry, 6th Edn., McGraw-Hill, 2008.

[9] W. Kemp, Organic Spectroscopy, 2nd Edn., Macmillan, 1987.

[10] F. Bernath, Spectra of Atoms and Molecules, 2nd Edn., Oxford University Press,2005.

[11] E.B. Wilson Jr., J.C. Decius, P.C. Cross, Molecular Vibrations: The Theory of Infrared and Raman Vibrational Spectra, Dover Pub., 1980.

[12] Online spectral databases including RIO-DB.

[13] P.S. Kalsi. Spectroscopy of Organic Compounds, 5th Edn., New Age International, 2004.

SEMESTER 4

ELECTIVE COURSES

(Any 3 courses to be opted from the following courses)

PG4ANL E01 ANALYTICAL PROCEDURES

Credit: 4 **Contact Lecture Hours: 90**

Module 1: Errors in Chemical Analysis (18 Hrs)

Systematic and random errors. Distribution of experimental results. Statistical treatment- standard deviation, variance, confidence limits, application of statistics to data treatment and evaluation, student-t and f tests, detection of gross errors, rejection of a result-Q test, estimation of detection limits. Least square method, correlation coefficient and its determination. Hypothesis testing using statistical analysis. Using spread sheets for plotting calibration curves. Quality assurance and control charts.

Module 2: Conventional Analytical Procedures (18 Hrs)

2.1 Gravimetry: Inorganic precipitating agents: NH_3, H_2S, H_2SO_4, H_2PtCl_6, $H_2C_2O_4$, $(NH_4)_2MoO_4$ and NH_4SCN. Organic precipitating agents: oxine, cupron, cupferron, 1-nitroso-l-naphthol, BPHA, dithiocarbamates, sodium tetra phenyl boron, nioxime and nitron.

2.2 Acid base titrations in non-aqueous media. Different solvents and their selection for a titration. Indicators for non-aqueous titrations. Applications. Precipitation reactions-titration curves, determination of end points (coloured precipitates, colored soluble compounds), adsorption indicators, turbidity methods. Typical examples.

2.3 Redox titrations: Variation of potential during redox titrations, formal potential, requirements of redox titrations, detection of end point, typical titrants, $KMnO_4$, $K_2Cr_2O_7$, Ce (IV).

2.4 Complexometric titrations: masking and demasking agents, selective demasking, metal ion indicators, theory of visual use of metal indicators, typical examples of titrants - murexide, eriochrome black T.

Module 3: Sampling **(18 Hrs)**

3.1 The basics and procedure of sampling, sampling statistics, sampling and the physical state, crushing and grinding, the gross sampling, size of the gross sample, sampling liquids, gas and solids (metals and alloys), preparation of a laboratory sample, moisture in samples-essential and non-essential water, absorbed and occluded water, determination of water (direct and indirect methods).

3.2 Decomposition and dissolution, source of error, reagents for decomposition and dissolution, microwave decompositions, combustion methods, uses of fluxes. Elimination of interference from samples-separation by precipitation, electrolytic precipitation, extraction and ion exchange. Distribution ratio and completeness of multiple extractions.

Module 4: Applied Analysis **(18 Hrs)**

4.1 Analytical procedures involved in environmental monitoring. Water quality-Drinking water standards, BOD, COD, DO, nitrite, nitrate, iron, fluoride. Analysis of metal and radioactive pollutants in effluents.

4.2 Soil- moisture, salinity, colloids, cation and anion exchange capacity. Measurement of soil solution pH, Chemical and biochemical processes that influence soil solution pH.

4.3 Air pollution monitoring sampling, collection of air pollutants-SO_2, NO_2, NH_3, O_3 analysis of NO_2, SO_2, H_2S, O_3, CO, CO_2, NH_3, PM10 and PM 2.5. Air pollution monitoring instruments and monitoring programs

4.4 Analysis of metals, alloys and minerals. Analysis of brass and steel. Analysis of limestone. Corrosion analysis - weight loss and impedance methods.

4.5 Food and drug analysis: Food adulteration – common adulterants in food, coding of food colours. Pesticide analysis in food products. Analysis of alcoholic beverages. Analysis of drugs and pharmaceuticals: Quality control. Official methods. Classical and modern methods of drug analysis.

Module 5: Nano Materials **(18 Hrs)**

5.1. General introduction to nano materials and emergence of nano technology. Moore's law. Graphene (elementary ideas only), synthesis properties and applications of fullerenes and carbon nano tubes, synthesis of nano particles of gold, silver, rhodium, palladium and platinum techniques of synthesis electroplating and electrophoretic deposition conversion through chemical reactions and lithography. Thin films, chemical vapour deposition and atomic layer deposition techniques. Applications of nanoparticles.

5.2. Diversity in nanosystems: self-assembled monolayers on gold-growth process and phase transitions. Gas phase clusters- formation, detection and analysis. Quantum dots- preparation, characterization and applications. Nanoshells- types of systems, characterization and application.

5.3. Evolving interfaces of nanotechnology- nanobiology, nanosensors, nanomedicines.

References

[1] J.M. Mermet, M. Otto, R. Kellner, Analytical chemistry, Wiley-VCH, 2004.

[2] D.A. Skoog, D.M. West, F.J. Holler, S.R. Crouch, Fundamentals of Analytical Chemistry, 8^{th} Edn., Saunders College Pub., 2007.

[3] Holme and H. Perk, 'Analytical Biochemistry', Longman Scientific and Technical, England, 3^{rd} Edn.

[4] British Pharmacopoeia, Her Majesty's Stationery Office, 1998.

[5] Official methods of analysis of the AOAC, Vol 17, 1994

[6] J.H. Kennedy, Analytical Chemistry: Principles, Saunders College Pub., 1990.

[7] J.G. Dick, Analytical Chemistry, R.E. Krieger Pub., 1978.

[8] G.H. Jeffery, J. Bassett, J. Mendham, R.C. Denney, Vogel's Text Book of Quantitative Chemical Analysis , 5^{th} Edn., John Wiley& sons,1989.

[9] S.E. Manahan, Environmental chemistry, 9^{th} Edn., CRC Press, 2010.

[10] C.L. Wilson, D.W. Wilson, Comprehensive Analytical Chemistry, Elsevier, 1982.

[11] G.D. Christian, J.E. O'Reilly, Instrumental Analysis, Allyn & Bacon, 1986.

[12] R.A. Day, A.L. Underwood, Quantitative Analysis, 6^{th} Edn., Prentice Hall, 1991.

[13] A.I. Vogel, A Textbook of Practical Organic Chemistry, Longman, 1974.

[14] D.C. Harris, Quantitative Chemical Analysis, 7^{th} Edn., W.H. Freeman & Co., 2011.

[15] T. Pradeep, Nano: the Essentials, Tata McGraw Hill, 2007.

[16] K.W. Kolasinski, Surface Science: Foundations of Catalysis and Nanoscience, 2^{nd} Edn., Wiley, 2009.

[17] F.W. Fifield, D. Kealey, Principles and Practice of Analytical Chemistry, Blackwell Science, 2000.

[18] W. Horwitz (Editor), Official Method of Analysis of AOAC International, 18^{th} Edn., AOAC, 2010

[19] British Pharmacopeia, TSO, 2012.

[20] B. K. Sharma. Environmental Chemistry, Goel Pub. Meerut.

[21] A. K. De Environmental Science Wily and Eastern Hd, N. Delhi.

PG4ANL E02 INSTRUMENTAL METHODS OF ANALYSIS

Credit: 4 **Contact Lecture Hours: 90**

Module 1: Introduction to Instrumental Methods (18 Hrs)

1.1 Electrical and nonelectrical data domains-transducers and sensors, detectors, examples for piezoelectric, pyroelectric, photoelectric, pneumatic and thermal transducers. Criteria for selecting instrumental methods - precision, sensitivity, selectivity, and detection limits.

1.2 Signals and noise: sources of noise, S/N ratio, methods of enhancing S/N ratio–hardware and software methods.

1.3 Electronics: transistors, FET, MOSFET, ICs, OPAMs. Application of OPAM in amplification and measurement of transducer signals.

Module 2: Molecular Spectral Measurements (18 Hrs)

2.1 UV-Vis spectroscopic instrumentation: types of optical instruments, components of optical instruments- sources, monochromators, detectors. Sample preparations. Instrumental noises. Applications in qualitative and quantitative analysis.

2.2 Molecular fluorescence and fluorometers: photoluminescence and concentration electron transition in photoluminescence, factors affecting fluorescence, instrumentation details. Fluorometric standards and reagents. Applications in qualitative and quantitative analysis,

2.3 IR spectrometry: instrumentation designs-various types of sources, monochromators, sample cell considerations, different methods of sample preparations, detectors of IR-NDIR instruments. FTIR instruments. Mid IR absorption spectrometry. Determination of path length. Application in qualitative and quantitative analysis.

2.4 Raman Spectrometric Instrumentation: sources, sample illumination systems. Application of Raman spectroscopy in inorganic, organic, biological and quantitative analysis.

2.5 NMR spectrometry-magnets, shim coils, sample spinning; sample probes (^{1}H, ^{13}C, ^{31}P). Principle of MRI.

Module 3: Atomic Spectral Measurements (18 Hrs)

Atomic emission and atomic absorption phenomena: comparison of relative merits and drawbacks. Instrumentation details of AAS. Atomisation methods -flame, electrothermal and plasma techniques, glow discharge and laser ablation, sources: HCL, EDL-TGL, wavelength choice detectors, use in qualitative and quantitative analysis, interferences in measurements-chemical, spectral, and instrumental background correction techniques. Atomic emission spectroscopy flame, arc, spark, plasma emissions (ICP and DCP), details of wave selection detection systems, applications.

Module 4: Atomic X-ray spectrometry (9 Hrs)

Emission of X-ray, absorption process, fluorescence, instrumentation: X-ray tube, radio isotope filters and monochromators, X-ray detectors and transducers, photon counting, gas filled transducers, Geiger tube, counters, signal processors. Application in quantitative and qualitative analysis. Diffraction methods.

Module 5: Mass Spectrometry (9 Hrs)

Ion sources - EI, CI, FI, MALDI, Electrospray and FAB, Instrumental components- mass analyzers, magnetic sector, double focussing, quadrupole, TOF, Ion trap, FT instruments. Applications in identification of pure compounds, molecular formula, compound identification from comparison spectra, analysis of mixturesby hyphenated methods, quantitative applications. Application of MS with GC, HPLC.

Module 6: Surface Study Techniques - Instrumentation and Applications (9 Hrs)

6.1 Spectroscopic methods: ISS, SIMS, ESCA, AES, AAS.

6.2 Microscopic methods: SEM, TEM, STM, AFM.

Module7: Research Methodology of Chemistry (9 Hrs)

7.1 The search of knowledge, purpose of research, scientific methods, role of theory, characteristics of research.

7.2 Types of research: fundamental research, applied research, historical and experimental research.

7.3 Chemical literature: primary, secondary and tertiary sources of literature. Classical and comprehensive reference. Literature databases: Science Direct, Sci Finder. Chemical Abstract.

7.4 Scientific writing: research reports, thesis, journal articles, books. Types of publications: articles, communications, reviews.

7.5 Important scientific and chemistry journals. Impact factor.

References

[1] D.A. Skoog, D.M. West, F.J. Holler, S.R. Crouch, Fundamentals of Analytical Chemistry, 8th Edn., Saunders College Pub., 2007.

[2] H.H. Willard, L.L. Merritt, J.A. Dean, Instrumental Methods of Analysis,5th Edn., Van Nostrand, 1974.47

[3] G.D. Christian, J.E. O'Reilly, Instrumental Analysis, Allyn & Bacon, 1986.

[4] W.W. Wendladt, Thermal Methods of Analysis, Interscience, 1964.

[5] T. Hatakeyama, F.X. Quinn, Thermal Analysis, John Wiley & Sons, 1999.

[6] H.F. Ebel, C. Bliefert and W.E. Russey, the Art of Scientific Writing, Wiley-VCH, 2004.

[7] F.A. Settle, Handbook of Instrumental Techniques for Analytical Chemistry, Prentice Hall PTR, 1997.

[8] R. Wiesendanger, Scanning Probe Microscopy and Spectroscopy, Cambridge University Press, 1994.

[9] R.L. Dominoswki, Research Methods, Prentice Hall, 1981.

[10] W.Best, J.V. Kahn, Research in Education, 10th Edn. Pearson/Allyn&Bacon, 2006.

[11] B.E. Cain, The Basis of Technical Communication, ACS, 1988

PG4ANL E03: MODERN ANALYTICAL TECHNIQUES ANDGREEN CHEMISTRY

Credit: 4 **Contact Lecture Hours: 90**

Module 1: Electrochemistry, Conductance and Potential measurements (18 Hrs)

1.1. Electrochemistry: Conductance measurements, results of conductance measurements, Debye-Huckel theory, Derivation of Debye-Huckel-Onsager equation, validity of DHO equation for aqueous and non aqueous solutions, Debye- Falkenhagen effect, conductance with high potential gradients, activity and activity coefficients in electrolytic solutions, ionic strength, Debye-Huckel limiting law and its various forms, qualitative and quantitative tests of Debye- Huckel limiting equation, deviations from the DHLL.

1.2 Potentiometry: techniques based on potential measurements, direct potentiometric systems, different types of indicator electrodes, limitations of glass electrode, applications in pH measurements, modern modifications, other types of ion selective electrodes, solid, liquid, gas sensing and specific types of electrodes, biomembrane, biological and biocatalytic electrodes as biosensors, importance of selectivity coefficients. CHEMFETS- importance of specially designed amplifier systems for ion selective electrode systems. Potentiometric titrations- types and applications.

Module 2: Electro Analytical Methods (18 Hrs)

2.1 Polarography and voltametric techniques: micro electrode and their specialities, potential and current variations at the micro electrode systems, DME. Polarographic maxima, quantitative polarography, differential pulse square wave polarographic techniques. Applications of polarography. Cyclic voltametry: fundamental studies, study of redox systems using cyclic voltametry.

2.2. Amperometry: Biamperometry, amperometric titrations. Coulometry-primary and secondary coulometry, advantages of coulometric titrations, applications. Principle of chronopotentiometry. Anodic stripping voltammetry- different types of electrodes and improvements of lower detection limits. Voltammetric sensors. Organic polarography.

Module 3: **Capillary Electrophoresis and Capillary Electro Chromatography (9 Hrs)**

3.1 Capillary electrophoresis-migration rates and plate heights, instrumentation, sample introduction, detection methods, applications. Capillary gel electrophoresis. Capillary isotachophoresis. Isoelectric focusing.

3.2 Capillary electro chromatography-packed columns. Micellar electro kinetic chromatography.

Module 4: **Thermal and Radiochemical Methods (9 Hrs)**

4.1 Thermogravimetry (TG), Differential Thermal Analysis (DTA) and Differential Scanning Calorimetry (DSC) and their instrumentation. Thermometric Titrations. Thermo Mechanical Analysis (TMA) and Dialatometric Analysis (DA)

4.2 Measurement of alpha, beta, and gamma radiations, neutron activation analysis and its applications. Principle and applications of isotope dilution methods, radiometric titrations.

Module 5: Chromatography (18 Hrs)

5.1 Liquid Chromatography: column efficiency, band broadening and the factors affecting it, particle size. HPLC- its instrumentation pumps, sample injection, columns, solvent selection and detectors. Partition chromatography- bonded phase.

5.2 GSC and GLC Instrumentation-preparation of column and column materials, temperature, effects, different types of detectors, capillary columns-bonded and cross linked phases, chiral stationary phases, selectivity factors, applications.

5.3 Size Exclusion Chromatography- columns and limits of permeation and exclusion, applications.

5.4 Supercritical fluid chromatography: properties of supercritical fluids, operating variables in instrumentation, stationary and mobile phases, comparison with the techniques, applications, supercritical fluid extraction, advantages, applications.

Module 6: Chemical safety and Green chemistry (18 Hrs)

6.1 Hazards of handling ordinary, corrosive and poisonous chemicals. Fire hazards. Handling carcinogens. Toxicology and residual analysis of Cd, Pb, Hg, As, Se and Pu (Atomic Absorption

Spectroscopy). Toxicology of benzene, halogenated hydrocarbons, aromatic amino compounds, benzopyrene and related compounds. Treatment of hazardous waste and their disposal.

6.3 Radiochemical wastes-technique of safe disposal of radiochemical wastes.

6.4 Good Laboratory Practices.

6.5 Principles of green chemistry, atom economy, principles of green organic synthesis, green alternatives of organic synthesis-coenzyme catalysed reactions, green alternatives of molecular rearrangements, electrophilic aromatic substitution reactions, oxidation-reduction reactions, clay catalysed synthesis, condensation reactions. Green photochemical reactions.

6.6 Green Solvents: ionic liquids, supercritical CO_2, fluorous chemistry.

6.7 General principles of microwave assisted organic synthesis.

References

[1] J.M. Mermet, M. Otto, R. Kellner, Analytical Chemistry, Wiley-VCH, 2004.

[2] D.A. Skoog, D.M. West, F.J. Holler, S.R. Crouch, Fundamentals of Analytical Chemistry, 8^{th} Edn., Saunders College Pub., 2007.

[3] J.G. Dick, Analytical Chemistry, R.E. Krieger Pub., 1978.

[4] J.H. Kennedy, Analytical Chemistry: Principles, Saunders College Pub., 1990.

[5] G.H. Jeffery, J. Bassett, J. Mendham, R.C. Denney, Vogel's Text Book of Quantitative Chemical Analysis , 5^{th} Edn., John Wiley& sons,1989.

[6] S.E. Manahan, Environmental Chemistry, 9^{th} Edn., CRC Press, 2010.

[7] C.L. Wilson, D.W. Wilson, Comprehensive Analytical Chemistry, Elsevier, 1982.

[8] G.D. Christian, J.E. O'Reilly, Instrumental Analysis, Allyn & Bacon, 1986.

[9] R.A. Day, A.L. Underwood, Quantitative Analysis, Prentice Hall, 1967.

[10] A.I. Vogel, A Textbook of Practical Organic Chemistry, Longman, 1974.

[11] H.A. Laitinen, W.E. Harris, Chemical Analysis, McGraw Hill, 1975.

[12] V.K. Ahluwalia, Green Chemistry: Environmentally Benign Reactions, CRC, 2008.

[13] F.W. Fifield, D. Kealey, Principles and Practice of Analytical Chemistry, Blackwell Science, 2000.

[14] W. Horwitz (Editor), Official Method of Analysis of AOAC International, 18^{th} Edn., AOAC, 2010

[15] British Pharmacopeia, TSO, 2012.

[16] V.K. Ahluwalia, Green Chemistry, Ane Books, 2009

[17] T. Pradeep, Nano: the Essentials, Tata McGraw Hill, 2007.

PG4ANL E04 - POLYMER CHEMISTRY

Credit: 4 **Contact Lecture Hours: 90**

Module 1: Introduction to Polymer Science (9 Hrs)

1.1 History of macromolecular science: monomers, functionality, degree of polymerization, classification of polymers based on origin, structure, backbone, branching, action of heat, ultimate form and use, tacticity and crystalline behaviour.

1.2 Primary bonds-molecular forces in polymers: dipole forces, induction forces, dispersion forces and H bond, dependence of physical properties on intermolecular forces. Polymer molecular weight-different averages, polydispersity index, molecular weight distribution curve, polymer fractionation. Methods for molecular weight determination: end group analysis, colligative property measurements, ultracentrifugation, vapour phase osmometry, viscometry, GPC, light scattering method. Monomers and structure of common polymers like PE, PP, PVC, PVAc, PVA, PMMA, PEMA, poly lactic acid, PET, PBT, PS, PTFE, PEI, nylon 6, nylon 66, nylon 612, Kevlar, PEEK, PES, PC, ABS, PAN, PEO, PPO, PEG, SAN, PCL, PLA, PHB, DGEBA, MF, UF, AF, PF, PU, NR, SBR, NBR, PB, butyl rubber, polychloroprene and thiokol rubber.

Module 2: Fundamentals of Polymerization (18 Hrs)

2.1 Addition polymerization, free radical addition polymerization, mechanism and kinetics of vinyl polymerization, kinetics of free radical addition polymerization, effect of temperature, pressure, enthalpies, entropies, free energies and activation energies on polymerization.

2.2 Ionic polymerization, common features of two types of ionic polymerization, mechanism and kinetics of cationic polymerization, expressions for overall rate of polymerization and the number average degree of polymerization, mechanism and kinetics of anionic polymerization, expressions for overall rate of polymerization and the average degree of polymerization, living polymers.

2.3 Mechanism of coordination polymerization, Ziegler-Natta polymerization, ring opening polymerization, mechanism of polymerization of cyclic amides.

2.4 Copolymerization, types of copolymers, the copolymer composition equation, reactivity ratio and copolymer structure-influence of structural effects on monomer reactivity ratios, the Q-e scheme, synthesis of alternating, block and graft copolymers.

2.5 Step reaction (condensation) polymerization, Carothers equation, mechanism of step reaction polymerization, kinetics of step reaction polymerization, number distribution and weight distribution functions, polyfunctional step reaction polymerization, prediction of gel point.

2.6 Controlled polymerization methods, nitroxide mediated polymerization, Ring Opening polymerization (ROP), Atom Transfer Radical Polymerization (ATRP), Reversible Addition Fragmentation Termination (RAFT).

Module 3: Properties of Polymers (18 Hrs)

3.1 Structure property relationship in polymers, transitions in polymers, first order and second order transitions in polymers, relationship between Tg and Tm, molecular motion and transitions, Boyer-Beamem rule, factors affecting glass transition temperature.

3.2 Rheological properties of polymers, Newtonian fluids, non-Newtonian fluids, pseudoplastic, thixotropy, St. Venant body, dialatant, complex rheological fluids, rheopectic fluids, time dependent fluids, time independent fluids, power law, Weissenberg effect, laminar flow, turbulent flow, die swell, shark skin, viscous flow.

3.3 Viscoelastic properties of polymers, viscoelasticity, Hooke's law, Newton's equation, viscoelastic models-time temperature equivalence, WLF equation, Boltzmann superposition principle, linear stress - strain relations for other types of deformation-creep, stress relaxation. Temperature dependence of viscosity. Transport in polymers - diffusion, liquid and gas transport, Fick's law, theories of diffusion.

Module 4: Stereochemistry and Conformation of Polymers (9 Hrs)

4.1 Stereoregular polymers, constitutional isomerism, positional isomerism and branching, optical isomerism, geometric isomerism, substitutional isomerism, configuration of polymer chains, infrared, Raman and NMR characterization, polymer conformation, chain end to end distance, random walks and random flights, self-avoiding walks.

Module 5: Morphology and Order in Crystalline Polymers (9 Hrs)

5.1 Polymer morphology, common polymer morphologies, structural requirements for crystallinity, degree of crystallinity, crystallisability- mechanism of crystallization, polymer single crystals, lamellar structure of polymers, fringed micelle concept, folded chain model, adjacent re-entry model, switchboard model.

5.2 Structure of polymers crystallised from melt, spherulitic morphology, mechanism of spherulite formation, theories of crystallisation kinetics, Avrami equation, Hoffman's nucleation theory, the entropic barrier theory, strain induced morphology, cold drawing, morphology changes during orientation, application of XRD, SEM and DSC in determining the crystallinity of polymers.

Module 6: Advances in Polymers (9 Hrs)

6.1 Specialty polymers, conducting polymers, high temperature polymers, flame resistant polymers, biopolymers and biomaterials, polymers in medicine, polymers for dental applications.

6.2 Carbon fibres. Synthesis, characterization and applications of carbon nanofibres.

Module 7: Dendrimers and Dendritic Polymers (18 Hrs)

7.1 Basic concepts and terminology: Dendrons, star shaped and starbust polymers, dendrimer formation and generations, various types of dendrimers.

7.2 Synthesis of dendrimers-convergent and divergent approaches, methods and mechanism. Properties of dendrimers- polydispersity, mechanical properties, viscoelastic properties. Determination of physical properties.

7.3 Characterisation of dendrimers: GPC, osmosis, TG, DSC, magnetic resonance spectroscopy (proton and carbon-13 NMR), mass spectral studies(MALDI and TOF).

7.4 Dendritic macromolecules: hypergrafted and hyperbranched polymers - definition and classification, synthesis-methods and mechanism, characterization, properties, applications

References

1. V.R. Gowariker, N.V. Viswanathan, J. Sreedhar, Polymer Science, New Age International, 2003.

2. F.W. Billmeyer Jr., Textbook of Polymer Science, 3rd Edn., Wiley-India, 2007.

3. L. H. Sperling, Introduction to Physical Polymer Science, 4thEdn, John Wiley & Sons, 2006.

4. J.M.G. Cowie, V. Arrighi, Polymers: Chemistry and Physics of Modern Materials, 3rd Edn., CRC Press, 2008.

5. D.I. Bower, An Introduction to Polymer Physics, Cambridge University Press, 2002.

6. M. Chanda, Introduction to Polymer Science and Chemistry: A Problem Solving approach, CRC/Taylor & Francis, 2006.

7. P.J. Flory, Principles of Polymer Chemistry, Cornell University Press, 1983.

8. J.R. Fried, Polymer Science and Technology, 2nd Edn., Prentice Hall, 2003.

9. G. Odian, Principles of Polymerization, 4th Edn., John Wiley & Sons, 2007

10. K.J. Saunders, Organic Polymer Chemistry, Chapmann & Hall, 1973.

11. K. Matyjaszewski, T.P. Davis, Handbook of Radical Polymerization, John Wiley & Sons, 2003.

12. H.R. Allock, F. W. Lampe, Contemporary Polymer Chemistry, Pearson/Prentice Hall, 2003.

PG4ANL E05 APPLIED ANALYSIS AND AQUATIC RESOURCES

Credit: 4 **Contact Lecture Hours: 90**

Module 1: Environmental Analysis (18 Hrs)

1.1 Water Analysis: sampling and preservation of water. Determination of pH, EC,TDS, DO, CO_2, alkalinity (carbonate, bicarbonate, hydroxide and total), salinity, chloride, fluoride, sulphate, H_2S, calcium, magnesium, sodium, potassium, iron (total ferrous and ferric), ammonia, nitrite, nitrate, phosphorous (total inorganic and organic), BOD, COD, phenols, surfactants, pesticides, E-Coli and total bacteria. Quality of water, standards of raw and treated water, objectives of waste water treatment. A brief idea of sedimentation, coagulation and flocculation, filtration, disinfection of water. Activated sludge process, trickling filters, sludge treatment and disposal. Softening of water, corrosion and its control. Removal of toxic compounds, refractory organics, and dissolved inorganic substances. Reverse osmosis.

1.2 Air Analysis: atmospheric pollution, classification of air pollutants, sources of air pollution and methods of control, sampling of aerosols, sampling of gaseous pollutants, analysis of SO_x, NO_x, CO-CO_2, hydrocarbons, particulates, effects of air pollutants on animals, ozone layer, chlorofluorocarbons, acid rain, greenhouse effect.

1.3 Soil/Sediment analysis: a brief idea of chemistry of soil. Trace element analysis in soil - B, Cd, Cu, Fe, Mn, Mo, Zn, Pb. Pesticides and pollution, classification and degradation of pesticides, methods of pesticides analysis. Sampling of soil, aquatic sediments, pH, electrical conductivity, redox potential, alkalinity, inorganic and organic contents.

1.4 Waste Management: waste management approaches - waste reduction, recycling, disposal. Management of hazardous wastes, household waste, municipal and industrial wastes-collection, transportation and disposal options.

Module 2: Biochemical and Clinical Analysis (9 Hrs)

2.1 Cell fractionation techniques-cell lysine: differential and density gradient centrifugation, salting in, salting out, dialysis, ultracentrifugation, electrophoretic techniques-polyacrilamide gel electrophoresis, SDS-PAGE, agrose gel electrophoresis.

2.2 Liver function tests, gastric function tests, kidney function tests and glucose tolerance tests. Screening of metabolic diseases.

Module 3: Forensic Analysis (18 Hrs)

3.1 Forensics-basic principles and significance, history and development. Crime-definition, crime scene, protection and recording of crime scene, physical clues, processing of crime scene.

3.2 Finger prints: classification, conventional methods of development of finger prints-fluorescent and chemical methods. Application of laser and other radiations to development of latent finger print. Foot prints, tyre marks, bite marks and lip prints.

3.3 Questioned Document Examination (QDE): forged documents and currency notes. UV counterfeit note detector.

3.4 Forensic Ballistics-fire arms, classification and characteristics, analysis of gunshot residues, mechanism of GSR, instrumental methods of GSR analysis.

3.5 Explosives: introduction, types, preliminary screening at crime scene, presumptive test (colour and spot test), micro chemical methods of analysis.

3.6 Fire Extinguishers and its chemistry, analysis of Arson exhibits by instrumental methods, management of flammable and combustible materials.

3.7 Counterfeit coins- AAS analysis, purity of Gold-analysis by XRF / EDXRF.

3.8 Forensic Toxicology: classification of poisons, estimation of poisons and drugs with chromatographic, neutron activation analysis and spectrophotometric methods.

Module 4: Food Chemistry and Food Analysis (36 Hrs)

4.1 Food chemistry: definition and importance. Water in food, water activity and shelf life of food. Carbohydrates-chemical reactions, functional properties of sugars and polysaccharides in foods. Lipids: classification and use of lipids in foods, physical and chemical properties, effects of processing on functional properties and nutritive value. Protein and amino acids-physical and chemical properties, distribution, amount and functions of proteins in foods, functional properties, effect of processing-loss of vitamins and minerals due to processing. Pigments in food, food flavours, browning reaction in foods. Enzymes in foods and food industry, bio-deterioration of foods, food contaminants, additives and toxicants.

4.2 Principles of food processing: scope and importance of food processing. Principles and methods of food preservation-freezing, heating, dehydration, canning, addition of additives, fermentation, irradiation, extrusion cooking, hydrostatic pressure cooking, dielectric heating, microwave processing, aseptic processing, hurdle technology, membrane technology. Storage of food-modified atmosphere packaging, refrigeration, freezing and drying of food, minimal processing, radiation processing.

4.3 Food microbiology: history of microbiology of food, microbial growth pattern, physical and chemical factors influencing destruction of micro-organisms. Types of micro-organisms normally associated with food-mold, yeast and bacteria. Micro-organisms in natural food products and their control. Contaminants of food-stuffs, vegetables, cereals, pulses, oil seeds, milk and meat during handling and processing. Biochemical changes caused by micro-organisms, deterioration of various types of food product. Food poisoning and microbial toxins, microbial food fermentation, standards for different foods. Food borne intoxicants and mycotoxins.

4.4 Advanced techniques of food analysis: role of analysis and various methods of sampling and analysis of results. Principles and application of flame photometry, atomic absorption, X-ray analysis, electrophoresis, mass spectroscopy, NMR, chromatography, refractometry, rheology, measurements, enzymatic methods, DSC, SEM, rapid methods of microbial analysis, immunoassays, ESR.

Module 5: Aquatic Resources (9 Hrs)

5.1 Aquatic resources: renewable and non-renewable resources-estimation, primary productivity, regional variations. Desalination: principles and applications of desalination-distillation, solar evaporation, freezing, electrodialysis, reverse osmosis, ion-exchange and hydrate formation methods. Relative advantages and limitations of the methods. Scale formation and its prevention in distillation process.

5.2 Non-renewable resources: inorganic chemicals from the sea-extraction and recovery of halides, magnesium, potassium, gold.

References

[1] B.B. Nanda, R.K. Tewari, Forensic Science in India: A Vision for the Twenty- first Century, Select Pub., 2001.

[2] A.S. Osborn, Questioned Documents, 2nd Edn., Rawman & Littlefield Pub., 1974.

[3] M.K. Mehta, Identification of Thumb Impression and Cross Examination of Finger Print Experts, N.M. Tripathi Pub., 1963.

[4] M. Johari, Identification of Firearms, Ammunition and Firearm Injuries, BPR&D, 1980.

[5] J.D. DeHaan, Kirk's Fire Investigation, 5th Edn., Prentice Hall, 2002.

[6] M. Prakash, C.K. Arora, Methods in Toxicology, Anmol Pub., 1998.

[7] P. Fellows, Food Processing Technology: Principles and Practice, CRC Press, 2000.

[8] P. Jelen, Introduction to Food Processing, Prentice Hall, 1995.

[9] P.M. Davidson, J.N. Sofos, A.L. Branen, Antimicrobials in Foods, 3rd Edn., CRC Press, 2005.

[10] J.M. Jay, Modern Food Microbiology, Springer, 1995.

[11] G.G. Birch, M. Spencer, A.G. Cameron, Food Science, 3rd Edn., Pergamon Press, 1986.

[12] J. A. Nathanson, Basic Environmental Technology, 5th Edn., Pearson Prentice Hall, 2007.

[13] C.W. Jefford, K.L. Rinehart, L.S. Shield, Pharmaceuticals and the Sea, Technomic Pub., 1988.

[14] E.D. Howe, Fundamentals of Water Desalination, M. Dekker, 1974.

[15] H-G. Heitmann, Saline Water Processing, VCH, 1990.

[16] G. M. Masters, W. Ela, Introduction to Environmental Engineering and Science, 3rd Edn., Prentice Hall,1998.

[17] C.S. Rao, Environmental Pollution Control Engineering, New Age International, 1995.

[18] Metcalf, Eddy, Waste Water Engineering, Tata McGraw Hill, 2003.

[19] H. Wright, A Hand book of Soil Analysis, Logos Press, 1994.

[20] T.G. Spiro, K. Purvis-Roberts, W.M. Stigliani, Chemistry of the Environment, University Science Books, 2011.

[21] N.P. Cheremisinoff, Biotechnology for Waste and Wastewater Treatment, William Andrew, 1996.

SEMESTERS 3 & 4

PG4ANL P04– INORGANIC CHEMISTRY PRACTICAL – 2

Credit: 3 **Contact Lab Hours: 54+54=108**

PART I

Estimation of simple binary mixtures (like Cu-Ni, Cu-Zn, Fe-Cr, Fe-Cu, Fe-Ni, Pb-Ca) of metallic ions in solution by volumetric and gravimetric methods.

PART II

Analysis of one of the alloys of brass, bronze and solder. Analysis of one of the ores from hematite, chromite, dolomite, monazite, illmenite.

References

[1] A.I. Vogel, A Text Book of Quantitative Inorganic Analysis, Longman, 1966.

[2] I.M. Koltoff, E.B. Sandell, Text Book of Quantitative Inorganic Analysis, 3rd Edn., Mc Millian, 1968.

[3] G. Pass, H. Sutcliffe, Practical Inorganic Chemistry, Chapman & Hall, 1974.

[4] N.H. Furman, Standard Methods of Chemical Analysis: Volume 1, Van Nostrand, 1966.

[5] F.J. Welcher, Standard Methods of Chemical Analysis: Vol. 2, R.E. Kreiger Pub., 2006.

PG4ANL P05 ORGANIC CHEMISTRY PRACTICAL - 2

Credit: 3 **Contact Lab Hours: 54+54=108**

PART I

A. Volumetric estimation of 1) Aniline 2) Phenol 3) glucose 4) Iodine value and saponification value of coconut oil

B. Colorimetric estimation of 1) Aniline 2) Glucose 3) Cholesterol 4) ascorbic acid 5) Streptomycin 6) Aspirin.

C. Estimation of the number of acetyl, methoxy, phenolic, amino, nitro, carboxyl, ester, ether and carbonyl groups in organic compounds.

PART II

Preparation of compounds by two stages.

1. Acetanilide- p-nitroacetanilide-- p-nitroaniline
2. Methyl benzoate-- -m-nitromethylbenzoate-- m-nitrobenzoic acid
3. Acetanilide- p-bromoacetanilide-- p-bromoaniline
4. Phenol-salicylaldehyde-coumarin
5. Benzophenone –benzophenone oxime- benzanilide
6. Aniline -2,4,6-tribromoaniline-1,3,5-tribromoaniline

PART III

1. Microwave assisted Organic Synthesis.
2. Preparation Involving by the Green alternatives of Chemical Methods.

PART IV

Prediction of FTIR, UV-Visible, ^{1}H and ^{13}C NMR spectra of the substrates and products at each stage of the products synthesized by the above methods.

PART V – Viva-Voce

References

[1] A.I. Vogel, A Textbook of Practical Organic Chemistry, Longman, 1974.

[2] A.I. Vogel, Elementary Practical Organic Chemistry, Longman, 1958.

[3] F.G. Mann and B.C Saunders, Practical Organic Chemistry, 4^{th} Edn., Pearson Education India, 2009.

[4] J.R. Adams, J.R. Johnson, J.F. Wilcox, Laboratory Experiments in Organic Chemistry, Macmillan, 1979.

[5] V.K. Ahluwalia, Green Chemistry: Environmentally Benign Reactions, Ane Books, 2009.

[6] Monograph on Green Chemistry Laboratory Experiments, Green Chemistry Task Force Committee, DST, 2009.

[7] R.M Silverstein, Spectrometric identification of Organic compounds

[8] F. G. Mann and B.C. Saunders, Practical Organic Chemistry, Pearson

[9] J. B. Cohen, Practical Organic Chemistry, Mc Graw Hill

[10] C.E Bella and DF Taber, Organic Chemistry Laboratory, Thomson

[11] P.F Shalz, J. Chem. Education, 1996, 173,267

[12] P.D.L Lampman and Chriz, Introduction to Organic Laboratory Techniques, College publishing,

[13] http://sdbs.riodb.aist.go.jp/sdbs/cgi-bin/direct_frame_top.cgi

PG4ANL P06 INSTRUMENTAL ANALYSIS PRACTICAL

Credit: 3 **Contact Lab Hours: 54+54=108**

Section A

I. Nephelometry

a. Determination of sulphate.

b. Determination of halides.

II. UV – Visible Spectrophotometry

1. Determination of absorption curve and concentration of a substance (Potassium nitrate)
2. Simultaneous determination of Ti^{3+} and V^{5+} spectrophotometrically by H_2O_2 method.
3. Spectrophotometric determination of the pK value of an indicator (the acid dissociation constant of methyl red)
4. Determination of phenols in water

III. Polarimetry

1. Kinetics of the inversion of sucrose in presence of HCl.
2. Determination of the concentration of a sugar solution
3. Determination of the concentration of HCl.
4. Determination of the relative strength of acids.

IV. Refractometry

1. Identification of pure organic liquids and oils.
2. Determination of molar refractions of pure liquids.
3. Determination of concentration of solutions (KCl-water, glycerol-water)
4. Determination of molar refraction of solids.
5. Study of complex formation between potassium iodide and mercuric iodide system.

Section B

V. Polarography and related experiments.

1. Determination of half wave potential.
2. Determination of Cd by (a) standard series (b) Standard addition (c) pilot ion method.
3. Determination of organic compounds.

VI. Conductivity measurements

1. Verification of Onsager equation.
2. Determination of the degree of ionization of weak electrolytes.
3. Determination of pKa values of organic acids.
4. Determination of solubility of sparingly soluble salts.
5. Titration of a mixture of acids against a strong base.
6. Titration of a dibasic acid against a strong base.

VII. Potentiometry

1. Determination of single electrode potentials (Cu and Zn)
2. Application of Henderson equation.
3. Potentiometric titrations, pH metric titrations.
4. Determination of the concentration of a mixture of Cl^- and I^- ions.

VIII. Electrogravimetric estimation of Cu, Ni, and Pb

IX. Flame Photometry

Determination of Na^+, Li^+, K^+ and Ca^{2+}.

The examination will be for 6 hours with one experiment each from section A and section B and will have equal weight.

References

[1] J.B. Yadav, Advanced Practical Physical Chemistry, Goel Publishing House, 2001.

[2] B. Viswanathan, Practical Physical Chemistry, Viva Pub., 2005.

[3] G.W. Garland, J.W. Nibler, D.P. Shoemaker, Experiments in Physical Chemistry, 8th Edn., McGraw Hill, 2009.

[4] A. Findlay, Practical Physical chemistry, Longman.

[5] F. Daniels et al Experimental Physical chemistry, McGraw Hill.

[6] Shoemaker, Garlands, Experiments in Physical chemistry, McGraw Hill.