DEPARTMENT OF CHEMISTRY

SYLLABUS FOR TWO YEAR POSTGRADUATE PROGRAMME
(FIRST AND SECOND SEMESTER)

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Content

PREFACE

"Education is not preparation for life; education is life itself."—John Dewey

The aim of imparting education is not only to increase the knowledge but also to create the possibilities for a student to invent and discover. The purpose of this syllabus is to establish minimum basic concepts for each course to meet the needs of all our students. All the elements in this syllabus amalgamate to bring out the best in every student and enable them to be on the path of continuous progress.

The syllabus is framed based on Learning Outcome Based Education (LOCF) –the spirit of NEP, 2020. The Post Graduate programmes offered by the college, presently, are :

Sl. No.	Discipline / Subject
1	Assamese
2	Chemistry
3	Economics
4	Education
5	Mathematics
6	Political Science
7	Zoology

Programme Overview & Eligibility

Category	Details
About the Programme	Provides advanced academic training in the concerned subject.
Who Can Apply	• Students successfully completing 3 years in the Four Year Undergraduate Programme (FYUGP) and satisfying minimum credit requirements. • Students successfully completing a 3-year Bachelor's degree and satisfying minimum credit requirements.

Course & Credit Structure

Parameter	Specification
Total Credits per Semester	20
Number of Courses per Semester	5
Credits Assigned per Course	4
Course Component Structures	L-T-0 (Lecture - Tutorial - Nil) L-0-P (Lecture - Nil - Practical) 0-0-P (Nil - Nil - Practical)

Course Level:

Year	Course Level
PG 1st Year	4 (400- 499)
PG 2nd Year	5 (500- 599)

Course Coding System

The format followed for all PG courses is XXX-ABCD. Here is how the code breaks down:

Code Position	Represents	Description
XXX	Subject Code	3-letter discipline identifier (e.g., CHE, MAT)
A	Semester Number	Identifies the current semester
B	Course Level	Identifies the academic level of the course
C	Course/Paper Number	Sequential number of the paper
D	Course Credit	Number of credits assigned to the paper

Example:

For a PG course in Chemistry offered in the First Semester and Third Semester, the course codes will be assigned as follows:

Course Paper	Semester	Course Code
Paper I	First	CHE-1414
Paper II	First	CHE-1424
Paper I	Third	CHE-3514
Paper II	Third	CHE-3524

LIST OF COURSES: POST GRADUATE PROGRAMME IN CHEMISTRY

Semester	Course Name	Course Code
1	**Research Methodology**	**CHE-1414**
	Organic Chemistry-IV	**CHE-1424**
	Inorganic Chemistry-IV	**CHE-1434**
	Physical Chemistry-IV	**CHE-1444**
	Quantum Chemistry	**CHE-1454**
2	**Organic Chemistry-V**	**CHE-2514**
	Inorganic Chemistry-V	**CHE-2524**
	Physical Chemistry-V	**CHE-2534**
	Spectroscopy	**CHE-2544**
	Green Chemistry	**CHE-2554**

PROGRAMME OUTCOMES

SPO-1 Knowledge: Learners are encouraged to apply the knowledge of mathematics and science fundamentals to various solutions of complex problems. As such, knowledge of the subject is the sole objective of any student learner. A student is exposed to a wide range of topics in various subjects and is given intensive training in each of the courses that have laboratory related work. The learner is encouraged to use various mathematical

acquired concepts and principles that help in studying various branches of sciences. At the end of the program, students are able to gain thorough knowledge in key areas in the subjects offered.

SPO-2 Problem Analyses: Well equipped with an understanding of the analytical methods involved, they are in a position to interpret and analyze results so obtained from experiments and draw suitable conclusions against their supported data acquired. At the end of the program, students will be able to identify, formulate and analyze scientific problems and reach concrete solutions using various principles of mathematics and sciences.

SPO-3 Designing Solutions: Having acquired knowledge of subjects, students are trained to think out of the box, design and conduct an experiment or a series of experiments that demonstrate their understanding of the methods and processes involved.

SPO-4 Modern tool usage: learners are trained to create, select, and apply appropriate techniques, resources and IT tools in the analysis and synthesis of data within limitations. (Outcome of final year project).

SPO-5 Effective Communication: Proficiency in speaking, reading, writing and listening in English and one Indian language and find meaning of the world by connecting people, ideas, books, media and technology.

SPO-6 Employability: This programme enables the learners to perform the jobs in diverse fields such as science, engineering, industries, survey, education, banking, development-planning, business, public service, self business etc. efficiently. They will also be able to appear for competitive examinations.

SPO-7 Ethics: While it is necessary to instil the spirit of competitiveness among students in a world of increasing competition, it is equally vital to develop a strong sense of ethics among learners that will help them develop some positive attitudes and values. This includes appreciation of the various principles and theories that evolved in science, the impact that science has on social, economical and environmental issues. One of the main objectives of any academic exercise, therefore, should be to

produce well-groomed individuals who understand the significance of ethical values and abide by them even in the most pressing circumstances. In this programme, this process is enabled through courses and facilitators who integrate the teaching of ethics in everyday pedagogy. As exercise, ethics in their professional as well as personal practices.

SPO-8 Environment and Sustainability: 'Environmental sustainability' has become the watchword of the 21st century. An increased engagement with environment related concerns is appearing tangibly on global fronts; academics cannot and should not remain quarantined from this massive development. Through classroom discussions and research projects, this programme facilitates active dialogues with factors which influence human-ecology interactions. As such, at the end of this programme students will be able to identify and analyze socio-political, cultural and economic problems which act as deterrents to environmental sustainability and provide creative solutions towards the same.

SPO-9 Soft-Skill Development: Apart from the attainment of knowledge and hands on skills in practical applicability of the subject, learners need to be equipped with soft-skills and values which will help them function effectively as an individual, and as a member or leader in diverse teams and in multidisciplinary groups. These soft skills include leadership, teamwork, project-management, positive outlook, innovative approaches and effective articulation. Several soft skill programs are organized for learners through various agencies that tie up with the state government. As such, at the end of this programme, students will be able to hone the soft-skills required in positively enhancing their academic, professional and personal pursuits towards self and societal advancement.

SPO-10 Science and Society: The learners are encouraged to apply logical reasoning based on the knowledge, skills, designing solutions to assess societal, health, safety issues and the responsibilities that go along with the scientific practice. As an extension activity to society, learners are encouraged to take up specific projects such as impact of salinity on fresh water wells in an adopted village, and provide effective solutions.

SPO-11 Life-long learning: With the pursuit of knowledge for either personal or professional reasons, learners are also encouraged to volunteer and be self motivated that not only enhances society values, active participation and personality development, but also enhances self-sustainability, competiveness and employability. As such, learners will be able to recognize the need for, and have the preparation and ability to engage in independent and life-long learning in every broad context of technological changes.

Programme Specific Outcomes

PSO No. & Name		Outcome
PSO-1	Basic Understanding	The learner will able to gain basic ideas about different branches of chemistry *viz.* organic, inorganic, physical, analytical and quantum chemistry.
PSO-2	Critical Thinking	The learner will be to analyze, interpret, evaluate and make judgement about the various concepts encountered in Chemistry.
PSO-3	Skill Enhancement	The learner will develop practical skills to work/ or to develop start-ups in different industrial fields like chemical, pharmaceutical, polymer, glass blowing, agro industry and others related to chemical sciences.
PSO-4	Communication Skill	The learner will gain communication skill to present their knowledge/expertise/skill in Chemistry in the form of project work, seminar presentation, poster presentation, wall magazine and other modes.
PSO-5	Digital Efficiency	The learner will be able to imply digital learning through different software packages like Google forms, docs, excel, Chem draw, ISIS draw, Origin, Gaussian etc. They will also able to search scientific literatures in different digital mediums.
PSO-6	Collective Effort	The learner will learn to complete common tasks or achieve common goals in an effective way through collaborative manner.
PSO-7	Exposure to Research Activities	The learner will get exposures to diverse research fields through project work, interactions with scientists/ researchers/scholars, institutional/industrial visits students outreach programmes, *etc*. which will incubate research aptitude in the students.
PSO-8	Employability Prospects	The learner will be able to gain knowledge and expertise to pursue a career in educational institutions, R&D organizations, *etc*. across the country and abroad.
PSO-9	Competency for Competitive Examinations	The learners will gain the confident to face the competitive exams like CUET, PGUET, JAM, NET, GATE, SLET, GRE, TOEFL, Civil services, etc.
PSO-10	Ethical Analysis	The learner will learn to make legitimate evidence based-decision making in a particular context, especially through the concepts of IPR like Patent, copyright, plagiarism, etc.

Course Learning Outcomes

Semester	Course Title & Course Code	Course Learning Outcome	
Semester 1	Research Methodology CHE-1414	CLO-1	The objectives of this course are to make the students aware of fundamental but mandatory ethical practices in chemistry, to introduce the concept of data analysis, to learn to perform literature survey in different modes, to make the students aware of safety handling and safe storage of chemicals, to make students aware about plagiarism and how to avoid it, and to teach the use of different e-resources.
		CLO-2	Student can have hands on training on various aspect of research including collecting journal articles and writing literature survey, preparing poster presentation, etc.
	Organic Chemistry-IV CHE-1424	CLO-1	The students will be able to critically analyze organic reaction mechanisms through a detailed understanding of kinetic and thermodynamic principles, including reaction profiles, isotope effects, and linear free energy relationships. They will gain in-depth knowledge of reactive intermediates. Additionally, students will develop a solid foundation in stereochemical principles.
		CLO-2	The students will be able to systematically analyze and identify components in a binary organic mixture using classical separation and identification techniques. They will also acquire practical experience in the extraction of natural products, specifically carotenoids, from plant sources.

	Inorganic Chemistry-IV CHE-1434	CLO-1	The students will be able to apply advanced concepts of inorganic, organometallic, and solid-state chemistry to explain the structure, bonding, synthesis, and reactivity of main group and transition metal compounds.
		CLO-2	The students will be able to interpret molecular structures and chemical behavior using principles of symmetry, group theory, and spectroscopic characterization.
	Physical Chemistry-IV CHE-1444	CLO-1	The objective of this course is to aware students on the detail of equillibrium, non-equillibrium and statistical thermodynamics. Also, to familiarize students with significance of polymer chemistry and data analysis. Moreover, the present course also enables students towards chemistry of natural products and basics of quantum chemistry.
		CLO-2	Student can perform hands-on training of various data analysis using MS Excel/origin. Student can also learn practically to determine the molecular weight of a polymer and various aspects of thermodynamics and phase equilibria.
	Quantum Chemistry CHE-1454	CLO-1	Upon completion of this course, students will be able to understand fundamental quantum concepts, operator theory, and the Schrödinger equation to describe atomic and molecular systems.
		CLO-2	The students will be able to apply quantum mechanical models and approximation methods (perturbation theory, Born-Oppenheimer approximation, MO theory) to solve atomic and molecular problems.

Semester 2	Organic Chemistry-V CHE-2514	CLO-1	The students will be able to analyze and predict the outcomes of key organic photochemical, oxidation-reduction and pericyclic reactions.
		CLO-2	The students will be able to carry out basic organic syntheses, including multi-step and multicomponent reactions. They will gain hands-on experience in natural product extraction, analysis, and biodiesel preparation. Additionally, students will develop skills in quantitative analysis using titrimetric and spectroscopic methods.
	Inorganic Chemistry-V CHE-2524	CLO-1	Apply group theory to analyze molecular symmetry, vibrations, and spectral transitions, Explain bonding and electronic spectra of transition metal complexes using crystal field and molecular orbital theories
		CLO-2	The students can have practical experience on advanced inorganic quantitative analysis
	Physical Chemistry-V CHE-2534	CLO-1	By studying this course student can able to: Apply steady-state approximation method toward various reaction, understand the kinetics of fast reaction, also understand the theory of molecular dynamics including transition state theory and its applications, Understand the electrochemical application for energy storage and energy conversion.
		CLO-2	Student can able to comprehend with advanced practical aspect of chemical kinetics and application of electrochemistry.
	Spectroscopy CHE-2544	CLO-1	By studying this course student can able to understand the various concepts used in the analysis of organic and inorganic molecules via various spectroscopic and spectrometric

			techniques.
		CLO-2	Student can get hands-on training on using NMR or IR or UV techniques to differentiate between organic molecules.
	Green Chemistry CHE-2554	CLO-1	Apart from introducing learners to the principles of green chemistry, this course will make them conversant with applications of green chemistry to organic synthesis. Students will be prepared for taking up entry level jobs in the chemical industry. They also will have the option of studying further in the area.
		CLO-2	The student will be able to apply the principles of green chemistry in organic synthesis and preparation of value-added chemicals.

Mapping of Programme Outcomes (PO) and Course Learning Outcomes (CLO)

Programme Outcome (PO)												
Course	CLO	SPO-1	SPO-2	SPO-3	SPO-4	SPO-5	SPO-6	SPO-7	SPO-8	SPO-9	SPO-10	SPO-11
CHE-1414	CLO-1	3	3	3	3	3	3	2	2	3	3	3
	CLO-2	3	3	3	3	3	3	2	3	3	3	3
CHE-1424	CLO-1	3	3	3	3	3	3	2	2	3	3	3
	CLO-2	3	3	3	3	3	3	2	3	3	3	3
CHE-1434	CLO-1	3	3	3	3	3	3	3	2	3	3	3
	CLO-2	3	3	3	3	3	3	3	2	3	3	3
CHE-1444	CLO-1	3	3	3	3	3	3	2	2	3	3	3
	CLO-2	3	3	3	3	3	3	2	2	3	3	3
CHE-1454	CLO-1	3	3	3	3	3	3	2	2	3	3	3
	CLO-2	3	3	3	3	3	3	2	2	3	3	3
CHE-2514	CLO-1	3	3	3	1	3	3	3	3	3	3	3
	CLO-2	3	3	3	2	3	3	2	3	3	3	3
CHE-2524	CLO-1	3	3	3	3	3	3	2	3	3	3	3
	CLO-2	3	3	3	3	3	3	3	3	3	3	3
CHE-2534	CLO-1	3	3	3	3	3	3	3	3	3	3	3
	CLO-2	3	3	3	3	3	3	3	3	3	3	3
CHE-2544	CLO-1	3	3	3	3	3	3	2	2	3	3	3
	CLO-2	3	3	3	3	3	3	2	2	3	3	3
CHE-2554	CLO-1	3	3	3	3	3	3	2	2	3	3	3
	CLO-2	3	3	3	3	3	3	2	2	3	3	3

Attributes:

Co-relation Levels

"1" : Minimum Co-relation

"2" : Moderate Co-relation

"3" : Maximum Co-relation

"-" : No Co-relation

Mapping of Programme Specific Outcomes (PSO) and Course Learning Outcomes (CLO)

		Programme Specific Outcome (PSO)									
Course	CLO	PSO-1	PSO-2	PSO-3	PSO-4	PSO-5	PSO-6	PSO-7	PSO-8	PSO-9	PSO-10
CHE-1414	CLO-1	3	3	2	2	3	3	2	3	3	1
	CLO-2	3	3	3	2	3	3	3	3	3	1
CHE-1424	CLO-1	3	3	2	2	3	3	2	3	3	1
	CLO-2	3	3	3	2	3	3	3	3	3	1
CHE-1434	CLO-1	3	3	2	2	1	3	2	2	3	1
	CLO-2	3	3	2	2	1	3	2	2	3	1
CHE-1444	CLO-1	3	3	2	2	3	3	3	3	3	2
	CLO-2	3	3	3	2	3	3	3	3	3	2
CHE-1454	CLO-1	3	3	2	2	3	3	3	3	3	2
	CLO-2	3	3	3	2	3	3	3	3	3	2
CHE-2514	CLO-1	3	3	3	2	3	3	2	3	3	1
	CLO-2	3	3	3	2	3	3	2	3	3	1
CHE-2524	CLO-1	3	3	2	2	3	3	2	3	3	2
	CLO-2	3	3	3	2	3	3	3	3	3	2
CHE-2534	CLO-1	3	3	1	2	3	3	3	2	3	1
	CLO-2	3	3	3	2	3	3	3	3	3	1
CHE-2544	CLO-1	3	3	2	2	3	3	2	3	3	2
	CLO-2	3	3	3	2	3	3	3	3	3	2
CHE-2554	CLO-1	3	3	2	2	3	3	2	3	3	2
	CLO-2	3	3	3	2	3	3	3	3	3	2

Attributes:

Co-relation Levels

"1" : Minimum Co-relation

"2" : Moderate Co-relation

"3" : Maximum Co-relation

"-" : No Co-relation

FIRST SEMESTER

COURSE NAME: RESEARCH METHODOLOGY

Course Code: CHE-1414

Total Credits: 4 (Theory: 3+Practical/Practice: 1)

Theory: 3 credits

Total Lectures: 45

Course Objectives:

The objectives of this course are to make the students aware of fundamental but mandatory ethical practices in chemistry, to introduce the concept of data analysis, to learn to perform literature survey in different modes, to make the students aware of safety handling and safe storage of chemicals, to make students aware about plagiarism and how to avoid it, and to teach the use of different e-resources.

Couse Learning Outcomes:

CLO-1: *By studying this course, students will be able to follow ethical practices in chemistry, do Data analysis, and literature survey in different modes, use e-resources, avoid plagiarism, understand the consequences and how to avoid*

CLO-2: *Student can have hands on training on various aspect of research including collecting journal articles and writing literature survey, preparing poster presentation, etc.*

Unit I: Scope of Research (5 **Lectures**)

Introduction, overview of research process: define research problem, review literature, formulate hypothesis, design research/experiment, collect and analyse data, interpret and report, scope and importance.

Unit II: Literature Survey, Databases and Research metrics **(15 Lectures)**

Print: Sources of information: Primary, secondary, tertiary sources; Journals: Journal abbreviations, **Digital**: Databases and their responsible use: Google Scholar, Web of science, Scopus, UGC INFONET, SciFinder, PubMed, ResearchGate, E-consortium, e-books; Search techniques: Phrase, Field, Boolean, Proximity, Concept, Limiting/Refining Search Results. **Research metrics**: Impact factor of Journal, h-index, i10 index, Citation index. Author identifiers/or profiles: ORCID, Google Scholar, ResearchGate, VIDWAN.

Unit III: Research and Publication ethics **(15 Lectures)**

Scientific Conduct: Ethics with respect to science and research, Scientific Misconducts: falsification, fabrication and plagiarism, similarity index, software tools for finding plagiarism (Turnitin, Urkundetc), redundant publications Publication Ethics: Introduction, COPE (Committee on Publication Ethics) guidelines; conflicts of interest, publication misconduct: problems that lead to unethical behaviour and vice versa, types, violation of publication ethics, authorship and contributorship, predatory publishers and journals

IPR - Intellectual property rights and patent law, commercialization, copy right, royalty, trade related aspects of intellectual property rights (TRIPS)

Unit IV: Statistical analysis for chemists **(10 Lectures)**

Types of data, data collection-Methods and tools, data processing, hypothesis testing, Normal and Binomial distribution, tests of significance: t-test, F-test, chi- square test, ANOVA, multiple range test, regression and correlation. Features of data analysis with computers and softwares -Microsoft Excel, Origin, SPSS.

Practical/Practice Credits: 01

Total Lectures: 15

1. Collection of journal articles on a particular topic using Google Scholar and creating a database.
2. Collection of journal articles on a particular topic using Science Direct and creating a database.
3. Collection of journal articles on a particular topic using Scopus and creating a database.
4. Drawing chemical structure, reactions and mechanisms using Chemsketch or ISIS draw or ChemDraw or any other software.
5. Collection of chemical structure using ChemSpider and creating a database.
6. Curve fitting using freely available softwares/apps (any one)
7. Making of power point presentation
8. Experimental learning of safe storage hazardous chemicals
9. Experimental learning of handling of hazardous chemicals
10. Technical writing on topics assigned.
11. Demonstration for checking of plagiarism using recommended software
12. Preparation of poster presentation.

Essential/recommended readings:

1. Dean, J. R., Jones, A. M., Holmes, D., Reed, R., Weyers, J. & Jones, A. (2011) Practical skills in chemistry. 2nd Ed. Prentice-Hall, Harlow.

2. Hibbert, D. B. & Gooding, J. J. (2006) Data analysis for chemistry. Oxford University Press.

3. Topping, J. (1984) Errors of observation and their treatment. Fourth Ed., Chapman Hall, London.

4. Harris, D. C. Quantitative chemical analysis. 6th Ed., Freeman (2007) Chapters 3-5.

5. Levie, R. de, how to use Excel in analytical chemistry and in general scientific data analysis. Cambridge Univ. Press (2001) 487 pages.

6. Chemical safety matters – IUPAC – IPCS, Cambridge University Press, 1992. OSU safety manual 1.01

COURSE NAME: Organic Chemistry-IV

COURSE CODE: CHE-1424

Total Credits: 4 (Theory: 3 + Practical: 1)

Theory: 3 Credits

Total Lectures: 45

Course Objective:

This course aims to provide students the with a detailed understanding of organic reaction mechanisms, including the structure, formation, and reactivity of key reactive intermediates such as carbanions, carbocations, carbenes, nitrenes, ylids, and radicals. It also aims to develop the ability to analyze kinetic and thermodynamic aspects of reactions, interpret linear free energy relationships, and apply stereochemical concepts in mechanistic contexts. The course emphasizes to develop practical skills of the students in qualitative analysis of binary organic mixtures and to introduce students to natural product chemistry through hands-on extraction techniques.

Course Learning Outcome:

CLO-1: *The students will be able to critically analyze organic reaction mechanisms through a detailed understanding of kinetic and thermodynamic principles, including reaction profiles, isotope effects, and linear free energy relationships. They will gain in-depth knowledge of reactive intermediates. Additionally, students will develop a solid foundation in stereochemical principles.*

CLO-2: *The students will be able to systematically analyze and identify components in a binary organic mixture using classical separation and identification techniques. They will also acquire practical experience in the extraction of natural products, specifically carotenoids, from plant sources.*

Unit I: Kinetics and Energetics of Reaction Mechanism (10 Lectures)

Reaction profiles for multistep reactions, Hammond postulate, Curtin-Hammett Principle; kinetic and thermodynamic control.

Linear free energy relationships (LFER): Hammett equation - substituent and reaction constants; kinetic isotope effects in organic reactions.

Unit II: Reaction Mechanisms & Intermediates: Structure & Reactivity I (13 Lectures)

Carbanions: enolates and enamines, Kinetic and thermodynamic enolates, lithium enolates in aldol and Michael reactions, alkylation and acylation of enolates; Name reactions under carbanion chemistry - Claisen, Dieckmann, Knoevenegal, Henry reaction, Nef reaction.

Ylids: Chemistry of phosphorous and sulfur ylids - Wittig and related reactions.

Carbocation: structure and stability of carbocations, classical and non-classical carbocations, neighbouring group participation and carbocation rearrangements, C-C bond formation involving carbocations, oxymercuration, halo-lactonisation.

Unit III: Reaction Mechanisms & Intermediates: Structure & Reactivity II (12 Lectures)

Carbenes and Nitrenes: Structure of carbenes, generation of carbenes, addition and insertion reactions. Structure of nitrene, generation and reactions of nitrene and related electron-deficient nitrogen intermediates, Tebbe olefination reactions.

Radicals: Generation of radical intermediates and its (a) addition to alkenes, alkynes (inter & intramolecular) for C-C bond formation and Baldwin‘s rules (b) fragmentation and rearrangements, McMurry coupling.

Unit IV: Stereochemistry (10 Lectures)

Classification of organic molecules into different Point Groups, R/S, E/Z nomenclature in C, N, S, P containing compounds; chirality in molecules devoid of chiral centers- allenes, spiranes and biphenyls (atropisomerism).

Concepts of stereogenic center – chirotopic and achirotopic center; homotopic and heterotopic ligands and faces (prostereoisomerism and prochirality, etc); optical purity and enantiomeric excess; conformations of cyclohexane and decalins.

Practical: 1 Credit

Total Lectures: 15

Qualitative analysis:

Binary mixture of organic compounds (solid-solid)

Experiments on Natural products:

Extraction of carotenoids from a natural source.

Books Recommended:

Theory:

1. F. A. Cary, R. I. Sundberg, Advanced Organic Chemistry, Part A and B, 5th Edition, Springer, 2009.
2. R. O. C. Norman, J. M. Coxon, Principles of Organic Synthesis, 3rd Edition, CRC Press, 2000.
3. J. Clayden, N. Greeves, S. Warren, Organic Chemistry, 2nd Edition, Oxford University Press, 2012.
4. E. V. Anslyn, D. A. Dougherty, Modern Physical Organic Chemistry, University Science Books, 2005.
5. E.L. Eliel, S. H. Wilen, Stereochemistry of Organic Compounds, Wiley Student Edition, Wiley-India, 2008 (Reprint).

Practical:

1. B. S. Furniss, A. J. Hannaford, P. W. G. Smith, Vogel's Textbook of Practical Organic Chemistry, Pearson, 2012.
2. V. K. Ahluwalia, S. Dhingra, Comprehensive Practical Organic Chemistry, University Press.
3. F. G. Mann, B. C. Saunders, Practical Organic Chemistry, 3rd Edition Longman, 1978.

COURSE NAME: Inorganic Chemistry - IV

COURSE CODE: CHE-1434

Total Credits: 4 (Theory: 3 + Practical: 1)

Theory: 3 Credits

Total Lectures: 45

Course Objective:

This course aims to provide an in-depth understanding of advanced inorganic and organometallic chemistry, focusing on the chemistry of s-, p-, d-, and f-block elements, their compounds, and applications in modern chemical systems. Students will gain knowledge of structure, bonding, reactivity, and synthetic strategies of main group and transition metal compounds, including their roles in catalysis and material science. The course also introduces concepts of solid-state chemistry and symmetry principles essential for interpreting molecular structures and bonding. The syllabus also includes advanced synthetic techniques of some important inorganic compounds.

Course Learning Outcomes:

CLO-1: *The students will be able to apply advanced concepts of inorganic, organometallic, and solid-state chemistry to explain the structure, bonding, synthesis, and reactivity of main group and transition metal compounds.*

CLO-2: *The students will be able to interpret molecular structures and chemical behavior using principles of symmetry, group theory, and spectroscopic characterization.*

Unit I: Chemistry of *s* and *p* block elements – III (12 Lectures)

Structure and bonding in metal borides, The hydroboration reaction, organoboranes including boronic acids, tetrahydridoborates – synthesis and synthetic use.

Preparation and reactivity of lithium aluminium hydride; alkyl aluminium compounds; chemistry of Al, Ga, In and Tl in +1 and +2 oxidation states.

Fullerenes and fullerides, nonmolecular compounds of carbon, organo compounds of Si, Ge, Sn and Pb; calixarenes, cryptands and crown ethers in complexation chemistry, metal chalcogenides, sulfur-nitrogen compounds

Organometallic compounds of Li, Be, Mg

Unit II: Transition elements (4*d* and 5*d* series) **(8 Lectures)**

Chemistry of the elements of the second and third transition series – general overview of compounds having the metals in their common oxidation states; halide containing clusters of niobium and tantalum; polyoxometallates of Mo and W; quadruple and quintuple M-M bonded compounds, the Creutz-Taube complex; $RuCl_2(PPh_3)_3$; osmium tetroxide; Vaska's compound; palladium complexes in the oxidation state 0; Pt(II,IV) linear chain compounds.

Unit III: Introduction to solid chemistry **(7 Lectures)**

Structure of simple solids – metals, alloys and compounds; common structure types. Synthesis of solid-state compounds - ceramic method, hydrothermal synthesis, CVD and intercalation methods. Characterization of solids.

Unit IV: Organometallic Chemistry – III **(12 Lectures)**

Synthesis, structure, bonding and reactivity of mono and polynuclear metal carbonyls. Substituted metal carbonyls. Vibrational spectra of metal carbonyls.

Types of M-C bonds, synthesis and reactivity of metal alkyls, carbenes, alkenes, alkynes, and arene complexes; metallocenes and bent metallocenes.

Reactions of organometallic complexes: substitution, oxidative addition, reductive elimination, insertion and deinsertion; ß – hydride elimination.

Unit V:Symmetry and Group Theory in Chemistry **(6 Lectures)**

Group and Matrices: Definitions and elements of group theory and matrix algebra

Molecular symmetry and symmetry groups: Symmetry elements and operations, classes of symmetry operations, symmetry and chirality, symmetry point groups, symmetry of the Platonic solids

Representation of Groups: Matrix notation for geometric transformations, reducible and irreducible representations, rules about irreducible representation as derived from great orthogonality theorem, relationship between reducible and irreducible groups, character tables.

Practical: 1 credit

Total Lecture: 15

Advanced Synthesis of Some Important Inorganic Compounds and their Isomers:

1. Synthesis of coordination compounds through ligand synthesis and spectroscopic characterization, *e.g.* preparation of bis (*N*,*N*-disalicylideneethylenediammine) (μ-aquadicobalt(II).
2. Solid phase synthesis of coordination compounds (*e.g.* Reinecke salt, trans-bisglycinatocopper (II)) and their properties.
3. Isomerism in coordination compounds. *e.g.* conversion of chloropentamminecobalt (III) chloride to nitro and nitroso isomers, *cis*- and *trans*-dichlorobis (ethylenediamine)cobalt(III) chloride etc.
4. Preparation of metal (II) isonicotinatetetrahydrates, characterization, use as precursors to metal oxides.
5. Synthesis of metal nanoparticles (Cu, Au, etc.), characterization and investigation of their optical properties.
6. Preparation of polyoxometallates (*e.g.*tetrabutylammoniumhexamolybdate (VI)), characterization.

Books Recommended:

Theory:

1. F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann; Advanced Inorganic Chemistry, 6thed. Wiley, 1999

2. P.W. Atkins, T. Overton, J. Rourke, M. Weller, F. Armstrong; Shriver &Atkins‘ Inorganic Chemistry, 5th ed. OxfordUniversity Press, 2010.

3. Fundamental Concepts of Inorganic Chemistry, Vols. 1-7, by A.K. Das and M. Das, CBS Publishers and Distributors, 2015

4. A. R. West, Solid State Chemistry and Its Application, Wiley Student Edition, John Wiley & Sons. 1998.

5. R. H. Crabtree, Organometallic Chemistry of the Transition Metals 2nd Ed. , John Wiley, 1993.

6. F. A. Cotton, Chemical Applications of Group Theory, 3rdEdition, Willey India Pvt. Ltd. 2008.

Practical:

1. J. Mendham, R. C. Denney, J. D. Barnes, M. Thomas, B. Sivasankar, Vogel‘s Textbook of Quantitative Chemical Analysis, 6th

Edition, Pearson, 2009.

2. G. Svehla, S. Mittal, Vogel's Qualitative Inorganic Analysis, Pearson Education, 7th Edition. 2013.

COURSE NAME: Physical Chemistry - IV

COURSE CODE: CHE-1444

Total Credits: 4 (Theory: 3 + Practical: 1)

Theory: 3 Credits

Total Lectures: 45

Course Objective:

The objective of this course is to aware students on the detail of equillibrium, non-equillibrium and statistical thermodynamics. Also, to familiarize students with significance of polymer chemistry and data analysis. Moreover, the present course also enables students towards chemistry of natural products and basics of quantum chemistry.

Course Learning Outcome:

CLO-1: *By studying this course student can able to differentiate fundamental aspect between equilibrium and non-equillibrium thermodynamics, also understand the importance of statistical mechanics in chemistry and can be able to analyse data and its concept to solve problems.*

CLO-2: *Student can perform hands-on training of various data analysis using MS Excel/origin. Student can also learn practically to determine the molecular weight of a polymer and various aspects of thermodynamics and phase equilibria.*

Unit I: Equilibrium and Non-equilibrium Thermodynamics (18 Lectures)

Laws of thermodynamics, state and path functions and their applications, Maxwell's relations; spontaneity and equilibria; Le-Chatelier principle

Non-ideal system: thermodynamics of real gases and gas mixtures, fugacity and its determination, non-ideal solutions, activity and activity coefficient-different scales of activity coefficient, electronic activity coefficients

Phase equilibrium: thermodynamic criteria of phase equilibrium, Gibbs phase rule and its application to three component systems- triangular plots- water- acetic acid –chloroform system, ammonium chloride-ammoniumsulphate-water system

Non-equilibrium thermodynamics: forced flows and entropy of production, coupled flows and phenomenological relations, Onsager reciprocal relations, thermodynamic effects- Seebeck and Peltier and Thomson effect

Unit II: Statistical Thermodynamics **(15 Lectures)**

Statistical mechanics of systems independent particles: Maxwell Boltzmann distribution, entropy and probability. Calculation of thermodynamic properties for independent particles,- molecular partition functions- evaluation of translational, rotational and vibrational and nuclear partition functions

Thermodynamic properties of monatomic and diatomic gases (Suckur-Tetrode equation)- calculation of partition functions, thermodynamic function, principles of equipartition, heat capacities (Einstein model and Debye modification), residual entropy, equilibrium constant

Unit III: Polymer Chemistry **(6 Lectures)**

Molecular weight of polymers, determination of molecular weight, kinetics of polymerization reaction, copolymerization, average dimension of polymer molecules, size exclusion chromatography

Unit IV: Sampling and Data Analysis: **(6 Lectures)**

Sampling of solid, liquid and gaseous samples, mean and standard deviation, absolute and relative errors, linear regression, covariance and correlation coefficient.

Practical: 1 Credit

Total Lecture: 15

(Students have to perform any five of the experiments mentioned below)

1. Least square fitting, linear and non-regression (Using Origin and MS Excel).
2. Boltzmann distribution plot.
3. Determination the molar mass of a polymer by viscometric method.
4. Study of the variation of surface tension of a solution of n-propyl alcohol/ethanol with concentration and determination of the limiting cross-sectional area of the alcohol molecule.
5. Determination of the partial molar volume of methanol/ethanol/formic acid by graphical method by determining the densities of solutions at different concentrations.
6. Study of the complex formation between Cu^{2+} ion and ammonia by distribution method and to find the composition of the complex.
7. To construct the phase diagram of 3 component system: triangular plots- water- acetic acid – chloroform system.

Books Recommended:

Theory:

1. P. Atkins, J. Paula, Physical Chemistry, 9th Edition, Oxford University Press, Oxford 2010.

2. I. R. Levine, Physical chemistry, 6th Edition, Mcgraw Hill Education, 2011.

3. D. A. McQuarrie, J. D. Simon, Physical Chemistry: A Molecular Approach, Viva Student Edition, 1st Edition, 2011.

4. D. A. McQuarrie, Statistical Mechanics, University Science Books, California, 2005.

5. J. Mendham, R. C. Denney, J. D. Barnes, M. Thomas, B. Sivasankar, Vogel's Textbook of Quantitative Chemical Analysis, 6thEdition, Pearson, 2009.

6. V. R. Gowarikar, N. V. Viwanathan, J. Sreedhar, Polymer Science, 1st Edition, New age International Publishers, 1986.

7. G. Odian, Principles of Polymerization, 4th Edition, Willy Student Edition, 2004.

Practical:

1. J. B. Yadav, Advanced Practical Physical Chemistry, Goel Publishing House, 27th Edison, 2008.

2. J. N. Gurtu and A. Gurtu, Advanced Physical Chemistry Experiments, PragatiPrakashan, 6th Edition, 2014.

3. M. Halpern, Experimental Physical Chemistry, 2nd Edition, Prentice Hall, Upper Saddle River, NJ 07458

COURSE NAME: Quantum Chemistry

COURSE CODE: CHE-1454

Total Credits: 4 (Theory: 3+Tutorial:1)

Theory: 3 Credits

Total Lectures: 45

Course Objective:

This course aims to provide students with a fundamental understanding of quantum mechanics, focusing on key concepts such as operators, wave functions, and the mathematical framework underpinning quantum systems. They will learn to solve energy eigen value equations for systems like the rigid rotor, H-atom, and molecular compounds, applying techniques such as molecular orbital theory. The course also covers approximate methods, including perturbation theory and the variation theorem, alongside the Born-Oppenheimer approximation for multi-electron systems. By the end, students will be equipped to analyze and solve complex quantum mechanical problems, particularly in the context of molecular and atomic systems.

Course Learning Outcome:

CLO-1: *Upon completion of this course, students will be able to understand fundamental quantum concepts, operator theory, and the Schrödinger equation to describe atomic and molecular systems.*

CLO-2: *The students will be able to apply quantum mechanical models and approximation methods (perturbation theory, Born-Oppenheimer approximation, MO theory) to solve atomic and molecular problems.*

Unit I: Operators and Wavepackets (15 Lectures)

Black-body radiation, photoelectric and Compton effects, duality of matter, atomic spectra, Dirac bra-ket notation.

Hermitian operators, matrix elements, The diagonalization of the Hamiltonian, wave-packets, wave functions of one particle and many particles system, the equation for the wave function, the separation of the Schrodinger equation

Born interpretation, expectation values of observable properties, complementarity and complementary observable, uncertainty principle, general angular momentum operators, step-up and step-down operators, theoretical basis of the *L-S* and *j-j* coupling schemes.

Unit II: Solutions of Eigen value equations **(10 Lectures)**

Solutions of the energy eigen value equations for particles in a ring, particle on a sphere, Rigid Rotor, The angular momentum, QM treatment of H-atom, QM treatment of harmonic oscillator

Free electron MO theory of benzene; HMO treatment for unsaturated carbon compounds

Unit III: Approximate Methods **(10 Lectures)**

Time-independent perturbation theory of a two level system (up to second order), the first order correction to the energy and wave function, perturbation theory for degenerate states, the second order correction to the energy

The variation theorem, linear variation function-secular equation, the Rayleigh ratio

Unit IV: Born-Oppenheimer Approximation **(10 Lectures)**

Born-Oppenheimer approximation, product wave-functions, complete many electron wave functions including electron spin, Pauli's anti-symmetry and exclusion principles, Singlet and triplet states, central field model of many electron atoms (He atom), Slater type orbitals, splitting of term energies in presence of electric and magnetic field (Stark effect and Zeeman effect)

Tutorial:1 credit

Total Lectures: 15

Books Recommended:

1. D. McQuarrie, Quantum Chemistry, Viva Student Edition, University Science Books, 2020.
2. P. Atkins, R. Friedman, Molecular Quantum Mechanics, 4th Edition, Oxford University Press, Oxford 2008.
3. I. N. Levine, Quantum Chemistry, 7th Edition, PHI Learning Pvt. Ltd., 2014.
4. David J. Griffiths, Introduction to Quantum Mechanics, 2nd edition, Pearson Education Ltd., 2014.

SECOND SEMESTER

COURSE NAME: Organic Chemistry-V

COURSE CODE: CHE-2514

Total Credits: 4 (Theory: 3 + Practical: 1)

Theory: 3 Credits

Total Lectures: 45

Course Objective:

This course aims to provide students with an in-depth understanding of advanced organic reaction mechanisms, with a focus on photochemical processes, selective oxidation and reduction techniques, and pericyclic reactions. The course aims to educate students with the theoretical foundation and practical insight needed to analyze complex organic transformations, interpret reaction stereochemistry and selectivity, and apply molecular orbital theory to predict reactivity and reaction pathways in organic synthesis. The course also tries to provide students with hands-on experience in multistep organic synthesis, natural product extraction and analysis, and quantitative estimation techniques.

Course Learning Outcome:

CLO-1: *The students will be able to analyze and predict the outcomes of key organic photochemical, oxidation-reduction and pericyclic reactions.*

CLO-2: *The students will be able to carry out basic organic syntheses, including multi-step and multicomponent reactions. They will gain hands-on experience in natural product extraction, analysis, and biodiesel preparation. Additionally, students will develop skills in quantitative analysis using titrimetric and spectroscopic methods.*

Unit I: Organic Photochemistry **(10 Lectures)**

Photophysical processes (basic ideas), chemiluminescence, photosensitization

Photochemistry of carbonyl compounds: α-cleavage, β-cleavage, intramolecular H-abstraction, addition to π-systems- Paterno-Buchi reaction; Photochemistry of olefins –photostereomutation of cis-trans isomers, optical pumping, cycloaddition, photochemistry of conjugated polyenes, photochemistry of vision

Photochemistry of enones; Photo-rearrangement reactions, di-π-methane rearrangement

Unit II: Oxidation Reactions **(9 Lectures)**

Metal based and non-metal based oxidations (Al, Ag, Hg, Ru, Se, DMSO, hypervalent iodine and TEMPO based reagents)

Sharpless asymmetric epoxidation, Baeyer-Villiger oxidation, Wacker oxidation, hydroboration-oxidation, Prevost reaction and Woodward modification

Unit III: Reduction Reactions **(12 Lectures)**

Catalytic hydrogenation (Pd/Pt/Rh/Ni). Wilkinson catalyst

Metal based reductions using Li/Na/Ca in liquid ammonia, Sodium, Magnesium, and Samarium (Birch, Acyloin formation, Pinacol formation, dehalogenations and deoxygenations)

Hydride transfer reagents from Group III and Group IV in reductions (L-selectride and K-selectride, DIBAL-H, and Red-Al, Meerwein-Pondorff-Verley reduction)

Unit IV: Pericyclic Reactions **(14 Lectures)**

MO symmetry, FMO of conjugated polyenes, Woodward-Hoffmann principle of conservation of orbital symmetry, allowed and forbidden reactions, stereochemistry of pericyclic reactions, orbital symmetry.

Cycloaddition reactions: 2+2, 4+2, 6+2 cycloadditions, 3+2 and 4+3 dipolar cycloadditions; regioselectivity of 4+2 cycloaddition reaction.

Sigmatropic rearrangement: (m+n) sigmatropic rearrangement of hydrogen and chiral alkyl groups; Divinylcyclopropane rearrangement

Electrocyclic reactions and cycloreversions: Conrotatory and disrotatory process, Stereoselectivity of the reactions.

Ene reactions: of 1,7-dienes, carbonyl enophiles, simple problems. Claisen rearrangement and its variants.

Practical: Credit 1

Total Lectures: 15

Organic Synthesis (2-steps):

1. Benzoin – Benzil – Benzilic acid: Base catalysed, rearrangement
2. Multicomponent reaction of aldehyde, β-keto ester and ammonia for the synthesis of dihydro-pyridine derivatives (Hantzsch Pyridine Synthesis)

Experiments on Natural products:

1. Extraction and phytochemical screening/analysis of Natural Products (A case study).
2. Conversion of Vegetable Oil to Biodiesel.

Quantitative analysis:

1. Estimation of sugars by redox titrimetric methods.
2. Spectroscopic methods for estimation of functional groups.

Books Recommended:

Theory:

1. F. A. Cary, R. I. Sundberg, Advanced Organic Chemistry, Part A and B, 5th Edition, Springer, 2009.
2. W. Carruthers and I. Coldham, Modern Methods of Organic Synthesis, First South Asian Edition, Cambridge University Press, 2005.
3. M. B. Smith, Organic Synthesis, 2nd Edition, McGraw-Hill Education, 2001.
4. J. Clayden, N. Greeves, S. Warren, Organic Chemistry, 2nd Edition, Oxford University Press, 2012.
5. T. H. Lowry, K. S. Richardson, Mechanism and Theory in Organic Chemistry, International Student Edition, Addison-Wesley Publishing, 1998.

Practical:

1. B. S. Furniss, A. J. Hannaford, P. W. G. Smith, Vogel‘s Textbook of Practical Organic Chemistry, Pearson, 2012.
2. V. K. Ahluwalia, S. Dhingra, Comprehensive Practical Organic Chemistry, University Press.
3. F. G. Mann, B. C. Saunders, Practical Organic Chemistry, 3rd Edition Longman, 1978.

COURSE NAME: Inorganic Chemistry-V

COURSE CODE: CHE-2524

Total Credits: 4 (Theory: 3 + Practical: 1)

Theory: 3 Credits

Total Lectures: 45

Course Objective:

The course aims to: Apply group theory to understand molecular symmetry, bonding, and spectroscopy, Explain electronic structures and spectra of transition metal complexes using CF and MO theories, Analyze magnetic properties of transition metal and lanthanide complexes, Understand principles and reactions in inorganic photochemistry, Explain nuclear reactions, radioactive decay, and applications of radiochemistry, Perform advanced inorganic analyses and apply computational tools to simple molecules

Course Learning Outcome:

CLO-1: *Apply group theory to analyze molecular symmetry, vibrations, and spectral transitions, Explain bonding and electronic spectra of transition metal complexes using crystal field and molecular orbital theories*

CLO-2: *The students can have practical experience on advanced inorganic quantitative analysis.*

Unit I: Symmetry and Group theory – II **(10 Lectures)**

Chemical application of group theory: Group Theory and Quantum Mechanics - wave functions as bases for irreducible representations, the direct product and its importance in predicting spectral transition probabilities.

Molecular vibrations - symmetry of normal vibrations, selection rules for fundamental vibrational (IR and Raman) transitions.

Symmetry properties of atomic orbitals, molecular orbitals for σ and π bonding in AB_4 molecules, MO treatment of the bonding in ferrocene. Ligand field states, construction of the correlation diagram for the d^2 configuration in an octahedral environment.

Crystallographic symmetry: Translational and point symmetry elements in crystal symmetry, glide planes and screw axes, the crystal systems, Bravais lattices, crystallographic point groups, space groups.

Unit II: Binding and electronic spectra of transition metal complexes (10 Lectures)

Jahn-Teller distortion, CFSE, pairing energy, low-spin and high-spin complexes; and molecular orbital (MO) theory of selected octahedral, tetrahedral complexes and other geometries, Walsh Diagram.

d-d transition, charge transfer transition, color, intensity and origin of spectra, interpretation, term symbols and splitting of terms different geometries, selection rules for electronic transitions, correlation, Tanabe-Sugano and Orgel diagrams, calculation of Dq, B and C, nephelauxetic ratio.

Unit III: Magnetic property (10 Lectures)

Magnetic properties of free ions, types of magnetic behaviour: dia-, para-, ferro- and antiferro-magnetism, temperature independent paramagnetism, magnetic susceptibility - Van Vleck equation, experimental measurement, magnetic moment - orbital contribution, quenching of contribution, effect of spin orbit coupling, spincrossover. Temperature dependence of magnetic susceptibility, exchange coupling effects. Magnetic properties of second and third transition series and lanthanides.

Unit IV: Inorganic photochemistry (5 Lectures)

Photo substitution and photoredox reactions of chromium, cobalt and ruthenium compounds, Ligand field and charge transfer state (Thexi & DOSENCO states), *cis-trans* isomerization, photocatalysis and solar energy conversion by ruthenium complexes.

Unit V:Nuclear and radiochemistry (10 Lectures)

Radioactive decay processes, Fermi theory, half-lives, auger effect. Nuclear reactions - notations, comparison with chemical reaction: Types of nuclear reactions. Applications of radioisotopes as tracers (activation and isotope dilution analysis). Age determination, radiolysis of water, units for measuring radiation absorbed by matter, radiation dosimetry. Radiation induced chemistry–sources of radiation, chemical effects produced by the absorption of ionizing radiation and high energy ions and electrons from accelerators - radiation induced synthesis of materials.

Practical: Credit 1

Total Lecture: 15

Advanced Inorganic Analysis:

1. Qualitative analysis (tertiary mixture, alloy, ore) (semi-micro technique to be preferred)
2. Quantitative analysis (binary mixture, alloy, ore) - Ca-Mg ore, Cu-Zn alloy, Pb-Sn alloy, Ni in an alloy etc.

3. Quantitative determination of components in food (Fe, Zn, I, Ca, etc.)
4. Construction of 3D computational models of simple molecules (NH_3, H_2O, H_2O_2, CH_4, C_2H_6) using Avogadro or ArgusLab or chemcraft or any similar software.

Books Recommended:

Theory:

1. F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann; Advanced Inorganic Chemistry, 6th ed. Wiley, 1999

2. P.W. Atkins, T. Overton, J. Rourke, M. Weller, F. Armstrong; Shriver &Atkins‘ Inorganic Chemistry, 5th ed. Oxford University Press, 2010.

3. Fundamental Concepts of Inorganic Chemistry, Vols. 1-7, by A.K. Das and M. Das, CBS Publishers and Distributors, 2015

4. J. E. Huheey, E. A. Keiter and R. L. Keiter; Inorganic Chemistry: Principles of Structure and Reactivity, 4th Ed. Pearson Education, 2006.

5. B. N. Figgis, M. A. Hitchman; Ligand Field theory and its Applications, Wiley India, 2010.

6. G. L. Miessler, D Tarr; Inorganic Chemistry. 3rd Ed., Pearson Education, 2004.

7. P. W. Atkins, T. Overton, J. Rourke, M. Weller, F. Armstrong; Shriver &Atkins‘ Inorganic Chemistry, 5th Ed. OxfordUniversity Press, 2010.

8. F. A. Cotton, Chemical Applications of Group Theory, 3rdEdition, Willey India Pvt. Ltd. 2008.

9. R. L. Dutta, A. Syamal, Elements of Magnetochemistry, 2nd Ed. Affiliated East-West Press Pvt. Ltd.-New Delhi, 2004.

10. D. M. Roundhill, Photochemistry and Photophysics of Metal Complexes; Plenum: New York, 1994.

Practical:

1. J. Mendham, R. C. Denney, J. D. Barnes, M. Thomas, B. Sivasankar, Vogel‘s Textbook of Quantitative Chemical Analysis, 6thEdition, Pearson, 2009.

2. G. Svehla, S. Mittal, Vogel's Qualitative Inorganic Analysis,Pearson Education, 7th Edition. 2013.

COURSE NAME: Physical Chemistry-V

COURSE CODE: CHE-2534

Total Credits: 4 (Theory: 3 + Practical: 1)

Theory: 3 Credits

Total Lectures: 45

Course Objective: *The objective of this course is to aware students to the advancement in chemical kinetics, molecular reaction dynamics. Also, to familiarize students with dynamic electrochemistry and application of electrochemistry.*

Course Learning Outcome:

CLO-1: *By studying this course student can able to apply steady-state approximation method toward various reaction, understand the kinetics of fast reaction, also understand the theory of molecular dynamics including transition state theory and its application, understand the electrochemical application for energy storage and energy conversion.*

CLO-2: *Student can able to comprehend with advanced practical aspect of chemical kinetics and application of electrochemistry.*

Unit I: Chemical Kinetics (8 Lectures)

Steady state approximation and its applications, Oscillating reactions, chemical Chaos, Belousov-Zhabotinski reaction, straight-chain reaction-hydrogen halogen reactions, alkane pyrolysis, Branching-chain reactions- the hydrogen-oxygen reaction, explosion limits, Enzyme catalyzed reactions, Michaelis-Menten mechanism- Lineweaver-Burk and Eadie plots, enzyme inhibition.

Unit II: Molecular Reaction Dynamics (7 Lectures)

Collisions of real molecules- trajectory calculations, Laser techniques, reactions in molecular beam, - reaction dynamics, Estimation of activation energy and calculation of potential energy surface- the transition state theory (TST) ofbimolecular gaseous reactions, statistical and thermodynamic formulations. Kinetics of reactions in solution diffusion controlled and chemically controlled reactions, TST of reactions in solution- Bronsted and Bjerrum equation, effect of ionic strength, kinetic salt effect.

Unit III: Study of Fast Reactions **(8 Lectures)**

Stopped flow technique, temperature and pressure jump methods, NMR studies in fast reactions, shock tube kinetics, relaxation kinetics, Linearized rate equation, relaxation time in single step fast reactions, determination of relaxation time.

Unit IV: Theories of Unimolecular Reactions **(6 Lectures)**

Theory of unimolecular reactions- Lindemann theoryand its limitations, Drawbacks of Lindemann theory- Hinselwood modification, RRK theory, slaters treatment, RRKM theory.

Unit V: Dynamic Electrochemistry (**10 Lectures**)

Ion-solvent interaction- the Born model, Thermodynamic parameters of ion solvent interactions-structural treatment, the ion-dipole model-its modifications, ion-quadrupole and ion-induced dipole interactions, Primary solution- determination of hydration number, compressibility method and viscosity-mobility method, Debye-Huckel theory of ion-ion interactions-derivation, validity and limitations.

Unit VI: Systems for Electro-chemical Energy Storage & Conversion **(6 Lectures)**

Batteries: Types of Batteries, Lead- acid batteries, Nickel-cadmium batteries and Li-ion batteries, Super capacitors: Electrical double layer capacitor, Pseudo-capacitor, Fuel Cells

Practical: Credit 1

Total Lectures: 15

(Students have to perform any five of the experiments mentioned below)

1. Study of the kinetics of reaction between iodine and acetone in acidic medium by half-life period method and determination of the order with respect to iodine and acetone.
2. Study of the autocatalytic reaction between oxalic acid and KMnO4 and determination of the order of the reaction.
3. Determination of the amount of each component of the following ternary mixture by conductometric titration. Hydrochloric acid, acetic acid and copper sulphate
4. Comparison of the relative strength of acetic acid and monochloroacetic acid by conductance measurement.
5. Determination of the degree of hydrolysis and hydrolysis constant of aniline hydrochloride /sodium acetate.
6. Determination of the dissociation constant of acetic acid by using Hendersen‘s equation

7. Finding the amount of the components of the following mixtures using pH metric titration: Hydrochloric acid + Acetic acid/oxalic acid

Books Recommended:

Theory:

1. P. Atkins and J. Paula, Physical Chemistry, 9th Edition, Oxford University Press, Oxford 2010.

2. I. R. Levine, Physical chemistry, 6th Edition, Mcgraw Hill Education, 2011.

3. K. J. Laidler, Chemical Kinetics,3rd Edition, Pearson, 2012.

4. J. O. Bockris, A. K. N. Reddy, Modern Electrochemistry Part 1, 2A and 2B, 2nd Edition, Springer

5. A. J. Bard, L. R. Faulkner, Electrochemical Methods Fundamentals and Applications, 2nd edition, Willy India, 2006.

Practical:

1. J. B. Yadav, Advanced Practical Physical Chemistry, Goel Publishing House, 27th Edison, 2008.

2. J. N. Gurtu and A. Gurtu, Advanced Physical Chemistry Experiments, PragatiPrakashan, 6th Edition, 2014.

3. M. Halpern, Experimental Physical Chemistry, 2nd Edition, Prentice Hall, Upper Saddle River, NJ 07458

COURSE NAME: Spectroscopy

COURSE CODE: CHE-2544

Total Credits: 4 (Theory: 3 + Practical: 1)

Theory: 3 Credits

Total Lectures: 45

Course Objective: *The objective of this course is to make students aware on the detail of NMR, EPR, Mossbauer Spectroscopy and Mass Spectrometry.*

Course Learning Outcome:

CLO-1: *By studying this course student can able to understand the various concepts used in the analysis of organic and inorganic molecules via various spectroscopic and spectrometric techniques.*

CLO-2: *Student can get hands-on training on using NMR or IR or UV techniques to differentiate between organic molecules.*

Unit I: NMR Spectroscopy (18 Lectures)

NMR phenomenon, Zeeman splitting, factors affecting sensitivity and resolution of a NMR spectrum, chemical shift tensor, spin-spin coupling, 1H NMR-inductive and anisotropic effects on chemical shifts (chemical and magnetic equivalence. First order patterns and J to structural correlations. Second order effects in AB, AX and ABX spin systems, simplification of second order spectrum using high magnetic field.

^{13}C NMR to structural correlations. Pulse and Fourier transformation in NMR. Dynamic processes by VT NMR- restricted rotation (DMF, annulenes and related systems), ring inversion (cyclohexane), degenerate rearrangement (bullvalene).

Unit II: ESR Spectroscopy (10 Lectures)

Its principle, hyperfine structure, ESR spectra of organic and inorganic compounds, ZFS, Kramer‘s degeneracy, determination of electronic structure, Zeeman splitting, g-values, hyperfine and super hyperfine coupling constants, practical considerations of measurements, and instrumentation.

Unit III: Mass Spectrometry (10 Lectures)

Mass spectrometry: basic principles, ionization techniques, isotope abundance, molecular ion, fragmentation processes of organic molecules, deduction of structure through mass spectral

fragmentation. ESI-MS and MALDI-MS-applications in biomolecules. Studies of inorganic/coordination and organometallic representative compounds. Instrumentation

Unit IV: Mössbauer Spectroscopy **(7 Lectures)**

Principles, instrumentation and applications.

Practical: 1 credit

Total Lectures: 15

1. To determine the concentration of chromium and manganese in a mixture of dichromate and permanganate by spectrophotometric method.
2. Determination of the composition of iron salicylic acid complex spectrophotometrically by Job's method of continuous variation.
3. Investigation of the complex ion formation between Ni^{2+} and o-phenanthroline by Job's method.
4. Differentiation between of benzoic acid and cinnamic acid by UV spectroscopy (Spectra to be provided).
5. Differentiation between of *o*-/*p*-hydroxybenzaldehyde by IR spectroscopy (Spectra to be provided).
6. Structure elucidation from simple proton and 13C NMR and Mass Spectrometry.

Books Recommended:

1. D.L. Pavia, G. M. Lampman, G. S. Kriz, Introduction to Spectroscopy, 4th Ed.,Cengage, 2001

2. R. S. Drago, Physical Methods in Chemistry, 1992

3. R. M Silverstein, F. X. Webster, D. J. Kiemle, D. L. Bryce, Spectrometric Identifications of Organic Compounds, 8th Edition,Wiley India Pvt. Ltd, 2015.

COURSE NAME: Green Chemistry

COURSE CODE: CHE-2554

Total Credits: 4 (Theory: 3 + Practical: 1)

Theory: 3 Credits

Total Lectures: 45

Course Objective: *The learners will be taught about the emerging discipline of green chemistry particularly to differentiate as to how the principles of green chemistry may be applied to organic synthesis.*

Course Learning Outcome:

CLO-1: *Apart from introducing learners to the principles of green chemistry, this course will make them conversant with applications of green chemistry to organic synthesis. Students will be prepared for taking up entry level jobs in the chemical industry. They also will have the option of studying further in the area.*

CLO-2: *The student will be able to apply the principles of green chemistry in organic synthesis and preparation of value-added chemicals.*

Unit I: Introduction to Green Chemistry (8 Lectures)

Introduction to Green Chemistry, some important environmental laws, pollution prevention Act of 1990, emergence of green chemistry, need for Green Chemistry. Goals of Green Chemistry. Limitations/ Obstacles in the pursuit of the goals of Green Chemistry. Green chemistry in sustainable development.

Unit II: Principles of Green Chemistry and Designing a Chemical synthesis (30 Lectures)

Twelve principles of Green Chemistry with their explanations and examples; Designing a Green Synthesis using these principles; Prevention of Waste/ byproducts; maximum incorporation of the materials used in the process into the final products (Atom Economy); prevention/ minimization of hazardous/ toxic products; designing safer chemicals – different basic approaches to do so; selection of appropriate auxiliary substances (solvents, separation agents), green solvents, solventless processes, immobilized solvents and ionic liquids; energy requirements for reactions - use of microwaves, ultrasonic energy; selection of starting materials; avoidance of unnecessary derivatization – careful use

of blocking/protecting groups; use of catalytic reagents (wherever possible) in preference to stoichiometric reagents; designing of biodegradable products; prevention of chemical accidents; strengthening/ development of analytical techniques to prevent and minimize the generation of hazardous substances in chemical processes.

Unit III: Future Trends in Green Chemistry (7 Lectures)

Oxidation reagents and catalysts; Biomimetic, multifunctional reagents; Solventless reactions; Green chemistry in sustainable development.

Practical: 1 credit

Total Lectures: 15

(Students have to perform any five of the experiments mentioned below)

1. Preparation and characterization by UV-Vis spectroscopy of nanoparticles of zinc using tea leaves/silvernanoparticles using plant extracts.
2. Preparation of biodiesel from commercial/waste cooking oil and characterization (TLC, pH, solubility).
3. Solid state synthesis of *N*-organophthalimide using phthalic anhydride and 3-amino benzoic acid.
4. Photochemical conversion of dimethyl maleate to dimethyl fumarate (*cis-trans* isomerisation)
5. Benzil- Benzilic acid rearrangement: Preparation of benzilic acid in solid state under solvent-free condition.
6. Preparation of dibenzalacetone by cross aldol condensation reaction using base catalysed green method.

Books Recommended

1. M. Lancaster, Green Chemistry: An Introductory Text, RSC, 2002
2. P.T. Anastas, J. C. Warner, Green Chemistry: Theory and Practice, Oxford University Press 2008
3. J. H. Clark, F. Deswarte, Introduction to Chemicals from Biomass, 2nd Edition, Wiley 2015

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