# दिल्ली विश्वविद्यालय UNIVERSITY OF DELHI

Bachelor of Science (Prog.) Industrial Chemistry

(Effective from Academic Year 2019-20)





## Revised Syllabus as approved by Academic Council

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Applicable for students registered with Regular Colleges, Non Collegiate Women's Education Board and School of Open Learning

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## Preamble

The objective of any programme at Higher Education Institute is to prepare their students for the society at large. The University of Delhi envisions all its programmes in the best interest of their students and in this endeavour, it offers a new vision to all its Under-Graduate courses. It imbibes a Learning Outcome-based Curriculum Framework (LOCF) for all its Under Graduate programmes.

The LOCF approach is envisioned to provide a focused, outcome-based syllabus at the undergraduate level with an agenda to structure the teaching-learning experiences in a more student-centric manner. The LOCF approach has been adopted to strengthen students' experiences as they engage themselves in the programme of their choice. The Under-Graduate Programmes will prepare the students for both, academia and employability.

Each programme vividly elaborates its nature and promises the outcomes that are to be

accomplished by studying the courses. The programmes also state the attributes that it offers to inculcate at the graduation level. The graduate attributes encompass values related to well-being, emotional stability, critical thinking, social justice and also skills for employability. In short, each programme prepares students for sustainability and life-long learning.

The new curriculum of B.Sc. (Prog.) with Industrial Chemistry offer courses in the areas of inorganic, organic, physical, materials, analytical and industrial chemistry. All the courses are having defined objectives and Learning Outcomes, which will help prospective students in choosing the elective courses to broaden their skills in the field of chemistry and interdisciplinary areas. The courses will train students with sound theoretical and experimental knowledge that suits the need of academics and industry. The courses also offers ample skills to pursue research as career in the filed of chemistry and allied areas. As usual, B.Sc. (Prog.) with Industrial Chemistry programme offered by one of the largest and oldest Departments in the country will continue to produce best minds to meet the demands of society.

The University of Delhi hopes the LOCF approach of the programme B.Sc (Prog.) with Industrial Chemistry will help students in making an informed decision regarding the goals that they wish to pursue in further education and life, at large.

## 1. Introduction to B.Sc. Programme with Industrial Chemistry

The choice based credit system (CBCS) offers flexibility of program structure while ensuring that students gets a strong foundation in the subject and gain in-depth knowledge of all aspects of the field. The learning outcome based curriculum framework is designed around the CBCS and is intended to suit the present day needs of the students in terms of securing their path towards higher studies or employment.

The B.Sc. Programme with Industrial Chemistry is of three year duration. Each year is called an academic year and is divided into two semesters. Thus there will be a total of six semesters. Each semester consists of sixteen weeks.

The teaching learning process involves theory classes (Periods) of an hour duration and practical classes of four hours duration. The curriculum will be delivered through various methods including chalk and talk, power point presentations, audio, video tools, E-learning/E-content, virtual laboratories, simulations, field trips/ Industry visits, seminars (talks by experts), workshops, projects, models and class discussions. The assessment broadly comprises of Internal Assessment (Continuous Evaluation) and End Semester Examination. Each theory paper carries100 marks with 25% marks for Internal Assessment and 75% for End Semester Examination. The internal assessment will be through MCQ, test, assignment, oral presentation, worksheets and short projects.

#### 2. Learning Outcome-based Curriculum Framework in B.Sc. (Prog.) with Industrial Chemistry

## 2.1 Nature and Extent of B.Sc. (Prog.) with Industrial Chemistry

The learning outcome - based approach for B.Sc. Prog. with Industrial Chemistry is to design curriculum framework to suit the requirements of the various industries. The course structure has been designed to allow flexibility in program and course content development while at the same time maintaining a basic uniformity in structure in comparison with other universities across the country. The core courses in Chemistry, Mathematics and Physics are designed to build strong foundation in theory and principles useful for practical applications. The core courses in Industrial Chemistry is designed to familiarize the students with the industrial processes involved in the commercial production of the products. The program also offers wide range of discipline specific electives, skill enhancement and compulsory Ability Enhancement and

Environmental Science courses to prepare students to improve their skills required in academic, research and in industrial projects.

## 2.2 Aims of the Bachelors Degree Programme in B.Sc. (Prog.) with Industrial Chemistry

Bachelor course in Industrial Chemistry offers the synergism of basic concepts of Chemistry with Industrial applications. The main objective of this degree course is to produce graduates with enhanced skills, knowledge and research aptitude to carry out higher studies or research and development in the various industrial areas. This degree course of Industrial Chemistry prepares the students for immediate entry to the workplace with sound theoretical, experimental knowledge in the area of fuels and energy, environment, health, foods, cosmetics, polymers and related multidisciplinary fields. Overall, the course offers basic foundation in chemistry, physics and maths which enables the students to understand the concepts in chemical processing, engineering and industrial development.

## 3. Graduate Attributes in B.Sc. (Prog.) with Industrial Chemistry

Some of the major attributions of an Industrial Chemistry graduate include:

- (i) Disciplinary Knowledge: In depth knowledge of basic and applied area of Industrial Chemistry. Capability to demonstrate knowledge and understanding of major chemistry concepts, theoretical principles and experimental findings and ability to use modern instrumentation techniques with chemical analysis and separation.
- (ii) Communication skills: Excellent communication skills to transmit complex technical information related to chemistry in a clear and concise written and verbal manner as oral presentations and compilation in the form of scientific reports.
- (iii) Critical thinking: Able to employ critical thinking and efficient problem solving skills in the basic areas of chemistry (analytical, organic, inorganic, physical and material). Students will become efficient in managerial skills, able to employ critical thinking, analytical reasoning, problems solving and interpretation and documentation of laboratory experiments at a level suitable to succeed at an entry-level position in chemical industry or a chemistry graduate program. They will be able to identify and explore new areas of research and planning, execute and report the results of an experiment or investigation, critical thinking and scientific inquiry in the performance, design.

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- (iv) Problem solving: Develop scientific logics and approaches towards problems with critical reasoning.
- (v) Analytical reasoning: Able to enhance the ability to assimilate, discuss scholarly articles and research papers showcasing interdisciplinary areas of industrial chemistry and capability for asking questions relating to issues and problems in the field of industrial chemistry.
- (vi) Research related skills: Will develop ability to scale up chemical products and techniques developed at laboratory to the industrial level. The course will take students beyond chemistry knowledge into the world of industrial professionals.
- (vii) Cooperation/Team work: Enabled with quality of team-work and strength of interacting with people from diverse backgrounds.
- (viii) Scientific reasoning: Advanced knowledge of fundamentals of industrial chemistry with enhanced command over modern scientific methods, techniques and chemical processes equipped with environment safety measures.
- (ix) Reflective thinking: Acquire skills not simply the ability to replicate techniques taught, but the ability to craft responses appropriate to the variety of circumstances in which they will find themselves.
- (x) Information/digital literacy:will learn how to develop Information & Digital Literacy Skills that will help them to achieve success in studies. Understand how to disseminate and communicate information in a professional way, including managing digital identity and building networks for learning and research.Understand how to use digital tools for referencing and attribution in order to avoid plagiarism.
- (xi) Self-directed learning: Cultivate independent thinking and able to integrate knowledge from other disciplines to fit into various industrial areas.
- (Xii) Multicultural competence:learn to observe, empathize, and appreciate other people's ways of doing things to become culturally competent. Learn about and become allies with people from other cultures, thereby broadening their understanding and ability to participate in a multicultural process.
- (xiii) Moral and ethical awareness/reasoning:students will be able to recognize the ethical component of complex situations. Acquired with awareness of work ethics and ethical issues in scientific research as well as plagiarism policies.
- (xiv) Leadership readiness/ qualities:Learn to think out of the box to come up with unique ideas and turn those ideas and goals into reality with team efforts.
- Lifelong learning:Students will be capable of self-paced and self-directed learning aimed at personal development and for improving knowledge/skill development. They will keep themselves updated with the best international practices and latest development in technologies, which will help them to gain a broader global perspective of the subject. Develop awareness of the role and importance of industrial chemistry in interdisciplinary research as well as in daily life.

## 4. Qualification Descriptors for Graduates in B.Sc. (Prog.) with Industrial Chemistry

The qualification description for B.Sc. (Prog.) with Industrial Chemistry include:

Demonstration of a clear and exhaustive understanding of the basic concepts of

- Industrial Chemistry, and an awareness of the emerging areas in the field.
- Acquisition of in-depth comprehension of the applied aspects of chemistry in daytoday life.
- Enhancement of ability to read, assimilate and discuss scholarly articles and research papers showcasingindustrial chemistry as well as interdisciplinary areas of sciences.
- Sharpening of critical thinking skills facilitating the application of knowledge gained in the field of industrial chemistry in the classroom to the practical solving of societal problems.
- Development of intellectual capabilities promoting the ability to formulate and test a hypothesis.
- Acquisition of practical laboratory skills, enabling the accurate design of an experiment and systematic collection of experimental data.
- Exhibition of ability to interpret and quantitatively analyze experimental data and maintain records of the same.
- Development of strong oral and written communication skills promoting the ability to present studies in the field of industrial chemistry using the concepts and knowledge acquired.
- Demonstration of the ability to work effectively and productively, independently or as part of a team.

#### 5. Programme Learning Outcomes in B.Sc. (Prog.) with Industrial Chemistry

On successful completion of the course of B. Sc. Programme with Industrial Chemistry, the student will be able to:

- Describe the chemical industry and identify the distinguishing features of its component,
- Explain the importance and roles of process optimization in chemical processing,
- Describe the industrial production of a number of important organic and inorganic compounds/chemicals,
- Evaluate environmental issues pertaining to the chemical industry,
- Use modern instrumentation techniques for chemical analysis and separation,
- Communicate the results of their work to chemists and non-chemists.

- Gain comprehensive knowledge of cutting-edge developments in a field of science by
   discussion and exchange of experiences and knowledge.
- Understand fundamental and applied aspects of organic, inorganic, physical and analytical chemistry as well as key major concepts, theoretical principles and experimental findings in industrial chemistrywill be covered.
- Develop proficiency in application of current aspects of industrial chemistry. Students
  will be able to use chemical techniques relevant to academia and industry, generic
  skills and global competencies including knowledge and skills that enable the students
  to undertake further studies in the field of industrial chemistry or a related field, and
  work in chemical and non chemical sector.
- Become efficient in using standard operating procedures and will be well versed with the regulations for safe handling and use of chemicals.
- Design, execute, record and analyse the results of chemical experiments.
- Undertake hands on lab work and practical activities and develop problem solving abilities required for successful career in pharmaceuticals, chemical industries, teaching research, environmental monitoring, product quality, food products, cosmetic industries, oils and lubricants industries, fuels, petrochemicals and energy sector, etc.
- Work effectively in a group in the classroom, laboratory, industries and field-based situations. They could interact with peers from diverse backgrounds with developed confidence to lead a team.
- Identify appropriate resources required for an assigned task/project to accomplish it.
- Identify the ethical and environmental dimensions of problems and issues facing chemists.
- Use modern library searching and retrieval methods to obtain information on a topic,
   relating to Industrial chemistry.
- Communicate and present their ideas effectively through power-point presentations and appropriate software for analysis of data.
- Find employment in government departments, research and development institutes, production, biotechnology, quality control, pharmaceutical industry, process industry, fertilizer production industry, plastics industry, pulp and paper industry, tanning

industry, consumer industry, oil and petroleum industry, textile industry, dyes and paints industry, cosmetics industry, cement industry, glass industry, water purification and waste water purification engineering including forensic science and patents, defence, education and research, and areas related to polymer chemistry.

 Further his/her career in higher studies such as masters in chemistry/ industrial chemistry/ biotechnology and allied courses. After their post-graduation, they may opt for Ph.D. in multidisciplinary areas.

## 6. Structure of the Programme in B.Sc. (Prog.) with Industrial Chemistry

The programme consists of core papers/ Discipline Specific Elective (DSE) papers of six credit each and Skill Enhancement Courses of four credit each. For theory classes, one credit indicates one-hour lecture per week while for practical, one credit indicates two hours practical laboratory session per week.

The program includes Core Courses (CC) and elective courses. The core courses are all compulsory courses. There are two kinds of elective courses: Discipline-Specific Elective (DSE), and Skill Enhancement Course (SEC). In addition, there are two compulsory Ability Enhancement Courses (AEC).

To acquire a degree in B.Sc. Prog. with Industrial Chemistry, a student must study twelve core courses, six Discipline Specific Elective courses, four Skill Enhancement courses and two compulsory Ability Enhancement Courses (AEC). The Core Courses, Discipline-Specific Electives are six credit courses. The Skill Enhancement Course are four-credit courses while the Ability Enhancement courses are four credit courses. A student has to earn a minimum of 132 credits to get a degree in B.Sc. Prog. with Industrial Chemistry.

The program offers Discipline-Specific Elective (DSE) papers in Chemistry, Industrial Chemistry and Mathophysics and the students must choose one from each of these in semesters V and VI. The students has to take four Skill Enhancement (SEC) Courses, two each from Chemistry and Industrial Chemistry in each of the semesters III, IV, V and VI which they can choose from the list of SEC courses offered by their college.

The student has to take two compulsory Ability Enhancement Courses (AECs): AE1 (Environmental Sciences) and AE2 (English Communication) one each in Semester I and II.

Scheme of B.Sc. (Prog.) withIndustrial Chemistry

Semester	CORE COURSE (12)*	Ability Enhancement Compulsory Course (AECC) (2)*	Skill Enhancement Course (SEC) (4)*	Elective: Discipline Specific DSE (6)*
I	C1, C2, C3	AECC-1		
II	C4, C5, C6	AECC-2		
III	C7, C8, C9		SEC-1	
IV	C10, C11, C12		SEC-2	
V			SEC-3	DSE-1, DSE-2, DSE-3
VI			SEC-4	DSE-4, DSE-5, DSE- 6

<sup>\*</sup>Number of Courses student has to study.

## 6.1 Semester-wise Distribution of Courses Under B.Sc. Prog. With Industrial Chemistry (CBCS) and Credit Distribution

1		Course name	Credits
_	Ability Enhancement	English/ MIL Communications/	4
	Compulsory Course-I	Environmental Science	
	Core Course Industrial	Industrial Chemicals and	4
	Chemistry-I	Environment	
	Core Course Industrial	Industrial Chemicals and	2
	Chemistry -I Practical	Environment	
	Core Course Chemistry-I	Atomic structure, bonding,	4
		General Organic Chemistry &	
		Aliphatic hydrocarbons	
	Core Course Chemistry-I	Atomic structure, bonding,	2
	Practical	General Organic Chemistry &	
		Aliphatic hydrocarbons	
	Core Course Mathophysics-I	Mechanics	4
	Core Course Mathophysics -I	Mechanics	2
	Practical		
II	Ability Enhancement	English/ MIL Communications/	4
	Compulsory Course-II	Environmental Science	
	Core Course Industrial	Fossil Fuels, Cleansing Agents	4
	Chemistry-II	and Food Additives	
	Core Course Industrial	Fossil Fuels, Cleansing Agents	2
	Chemistry -II Practical	and Food Additives	
	Core Course Chemistry –II	Chemical Energetics, Equilibria	4
		& Functional Group Organic	
		Chemistry-1	
	Core Course Chemistry-II	Chemical Energetics, Equilibria	2
	Practical	& Functional Group Organic	
		Chemistry-1	
	Core Course Mathophysics-II	Calculus and Matrices	4
	Core Course Mathophysics-II	Calculus and Matrices	2
	Practical		
III	Core Course Industrial	Industrial Chemistry-Inorganic	4
	Chemistry -III	Materials	
	Core Course Industrial	Industrial Chemistry-Inorganic	2
	Chemistry - III Practical	Materials	
	Core Course Chemistry – III	Solutions, Phase Equilibria,	4
		Conductance, Electrochemistry	

		& Functional Group Organic	
		Chemistry -II	
	Core Course Chemistry - III	Solutions, Phase Equilibria,	2
	Practical	Conductance, Electrochemistry	_
	- Fuelisai	& Functional Group Organic	
		Chemistry –II	
	Core Course Mathophysics-III	Algebra	6
	Skill Enhancement Course-I	SEC-1	2
	Skill Enhancement Course –I	SEC-1	2
	Practical*	520-1	
IV	Core Course Industrial	Pharmaceuticals, Fermentation,	4
	Chemistry –IV	Pesticides & Perfumes	
	Core Course Industrial	Pharmaceuticals, Fermentation,	2
	Chemistry- IV Practical	Pesticides & Perfumes	
	Core Course Chemistry-IV	Chemistry of s- and p- block	4
	,	elements, States of matter &	
		Chemical kinetics	
	Core Course Chemistry-IV	Chemistry of s- and p- block	2
	Practical	elements, States of matter &	
		Chemical kinetics	
	Core Course Mathophysics-IV	Wave and Optics	6
	Skill Enhancement Course-II	SEC-2	2
	Skill Enhancement Course-II	SEC-2	2
	Practical *		
V	Discipline Specific Elective -1	Industrial Chemistry (DSE-1)	4
	Discipline Specific Elective -1	Industrial Chemistry (DSE-1)	2
	Practical *		
	Discipline Specific Elective –I	Chemistry (DSE-2)	4
	Discipline Specific Elective –I	Chemistry (DSE-2)	2
	Practical *		
	Discipline Specific Elective –I	Mathophysics – Physics (DSE-3)	6
	Skill Enhancement Course-III	SEC-3	2
	Skill Enhancement Course-III	SEC-3	2
	Practical *		
VI	Discipline Specific Elective –II	Industrial Chemistry (DSE-4)	4
	Discipline Specific Elective –II	Industrial Chemistry (DSE-4)	2
	Practical *		
	Discipline Specific Elective –II	Chemistry(DSE-5)	4
	Discipline Specific Elective –II	Chemistry (DSE-5)	2
	Practical *		

Discipline Specific Elective -II	Mathophysics – Maths (DSE-6)	6
Skill Enhancement Course-IV	SEC-4	2
Skill Enhancement Course-IV	SeC-4	2
Practical *		
	Total Credits	132

<sup>\*</sup>SEC- Papers having only theory will be of 4 Credits in total i.e. no practical class.

Note: Wherever there is a practical there will be no tutorial and vice-versa. The size of the group for chemistry practical papersis recommended to be maximum of 15 to 20 students.

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## **6.2 Details of Courses**

## **CORE COURSES: Industrial Chemistry**

- I. Industrial Chemicals and Environment
- II. Industrial Chemistry -Fossil Fuels, Cleansing Agents and Food Additives
- III. Industrial Chemistry-Inorganic Materials
- IV. Industrial Chemistry Pharmaceuticals, Fermentation, Pesticides & Perfumes

## **CORE COURSES: Chemistry**

- Atomic Structure, Bonding, General Organic Chemistry & Aliphatic Hydrocarbons
- 2. Chemical Energetics, Equilibria & Functional Group Organic Chemistry-I
- 3. Solutions, Phase Equilibrium, Conductance, Electrochemistry & Functional Group Organic Chemistry-II
- 4. Chemistry of s- and p-block elements, States of matter & Chemical kinetics

## **CORE COURSES: Mathophysics**

- 1. Mechanics
- 2. Calculus and Matrices
- 3. Algebra
- 4. Wave and Optics

## **DISCIPLINE SPECIFIC ELECTIVES: Industrial Chemistry (Any two)**

- 1. Green Chemistry
- 2. Analytical Methods in Chemistry
- 3. Polymer Chemistry
- 4. Molecules of life
- 5. Dissertation

## **DISCIPLINE SPECIFIC ELECTIVES Chemistry (Any two)**

- Chemistry of d-Block elements, Quantum Chemistry & Spectroscopy (Compulsory Chemistry DSE-I)
- Organometallics, Bio-inorganic Chemistry, Polynuclear Hydrocarbons and UV,
   IR Spectroscopy
- 3. Applications of Computers in Chemistry
- 4. Molecular Modelling & Drug Design

- 5. Novel Inorganic Solids
- 6. Research Methodology for Chemistry
- 7. Dissertation

## **DISCIPLINE SPECIFIC ELECTIVES Mathophysics**

(One each from Maths and Physics)

- 1. Electricity and Magnetism
- 2. Elements of Modern Physics
- 3. Medical Physics
- 4. Differential Equations
- 5. Calculus and Geometry

## SKILL ENHANCEMENT COURSE Chemistry (Any two)

- 1. IT Skills for Chemists
- 2. Basic Analytical Chemistry
- 3. Chemical Technology and Society
- 4. Cheminformatics
- 5. Analytical Clinical Biochemistry
- 6. Green Methods in Chemistry

## **SKILL ENHANCEMENT COURSE Industrial Chemistry (Any two)**

- 1. Instrumental Methods of Analysis
- 2. Business Skills for Chemist
- 3. Intellectual Property Rights
- 4. Pharmaceuticals Chemistry
- 5. Pesticide Chemistry
- 6. Fuel Chemistry
- 7. Basic Principles and Laboratory Operations

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## 7. Teaching-Learning Process

A student-centered approach, which actively engages the students in the learning process is critical of skills which result in healthy behavior are to be fostered and developed.

The B. Sc. Program with Industrial Chemistry course aims to make the students proficient in industrial chemistry through the transfer of knowledge in the classroom as well as in the laboratory. Industrial Chemistry program is designed to encourage the learning strategies that could be incorporated in a comprehensive approach that includes self-directed learning, cooperative learning, and peer education. In the classroom this will be done through blackboard and chalk lectures, charts, power point presentations, and the use of audio visual resources that are available on the internet such as virtual lab. The process of effective learning to a great extent will be based on teacher's experiences, identifying the slow learners and individual attention of the teacher towards them. A variety of approaches to teachinglearning process, including lectures, seminars, tutorials, workshops, peer teaching and learning, practicum and project-based learning, field-based learning, substantial laboratorybased practical component and experiments, open-ended project work, technology-enabled learning, internship in industry and research establishments will be adopted. Problem-solving skills and higher-order skills of reasoning and analysis will be encouraged through teaching strategies. A feedback method with more anonymity will be preferred. An interactive mode of teaching will be used. The students will be encouraged to participate in the discussions and deliver seminars on the course related topics. A problem solving approach will be adopted wherever suitable. In the laboratory, the students will first learn good laboratory practice and then get hands on training on basic instrumentation techniques and methods. Emphasis on laboratory work is particularly important keeping in mind the practical nature of the subject, and the time devoted to practical will enable the students to better correlate understand the applications of theoretical understandings. The students will participate in field trips to various industries that will facilitate their understanding of the practical aspects of the program and enable them to gain exposure to future places/ areas of employment.

#### 8. Assessment Methods

The assessment of students achievements in Industrial Chemistry will be aligned with the course/program learning outcomes and the academic and professional skills that the program is designed to develop. The students will be assessed over the duration of the program by

many different methods. A variety of appropriate assessment methods within the disciplinary area of industrial chemistry will be used. Learning outcomes will be assessed using the following direct measures:

- Oral and written examinations,
- Closed book and open book tests,
- Classroom quiz,
- Focused group discussion,
- Short objective type quizzes,
- Group discussion and presentations,
- Assignments,
- Problem-solving exercises,
- Experimental design planning,
- Execution of experiments,
- Observation of practical skills,
- Individual project reports,
- Seminar presentation,
- Case study presentations,
- Viva voce interviews,
- Computerized adaptive testing,
- Literature surveys and evaluations,
- Outputs from collaborative work,
- Portfolios on industrial visits undertaken,
- Preparation of reports,
- Presentation of practical records.

Exposure with different colleges and universities from different parts of the nation will be provided to students. Besides standardized tests, interim benchmarks, daily assessments, observations, interaction and formal assessments of each student will be done to enhance his/her overall performance.

Overall, a wide range of assessment approaches those aim to break the monotony of having a single assessment method will be followed.

## **CORE COURSE**

## **SEMESTER 1**

Course Code: CC – IC1:CORE COURSE INDUSTRIAL CHEMISTRY-1

**Course Title: Industrial Chemicals & Environment** 

Total Credits: 06 (Credits: Theory-04, Practical-02)

(Total Lectures: Theory- 60, Practical-60)

## **Objectives**

The aim of this course is to make students aware of different industrial processes in detail. This course is basically designed to understand the chemistry of the industrial processes like Purification techniques, handling of important gases, acids, bases, pollutants, Industrial effluent and water treatment. The analytical approach of this course is to enhance the reasoning and to understand the mechanical part of the industry. The aim of this course is that the students will learn the conventional and latest techniques used in abatement of environmental pollution (air, water and industrial effluents).

## **Learning Outcomes**

## By the end of the course, the students will be able to:

- Know the various purification techniques used in industries like distillation, absorption, adsorption and solvent extraction.
- Understand the production, storage and handling of important gases like-oxygen, argon, helium, hydrogen and acetylene.
- Understand and develop efficacy in handling and preparation of frequently used inorganic chemicals like acids, bases, oxidizing and disinfecting chemicals.
- Learn major causes of air pollution, its control and alarming problem of global warming.
- Know qualitative and quantitative measurements of water treatment, conservation and handling of industrial effluent.

## Unit 1

## **Chemical Technology**

Basic principles of distillation, solvent extraction, solid-liquid leaching and liquid-liquid extraction, separation by absorption and adsorption. An introduction into the scope of different types of equipment needed in chemical technology, including reactors, distillation columns, extruders, pumps, mills, emulgators. Scaling up operations in chemical industry.

(Lectures: 15)

#### Unit 2

## **Industrial Gases and Inorganic Chemicals**

(a) Industrial Gases: Large scale production, uses, storage and hazards in handling of the following gases: oxygen, nitrogen, argon, neon, helium, hydrogen, acetylene, carbon monoxide, chlorine, fluorine, sulphur dioxide and phosgene. (b) Inorganic Chemicals: Industrial preparation with the help of flowchart, application, analysis and hazards in handling the following chemicals: hydrochloric acid, nitric

acid, sulphuric acid, caustic soda, common salt, borax, bleaching powder, sodium thiosulphate, hydrogen peroxide, potash alum, chrome alum, potassium dichromate and potassium permanganate.

(Lectures: 20)

## Unit 3

## **Environment**

- (a) Air Pollution: Pollutants and their sources, pollution by  $SO_2$ ,  $CO_2$ ,  $CO_3$ ,  $CO_4$ ,  $CO_5$ ,  $CO_5$ ,  $CO_5$ ,  $CO_6$ ,  $CO_6$ ,  $CO_7$ ,  $CO_8$ ,
- (b) Water pollution and Water Quality Standards: Pollutants and their sources, Effluent treatment plants (primary, secondary and tertiarytreatment). Industrial effluent from the following industries and their treatment: electroplating, textile, tannery, dairy, petroleum and petrochemicals, agrochemicals, fertilizer. Sludge disposal. Industrial waste management, incineration of waste. Water treatmentand purification (reverse osmosis, electro dialysis, ion exchange). Water quality parameters for waste water, industrial water and domestic water.

(Lectures: 25)

## **Practical**

## (Credits: 02, Laboratory periods: 60)

- 1. Determination of dissolved oxygen in water.
- 2. Determination of Chemical Oxygen Demand (COD)
- 3. Determination of Biological Oxygen Demand (BOD)
- 4. Percentage of available chlorine in bleaching powder.
- Measurement of chloride, sulphate and salinity of water samples by simple titration method. (AgNO<sub>3</sub>and potassium chromate)
- 6. Estimation of total alkalinity of water samples (CO<sub>3</sub><sup>2-</sup>, HCO<sub>3</sub><sup>-</sup>) using double titration method.
- 7. Isolation of compound using solvent extraction method.
- 8. A survey based study on common bio-indicators of pollution and SPM in air samples.
- 9. Preparation of borax and boric acid.
  - 1. Stocchi, E.(1990), Industrial Chemistry, Vol -I, Ellis Horwood Ltd. UK.
  - Kent, J. A. (ed) (1997), Riegel's Handbook of Industrial Chemistry, CBS Publishers, New Delhi.
  - Pani, B. (2017), Textbook of Environmental Chemistry, I.K. International Publishing House.
  - 4. De, A. K. (2012), Environmental Chemistry, New Age International Pvt, Ltd, New Delhi.
  - 5. Khopkar, S.M.(2010), **Environmental Pollution Analysis**, New Age International Publisher.

## **Teaching Learning process**

To accomplish a goal, it is very important to learn in a strategic manner. There are different components of learning and the capacity of each learner varies. 'How' to teach and 'What' to teach in the defined curriculum not only depends on the content and the knowledge of the teacher but critically more so on designing, i.e. how to introduce the concept to the students in a very effective way. Different ways of teaching include classical board teaching method, visual conceptual method, application based practical demonstration of the concept etc. In fact the pedagogy is to make a class interesting and thus learning becomes enjoyable.

## **Assessment Methods**

The effectiveness of learning can be judged by assessing the students. Assessment can be in form of gradedassignments, conventional class tests, class seminars by students on course topics with a view

to strengthening the content through width and depth, end semester university examination for theory and practical.

## **Keywords**

Industrial Chemicals, Purification techniques, Handling of acids and bases, Air pollutants, Industrialeffluents.

Course Code: CC - C1:CORE COURSE CHEMISTRY-1

Course Title: Atomic Structure, Bonding, General Organic Chemistry &

**Aliphatic Hydrocarbons** 

Total Credits: 06 (Credits: Theory-04, Practical-02)

(Total Lectures: Theory- 60, Practical-60)

## **Objectives:**

The course reviews the structure of the atom, which is a necessary pre-requisite in understanding the nature of chemical bonding in compounds. It provides basic knowledge about ionic, covalent and metallic bonding and explains that chemical bonding is best regarded as a continuum between the three cases. It discusses the Periodicity in properties with reference to the *s* and *p* block, which is necessary in understanding their group chemistry. The course is also infused with the recapitulation of fundamentals of organic chemistry and the introduction of a new concept of visualizing the organic molecules in a three-dimensional space. To establish the applications of these concepts, the classes of alkanes, alkenes, alkynes and aromatic hydrocarbons are introduced. The constitution of the course strongly aids in the paramount learning of the concepts and their applications.

## **Learning Outcomes:**

## By the end of the course, the students will be able to:

- Solve the conceptual questions using the knowledge gained by studying the quantum mechanical model of the atom, quantum numbers, electronic configuration, radial and angular distribution curves, shapes of s, p, and d orbitals, and periodicity in atomic radii, ionic radii, ionization energy and electron affinity of elements.
- Draw the plausible structures and geometries of molecules using radius ratio rules, VSEPR theory and MO diagrams (homo- & hetero-nuclear diatomic molecules).
- Understand and explain the differential behavior of organic compounds based on fundamental concepts learnt.
- Formulate the mechanism of organic reactions by recalling and correlating the fundamental properties of the reactants involved.
- Learn and identify many organic reaction mechanisms including free radical substitution, electrophilic addition and electrophilic aromatic substitution.

## Section A: Inorganic Chemistry (Lectures:30)

## Unit 1

## **Atomic Structure**

Review of: Bohr's theory and its limitations, Heisenberg uncertainty principle, Dual behaviour of matter and radiation, De-Broglie's relation, Hydrogen atom spectra, need of a new approach to atomic

structure. What is Quantum mechanics? Time independent Schrodinger equation and meaning of various terms in it. Significance of  $\psi$  and  $\psi^2$ , Schrödinger equation for hydrogen atom, radial and angular parts of the hydogenic wave functions (atomic orbitals) and their variations for 1s, 2s, 2p, 3s, 3p and 3d orbitals (Only graphical representation), radial and angular nodes and their significance, radial distribution functions and the concept of the most probable distance with special reference to 1s and 2s atomic orbitals. Significance of quantum numbers, orbital angular momentum and quantum numbers  $m_1$  and  $m_2$ . Shapes of s, p and d atomic orbitals, nodal planes, discovery of spin, spin quantum number (s) and magnetic spin quantum number ( $m_2$ ).

Rules for filling electrons in various orbitals, electronic configurations of the atoms, stability of half-filled and completely filled orbitals, concept of exchange energy, relative energies of atomic orbitals, anomalous electronic configurations.

(Lectures: 14)

## Unit 2

## **Chemical Bonding and Molecular Structure**

lonic Bonding: General characteristics of ionic bonding, energy considerations in ionic bonding, lattice energy and solvation energy and their importance in the context of stability and solvability of ionic compounds, statement of Born-Landé equation for calculation of lattice energy (no derivation), Born-Haber cycle and its applications, covalent character in ionic compounds, polarizing power and polarizability, Fajan's rules. Ionic character in covalent compounds, bond moment, dipole moment and percentage ionic character.

Covalent bonding: VB Approach: Shapes of some inorganic molecules and ions on the basis of VSEPR (H<sub>2</sub>O, NH<sub>3</sub>, PCl<sub>5</sub>, SF<sub>6</sub>, ClF<sub>3</sub>, SF<sub>4</sub>) and hybridization with suitable examples of linear, trigonal planar, square planar, tetrahedral, trigonal bipyramidal and octahedral arrangements.

Concept of resonance and resonating structures in various inorganic and organic compounds.

MO Approach: Rules for the LCAO method, bonding and antibonding MOs and their characteristics for s-s, s-p and p-p combinations of atomic orbitals, nonbonding combination of orbitals, MO treatment of homonuclear diatomic molecules of 1<sup>st</sup> and 2<sup>nd</sup> periods (including idea of s-p mixing) and heteronuclear diatomic molecules such as CO, NO and NO<sup>+</sup>.

(Lectures: 16)

## Section B: Organic Chemistry (Lectures:30)

## Unit 3

## **Fundamentals of Organic Chemistry**

Electronic displacements: Inductive effect, electromeric effect, resonance, hyperconjugation. Cleavage of bonds: homolysis and heterolysis. Reaction intermediates: carbocations, carbanions and free radicals. Electrophiles and nucleophiles, Aromaticity: benzenoids and Hückel's rule.

(Lectures: 08)

## Unit 4

#### Stereochemistry

Conformations with respect to ethane, butane and cyclohexane, interconversion of Wedge Formula, Newmann, Sawhorse and Fischer representations, concept of chirality (upto two carbon atoms).

configuration: geometrical and optical isomerism; enantiomerism, diastereomerism and meso compounds). Threo and erythro; D and L; cis - trans nomenclature; CIP Rules: R/S (for upto 2 chiral carbon atoms) and E/Z nomenclature (for upto two C=C systems).

(Lectures: 10)

#### Unit 5

## **Aliphatic Hydrocarbons**

Functional group approach for the following reactions: preparations, physical property & chemical reactions to be studied with mechanism in context to their structure.

#### Alkanes:

Preparation: catalytic hydrogenation, Wurtz reaction, Kolbe's synthesis, Grignard reagent.

Reactions: Free radical substitution: Halogenation.

#### Alkenes:

Preparation: Elimination reactions: Dehydration of alcohols and dehydrohalogenation of alkyl halides (Saytzeff's rule); cis alkenes (Partial catalytic hydrogenation) and trans alkenes (Birch reduction).

Reactions: cis-addition (alk. KMnO<sub>4</sub>) and trans-addition (bromine), addition of HX (Markownikoff's and anti-Markownikoff's addition), Hydration, Ozonolysis, oxymecuration-demercuration, Hydroboration-oxidation.

## Alkynes:

Preparation: Acetylene from CaC<sub>2</sub> and conversion into higher alkynes; by dehalogenation of tetrahalides and dehydrohalogenation of vicinal-dihalides.

Reactions: formation of metal acetylides and acidity of alkynes, addition of bromine and alkaline KMnO<sub>4</sub>, ozonolysis and oxidation with hot alk. KMnO<sub>4</sub>. Hydration to form carbonyl compounds

(Lectures: 12)

## **Practical:**

(Credits: 2, Laboratory periods: 60)

Section A: Inorganic Chemistry - Volumetric Analysis

- 1. Estimation of oxalic acid by titrating it with KMnO<sub>4</sub>.
- 2. Estimation of Mohr's salt by titrating it with KMnO<sub>4</sub>.
- 3. Estimation of water of crystallization in Mohr's salt by titrating with KMnO<sub>4</sub>.
- 4. Estimation of Fe (II) ions by titrating it with K<sub>2</sub>Cr<sub>2</sub>O<sub>7</sub> using internal indicator.
- 5. Estimation of Cu (II) ions iodometrically using Na<sub>2</sub>S<sub>2</sub>O<sub>3</sub>.

## Section B: Organic Chemistry

- 1. Purification of organic compound by crystallisation (from water and alcohol) and distillation.
- 2. Criteria of purity: Determination of M.P./B.P.
- 3. Separation of mixtures by chromatography: Measure the Rf value in each case (combination of two compounds to be given)
- a) Identify and separate the components of a given mixture of 2 amino acids (glycine, aspartic acid, glutamic acid, tyrosine or any other amino acid) by radial/ascending paper chromatography.
- b) Identify and separate the sugars present in the given mixture by radial/ascending paper chromatography.

#### References:

## Theory:

- 1. Lee., J. D.(2010), A new Concise Inorganic Chemistry, Pearson Education.
- 2. Huheey, J.E.; Keiter, E.; Keiter, R. (2009), Inorganic Chemistry: Principles of Structure and Reactivity, Pearson Publication.
- 3. Atkins, P.W.; Overton, T.L.; Rourke, J.P.; Weller, M.T.; Armstrong, F.A.(2010), Shriver and Atkin's Inorganic Chemistry, Oxford
- 4. Sykes, P.(2005), A Guide Book to Mechanism in Organic Chemistry, Orient Longman.
- 5. Eliel, E. L. (2000), Stereochemistry of Carbon Compounds, Tata McGraw Hill.
- 6. Morrison, R. N.; Boyd, R. N. **Organic Chemistry**, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- 7. Bahl, A; Bahl, B. S. (2012), Advanced Organic Chemistry, S. Chand.

#### Practical:

- 1. Jeffery, G.H.; Bassett, J.; Mendham, J.; Denney, R.C.(1989), Vogel's Textbook of Quantitative Chemical Analysis, 5th Edn., John Wiley and Sons Inc,.
- 2. Furniss, B.S.; Hannaford, A.J.; Smith, P.W.G.; Tatchell, A.R. (2012), Vogel's Textbook of Practical Organic Chemistry. Pearson.
- 3. Mann, F.G.; Saunders, B.C.(2009), Practical Organic Chemistry, Pearson Education.

## **Teaching Learning Process:**

- · Lectures in class rooms
- Peer assisted learning.
- Hands-on learning using 3-D models, videos, presentations, seminars
- Technology driven learning.
- Industry visits

## **Assessment Methods:**

Assessmentwill be done on the basis of regular class test, presentations and assignments as a part of internal assessment during the course as per the curriculum. End semester university examination will be held for both theory and practical. In practical, assessment will be done based on continuous evaluation, performance in the experiment on the date of examination and viva voce.

## **Keywords**

Atomic structures, Quantum numbers, Lattice energy, Electronic effects, Stereochemistry, Chemistry of aliphatic hydrocarbons.

## **SEMESTER II**

Course Code: CC – IC2:CORE COURSE INDUSTRIAL CHEMISTRY-2

Course Title: Industrial Chemistry-Fossil Fuels, Cleansing Agents and Food

**Additives** 

Total Credits: 06 (Credits: Theory-04, Practical-02)

(Total Lectures: Theory- 60, Practical-60)

## **Course Objective**

After studying this course, student shall be able to understand the different aspects of industrial processes of fossil fuels in detail. Sensible use of limited resources of non-renewable energy and technology investment in improving the production of renewable cleaner energy sources. The analytical approach of this course is to enhance the reasoning and to understand the mechanical part of the industry.

## **Course Learning Outcomes**

#### By the end of the course, the students will be able to:

- Know about fuels, composition, carbonization of coal, gasification, liquefaction, and coal tar based chemicals and layout for key processes in oil refining.
- Understand the role of petroleum and petrochemical industry, composition, applications, process-cracking. Increasing demand of non-petroleum fuels, synthetic fuels. Petrochemical.
- Understand different fossil fuel products and processes, types of lubricants their property based on viscosity index, cloud point, pore point and applications of lubricant in Industry.
- Know types of oils, fat splitting, familiarized with rancidity, saponification value, iodine number, Superiority of synthetic detergent and role of Surfactants.
- Know merits and demerits of synthetic and natural colouring, flavouring and sweetening agents as food additives.

#### Unit 1

**Fuel Chemistry:** Review of energy sources (renewable and non-renewable). Classification of fuels and their calorific value.

- (a) Coal: Introduction of coal, uses of coal (fuel and non-fuel) in various industries (atleast three examples), its types and composition, carbonization of coal. Coal gas, producer gas and water gas—composition and their uses. Industrial methods for the fractionation of coal tar, uses of coal tar based chemicals, Requisites of a good metallurgical coke, Industrial method with flowchart for the coal gasification (Hydro and Catalytic gasification), Coal liquefaction and Solvent refining.
- (b) **Petroleum and Petrochemical Industry**: Composition of crude petroleum, Refining and different types of petroleum products and their applications. Fractional distillation (principle and process), Cracking (thermal and catalytic cracking), Reforming petroleum and non-petroleum fuels (LPG, CNG, LNG, bio-gas, fuels derived from biomass), fuel from waste, synthetic fuels (gaseous and liquids), clean fuels. Petrochemicals: Vinyl acetate, Propylene oxide, Isoprene, Butadiene, Toluene and Xylene.

(c) **Lubricants**: Classification and properties of lubricants- (viscosity index, cloud point, pore point), lubricating oils (conducting and non-conducting) solid and semisolid lubricants, synthetic lubricants.

(Lectures: 40)

#### Unit 2

**Oils and Fats**: Classification of oils, fat splitting, distillation of completely miscible and non-miscible oils, hydrogenation of oils, rancidity, saponification value, iodine number, acid value, soap and synthetic detergent, preparation of soap and detergent, different types of soap and their composition, surfactants (LAS, ABS, LABS), detergent binders and builders.

(Lectures: 15)

## Unit 3

Food additives: A general study of food flavours, colours and preservatives, artificial sweeteners

(Lectures: 5)

#### **Practical**

## (Credits: 02, Laboratory periods: 60)

- 1. Determination of alkali in water samples and soaps.
- 2. Extraction of essential oils from flowers and fruits by soxhlet extraction method.
- 3. Extraction of natural coloring and flavoring agent from flowers and fruits.
- 4. Determination of iodine value of the oils/ fats.
- 5. Determination of saponification value of the oils/ fats.
- 6. Determination of acid value of the oils/ fats.
- 7. Testing of turmeric powder, milk and mustard oil for adulterants.
- 8. Estimation of glucose in food samples.
- 9. Estimation of hardness of water by titration with soap solution.
- 10. Preparation of soap.

## References

- Vermani, O. P.; Narula, A. K. (2004), Industrial Chemistry, Galgotia Publications Pvt. Ltd., New Delhi
- 2. Bhatia, S. C. (2004), Chemical Process Industries, Vol. I & II, CBS Publishers, New Delhi.
- 3. Jain, P. C.; Jain, M. (2013), Engineering Chemistry, Dhanpat Rai & Sons, Delhi.
- Gopalan, R. Venkappayya, D.; Nagarajan, S. (2004), Engineering Chemistry, Vikas Publications.
- 5. Sharma, B. K. (1997), Engineering Chemistry, Goel Publishing House, Meerut

## **Teaching Learning process**

To accomplish a goal, it is very important to learn in a strategic manner. There are different components of learning and the capacity of each learner varies. 'How' to teach and 'What' to teach in the defined curriculum not only depends on the content and the knowledge of the teacher but critically more so on designing, i.e. how to introduce the concept to the students in a very effective way. Different ways of teaching include classical board teaching method, visual conceptual method, application based practical demonstration of the concept etc. In fact the pedagogy is to make a class interesting and thus learning becomes enjoyable.

## **Assessment Methods**

The effectiveness of learning can be judged by assessing the students. Assessment can be in form of gradedassignments, conventional class tests, class seminars by students on course topics with a view to strengthening the content through width and depth, end semester university examination for theory and practical.

## **Keywords**

Renewable and non-renewable resources, Synthetic fuels, calorific value, Refining, Cracking, Petrochemicals, Lubricants, Rancidity, Synthetic Detergents, Food additives.

Course Code: CC - C2:CORE COURSE CHEMISTRY-2

Course Title: Chemical Energetics, Equilibria and Functional Group Organic

**Chemistry-I** 

Total Credits: 06 (Credits: Theory-04, Practical-02)

(Total Lectures: Theory- 60, Practical-60)

## **Objectives:**

The objective of this paper is to develop basic understanding of the chemical energetics, laws of thermodynamics, chemical and ionic equilibrium. It provides basic understanding of the behaviour of electrolytes and their solutions. It acquaints the students with the functional group approach to study organic chemistry. To establish applications of this concept structure, methods of preparation and reactions for the following classes of compounds: Aromatic hydrocarbons, alkyl and aryl halides, alcohols, phenols and ethers, aldehydes and ketones are described. This course helps the students to relate the structure of an organic compound to its physical and chemical properties.

## **Learning Outcomes:**

## By the end of this course, students will be able to:

- Understand the laws of thermodynamics, thermochemistry and equilibria.
- Understand concept of pH and its effect on the various physical and chemical properties
  of the compounds.
- Use the concepts learnt to predict feasibility of chemical reactions and to study the behaviour of reactions in equilibrium.
- Understand the fundamentals of functional group chemistry through the study of methods of preparation, properties and chemical reactions with underlying mechanism.
- Use concepts learnt to understand stereochemistry of a reaction and predict the reaction outcome
- Design newer synthetic routes for various organic compounds.

## Section A: Physical Chemistry (Lectures:30)

## Unit 1

## **Chemical Energetics**

Review of thermodynamics and the laws of thermodynamics, important principles and definitions of thermochemistry, concept of standard state and standard enthalpies of formations, integral and differential enthalpies of solution and dilution, calculation of bond energy, bond dissociation energy and resonance energy from thermochemical data, variation of enthalpy of a reaction with temperature – Kirchhoff's equation., statement of third law of thermodynamics and calculation of absolute entropies of substances.

(Lectures: 8)

## Unit 2

## **Chemical Equilibrium**

Free energy change in a chemical reaction, Thermodynamic derivation of the law of chemical equilibrium, distinction between G and Go, Le Chatelier's principle, relationships between Kp, Kc and Kx for reactions involving ideal gases.

(Lectures: 8)

## Unit 3

## Ionic Equilibria

Strong, moderate and weak electrolytes, degree of ionization, factors affecting degree of ionization,Ostwald's dilution law, ionization constant and ionic product of water, ionization of weak acids and bases, pH scale, common ion effect, salt hydrolysis-calculation of hydrolysis constant, degree of hydrolysis and pH for different salts. Buffer solutions,Henderson-Hasselbach equation.Solubility and solubility product of sparingly soluble salts – applications of solubility product principle

(Lectures: 14)

## Section B: Organic Chemistry (Lectures: 30)

## Unit 4

#### **Aromatic Hydrocarbons**

Structure and aromatic character of benzene.

Preparation: methods of preparation of benzene from phenol, benzoic acid, acetylene and benzene sulphonic acid.

Reactions: electrophilic substitution reactions in benzene citing examples of nitration, halogenation, sulphonation and Friedel-Craft's alkylation and acylation with emphasis on carbocationic rearrangement, side chain oxidation of alkyl benzenes.

(Lectures: 5)

## Unit 5

## Alkyl and Aryl Halides

A) Alkyl halides (upto 5 carbons):

Structure of haloalkanes and their classification as 1°, 2° & 3°.

Preparation: starting from alcohols (1°, 2° & 3°) and alkenes with mechanisms.

Reactions: Nucleophilic substitution reactions with mechanism and their types ( $S_N1$ ,  $S_N2$  and  $S_Ni$ ), competition with elimination reactions (elimination vs substitution), nucleophilic substitution reactions with specific examples from: hydrolysis, nitrite & nitro formation, nitrile & isonitrile formation and Williamson's ether synthesis.

B) Haloarenes:

Structure and resonance

Preparation: Methods of preparation of chloro, bromo & iodobenzene from benzene (electrophilic substitution), from phenols (nucleophilic substitution reaction) and from aniline (Sandmeyer and Gattermann reactions).

Reaction: Nucleophilic aromatic substitution by OH group (Bimolecular Displacement Mechanism), Effect of nitro substituent on reactivity of haloarenes, Reaction with strong bases NaNH<sub>2</sub>/NH<sub>3</sub> (elimination-addition mechanism involving benzyne intermediate), relative reactivity and strength of C-X bond in alkyl, allyl, benzyl, vinyl and aryl halides.

(Lectures:11)

#### Unit 6

## Alcohols, Phenols, Ethers, Aldehydes and Ketones (Aliphatic and Aromatic)

A) Alcohols (upto 5 Carbon):

Structure and classification of alcohols as 1°, 2° & 3°.

Preparation: Methods of preparation of 1°, 2° & 3° by using Grignard reagent, ester hydrolysis and reduction of aldehydes, ketones, carboxylic acids and esters.

Reactions: Acidic character of alcohols and reaction with sodium, with HX (Lucas Test), esterification, oxidation (with PCC, alkaline KMnO<sub>4</sub>, acidic K<sub>2</sub>Cr<sub>2</sub>O<sub>7</sub> and conc. HNO<sub>3</sub>), Oppeneauer Oxidation.

- B) Diols (upto 6 Carbons): Oxidation and Pinacol-Pinacolone rearrangement.
- C) Phenols: acidity of phenols and factors affecting their acidity.

Preparation: Methods of preparation from cumene, diazonium salts and benzene sulphonic acid.

Reactions: Directive influence of OH group and Electrophilic substitution reactions, viz. nitration, halogenation, sulphonation, Reimer-Tiemann reaction, Gattermann–Koch reaction, Houben-Hoesch condensation, reaction due to OH group: Schotten-Baumann reaction

D) Ethers (Aliphatic & Aromatic):

Williamson's ether synthesis, Cleavage of ethers with HI

E) Aldehydes and ketones (Aliphatic and Aromatic):

Preparation: from acid chlorides and from nitriles.

Reactions: Nucleophilic addition, nucleophilic addition – elimination reaction including reaction with HCN, ROH, NaHSO $_3$ , NH $_2$ -G derivatives. Iodoform test, Aldol Condensation, Cannizzaro's reaction, Wittig reaction, Benzoin condensation. Clemmensen reduction, Wolff Kishner reduction, Meerwein-Pondorff Verley reduction.

(Lectures:14)

## **Practical:**

(Credits: 2, Laboratory periods: 60)

**Section A: Physical Chemistry** 

## **Energetics:**

- 1. Determination of heat capacity of calorimeter.
- 2. Determination of enthalpy of neutralization of hydrochloric acid with sodium hydroxide.
- 3. Determination of integral enthalpy of solution of salts (KNO<sub>3</sub>, NH<sub>4</sub>Cl).
- 4. Determination of enthalpy of hydration of copper sulphate.

## Ionic equilibria:

 Preparation of buffer solutions: (i) Sodium acetate-acetic acid or (ii) Ammonium chloride-ammonium acetate. Measurement of the pH of buffer solutions and comparison of the values with theoretical values.

## **Section B: Organic Chemistry**

**Preparations:** (Mechanism of various reactions involved to be discussed)

(Recrystallization, determination of melting point and calculation of quantitative yields to be done in all cases)

- 1. Bromination of phenol/aniline
- 2. Benzoylation of amines/phenols
- 3. Oxime of aldehydes and ketones
- 4. 2,4-dinitrophenylhydrazone of aldehydes and ketones
- 5. Semicarbazone of aldehydes and ketones

## **References:**

## Theory:

- 1. Castellan, G. W. (2004), Physical Chemistry, Narosa.
- Kapoor, K.L. (2015), A Textbook of Physical Chemistry, Vol 1, 6<sup>th</sup> Edition, McGraw Hill Education.
- 3. Kapoor, K.L.(2015), **A Textbook of Physical Chemistry**, Vol 2, 6<sup>th</sup> Edition,McGraw Hill Education.

- 4. Rastogi, R.P.; Mishra,R.R. (2009), **Chemical Thermodynamics**, 6<sup>th</sup> Edition, Vikas Publishing House Pvt. Ltd.
- 5. B.R.Puri, L.R.Sharma, M.S.Pathania, (2017), **Principles of Physical Chemistry**, Vishal Publishing Co.
- Finar, I. L. Organic Chemistry (Volume 1 & 2), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- 7. Morrison, R. N.; Boyd, R. N. **Organic Chemistry**, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- 8. Bahl, A; Bahl, B. S. (2012), Advanced Organic Chemistry, S. Chand.

## Practical:

- Khosla, B.D.; Garg, V.C.; Gulati, A.(2015), Senior Practical Physical Chemistry, R. Chand & Co.
- 2. Furniss, B.S.; Hannaford, A.J.; Smith, P.W.G.; Tatchell, A.R. (2012), Vogel's Textbook of Practical Organic Chemistry, Pearson.
- 3. Mann, F.G.; Saunders, B.C. (2009), Practical Organic Chemistry, Pearson Education.

## **Additional Resources:**

- 1. Mahan, B. H.(2013), University Chemistry, Narosa.
- 2. Barrow, G.M. (2006). Physical Chemistry, 5th Edition, McGraw Hill.

## **Teaching Learning Process:**

- The teaching learning process will involve the blended learning technique along with traditional chalk and black board method wherever required.
- Certain topics like stereochemistry of nucleophilic substitution, elimination reactions and their underlying stereochemistry, where traditional chalk and talk method may not be able to convey the concept, are especially taught through audio-visual aids.
- Students are encouraged to participate actively in the classroom through regular presentations on curriculum based topics.

## **Assessment Methods:**

Assessmentwill be done on the basis of regular class test, presentations and assignments as a part of internal assessment during the course as per the curriculum. End semester university examination will be held for both theory and practical. In practical, assessment will be done based on continuous evaluation, performance in the experiment on the date of examination and viva voce.

## **Keywords:**

Chemical energetics, Feasibility of reaction, Hydrocarbons, Haloalkanes and haloarenes, Alcohols, Phenols and Ethers, Aldehydes and Ketones.

B.Sc. Industrial Chemistry University of Delhi

## **SEMESTER III**

Course Code: CC – IC3: CORE COURSE INDUSTRIAL CHEMISTRY-3

**Course Title: Industrial Chemistry-Inorganic Materials** 

Total Credits: 06 (Credits: Theory-04, Practical-02)

(Total Lectures: Theory- 60, Practical-60)

## **Course Objective**

The paper imparts basic knowledge of chemistry of inorganic materials such as silicates, non-silicates, ceramics, cement. This paper is designed in such a way that it will enrich students with the knowledge of various type of surface coatings, fillers, thinners, enamels, emulsifying agents. The paper has been drafted to impart the theoretical and practical knowledge of estimation and determination of various industrially important chemicals.

## **Course Learning Outcomes**

## By the end of this course, students will be able to:

- Establish an appreciation of the role of inorganic chemistry in the chemical sciences.
- Gain sound knowledge of inorganic materials like silicates, ceramics and cement.
- Develop skills to estimate various components of fertilizers.
- Understand the ethical, historic, philosophical, and environmental dimensions of problems and issues facing industrial chemists.
- Get skilled in scientific method of planning, developing, conducting, reviewing and reporting experiments.
- Identify various concepts of industrial metallurgy which will help them to explore new innovative areas of research.
- Know scientific methods employed in inorganic chemistry.

## Unit 1

#### Silicate Industries

- (a) Glass: Glassy state and its properties, Classification (silicate and non-silicate glasses). Manufacture and processing of glass. Composition and properties of the following: Soda lime glass, lead glass, armoured glass, safety glass, borosilicate glass, fluorosilicate, coloured glass and photosensitive glass.
- (b) Ceramics: Ceramic, their types and manufacture. High technology ceramics and their applications, super conducting and semi conducting oxides, fullerenes carbon nanotubes and carbon fiber, clays and feldspar.
- (c) Cement: Classification of cement, ingredients and their role. Manufacture of cement and the setting process, quick setting cements

(Lectures: 18)

## Unit 2

## **Surface Coatings**

Objectives of surface coatings, preliminary treatment of surface and classification of surface coatings.

Paints and pigments - formulation, composition and related properties. Oil paint, Vehicle oils, modified oils, Pigments, toners and lakes pigments, fillers, thinners, enamels, emulsifying agents. Special paints (heat retardant, fire retardant, eco- friendly and plastic paint), wax polish, water and oil paints, additives.

Metallic coatings (electrolytic and electroless), metal spraying and anodizing.

(Lectures: 12)

#### Unit 3

#### **Batteries**

Primary and secondary batteries, battery components and their role and characteristics of battery. Working of following batteries: Pb acid, Li-Battery, solid state electrolyte battery.

Fuel Cells, Solar cell and polymer cell.

(Lectures: 10)

## Unit 4

#### **Alloys**

Classification of alloys, ferrous and non-ferrous alloys, specific properties of elements in alloys.

Industrial manufacture of steel (removal of silicon decarbonization, demagnetization, desulphurization dephosphorisation) and surface treatment (argon treatment, heat treatment, nitriding, carburizing).

Composition and properties of different types of steel.

(Lectures: 10)

## Unit 5

## **Industrial Metallurgy**

Preparation of metals (ferrous and nonferrous) and ultra pure metals for semiconductor technology.

(Lectures: 2)

#### Unit 6

#### **Fertilizers**

Different types of fertilizers (N, P and K). Importance of fertilizers, chemistry involved in the manufacture of the following fertilizers: urea, ammonium nitrate, calcium ammonium nitrate, ammonium phosphates, superphosphate of lime, potassium chloride and potassium nitrate.

(Lectures: 8)

## **Practical:**

#### (Credits: 2, Laboratory periods: 60)

- 1. Preparation of carbon nanotubes (CNTs).
- 2. Preparation of paints.
- 3. Determination of metal ions using complexometric titration.
- 4. Analysis of (Cu, Ni) (Cu, Zn) in alloy or synthetic samples.
- 5. Preparation of pigment (zinc oxide).
- 6. Study the loss of raw iron in acidic medium.
- 7. Study the loss of raw iron in basic medium.
- 8. Detection of constituents of Ammonium Sulphate fertilizer (Ammonium and Sulphate ions) by qualitative analysis and determine its free acidity.
- Detection of constituents of CAN fertilizer (Calcium, Ammonium and Nitrate ions) fertilizer and estimation of Calcium content.
- 10. Detection of constituents of Superphosphate fertilizer (Calcium and Phosphate ions) and estimation of phosphoric acid content.

11. Detection of constituents of Dolomite (Calcium, Magnesium and carbonate ions) and determination of composition of Dolomite (Complexometric titration).

## References

- 1. Stocchi, E.(1990), Industrial Chemistry, Vol -I, Ellis Horwood Ltd. UK.
- 2. Felder, R. M.; Rousseau, R. W. (2015), **Elementary Principles of Chemical Processes**, Wiley Publishers, New Delhi.
- 3. Kingery, W. D.;Bowen, H. K.;Uhlmann, D. R. (1976), Introduction to Ceramics, Wiley Publishers, New Delhi.
- Kent, J. A. (ed) (1997), Riegel's Handbook of Industrial Chemistry, CBS Publishers, New Delhi.
- 5. Jain, P. C.; Jain, M. (2013), Engineering Chemistry, Dhanpat Rai & Sons, Delhi.

## **Teaching Learning process**

To accomplish a goal, it is very important to learn in a strategic manner. There are different components of learning and the capacity of each learner varies. 'How' to teach and 'What' to teach in the defined curriculum not only depends on the content and the knowledge of the teacher but critically more so on designing, i.e. how to introduce the concept to the students in a very effective way. Different ways of teaching include classical board teaching method, visual conceptual method, application based practical demonstration of the concept etc. In fact the pedagogy is to make a class interesting and thus learning becomes enjoyable.

## **Assessment Methods**

The effectiveness of learning can be judged by assessing the students. Assessment can be in form of gradedassignments, conventional class tests, class seminars by students on course topics with a view to strengthening the content through width and depth, end semester university examination for theory and practical.

## **Keywords**

Glass, Ceramics, Cements, Surface coatings, Alloys, Primary and Secondary batteries, Fullerenes.

Course Code: CC - C3: CORE COURSE CHEMISTRY-3

Course Title: Solutions, Phase Equilibrium, Conductance, Electrochemistry

and Functional Group Organic Chemistry-II

Total Credits: 06 (Credits: Theory-04, Practical-02)

(Total Lectures: Theory- 60, Practical-60)

## **Objectives:**

The students will learn about ideal and non-ideal solutions, Raoult's law, partially miscible and immiscible solutions and their applications. The student will also learn about equilibrium between phases with emphasis on one component and simple eutectic systems. In electrochemical cells the students will learn about electrolytic and galvanic cells, measurement of conductance and its applications, measurement of emf and its applications. The topics of carbohydrates, amino acids,

peptides and proteins are introduced through some specific examples. A relationship between structure, reactivity and biological properties of biomolecules is established through the study of these representative biomolecules.

## **Learning Outcomes:**

## By the end of the course, the students will be able to:

- Explain the concepts of different types of binary solutions-miscible, partially miscible and immiscible along with their applications.
- Explain the thermodynamic aspects of equilibria between phases and draw phase diagrams of simple one component and two component systems.
- Explain the factors that effect conductance, migration of ions and application of conductance measurement.
- Understand different types of galvanic cells, their Nernst equations, measurement of emf, calculations of thermodynamic properties and other parameters from the emf measurements.
- Understand and demonstrate how the structure of biomolecules determines their chemical properties, reactivity and biological uses.
- Design newer synthetic routes for various organic compounds.

## Section A: Physical Chemistry (Lectures:30)

## Unit 1

#### **Solutions**

Thermodynamics of ideal solutions: Ideal solutions and Raoult's law, deviations from Raoult's law-non-ideal solutions. Vapour pressure, composition and temperature-composition curves of ideal and non-ideal solutions. Distillation of solutions, Lever rule, Azeotropes. Partial miscibility of liquids: Critical solution temperature; effect of impurity on partial miscibility of liquids. Immiscibility of liquids: principle of steam distillation, Nernst distribution law and its applications, solvent extraction.

(Lectures: 6)

## Unit 2

## **Phase Equilibrium**

Phases, components and degrees of freedom of a system, criteria of phase equilibrium, Gibbs phase rule and its thermodynamic derivation, derivation of Clausius- Clapeyron equation and its importance in phase equilibria, phase diagrams of one component systems (water and sulphur) and two component systems involving eutectics, congruent and incongruent melting points (lead-silver, FeCl<sub>3</sub>-H<sub>2</sub>O and Na-K only).

(Lectures: 6)

## Unit 3

#### Conductance

Conductivity, equivalent and molar conductivity and their variation with dilution for weak and strong electrolytes, Kohlrausch Law of independent migration of ions, transference number and its experimental determination using Hittorf and moving boundary methods, Ionic mobility, applications of conductance measurements: determination of degree of ionization of weak electrolytes, solubility and

solubility products of sparingly soluble salts, ionic product of water, hydrolysis constant of a salt. Conductometric titrations (only acid-base).

(Lectures: 8)

## Unit 4

## Electrochemistry

Reversible and irreversible cells, concept of EMF of a cell, measurement of EMF of a cell, Nernst equation and its importance, types of electrodes, standard electrode potential, electrochemical series. thermodynamics of a reversible cell, calculation of thermodynamic properties: G, H and S from EMF data. Calculation of equilibrium constant from EMF data, concentration cells with transference and without transference, liquid junction potential and salt bridge, pH determination using hydrogen electrode and quinhydrone electrode, Potentiometric titrations-qualitative treatment (acid-base and oxidation-reduction only).

(Lectures: 10)

## Section B: Organic Chemistry (Lectures:30)

## Unit 5

Functional group approach for the following reactions: Preparations, physical & chemical properties to be studied in context to their structure with mechanism.

## A) Carboxylic acids and their derivatives (aliphatic and aromatic)

Preparation: Acidic and alkaline hydrolysis of esters.

Reactions: Hell-Volhard Zelinsky reaction, acidity of carboxylic acids, effect of substitution on acid strength.

Carboxylic acid derivatives (aliphatic):

Preparation: Acid chlorides, anhydrides, esters and amides from acids and their interconversion, Claisen condensation.

Reactions: Relative reactivities of acid derivatives towards nucleophiles, Reformatsky reaction, Perkin condensation.

## B) Amines (aliphatic & aromatic) and Diazonium Salts

#### **Amines**

Preparation: from alkyl halides, Gabriel's Phthalimide synthesis, Hofmann Bromamide reaction.

Reactions: Hofmann vs Saytzeff elimination, carbylamine test, Hinsberg test, reaction with HNO<sub>2</sub>, Schotten-Baumann reaction. Electrophilic substitution (case aniline): nitration, bromination, sulphonation, basicity of amines.

Diazonium salt

Preparation: from aromatic amines

Reactions: conversion to benzene, phenol and dyes.

(Lectures: 13)

#### Unit 6

#### Amino Acids, Peptides and Proteins

Zwitterion, isoelectric point and electrophoresis

Preparation of amino acids: Strecker synthesis and using Gabriel's phthalimide synthesis.

Reactions of amino acids: ester of -COOH group, acetylation of -NH<sub>2</sub> group, complexation with Cu<sup>2+</sup> ions, ninhydrin test.

Overview of Primary, Secondary, Tertiary and Quaternary Structure of proteins.

Determination of primary structure of peptides by degradation Edmann degradation (N- terminal) and C-terminal (thiohydantoin and with carboxypeptidase enzyme). Synthesis of simple peptides (upto dipeptides) by N-protection (t-butyloxycarbonyl and phthaloyl) & C- activating groups and Merrifield solid-phase synthesis.

(Lectures: 9)

#### B) Carbohydrates

Classification, and general properties, glucose and fructose (open chain and cyclic structure), determination of configuration of monosaccharides, absolute configuration of glucose and fructose, mutarotation, ascending and descending in monosaccharides. Structure of disaccharides (sucrose, cellobiose, maltose, lactose) and polysaccharides (starch and cellulose) excluding their structure elucidation.

(Lectures:8)

#### **Practical:**

(Credits: 2, Laboratory periods: 60)

Section A: Physical Chemistry

## Phase Equilibria

- 1. Construction of the phase diagram of a binary system (simple eutectic) using cooling curves.
- 2. Determination of critical solution temperature and composition of phenol water system and study the effect of impurities on it.

#### Conductance

- 1. Determination of cell constant.
- Determination of equivalent conductance, degree of dissociation and dissociation constant of a weak acid.
- 3. Perform the following conductometric titrations:
  - a) Strong acid vs strong base
  - b) Weak acid vs strong base.

#### **Potentiometry**

Perform the potentiometric titrations of (i) Strong acid vs strong base and (ii) Weak acid vs strong base.

#### **Section B: Organic Chemistry**

Systematic qualitative analysis of organic compounds possessing monofunctional groups (Alcohols, Phenols, Carbonyl, -COOH). (Including Derivative Preparation).

#### **References:**

- 1. Barrow, G.M. (2006), **Physical Chemistry**, 5<sup>th</sup> Edition,McGraw Hill.
- 2. Castellan, G.W. (2004), Physical Chemistry, Narosa.
- 3. Kapoor, K.L. (2015), A Textbook of Physical Chemistry, Vol 1, 6th Edition, McGraw Hill Education.
- Kapoor, K.L. (2013), A Textbook of Physical Chemistry, Vol 3, 3<sup>rd</sup> Edition, McGraw Hill Education.
- 5. B.R.Puri, L.R.Sharma, M.S.Pathania, (2017), **Principles of Physical Chemistry**, Vishal Publishing Co.
- 6. Morrison, R. N.; Boyd, R. N. **Organic Chemistry**, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- 7. Finar, I. L. **Organic Chemistry** (Volume 1 & 2), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).

# **Teaching Learning Process:**

- Teaching Learning Process for the course is visualized as largely student-focused.
- Transaction through an intelligent mix of conventional and modern methods.
- Engaging students in cooperative learning.
- Learning through quiz design.
- Problem solving to enhance comprehension.

#### **Assessment Methods:**

Assessmentwill be done on the basis of regular class test, presentations and assignments as a part of internal assessment during the course as per the curriculum. End semester university examination will be held for both theory and practical. In practical, assessment will be done based on continuous evaluation, performance in the experiment on the date of examination and viva voce.

# **Keywords:**

Raoult's law, Lever rule, azeotropes, critical solution temperature, transference number, EMF, Carboxylic acids and derivatives, Amines and diazonium salts, Polynuclear and heterocyclic compounds.

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# **SEMESTER IV**

Course Code: CC – IC4: CORE COURSE INDUSTRIAL CHEMISTRY-4
Course Title: Pharmaceuticals, Fermentation, Pesticides and Perfumes

Total Credits: 06 (Credits: Theory-04, Practical-02)

(Total Lectures: Theory- 60, Practical-60)

# **Course Objective**

The objectives of this paper are to provide basic knowledge of chemistry of pharmaceuticals, cosmetics, perfumes and pesticides considering their importance for human beings. This paper designed in a manner that it forms a cardinal part of the learning of industrial chemistry for the students. The paper has been designed to impart the theoretical and practical knowledge on the basic chemistry and uses of various pharmaceuticals, cosmetic products and pesticides.

# **Course Learning Outcomes**

#### By the end of the course, the students will be able to:

- Have sound knowledge of pharmaceuticals, cosmetics, perfumes and pesticides.
- Become well equipped to design, carry out, record and analyze the industrial preparations
- Understand the ethical, historic, philosophical, and environmental dimensions of problems and issues facing industrial chemists.
- Become skilled in problem solving, critical thinking and analytical reasoning.
- Identify and solve chemical problems and explore new innovative areas of research.
- Know the proper procedures and regulations for safe handling and use of chemicals and can follow the proper procedures.

## Unit 1

#### **Drugs and Pharmaceuticals**

Drug discovery, design and development; Retrosynthetic approach (with any two examples).

Synthesis of the representative drugs of the following classes: analgesics, antipyretics, anti-inflammatory agents (Aspirin, Paracetamol. Ibuprofen), antibiotics (Penicillin, Cephalosporin, Chloromycetin, Streptomycin and Chloramphenicol); antibacterial and antifungal agents (Sulphonamides, Sulphanethoxazol, Sulphacetamide, Trimethoprim); antiviral agents (Acyclovir). Central Nervous System agents (Phenobarbital, Diazepam), Cardiovascular drugs (Glyceryl trinitrate), antileprosy drug (Dapsone), HIV-AIDS related drugs (AZT- Zidovudine).

(Lectures: 20)

#### Unit 2

# **Cosmetics and Perfumes**

Introduction to cosmetics and perfumes, preparation and uses of the following: Hair dye, hair spray. Shampoo. Sun-tan lotions, face powder, lipsticks. talcum powder, nail enamel, creams (cold, vanishing and shaving creams), antiperspirants and artificial flavours.

Essential oils and their importance in cosmetic industries with reference to Eugenol. Geraniol, Sandalwood oil, Eucalyptus, Rose oil, Jasmone, Civetone, Muscone

(Lectures: 15)

#### Unit 3

#### **Pesticides**

Introduction to pesticides (natural and synthetic), benefits and adverse effects, changing concepts of pesticides.

Structure activity relationship, synthesis and technical manufacture, uses of representative pesticides in the following classes: Organochlorines (DDT, Gammaxene), Organophosphates (Malathion, Parathion), Carbamates (Carbofuran and carbaryl), Quinones (Chloranil), Anilides (Alachlor and Butachlor).

(Lectures: 15)

## Unit 4

#### **Fermentation**

Aerobic and anaerobic fermentation. Production of (i) Ethyl alcohol and citric acid; (ii) Lysine, Glutamic acid, Vitamin B2, Vitamin B12, Vitamin C.

(Lectures: 10)

## **Practical**

# (Credits: 02, Laboratory periods: 60)

- 1. Preparation of talcum powder.
- 2. Preparation of shampoo.
- 3. Preparation of nail enamel
- 4. Preparation of hair remover.
- 5. Preparation of face cream.
- 6. Preparation of Aspirin and its analysis.
- 7. Preparation of nail polish and nail polish remover.
- 8. To calculate acidity/alkalinity in given sample of pesticide formulations as per BIS specifications.
- 9. Preparation of Antacid.
- 10. Preparation of paracetamol.
- 11. Estimation of free acidity in ammonium sulphate fertilizers

#### References

- Vermani, O. P.; Narula, A. K. (2004), Industrial Chemistry, Galgotia Publications Pvt. Ltd., New Delhi.
- 2. Bhatia, S. C. (2004), Chemical Process Industries, Vol. I & II, CBS Publishers, New Delhi.
- 3. Barel, A.O.; Paye, M.; Maibach, H.I.(2014), Handbook of Cosmetic Science and Technology, CRC Press.
- Gupta, P.K.: Gupta, S.K. (2011). Pharmaceutics and Cosmetics. Pragati Prakashan
- 5. Butler, H. (2000), Poucher's Perfumes, Cosmetic and Soap, Springer

# **Teaching Learning process**

To accomplish a goal, it is very important to learn in a strategic manner. There are different components of learning and the capacity of each learner varies. 'How' to teach and 'What' to teach in the defined curriculum not only depends on the content and the knowledge of the teacher but critically more so on designing, i.e. how to introduce the concept to the students in a very effective way. Different ways of teaching include classical board teaching method, visual conceptual method, application based practical demonstration of the concept etc. In fact the pedagogy is to make a class interesting and thus learning becomes enjoyable.

#### **Assessment Methods**

The effectiveness of learning can be judged by assessing the students. Assessment can be in form of gradedassignments, conventional class tests, class seminars by students on course topics with a view to strengthening the content through width and depth, end semester university examination for theory and practical.

# **Keywords**

Drugs, Pharmaceuticals, Pesticides, Cosmetic Products, Perfumes, Flavours, Ingredients, Formulations, Raw materials.

Course Code: CC – C4: CORE COURSE CHEMISTRY-4

Course Title: Chemistry of s- and p-Block Elements, States of Matter and

**Chemical Kinetics** 

Total Credits: 06 (Credits: Theory-04, Practical-02)

(Total Lectures: Theory- 60, Practical-60)

# **Objectives:**

The objective of this paper is to provide basic understanding of the fundamental principles of metallurgy through study of the methods of extraction of metals, recovery of the by-products during extraction, applications of metals, alloy behaviour and their manufacturing processes. The course illustrates the diversity and fascination of inorganic chemistry through the study of properties and utilities of s- and p-block elements and their compounds. The students will learn about the properties of ideal and real gases and deviation from ideal behaviour, properties of liquid, types of solids with details about crystal structure. The student will also learn about the reaction rate, order, activation energy and theories of reaction rates.

# **Learning Outcomes:**

#### By the end of the course, the students will be able to:

- Understand the chemistry and applications of s- and p-block elements.
- Derive ideal gas law from kinetic theory of gases and explain why the real gases deviate from ideal behaviour.
- Explain Maxwell-Boltzmann distribution, critical constants and viscosity of gases.
- Explain the properties of liquids especially surface tension and viscosity.
- Explain symmetry elements, crystal structure specially NaCl, KCl and CsCl
- Define rate of reactions and the factors that affect the rates of reaction.
- Understand the concept of rate laws e.g., order, molecularity, half-life and their determination
- Learn about various theories of reaction rates and how these account for experimental observations.

Section A: Inorganic Chemistry (Lectures:30)

#### Unit 1

## **General Principles of Metallurgy**

Chief modes of occurrence of metals based on standard electrode potentials. Ellingham diagrams for reduction of metal oxides using carbon as reducing agent.

Hydrometallurgy with reference to cyanide process for silver and gold, Methods of purification of metals (Al, Pb, Ti, Fe, Cu, Ni, Zn): electrolytic, oxidative refining, van Arkel-de Boer process, Mond's process and Zone Refining.

(Lectures: 4)

## Unit 2

## s- and p- block elements

Periodicity in s- and p-block elements with respect to electronic configuration, atomic and ionic size, ionization enthalpy, electronegativity (Pauling, Muliken, and Allred-Rochow scales). Allotropy in C, S, and P. Oxidation states with reference to elements in unusual and rare oxidation states like carbides and nitrides), inert pair effect, diagonal relationship and anomalous behaviour of first member of each group. ,compounds of s- and p-block elements, diborane and concept of multicentre bonding. Structure, bonding and their important properties like oxidation/reduction, acidic/basic nature of the following compounds and their applications in industrial and environmental chemistry. Hydrides of nitrogen (NH<sub>3</sub>, N<sub>2</sub>H<sub>4</sub>, N<sub>3</sub>H, NH<sub>2</sub>OH) Oxoacids of P, S and Cl, Halides and oxohalides: PCl<sub>3</sub>, PCl<sub>5</sub>, SOCl<sub>2</sub> and SO<sub>2</sub>Cl<sub>2</sub>.

(Lectures: 26)

## Section B: Physical Chemistry (Lectures:30)

#### Unit 3

#### **Kinetic Theory of Gases**

Postulates of kinetic theory of gases and derivation of the kinetic gas equation, deviation of real gases from ideal behaviour, compressibility factor, causes of deviation, van der Waals equation of state for real gases. Boyle temperature (derivation not required), critical phenomena, critical constants and their calculation from van der Waals equation, Andrews isotherms of CO<sub>2</sub>, Maxwell Boltzmann distribution laws of molecular velocities and molecular energies (graphic representation – derivation not required) and their importance. Temperature dependence of these distributions, most probable, average and root mean square velocities (no derivation), collision cross section, collision number, collision frequency, collision diameter and mean free path of molecules, viscosity of gases and effect of temperature and pressure on coefficient of viscosity (qualitative treatment only).

(Lectures: 10)

#### Unit 4

# Liquids

Surface tension and its determination using stalagmometer, Viscosity of a liquid and determination of coefficient of viscosity using Ostwald viscometer, effect of temperature on surface tension and coefficient of viscosity of a liquid (qualitative treatment only).

(Lectures: 3)

# Unit 5

#### **Solids**

Forms of solids, symmetry elements, unit cells, crystal systems, Bravais lattice types and identification of lattice planes. Laws of crystallography - law of constancy of interfacial angles.

Law of rational indices, Miller indices. X–ray diffraction by crystals, Bragg's law, structures of NaCl, KCl and CsCl (qualitative treatment only), defects in crystals. Glasses and liquid crystals.

(Lectures: 6)

#### Unit 6

#### **Chemical Kinetics**

The concept of reaction rates, effect of temperature, pressure, catalyst and other factors on reaction rates. Order and molecularity of a reaction, derivation of integrated rate equations for zero, first and second order reactions (both for equal and unequal concentrations of reactants), half—life of a reaction, general methods for determination of order of a reaction, Concept of activation energy and its calculation from Arrhenius equation.

Theories of reaction rates: Collision theory and activated complex theory of bi-molecular reactions. Comparison of the two theories (qualitative treatment only)

(Lectures: 11)

# **Practical:**

#### (Credits: 2, Laboratory periods: 60)

#### **Section A: Inorganic Chemistry**

Semi-micro qualitative analysis of mixtures using  $H_2S$  or any other scheme- not more than four ionic species (two anions and two cations and excluding insoluble salts) out of the following:

Cations: NH<sub>4</sub>+, Pb<sup>2+</sup>, Bi<sup>3+</sup>, Cu<sup>2+</sup>, Cd<sup>2+</sup>, Fe<sup>3+</sup>, Al<sup>3+</sup>, Co<sup>2+</sup>, Ni<sup>2+</sup>, Mn<sup>2+</sup>, Zn<sup>2+</sup>, Ba<sup>2+</sup>, Sr<sup>2+</sup>, Ca<sup>2+</sup>, K<sup>+</sup>

Anions: CO<sub>3</sub><sup>2-</sup>, S<sup>2-</sup> , SO<sub>3</sub><sup>-</sup> , NO<sub>2</sub><sup>-</sup> , CH<sub>3</sub>COO<sup>-</sup>, Cl<sup>-</sup>, Br<sup>-</sup>, l<sup>-</sup>, NO<sub>3</sub><sup>-</sup>, SO<sub>4</sub><sup>2-</sup> , PO<sub>4</sub><sup>3-</sup> , BO<sub>3</sub><sup>3-</sup> , C<sub>2</sub>O<sub>4</sub><sup>2-</sup>, F<sup>-</sup>.

(Spot tests should be carried out wherever feasible)

#### **Section B: Physical Chemistry**

1. Surface tension measurement (use of organic solvents excluded):

Determination of the surface tension of a liquid or a dilute solution using a stalagmometer.

- 2. Viscosity measurement (use of organic solvents excluded):
  - a) Determination of the relative and absolute viscosity of a liquid or dilute solution using an Ostwald viscometer.

- b) Study of the variation of viscosity of an aqueous solution with concentration of solute.
- 3. Chemical Kinetics

Study the kinetics of the following reactions by integrated rate method:

- a) Acid hydrolysis of methyl acetate with hydrochloric acid.
- b) Compare the strength of HCl and H<sub>2</sub>SO<sub>4</sub> by studying the kinetics of hydrolysis methyl acetate.

## References:

#### Theory:

- 1. Lee., J. D.(2010), A new Concise Inorganic Chemistry, Pearson Education.
- 2. Atkins, P.W.; Overton, T.L.; Rourke, J.P.; Weller, M.T.; Armstrong, F.A. (2010), Shriver and Atkin's Inorganic Chemistry, Oxford.
- 3. Miessler, G. L.; Tarr, D.A.(2014), Inorganic Chemistry, Pearson.
- 4. Cotton, F.A.; Wilkinson, G.; Gaus, P.L. (1995), **Basic Inorganic Chemistry**, 3<sup>rd</sup> Edition, Wiley India.
- 5. Castellan, G. W.(2004), Physical Chemistry, Narosa.
- Kapoor, K.L. (2015), A Textbook of Physical Chemistry, Vol.1, 6th Edition, McGraw Hill Education.
- Kapoor, K.L. (2015), A Textbook of Physical Chemistry, Vol.5,3<sup>rd</sup> Edition, McGraw Hill Education.
- 8. B.R.Puri, L.R.Sharma, M.S.Pathania, (2017), **Principles of Physical Chemistry**, Vishal Publishing Co.

#### Practical:

- 1. Svehla, G. (1996), Vogel's Qualitative Inorganic Analysis, Prentice Hall.
- Khosla, B.D.; Garg, V.C.; Gulati, A.(2015), Senior Practical Physical Chemistry, R. Chand & Co.

# **Teaching Learning Process:**

- Through chalk and talk method.
- Revising and asking questions from students at the end of class
- Motivating students to do some activity related to the topic
- Power point presentation
- Correlating the topic with real life cases.
- Quiz contest among students on important topic.

## **Assessment Methods:**

- 1. Graded assignments
- 2. Conventional class tests
- 3. Class seminars by students on course topics with a view to strengthening the content through width and depth
- 4. Quizzes
- 5. End semester university examination.

#### **Keywords:**

Metallurgy, Periodicity, Anomalous behaviour, Ellingham diagrams, Hydrometallurgy, Allotropy, Diagonal relationship, Multicentre bonding, Ideal/real gases, Surface tension, Viscosity, Crystal systems, Rate Law, Rate constant.

# DISCIPLINE SPECIFIC ELECTIVE COURSES (DSE) INDUSTRIAL CHEMISTRY

Course Code: INDUSTRIAL CHEMISTRY -DSE-1

**Course Title: Green Chemistry** 

Total Credits: 06 (Credits: Theory-04, Practical-02)

(Total Lectures: Theory- 60, Practical-60)

# **Objectives:**

Today's society is moving towards becoming more and more environmentally conscious. There is rising concern of environmental pollution, depleting resources, climate change, ozone depletion, heaps and heaps of landfills piling up, legislation which is getting stringent with strict environmental laws,, rising cost of waste deposits and so on. We are faced with a challenge to work towards sustainable practices. Green chemistry has arisen from these concerns. It is not a new branch of chemistry but the way chemistry should be practiced. Innovations and applications of green chemistry in education has helped companies not only gain environmental benefits but at the same time achieve economic and societal goals also. This is possible because these undergraduate students are ultimate scientific community of tomorrow.

# **Learning Outcomes:**

#### By the end of this course, students will be able to:

- 1. Understand the twelve principles of green chemistry and will build the basic understanding of toxicity,hazard and risk of chemical substances.
- 2. Understand stoichiometric calculations and relate them to green chemistry metrics. They will learn about atom economy and how it is different from percentage yield.
- 3. Learn to design safer chemical ,products and processes that are less toxic,than current alternatives. Hence,they will understand the meaning of inherently safer design for accident prevention and the principle "what you don't have can't harm you"
- 4. Understand benefits of use of catalyst and bio catalyst, use of renewable feed stock which helps in energy efficiency and protection of the environment, renewable energy sources, importance led reactions in various green solvents.
- 5. Appreciate the use of green chemistry in problem solving skills, critical thinking and valuable skills to innovate and find out solution to environmental problems. Thus the students are able to realise that chemistry can be used to solve rather than cause environmental problems.
- 6. Green chemistry is a way to boost profits, increase productivity and ensure sustainability with absolute zero waste. Success stories and real world cases also motivate them to practice green chemistry. These days customers are demanding to know about a product: Is it green? Does it contribute to global warming? Was it made from non depletable resources? Students have many career opportunities as "green" is the path to success.

## Unit 1

**Introduction to Green Chemistry** 

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What is 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.

(Lectures:5)

#### Unit 2

# Principles of Green Chemistry and Designing a Chemical synthesis

Twelve principles of Green Chemistry and their explanation with examples

Special emphasis on the following:

- Prevention of Waste/ by products; maximum incorporation of the materials used in the process into the final products, Environmental impact factor, waste or pollution prevention hierarchy
- Green metrics to assess greenness of a reaction, e.g. Atom Economy, calculation of atom economy of the rearrangement, addition, substitution and elimination reactions.
- Prevention/ minimization of hazardous/ toxic products reducing toxicity
- Risk = (function) hazard x exposure
- Designing safer chemicals with minimum toxicity yet has the ability to perform the desired functions
- Green solvents: super critical fluids with special reference to carbon dioxide, water as a solvent for
  organic reactions, ionic liquids, fluorous biphasic solvent, PEG, solventless processes, solvents
  obtained from renewable resources and how to compare greenness of solvents
- Energy requirements for reactions alternative sources of energy: use of microwaves , ultrasonic energy and photochemical energy
- Selection of starting materials; should be renewable rather than depleting, Illustrate with few examples such as biodiesel and polymers from renewable resources (such as green plastic)
- Avoidance of unnecessary derivatization careful use of blocking/protecting groups
- Use of catalytic reagents (wherever possible) in preference to stoichiometric reagents; catalysis and green chemistry, comparison of heterogeneous and homogeneous catalysis, biocatalysis, asymmetric catalysis and photocatalysis.
- Design for degradation: A product should not persist after the commercial function is over e.g. soaps and detergents, pesticides and polymers
- Strengthening/ development of analytical techniques to prevent and minimize the generation of hazardous substances in chemical processes.
- Prevention of chemical accidents designing greener processes, inherent safer design, principle of ISD "What you don't have cannot harm you", greener alternative to Bhopal Gas Tragedy (safer route to carcarbaryl) and Flixiborough accident (safer route to cyclohexanol) subdivision of ISD, minimization, simplification, substitution, moderation and limitation.

(Lectures:25)

#### Unit 3:

#### **Examples of Green Synthesis/ Reactions**

- Green Synthesis of the following compounds: adipic acid, catechol, disodium iminodiacetate (alternative to Strecker synthesis).
- Green Reagents: Non-phosgene Isocyanate Synthesis, Selective Methylation using dimethylcarbonate.
- Microwave assisted solvent free synthesis of copper phthalocyanine
- Microwave assisted reactions in water: Hofmann Elimination, methyl benzoate to benzoic acid and Decarboxylation reaction
- Ultrasound assisted reactions: sonochemical Simmons-Smith Reaction (Ultrasonic alternative to Iodine)

(Lectures:10)

# Unit 4

#### Real world case studies based on the Presidential green chemistry awards of EPA

- Surfactants for Carbon Dioxide replacing smog producing and ozone depleting solvents with CO<sub>2</sub> for precision cleaning and dry cleaning of garments.
- A new generation of environmentally advanced wood preservatives: Getting the chromium and Arsenic
  out of pressure treated wood.
- An efficient, green synthesis of a compostable and widely applicable plastic (polylactic acid) made from corn.
- Healthier Fats and oils by Green Chemistry: Enzymatic Inter esterification for production of No Trans-Fats and Oils.
- Development of Fully Recyclable Carpet: Cradle to Cradle Carpeting.
- Using a naturally occurring protein to stimulate plant growth, improve crop quality, increase yields, and suppress disease.

(Lectures:10)

#### Unit 5

#### **Future Trends in Green Chemistry**

Oxidation reagents and catalysts; Biomimcry and green chemistry, Biomimetic, Multifunctional Reagents; mechanochemical and solvent free synthesis of inorganic complexes; co crystal controlled solid state synthesis (C²S³); Green chemistry in sustainable development.

(Lectures:10)

#### **Practical:**

#### (Credits: 2, Laboratory periods: 60)

## **Chemistry Lab- Green chemistry**

Characterization by m. pt., U.V.-Visible spectroscopy, IR spectroscopy, and any other specific method should be done (wherever applicable).

# Safer starting materials

1. Preparation and characterization of nanoparticles of gold using tea leaves/silver nanoparticles using plant extracts.

#### Using renewable resources

2. Preparation of biodiesel from waste cooking oiland characterization (TLC, pH, Solubility, Combustion Test, Density, Viscosity, Gel Formation at Low Temperature and IR can be provided).

## Use of enzymes as catalysts

- 3. Benzoin condensation using Thiamine Hydrochloride as a catalyst instead of cyanide.

  Alternative green solvents
- 4. Extraction of D-limonene from orange peel using liquid CO<sub>2</sub> prepared form dry ice.
- 5. Mechanochemical solvent free, solid—solid synthesis of azomethine using p- toluidine and o-vanillin/p-vanillin (various other combinations of primary amine and aldehyde can also be tried).

#### Alternative sources of energy

- 6. Solvent free, microwave assisted one pot synthesis of phthalocyanine complex of copper(II).
- 7. Photoreduction of benzophenone to benzopinacol in the presence of sunlight.

#### Reducing waste

8. Designing and conducting an experiment by utilizing the products and by products obtained in above preparations which become waste otherwise if not used. This is done by critical thinking and literature survey.

Some representative examples:

- Use of nanoparticles as catalyst for a reaction
- Benzoin converted into Benzil and Benzil into Benzilic acid by a green method
- Use of azomethine for complex formation
- Rearrangement reaction from Benzopinacol to Benzopinacolone
- Conversion of byproduct of biodiesel to a useful product
- Students should be taught to do spot tests for qualitative inorganic analysis for cations and anions, and qualitative organic analysis for preliminary test and functional group analysis.

## **References:**

# Theory:

- 1. Anastas, P.T.; Warner, J.C.(1998), Green Chemistry, Theory and Practice, Oxford University Press.
- 2. Lancaster, M.(2016), Green Chemistry An Introductory Text. 2nd Edition, RSC Publishing.
- Cann ,M. C.; Connely, M. E. (2000), Real-World cases in Green Chemistry, American Chemical Society, Washington.
- 4. Matlack, A.S.(2001), Introduction to Green Chemistry, Marcel Dekker.
- 5. Alhuwalia, V. K.; Kidwai, M.R. (2005), New Trends in Green chemistry, Anamalaya Publishers.

## **Practical:**

- 1. Kirchoff, M.; Ryan, M.A. (2002), **Greener approaches to undergraduate chemistry experiment.** American Chemical Society, Washington DC.
- 2. Sharma, R.K.; Sidhwani, I.T.; Chaudhari, M.K.(2013), **Green Chemistry Experiments: A monograph**, I.K. International Publishing House Pvt Ltd. New Delhi.
- 3. Pavia, D.L.; Lamponam, G.H.; Kriz, G.S.W. B.(2006), Introduction to organic Laboratory Technique-A Microscale approach, 4<sup>th</sup> Edition, Brrooks-Cole Laboratory Series for Organic chemistry.
- 4. Wealth from Waste: A green method to produce biodiesel from waste cooking oil and generation of useful products from waste further generated. Indu Tucker Sidhwani et al. University of Delhi, Journal of Undergraduate Research and Innovation, Volume 1, Issue 1,February 2015, ISSN: 2395-2334.
- 5. Sidhwani, Tucker I.; Chowdhury, S. Greener alternatives to Qualitative Analysis for Cations without H<sub>2</sub>S and other sulfur containing compounds, J. Chem. Educ. 2008, 85, 1099.
- 6. Sidhwani, Tucker I.; Chowdhury, S. et al., DU Journal of Undergraduate Research and Innovation2016, Volume 2, Issue 2, 70-79.
- 7. Dhingra, S., ;Angrish, C. Qualitative organic analysis: An efficient, safer, and economical approach to preliminary tests and functional group analysis. *Journal of Chemical Education*, 2011, 88(5), 649-651.

# **Teaching Learning Process:**

- Conventional chalk and board teaching
- Power point presentations
- Interactive sessions
- Literature survey and critical thinking to design to improve a traditional reaction and problem solving

- Visit to a green chemistry lab
- Some motivating short movies in green chemistry especially in bio mimicry

#### **Assessment Methods:**

- Presentation by students
- Class Test
- Written Assignment
- End Semester University Theory and Practical Exams

## **Keywords:**

Green chemistry, Twelve principles of green chemistry, Atom economy, Waste minimization, Green metric, Green solvents, Solvent free, Catalyst, Bio-catalyst, Renewable energy sources, Hazardous, Renewable feedstock, Ionic liquids, Supercritical fluids, Inherent safer design, Green synthesis, Cocrystal controlled solid state synthesis, Sustainable development, Presidential green chemistry awards.

Course Code: INDUSTRIAL CHEMISTRY -DSE-2 Course Title: Analytical Methods in Chemistry

Total Credits: 06 (Credits: Theory-04, Practical-02)

(Total Lectures: Theory- 60, Practical-60)

# **Objectives:**

The objective of this course is to make student aware of the concept of sampling, Accuracy, Precision, Statistical test data-F, Q and t test. The course exposes students to the laws of spectroscopy and selection rules governing the possible transitions in the different regions of the electromagnetic spectra. Thermal and electroanalytical methods of analysis are also dealt with. Students are exposed to important separation methods like solvent extraction and chromatography. The practicals expose students to latest instrumentation and they learn to detect analytes in a mixture.

#### **Learning Outcomes:**

#### By the end of this course, students will be able to:

- 1. Perform experiment with accuracy and precision.
- 2. Develop methods of analysis for different samples independently.
- 3. Test contaminated water samples.
- 4. Understand basic principle of instrument like Flame Photometer, UV-vis spectrophotometer.
- 5. Learn separation of analytes by chromatography.
- 6. Apply knowledge of geometrical isomers and keto-enol tautomers to analysis.
- 7. Determine composition of soil.
- 8. Estimate macronutrients using Flame photometry.

#### Unit 1

#### Qualitative and quantitative aspects of analysis:

Sampling, evaluation of analytical data, errors, accuracy and precision, methods of their expression.

Normal law of distribution of indeterminate errors, statistical test of data; F, Q and t test, rejection of data, and confidence intervals.

(Lectures: 5)

#### Unit 2

## Optical methods of analysis

Origin of spectra, interaction of radiation with matter, fundamental laws of spectroscopy and selection rules

UV-Visible Spectrometry: Basic principles of instrumentation (choice of source, monochromator and detector) for single and double beam instrument; Transmittance. Absorbance and Beer-Lambert law

Basic principles of quantitative analysis: estimation of metal ions from aqueous solution, geometrical isomers, keto-enol tautomers.

Flame Atomic Absorption and Emission Spectrometry: Basic principles of instrumentation (choice of source, monochromator, detector, choice of flame and Burner designs). Techniques of atomization and sample introduction; Method of background correction, sources of chemical interferences and their method of removal, Techniques for the quantitative estimation of trace level of metal ions from water samples.

(Lectures: 25)

#### Unit 3

#### Thermal methods of analysis:

Theory of thermogravimetry (TG) and basic principle of instrumentation of thermal analyser. Techniques for quantitative estimation of Ca and Mg from their mixture.

(Lectures: 5)

# Unit 4

## **Electroanalytical methods**

Classification of electroanalytical methods, basic principle of pH metric, potentiometric and conductometric titrations. Techniques used for the determination of equivalence points. Techniques used for the determination of pKa values.

(Lectures:10)

## Unit 5

#### Separation techniques

Solvent extraction: Classification, principle and efficiency of the technique.

Mechanism of extraction: extraction by solvation and chelation, Technique of extraction: batch, continuous and counter current extractions, Qualitative and quantitative aspects of solvent extraction:

extraction of metal ions from aqueous solution, extraction of organic species from the aqueous and non-aqueous media.

Chromatography: Classification, principle and efficiency of the technique, Mechanism of separation: adsorption, partition &ion-exchange, Development of chromatograms: frontal, elution and displacement methods.

(Lectures:15)

#### **Practical:**

# (Credits: 2, Laboratory periods: 60)

- 1. Separation of mixtures by paper chromatography and reporting the R<sub>f</sub> values:
  - (i)  $Co^{2+}$  and  $Ni^{2+}$ .
  - (ii) Amino acids present in the given mixture.
- Solvent Extractions
  - (i) To separate a mixture of Ni<sup>2+</sup> & Fe<sup>2+</sup> by complexation with DMG and extracting the Ni<sup>2+</sup> DMG complex in chloroform, and determine its concentration by spectrophotometry.
- 3. Analysis of soil:
  - (i) Determination of pH of soil.
  - (ii) Total soluble salt
  - (iii) Estimation of calcium and magnesium
  - (iv) Qualitative detection of nitrate and phosphate
- 4. Ion exchange:
  - (i) Determination of exchange capacity of cation exchange resins and anion exchange resins.
  - (ii) Separation of amino acids from organic acids by ion exchange chromatography.
- 5. Spectrophotometry
  - (i) Verification of Lambert-Beer's law and determination of concentration of a coloured species (CuSO<sub>4</sub>, KMnO<sub>4</sub>, CoCl<sub>2</sub>, CoSO<sub>4</sub>)
  - (ii) Determination of concentration of coloured species via following methods;
    - (a) Graphical method, (b) Epsilon method, (c) Ratio method, (iv) Standard addition method

# **References:**

## Theory:

- Willard, H.H.(1988), Instrumental Methods of Analysis, 7th Edition, Wardsworth Publishing Company.
- 2. Christian, G.D.(2004), Analytical Chemistry, 6th Edition, John Wiley & Sons, New York.
- 3. Harris, D. C.(2007), Quantitative Chemical Analysis, 6th Edition, Freeman.
- 4. Khopkar, S.M. (2008), **Basic Concepts of Analytical Chemistry**, New Age International Publisher.
- 5. Skoog, D.A.; Holler F.J.; Nieman, T.A. (2005), **Principles of Instrumental Analysis,** Thomson Asia Pvt. Ltd.

# **Practical:**

1. Jeffery, G.H.; Bassett, J.; Mendham, J.; Denney, R.C.(1989), Vogel's Textbook of Quantitative Chemical Analysis, John Wiley and Sons.

# **Teaching Learning Process:**

- Teaching through audio-visual aids.
- Students are encouraged to participate actively in the classroom through regular presentations on curriculum based topics.
- As the best way to learn something is to do it yourself, practicals are planned in such a way so as to reinforce the topics covered in theory.

# **Assessment Methods:**

- · Presentations by individual student/ small group of students
- Class tests at periodic intervals.
- Written assignment(s)
- Objective type chemical guizzes based on contents of the paper.
- End semester university theory and practical examination.

# **Keywords:**

Separation techniques, Solvent extraction, Ion-exchange, Optical methods, Flame Atomic Absorption and Emission Spectrometry, indeterminate errors, statistical test of data; F, Q and t tests. TGA.

Course Code: INDUSTRIAL CHEMISTRY -DSE-3

**Course Title: Polymer Chemistry** 

Total Credits: 06 (Credits: Theory-04, Practical-02)

(Total Lectures: Theory- 60, Practical-60)

# **Objectives:**

The primary objective of this paper is to help the student to know about the synthesis, properties and applications of polymers.

# **Learning Outcomes:**

# By the end of this course, students will be able to:

- Know about history of polymeric materials and their classification
- Learn about different mechanisms of polymerization and polymerization techniques
- Evaluate kinetic chain length of polymers based on their mechanism
- Differentiate between polymers and copolymers
- · Learn about different methods of finding out average molecular weight of polymers
- Differentiate between glass transition temperature (Tg) and crystalline melting point (Tm)
- Determine Tg and Tm
- Know about solid and solution properties of polymers
- Learn properties and applications of various useful polymers in our daily life.

This paper will give glimpse of polymer industry to the student and help them to choose their career in the field of polymer chemistry.

#### Unit 1

## Introduction and history of polymeric materials:

History of polymeric materials, Different schemes of classification of polymers, Polymer nomenclature, Molecular forces and chemical bonding in polymers, Texture of Polymers

#### Functionality and its importance:

Criteria for synthetic polymer formation, classification of polymerization processes, Relationships between functionality, extent of reaction and degree of polymerizationBifunctional systems, Polyfunctional systems

(Lectures: 12)

# Unit 2

# **Kinetics of Polymerization**

Mechanism of step growth polymerization, kinetics of step growth, radical chain growth, ionic chain (both cationic and anionic), Mechanism and kinetics of copolymerization, polymerization techniques

(Lectures: 8)

# Unit 3

Glass transition temperature (Tg) and determination of Tg, Free volume theory, WLF equation, Factors affecting glass transition temperature (Tg).

Crystallization and crystallinity: Determination of crystalline melting point and degree of crystallinity, Morphology of crystalline polymers, Factors affecting crystalline melting point.

Nature and structure of polymers-Structure Property relationships

(Lectures: 14)

#### Unit 4

**Determination of molecular weight of polymers (M\_n, M\_w, etc.)** by end group analysis, viscometry, light scattering and osmotic pressure methods. Molecular weight distribution and its significance. Polydispersity index

#### **Polymer Solution**

Criteria for polymer solubility and Solubility parameter, Thermodynamics of polymer solutions, entropy, enthalpy and free energy change of mixing of polymers solutions.

#### **Polymer Degradation**

Thermal, oxidative, hydrolytic and photodegradation

(Lectures: 16)

#### Unit 5

#### **Properties of Polymers**

(Physical, thermal, Flow & Mechanical Properties) Brief introduction to preparation, structure, properties and application of the following polymers: polyolefins, polystyrene and styrene copolymers, poly(vinyl chloride) and related polymers, poly(vinyl acetate) and related polymers, acrylic polymers, fluoro polymers, polyamides and related polymers. Phenol formaldehyde resins (Bakelite, Novolac), polyurethanes, silicone polymers, polydienes, Polycarbonates, Conducting Polymers: polyacetylene, polyaniline, poly(p-phenylene sulphide, polypyrrole, polythiophene

(Lectures: 10)

## **Practical:**

(Credits: 2, Laboratory periods: 60) Chemistry Lab: Polymer chemistry

#### Polymer synthesis

- Free radical solution polymerization of styrene (St) / Methyl Methacrylate (MMA)/MethylAcrylate (MA).
- 2. Preparation of nylon 6,6
- 3. Redox polymerization of acrylamide
- 4. Precipitation polymerization of acrylonitrile
- 5. Preparation of urea-formaldehyde resin
- **6.** Preparations of novalac resin/resold resin.
- 7. Microscale Emulsion Polymerization of Poly(methylacrylate).

#### Polymer characterization

- 1. Determination of molecular weight of polyvinyl propylidene in water by viscometry:
- 2. Determination of the viscosity-average molecular weight of poly(vinyl alcohol) (PVOH) and the fraction of head-to-head monomer linkages in the polymer.
- 3. Determination of molecular weight by end group analysis of polymethacrylic acid.

# Polymer analysis

- 1. Estimation of the amount of HCHO in the given solution by sodium sulphite method
- 2. IR studies of polymers
- 3. DSC (Differential Scanning Calorimetry) analysis of polymers
- 4. TG-DTA (Thermo-Gravimetery-Differential Thermal Analaysis) of polymers

#### **Suggested Additional Experiment:**

- 1. Purification of monomer.
- 2. Emulsion polymerization of a monomer.

#### **References:**

#### Theory:

- 1. Carraher, C. E. Jr. (2013), Seymour's Polymer Chemistry, Marcel Dekker, Inc.
- 2. Odian, G. (2004), Principles of Polymerization, John Wiley.
- 3. Billmeyer, F.W. (1984), Text Book of Polymer Science, John Wiley.
- 4. Ghosh, P. (2001), Polymer Science & Technology, Tata Mcgraw-Hill.
- 5. Lenz, R.W. (1967), Organic Chemistry of Synthetic High Polymers, Intersecience (Wiley).

#### Practical:

- Allcock, H.R.; ; Lampe, F. W.; Mark, J. E. (2003), Contemporary Polymer Chemistry, Prentice-Hall.
- Fried, J.R. (2003), Polymer Science and Technology, Prentice-Hall.
- Munk, P.; Aminabhavi, T. M. (2002), Introduction to Macromolecular Science, John Wiley & Sons.
- 4. Sperling, L.H.(2005), Introduction to Physical Polymer Science, John Wiley & Sons.

# **Teaching-Learning Process:**

- Teaching learning process for the course is visualized as largely student-focused.
- Transaction through an intelligent mix of conventional and modern methods.
- Engaging students in cooperative learning.
- Learning through quiz design.
- Problem solving to enhance comprehension.

## **Assessment Methods:**

Assessmentwill be done on the basis of regular class test, presentations and assignments as a part of internal assessment during the course as per the curriculum. End semester university examination will be held for both theory and practical. In practical, assessment will be done based on continuous evaluation, performance in the experiment on the date of examination and viva voce.

# **Keywords:**

Bonding, Texture, Polymerization, Degradation, Polymer solution, Crystallization, Properties, Applications.

Course Code: INDUSTRIAL CHEMISTRY -DSE-4

**Course Title: Molecules of Life** 

Total Credits: 06 (Credits: Theory-04, Practical-02)

(Total Lectures: Theory- 60, Practical-60)

# **Objectives:**

The objective of this course is to deliver information about biochemically significant features of the chemistry of carbohydrates, proteins, enzymes, nucleic acids and lipids, using suitable examples. This includes classification, reaction chemistry and biological importance of these biomolecules. This course extends the knowledge gained from synthetic organic chemistry to chemistry of biomolecules. Key emphasis is placed on understanding the structural principles that govern reactivity/physical /biological properties of biomolecules as opposed to learning structural detail.

# **Learning Outcomes:**

# By the end of the course, the students will be able to:

- 1. Learn and demonstrate how the structure of biomolecules determines their chemical properties, reactivity and biological uses.
- 2. Gain an insight into mechanism of enzyme action and inhibition.
- 3. Understand the basic principles of drug-receptor interaction and SAR.
- 4. Understand biological processes like replication, transcription and translation.
- 5. Demonstrate an understanding of metabolic pathways, their inter-relationship, regulation and energy production from biochemical processes.

#### Unit 1

#### Carbohydrates

Classification of carbohydrates, reducing and non-reducing sugars, biological functions, general properties and reactions of glucose and fructose, their open chain structure, epimers, mutarotation and anomers, reactions of monosaccharides, determination of configuration of glucose (Fischer proof), cyclic structure of glucose. Haworth projections. Cyclic structure of fructose. Linkage between monosaccharides: structure of disaccharides (sucrose, maltose, lactose) and polysaccharides (starch and cellulose) excluding their structure elucidation.

(Lectures: 10)

#### Unit 2

#### **Amino Acids, Peptides and Proteins**

Classification of amino acids and biological uses of amino Acids, peptides and proteins. Zwitterion structure, isoelectric point and correlation to acidity and basicity of amino acids. Determination of primary structure of peptides, determination of N-terminal amino acid (by DNFB and Edman method) and C—terminal amino acid (by thiohydantoin and with carboxypeptidase enzyme). Synthesis of simple peptides (up to dipeptides) by N-protection (t-butyloxycarbonyl and phthaloyl) & C-activating groups and Merrifield solid phase synthesis, Overview of primary, secondary, tertiary and quaternary structure of proteins, denaturation of proteins.

(Lectures: 12)

## Unit 3

# Enzymes and correlation with drug action

Classification of enzymes and their uses(mention Ribozymes). Mechanism of enzyme action, factors affecting enzyme action, Coenzymes and cofactors and their role in biological reactions, specificity of enzyme action(including stereospecificity), enzyme inhibitors and their importance, phenomenon of

inhibition (Competitive and non-competitive inhibition including allosteric inhibition). Drug action-receptor theory. Structure – activity relationships of drug molecules, binding role of –OH group,-NH<sub>2</sub> group, double bond and aromatic ring.

(Lectures: 10)

#### Unit 4

#### **Nucleic Acids**

Components of Nucleic acids: Adenine, guanine, thymine ,cytosine and uracil (structure only), other components of nucleic acids, nucleosides and nucleotides (nomenclature), structure of polynucleotides; structure of DNA (Watson-Crick model) and RNA(types of RNA),difference between DNA and RNA, genetic code, biological roles of DNA and RNA: replication, transcription and translation.

(Lectures: 10)

#### Unit 5

#### Lipids

Introduction to lipids, classification. Oils and fats: Common fatty acids present in oils and fats, Omega-3&6 fatty acids, trans fats, hydrogenation, hydrolysis, acid value, saponification value, iodine number. Biological importance of triglycerides, phospholipids, glycolipids, and steroids (cholesterol).

(Lectures: 8)

# Unit 6

#### **Concept of Energy in Biosystems**

Calorific value of food. Standard caloric content of carbohydrates, proteins and fats. Oxidation of foodstuff (organic molecules) as a source of energy for cells. Introduction to metabolism (catabolism, anabolism), ATP: the universal currency of cellular energy, ATP hydrolysis and free energy change. Conversion of food into energy. Outline of catabolic pathways of carbohydrate- glycolysis, fermentation and Krebs cycle. Overview of catabolic pathways of fats and proteins. Interrelationships in the metabolic pathways of proteins, fats and carbohydrates.

(Lectures: 10)

#### **Practical:**

#### (Credits: 2, Laboratory periods: 60)

- 1. Separation of amino acids by paper chromatography
- 2. Study of titration curve of glycine and determination of its isoelectric point.
- 3. Estimation of proteins by Lowry's method
- 4. Action of salivary amylase on starch
- 5. Effect of temperature on the action of salivary amylase on starch.
- 6. To determine the saponification value of an oil/fat.

- 7. To determine the iodine value of an oil/fat
- 8. Qualitative tests for carbohydrates- Molisch test Barfoed's reagent test, rapid furfural test, Tollen's test and Fehling solution test(Only these tests are to be done in class)
- 9. Qualitative tests for proteins
- 10. Extraction of DNA from onion/cauliflower

#### **References:**

#### Theory:

- 1. Finar, I. L. **Organic Chemistry** (Volume 1 & 2), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- 2. Morrison, R. N.; Boyd, R. N. **Organic Chemistry**, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- 3. Berg, J. M.; Tymoczko, J. L.; Stryer, L.(2002), Biochemistry, W. H. Freeman.

#### Practical:

- 1. Furniss, B.S.; Hannaford, A.J.; Smith, P.W.G.; Tatchell, A.R. (2012), Vogel's Textbook of Practical Organic Chemistry, Pearson.
- Manual of Biochemistry Workshop, 2012, Department of Chemistry, University of Delhi.

# **Teaching Learning Process:**

- The teaching learning process will involve the traditional chalk and black board method. Along with pedagogy of flipped classroom
- Certain topics like mechanism of enzyme action and enzyme inhibition, transcription and translation etc. where traditional chalk and talk method may not be able to convey the concept, are taught through audio-visual aids.
- Students are encouraged to participate actively in the classroom through regular presentations on curriculum based topics, peer assessment, designing games based on specific topics etc.
- As the best way to learn something is to do it yourself, practicals are planned in such a way so as to reinforce the topics covered in theory.

#### **Assessment Methods:**

- · Graded assignments
- Conventional class tests
- Class seminars by students on course topics with a view to strengthening the content through width and depth
- Quizzes
- End semester university examination.

## **Keywords:**

Biomolecules, Enzymes, Mechanism of enzyme action and inhibition, SAR, Drug Receptor Theory, Energy concept in biological system, Catabolic pathways and their inter-relationship.

B.Sc. Industrial Chemistry University of Delhi

Course Code: INDUSTRIAL CHEMISTRY -DSE-5

**Course Title: Dissertation** 

**Total Credits: 06** 

# **Objectives:**

The key objective of introducing the dissertation at UG students is to make them able to find a problem and understand logically with the books and publishing houses. This will make them capable of to search literature available in print as well electronic research/journals, Plan experiments and the most important is the recording of observations, their analysis.

# **Learning Outcomes**

At the end of this course, students will be able to;

- Survey and study of published literature on the assigned topic;
- Work out a preliminary approach to the problem relating to the assigned topic;
- Design a preliminary experiment;
- Prepare a written report on the study conducted for presentation;
- Make oral presentation of the work.

#### **Contents**

- Refer literature from different Publishing and SciFinder,
- Generate a time based feasible problem,
- Design a route to achieve the objective in the problem,
- Perform experiments, note the observations & their analysis,
- Result & discussion,
- Writing dissertation and prepare presentation.

The object of dissertation work is to enable the student to take up investigative study in the broad field of Chemistry/ Industrial Chemistry, either fully theoretical/ experimental or involving both theoretical and experimental work to be assigned by the Department on an individual basis or two/ three students in a group, under the guidance of a Supervisor.

#### **Assessment**

Continuous evaluation (IA) : 25%

(Regularity, understanding of concept)

Experimental/ Theoretical work performed : 30%
Dissertation report submitted : 30%
Presentation : 15%

## Suggested Reading:

 Research Methodology: Methods and techniques by C.R. Kothari and Gaurav Garg. New Age International, India. 2018.

# DISCIPLINE SPECIFIC ELECTIVE COURSES (DSE) CHEMISTRY

**Course Code: CHEMISTRY -DSE-1** 

Course Title: Chemistry of d-Block Elements, Quantum Chemistry and

**Spectroscopy** 

Total Credits: 06 (Credits: Theory-04, Practical-02)

(Total Lectures: Theory- 60, Practical-60)

# **Objectives:**

The objective of this course is to introduce the students to d and f block elements and highlights the concept of horizontal similarity in a period and stresses on their unique properties. It familiarizes them with coordination compounds which find manifold applications in diverse fields. This course also disseminates the concepts and methodology of quantum mechanics, its applications to spectroscopy and establishes relation between structure determination and spectra.

# **Learning Outcomes:**

#### By the end of the course, the students will be able to:

- Understand chemistry of d and f block elements, Latimer diagrams, properties of coordination compounds and VBT and CFT for bonding in coordination compounds
- Understand basic principles of quantum mechanics: operators, eigen values, averages, probability distributions.
- Understand and use basic concepts of microwave, IR and UV-VIS spectroscopy for interpretation of spectra.
- Explain Lambert-Beer's law, quantum efficiency and photochemical processes.

#### Section A: Inorganic Chemistry (Lectures:30)

# Unit 1

## Transition Elements (3d series)

General properties of elements of 3d series with special reference to electronic configuration, variable valency, colour, magnetic and catalytic properties and ability to form complexes. A brief introduction to Latimer diagrams (Mn, Fe and Cu) and their use to identify oxidizing, reducing species and species which disproportionate. Calculation of skip step potentials.

Lanthanoids and actinoids: Electronic configurations, oxidation states displayed. A very brief discussion of colour and magnetic properties. Lanthanoid contraction(causes and consequences), separation of lanthanoids by ion exchange method.

(Lectures: 10)

#### Unit 2

## **Coordination Chemistry**

Brief discussion with examples of types of ligands, denticity and concept of chelate. IUPAC system of nomenclature of coordination compounds (mononuclear and binuclear) involving simple monodentate and bidentate ligands. Structural and stereoisomerism in complexes with coordination numbers 4 and 6

(Lectures: 6)

## Unit 3

#### Bonding in coordination compounds

Valence Bond Theory (VBT): Salient features of theory, concept of inner and outer orbital complexes of Cr, Fe, Co and Ni. Drawbacks of VBT.

## **Crystal Field Theory**

Splitting of d orbitals in octahedral symmetry. Crystal field effects for weak and strong fields. Crystal field stabilization energy (CFSE), concept of pairing energy. Factors affecting the magnitude of  $\Delta$ . Spectrochemical series. Splitting of d orbitals in tetrahedral symmetry. Comparison of CFSE for octahedral and tetrahedral fields, tetragonal distortion of octahedral geometry. Jahn-Teller distortion, square planar coordination.

(Lectures: 14)

## Section B: Physical Chemistry (Lectures:30)

#### Unit 4

#### **Quantum Chemistry**

Postulates of quantum mechanics, quantum mechanical operators.

Free particle. Particle in a 1-D box (complete solution), quantization, normalization of wave functions, concept of zero-point energy.

Rotational Motion: Schrödinger equation of a rigid rotator and brief discussion of its results (solution not required). Quantization of rotational energy levels.

Vibrational Motion: Schrödinger equation of a linear harmonic oscillator and brief discussion of its results (solution not required). Quantization of vibrational energy levels.

(Lectures: 12)

#### Unit 5

## **Spectroscopy**

Spectroscopy and its importance in chemistry. Wave-particle duality. Link between spectroscopy and quantum chemistry. Electromagnetic radiation and its interaction with matter.

Types of spectroscopy. Difference between atomic and molecular spectra. Born- Oppenheimer approximation: Separation of molecular energies into translational, rotational, vibrational and electronic components.

Microwave (pure rotational) spectra of diatomic molecules. Selection rules. Structural information derived from rotational spectroscopy.

IR Spectroscopy: Selection rules, IR spectra of diatomic molecules. Structural information derived from vibrational spectra. Vibrations of polyatomic molecules. Group frequencies. Effect of hydrogen bonding (inter- and intramolecular) and substitution on vibrational frequencies.

Electronic Spectroscopy: Electronic excited states. Free electron model and its application to electronic spectra of polyenes. Colour and constitution, chromophores, auxochromes, bathochromic and hypsochromic shifts.

(Lectures: 12)

#### Unit 6

## **Photochemistry**

Laws of photochemistry. Lambert-Beer's law. Fluorescence and phosphorescence. Quantum efficiency and reasons for high and low quantum yields. Primary and secondary processes in photochemical reactions. Photochemical and thermal reactions. Photoelectric cells.

(Lectures: 6)

#### **Practical:**

## (Credits: 2, Laboratory periods: 60)

# **Section A: Inorganic Chemistry**

- 1. Estimation of the amount of nickel present in a given solution as bis (dimethylglyoximato) nickel(II) or aluminium as oxinate in a given solution gravimetrically.
- 2. Estimation of (i) Mg<sup>2+</sup> or (ii) Zn<sup>2+</sup> by complexometric titrations using EDTA.
- 3. Estimation of total hardness of a given sample of water by complexometric titration.
- 4. Determination of the composition of the Fe<sup>3+</sup> salicylic acid complex / Fe<sup>2+</sup> phenanthroline complex in solution by Job's method.

## **Section B: Physical Chemistry**

# **UV/Visible spectroscopy**

- Study the 200-500 nm absorbance spectra of KMnO<sub>4</sub> and K<sub>2</sub>Cr<sub>2</sub>O<sub>7</sub> (in 0.1 M H<sub>2</sub>SO<sub>4</sub>) and determine the λ<sub>max</sub> values. Calculate the energies of the two transitions in different units (J molecule<sup>-1</sup>, kJ mol<sup>-1</sup>, cm<sup>-1</sup>, eV).
- 2. Study the pH-dependence of the UV-Vis spectrum (200-500 nm) of K<sub>2</sub>Cr<sub>2</sub>O<sub>7</sub>
- 3. Record the 200-350 nm UV spectra of the given compounds (acetone, acetaldehyde, 2-propanol, acetic acid) in water. Comment on the effect of structure on the UV spectra of organic compounds.

## Colorimetry

1. Verify Lambert-Beer's law and determine the concentration of CuSO<sub>4</sub>/KMnO<sub>4</sub>/K<sub>2</sub>Cr<sub>2</sub>O<sub>7</sub>/CoSO<sub>4</sub> in a solution of unknown concentration

**Chemical Kinetics**; Study the kinetics of the following reactions.

- 1. Initial rate method: lodide-persulphate reaction
- 2. Integrated rate method: Saponification of ethyl acetate.

### **References:**

## Theory:

- 1. Atkins, P.W.; Overton, T.L.; Rourke, J.P.; Weller, M.T.; Armstrong, F.A.(2010), Shriver and Atkins Inorganic Chemistry, W. H. Freeman and Company.
- 2. Miessler, G. L.; Fischer P.J.; Tarr, D.A.(2014), Inorganic Chemistry, Pearson.
- 3. Huheey, J.E.; Keiter, E.A., Keiter; R.L., Medhi, O.K. (2009), Inorganic Chemistry- Principles of Structure and Reactivity, Pearson Education.
- 4. Pfennig, B. W.(2015), Principles of Inorganic Chemistry. John Wiley & Sons.
- Kapoor, K.L. (2015), A Textbook of Physical Chemistry, Vol.4, 5th Edition, McGraw Hill Education.
- Kapoor, K.L. (2015), A Textbook of Physical Chemistry, Vol.5, 3<sup>rd</sup> Edition, McGraw Hill Education.
- 7. B.R.Puri, L.R.Sharma, M.S.Pathania, (2017), **Principles of Physical Chemistry**, Vishal Publishing Co.

#### Practical:

- 1. Jeffery, G.H.; Bassett, J.; Mendham, J.; Denney, R.C.(1989), Vogel's Textbook of Quantitative Chemical Analysis, John Wiley and Sons.
- 2. Marr, G.; Rockett, B.W. (1972), Practical Inorganic Chemistry, Van Nostrand Reinhold.
- Khosla, B.D.; Garg, V.C.; Gulati, A.(2015), Senior Practical Physical Chemistry, R. Chand & Co.

#### **Additional Resources:**

1. Castellan, G. W.(2004), Physical Chemistry, Narosa.

# **Teaching Learning Process:**

- Lectures to introduce a topic and give its details.
- Discussions so that the student can internalize the concepts.
- Problem solving to make the student understand the working and application of the concepts.

# **Assessment Methods:**

- · Graded assignments
- Conventional class tests
- Class seminars by students on course topics with a view to strengthening the content through width and depth
- Quizzes
- End semester university examination.

# **Keywords:**

d-block elements, Actinoids, Lanthinoids, VBT, Crystal field theory, Splitting of d levels, Coordination compounds, Quantisation, Selection rules, Schrodinger equation, Operator, Spectrum, Quantum efficiency, Fluorescence.

Course Code: CHEMISTRY -DSE-2

Course Title: Organometallics, Bioinorganic Chemistry, Polynuclear

Hydrocarbons and UV, IR Spectroscopy

Total Credits: 06 (Credits: Theory-04, Practical-02)

(Total Lectures: Theory- 60, Practical-60)

# **Objectives:**

The purpose of the course is to introduce students to some important 3d metals and their compounds which they are likely to come across. Students learn about organometallic compounds and bioinorganic chemistry which are currently frontier areas of chemistry providing an interface between organic chemistry, inorganic Chemistry and biology. The functional group approach to organic chemistry introduced in the previous courses is reinforced through the study of the chemistry of carboxylic acids and their derivatives, Amines and diazonium salts, active methylene compounds. The students will also be introduced to the chemistry and applications of polynuclear hydrocarbons and heterocyclic compounds. The learners are introduced to spectroscopy, an important analytical tool which allows identification of organic compounds by correlating their spectra to structure.

# **Learning Outcomes:**

#### By the end of the course, the students will be able to:

- Understand the chemistry and applications of 3d elements including their oxidation states and important properties of the familiar compounds potassium dichromate, potassium permanganate and potassium ferrocyanide
- Use IR data to explain the extent of back bonding in carbonyl complexes
- Get a general idea of toxicity of metal ions through the study of Hg<sup>2+</sup> and Cd<sup>2+</sup> in the physiological system
- Understand the fundamentals of functional group chemistry, polynuclear hydrocarbons and heterocyclic compounds through the study of methods of preparation, properties and chemical reactions with underlying mechanism.
- Gain insight into the basic fundamental principles of IR and UV-Vis spectroscopic techniques.
- Use basic theoretical principles underlying UV-visible and IR spectroscopy as a tool for functional group identification in organic molecules.

#### Section A: Inorganic Chemistry (Lectures:30)

#### Unit 1

# Chemistry of 3d metals

General discussion of 3d metals. Oxidation states displayed by Cr. Fe, Co, Ni and Cu.

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A study of the following compounds (including preparation and important properties):

 $K_2Cr_2O_7$ ,  $KMnO_4$ ,  $K_4[Fe(CN)_6]$ .

(Lectures: 6)

#### Unit 2

#### **Organometallic Compounds**

Definition and classification with appropriate examples based on nature of metal-carbon bond (ionic, s, p and multicentre bonds). Structure and bonding of methyl lithium and Zeise's salt. Structure and physical properties of ferrocene. 18-electron rule as applied to carbonyls. Preparation, structure, bonding and properties of mononuclear and polynuclear carbonyls of 3d metals.  $\pi$ -acceptor behaviour of carbon monoxide (MO diagram of CO to be discussed), synergic effect and use of IR data to explain extent of back bonding.

(Lectures: 12)

## Unit 3

# **Bio-Inorganic Chemistry**

A brief introduction to bio-inorganic chemistry. Role of metal ions present in biological systems with special reference to Na<sup>+</sup>, K<sup>+</sup> and Mg<sup>2+</sup> ions: Na/K pump; Role of Mg<sup>2+</sup> ions in energy production and chlorophyll. Brief introduction to oxygen transport and storage (haemoglobin-myoglobin system). Brief introduction about toxicity of metal ions (Hg<sup>2+</sup>and Cd<sup>2+</sup>).

(Lectures: 12)

#### Section B: Organic Chemistry (Lectures:30)

#### Unit 4

#### Polynuclear and heteronuclear aromatic compounds:

Structure elucidation of naphthalene, preparation and properties of naphthalene and anthracene. Preparation and Properties of the following compounds with reference to electrophilic and nucleophilic substitution: furan, pyrrole, thiophene, and pyridine.

(Lectures: 13)

#### Unit 5

## Active methylene compounds

Preparation: Claisen ester condensation. Keto-enol tautomerism.

Reactions: Synthetic uses of ethylacetoacetate (preparation of non-heteromolecules having up to 6 carbons).

(Lectures: 5)

# Unit 6

UV-Visible and infrared spectroscopy and their application to simple organic molecules.

Electromagnetic radiations and their properties; double bond equivalence and hydrogen deficiency.

UV-Visible spectroscopy (electronic spectroscopy): General electronic transitions,  $\lambda_{\text{max}}$  & $\epsilon_{\text{max}}$ , chromophores & auxochromes, bathochromic & hypsochromic shifts. Application of Woodward rules for calculation of  $\lambda_{\text{max}}$  for the following systems: conjugated dienes - alicyclic, homoannular and heteroannular;  $\alpha,\beta$ -unsaturated aldehydes and ketones, charge transfer complex.

Infrared (IR) Spectroscopy: Infrared radiation and types of molecular vibrations, significance of functional group & fingerprint region. IR spectra of alkanes, alkenes, aromatic hydrocarbons (effect of conjugation and resonance on IR absorptions), simple alcohols (inter and intramolecular hydrogen bonding and IR absorptions), phenol, carbonyl compounds, carboxylic acids and their derivatives (effect of substitution on >C=O stretching absorptions).

(Lectures: 12)

# **Practical:**

(Credits: 2, Laboratory periods: 60)

## Section A: Inorganic Chemistry

1. Separation of mixtures of two ions by paper chromatography and measurement of R<sub>N</sub>alue in each case:

$$(Fe^{3+}, Al^{3+} \text{ and } Cr^{3+}) \text{ or } (Ni^{2+}, Co^{2+}, Mn^{2+} \text{ and } Zn^{2+})$$

- 2.Preparation of any two of the following complexes and measurement of their conductivity:
- (i) tetraamminecopper (II) sulphate (ii) potassium trioxalatoferrate (III) trihydrate.

Compare the conductance of the complexes with that of M/1000 solution of NaCl, MgCl<sub>2</sub> and LiCl<sub>3</sub>.

#### **Section B: Organic Chemistry**

- 1. Detection of extra elements
- 2. Systematic qualitative analysis of organic compounds possessing monofunctional groups: amide, amines, halo-hydrocarbons and carbohydrates (Including Derivative preparation)
- 3. Identification of simple organic compounds containing the above functional groups by IR spectroscopy through examination of spectra (spectra to be provided).

# **References:**

## Theory:

- 1. Huheey, J.E.; Keiter, E.A.; Keiter; R. L.; Medhi, O.K. (2009), Inorganic Chemistry- Principles of Structure and Reactivity, Pearson Education.
- 2. Lee., J. D.(2010), A new Concise Inorganic Chemistry, Pearson Education.
- Douglas, B.E.; McDaniel, D.H.; Alexander, J.J. (1994), Concepts and Models of Inorganic Chemistry, John Wiley & Sons.
- 4. Atkins, P.W.; Overton, T.L.; Rourke, J.P.; Weller, M.T.; Armstrong, F.A. (2010), Shriver and Atkins Inorganic Chemistry, 5th Edn, W. H. Freeman and Company, 41 Madison Avenue, New York, NY.
- 5. Finar, I. L. **Organic Chemistry** (Volume 1 & 2), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).

- 6. Morrison, R. N.; Boyd, R. N. **Organic Chemistry**, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- 7. Bahl, A; Bahl, B. S. (2012), Advanced Organic Chemistry, S. Chand.

#### **Practical:**

- 1. Ahluwalia, V.K.; Dhingra, S.; Gulati, A.(2005), College Practical Chemistry, University Press (India) Ltd.
- 2. Ahluwalia, V.K.; Dhingra, S.(2004), Comprehensive Practical Organic Chemistry: Qualitative Analysis, University Press.
- 3. Vogel, A.I.(1972), Textbook of Practical Organic Chemistry, Prentice Hall.
- 4. Svehla, G. (1996), Vogel's Qualitative Inorganic Analysis, Prentice Hall.

#### **Additional Resources:**

- 1. Cotton, F. A.; Wilkinson, G.; Gaus, P.L. (1995), **Basic Inorganic Chemistry**, 3<sup>rd</sup> Edition, John Wilev.
- 2. Sharpe, A.G.(2005), **Inorganic Chemistry**, Pearson Education.
- 3. Greenwood, N.N.; Earnshaw, A.(1997), Chemistry of the Elements, Elsevier.
- 4. Silverstein, R.M.; Bassler, G.C.; Morrill, T.C. (1991), Spectroscopic Identification of Organic Compounds, John Wiley & Sons.
- 5. Dyer, J.R.(1978), Applications of Absorption Spectroscopy of Organic Compounds, Prentice Hall.

# **Teaching Learning Process:**

- Teaching Learning Process for the course is visualized as largely student-focused.
- Transaction through an intelligent mix of conventional and modern methods.
- Engaging students in cooperative learning.
- Learning through quiz design.
- Problem solving to enhance comprehension.

#### **Assessment Methods:**

Assessmentwill be done on the basis of regular class test, presentations and assignments as a part of internal assessment during the course as per the curriculum. End semester university examination will be held for both theory and practical. In practical, assessment will be done based on continuous evaluation, performance in the experiment on the date of examination and viva voce.

# **Keywords:**

3d metals; Organometallic Chemistry; Metal Carbonyl; Ferrocene; 18-electron rule; Synergic bonding; Bioinorganic chemistry; Sodium potassium pump; Haemoglobin-myoglobin system; Biomolecules, UV-visible spectroscopy; IR spectroscopy; Charge transfer spectra.

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Course Code: CHEMISTRY -DSE-3

**Course Title: Applications of Computers in Chemistry** 

Total Credits: 06 (Credits: Theory-04, Practical-02)

(Total Lectures: Theory- 60, Practical-60)

# **Objectives:**

The aim of this paper is to make the students learn the working of computer and its applications in chemistry via programming language, QBASIC and use of software as a tool to understand chemistry, and solve chemistry based problems.

# **Learning Outcomes:**

#### By the end of the course, the students will be able to:

- Have knowledge of most commonly used commands and library functions used in QBASIC programming.
- 2. Develop algorithm to solve problems and write corresponding programs in BASIC for performing calculations involved in laboratory experiments and research work.
- 3. Use various spreadsheet software to perform theoretical calculations and plot graphs

#### Unit 1

#### **Basic Computer system (in brief)**

Hardware and Software; Input devices, Storage devices, Output devices, Central Processing Unit (Control Unit and Arithmetic Logic Unit); Number system (Binary, Octal and Hexadecimal Operating System); Computer Codes (BCD and ASCII); Numeric/String constants and variables. Operating Systems (DOS, WINDOWS, and Linux); Software languages: Low level and High Level languages (Machine language, Assembly language; QBASIC, FORTRAN and C++); Compiled versus interpreted languages. Debugging Software Products (Office, chemsketch, scilab, matlab, and hyperchem), internet application

(Lectures: 5)

## Unit 2

#### Use of Programming Language for solving problems in Chemistry

Computer Programming Language- QBASIC, (for solving some of the basic and complicated chemistry problems). QB4 version of QBASIC can be used.

Programming Language – QBASIC; arithmetic expressions, hierarchy of operations, inbuilt functions. Syntax and use of the following QBASIC commands: INPUT and PRINT; GOTO, If, ELSEIF, THEN and END IF; FOR and NEXT; Library Functions (ABS, ASC, CHR\$, EXP,INT, LOG, RND, SQR,TAB and trigonometric Functions), DIM, READ, DATA, REM, RESTORE, DEF FNR, GOSUB, RETURN, SCREEN, VIEW, WINDOW, LINE, CIRCLE, LOCATE, PSET

Simple programs using above mentioned commands.

Solution of quadratic equation, polynomial equations (formula, iteration, Newton – Raphson methods, binary bisection and Regula Falsi); Numerical differential, Numerical integration (Trapezoidal and Simpson's rule), Simultaneous equations, Matrix addition and multiplication, Statistical analysis.

QBASIC programs for Chemistry problems - Example: plotting van der Waals Isotherms (Simple Problem, available in general text books) and observe whether van der Waal gas equation is valid at temperatures lower than critical temperature where we require to solve a cubic equation and calculation of area under the curves (Complicated Problem, not available in general text books).

(Lectures: 40)

# Unit 3

#### **Use of Software Products**

Computer Software like Scilab, Excel, LibreOffice and Calc, to solve some of the plotting or calculation problems, Handling of experimental data

(Lectures: 15)

## **Practical:**

# (Credits: 2, Laboratory periods: 60)

#### Computer programs using QBASIC based on numerical methods

- 1. Roots of equations: (e.g. volume of gas using van der Waals equation and comparison with ideal gas, pH of a weak acid).
- 2. Numerical differentiation (e.g., change in pressure for small change in volume of a van der Waals gas, potentiometric titrations).
- 3. Numerical integration (e.g. entropy/ enthalpy change from heat capacity data).
- 4. Probability distributions (gas kinetic theory) and mean values.
- 5. Mean, standard deviation and Least square curve fitting method for linear equation.
- 6. Matrix operations: addition, multiplication and transpose
- 7. Graphic programs related to Chemistry problems. e.g. van der Waals isotherm, Compressibility versus pressure curves, Maxwell distribution curves, concentration-time graph, pH metric titration curve, conductometric titration curves, Lambert Beer's law graph, s, p, d orbital shapes, radial distribution curves, particle in one dimensional box.

#### **Use of Software Products**

- 1. Computer Software like Scilab and Excel, etc for data handling and manipulation.
- 2. Simple exercises using molecular visualization software.
- 3. Open source chemistry software to draw structures.

## **References:**

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## Theory:

- 1. McQuarrie, D. A.(2008), Mathematics for Physical Chemistry, University Science Books.
- 2. Mortimer, R.(2005), Mathematics for Physical Chemistry, 3rd Edition, Elsevier.
- 3. Steiner, E.(1996), The Chemical Maths Book, Oxford University Press.
- 4. Yates, P. (2007), Chemical Calculations, CRC Press.
- 5. Harris, D. C. (2007), Quantitative Chemical Analysis, 6th Edition, Freeman, Chapters 3-5.

#### Practical:

- 1. Levie, R.D.(2001), How to use Excel in analytical chemistry and in general scientific data analysis, Cambridge University Press.
- 2. Noggle, J. H.(1985), Physical Chemistry on a Microcomputer, Little Brown & Co.
- 3. Venit, S.M.(1996), Programming in BASIC: Problem solving with structure and style, Jaico Publishing House.

# **Teaching Learning Process:**

Conventional methods of teaching i.e. lectures, PPTs, Complete demonstrations of computer systems in chemistry using QBASIC -a DOS based language. Using DOSBOX emulator for different operating systems and running QB45 in it can solve this problem. Another version that runs on WINDOWS is QB64. This is compatible with most of the QBASIC commands.

#### **Assessment Methods:**

- The students to be assigned projects based on chemistry problems done in class or in practical classes and use BASIC program to solve it. The projects to be a part of internal assessment.
- Presentation
- Test
- Semester end examination

# **Keywords:**

Hardware, software, programming language, ASCII, BCD, QBASIC, Library commands, mathematical operators, QBASIC commands.

Course Code: CHEMISTRY -DSE-4

**Course Title: Molecular Modelling and Drug Design** 

Total Credits: 06 (Credits: Theory-04, Practical-02)

(Total Lectures: Theory- 60, Practical-60)

# **Objectives:**

Objective of this course is to make students learn the theoretical background of principles of computational techniques in molecular modelling, evaluation and applications of different methods for various molecular systems, energy minimization techniques, analysis of Mulliken Charge & ESP Plots and elementary idea of drug design.

# **Learning Outcomes:**

## By the end of this course, students will be able to:

- Understand theoretical background of computational techniques and selective application to various molecular systems.
- Learn Energy minimization methods through use of different force fields.
- Learn ESP Plots by suitable soft wares, electron rich and electron deficient sites,
- Compare computational and experimental results and explain deviations.
- Carry out Molecular dynamics (MD) and Monte Carlo (MC) simulations on several molecules and polymers.
- Learn QSAR properties and their role in molecular modelling, cheminformatics and drug discovery.
- Perform Optimization of geometry parameters of a molecule (such as shape, bond length and bond angle) through use of software like Chem Sketch and Argus Lab in interesting hands-on exercises.

#### Unit 1

**Introduction:** Overview of Classical and Quantum Mechanical Methods (Ab initio, Semi-empirical, Molecular Mechanics, Molecular Dynamics and Monte Carlo) General considerations.

Coordinate systems: Cartesian and Internal Coordinates, Bond lengths, bond angles and torsion angles, Writing Z -matrix (ex: methane, ethane, ethene, ethyne, water,  $H_2O_2$ .

(Lectures: 8)

## Unit 2

**Potential Energy Surfaces:** Intrinsic Reaction Coordinates, Stationary points, Equilibrium points – Local and Global minima, concept of transition state with examples: Ethane, propane, butane, cyclohexane. Meaning of rigid and relaxed PES.

Applications of computational chemistry to determine reaction mechanisms.

**Energy Minimization and Transition State Search:** Geometry optimization, Methods of energy minimization: Multivariate Grid Search, Steepest Descent Method, Newton-Raphson method and Hessian matrix.

(Lectures: 12)

#### Unit 3

**Molecular Mechanics:** Force Fields, Non-bonded interactions (van der Waals and electrostatic), how to handle torsions of flexible molecules, van der Waals interactions using Lennard-Jones potential, hydrogen bonding interactions, electrostatic term, Parameterization. Applications of MM, disadvantages, Software, Different variants of MM: MM1, MM2, MM3, MM4, MM+, AMBER, BIO+, OPLS.GUI.

(Lectures: 10)

# Unit 4

**Molecular Dynamics:** Radial distribution functions for solids, liquids and gases, intermolecular Potentials (Hard sphere, finite square well and Lennard-Jones potential), concept of periodic box, ensembles (microcanonical, canonical, isothermal – isobaric), Ergodic hypothesis. Integration of

Newton's equations (Leapfrog and Verlet Algorithms), Rescaling, Simulation of Pure water – Radial distribution curves and interpretation, TIP & TIP3P, Typical MD simulation

Brief introduction to Langevin and Brownian dynamics

Monte Carlo Method: Metropolis algorithm.

(Lectures: 10)

#### Unit 5

**Huckel MO** with examples: ethane, propenyl, cyclopropenyl systems, Properties calculated – energy, charges, dipole moments, bond order, electronic energies, resonance energies, Oxidation and reduction (cationic and anionic species of above systems)

Extension to Extended Huckel theory and PPP methods

**Ab-initio** methods: Writing the Hamiltonian of a system, Brief recap of H – atom solution, Units in quantum mechanical calculations, Born-Oppenheimer approximation (recap), Antisymmetry principle, Slater determinants, Coulomb and Exchange integrals,

Examples of He atom and hydrogen molecule, Hartree-Fock method

Basis sets, Basis functions, STOs and GTOs, diffuse and polarization functions. Minimal basis sets

Advantages of ab initio calculations, Koopman's theorem, Brief idea of Density Functional Theory

(Lectures: 12)

#### Unit 6

**Semi-empirical methods:** Brief idea of CNDO, INDO, MINDO/3, MNDO, AM1, PM3 methods. Other file formats – PDB. Visualization of orbitals – HOMO, LUMO, ESP maps.

**QSAR:** Structure-activity relationships. Properties in QSAR (Partial atomic charges, polarizabilities, volume and surface area, log P, lipophilicity and Hammet equation and applications, hydration energies, refractivity). Biological activities (LD50, IC50, ED50.)

(Lectures: 8)

# **Practical:**

#### (Credits: 2, Laboratory periods: 60)

- 1. Plotting a 3D graph depicting a saddle point in a spreadsheet software.
- 2. Determine the enthalpy of isomerization of cis and trans 2-butene.
- 3. Determine the heat of hydrogenation of ethylene.
- 4. Compare the optimized C-C bond lengths and Wiberg bond orders in ethane, ethene, ethyne and benzene using PM3. Is there any relationship between the bond lengths and bond orders? Visualize the highest occupied and lowest unoccupied molecular orbitals of ethane, ethene, ethyne, benzene and pyridine.

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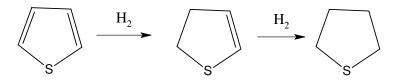
- 5. Perform a conformational analysis of butane.
- 6. Compare the basicities of the nitrogen atoms in ammonia, methylamine, dimethylamine and trimethylamine by comparison of their Mulliken charges and ESP maps.
- 7. Compare the gas phase basicities of the methylamines by comparing the enthalpies of the following reactions:

 $BH^+ + NH_3 \rightarrow B + NH_4^+$ 

where  $B = CH_3NH_2$ ,  $(CH_3)_2NH$ ,  $(CH_3)_3N$ 

- 8. Arrange 1-hexene, 2-methyl-2-pentene, (E)-3-methyl-2-pentene, (Z)-3-methyl-2-pentene, and 2,3-dimethyl-2-butene in order of increasing stability.
- 9. Compare the optimized bond angles H<sub>2</sub>O, H<sub>2</sub>S, H<sub>2</sub>Se using PM3.
- 10. Compare the HAH bond angles for the second row hydrides (BeH<sub>2</sub>, CH<sub>4</sub>, NH<sub>3</sub>, H<sub>2</sub>O) and compare with the results from qualitative MO theory.
- 11. (a) Compare the shapes of the molecules: 1-butanol, 2-butanol, 2-methyl-1-propanol, and 2-methyl-2-propanol. Note the dipole moment of each molecule. (b) Show how the shapes affect the trend in boiling points: (118 °C, 100 °C, 108 °C, 82 °C, respectively).
- 12. Compute the resonance energy of benzene by comparison of its enthalpy of hydrogenation with that of cyclohexene.
- 13. Plot the electrostatic potential mapped on electron density for benzene and use it to predict the type of stacking in the crystal structure of benzene dimer.
- 14. Predict the aromaticity of thiophene with respect to benzene by comparing the enthalpies of the following reactions:
  - (a) Hydrogenation of benzene to 1,3-cyclohexadiene and then 1,3-cyclohexadiene to cyclohexene.

(b)



15. Docking of Sulfonamide-type D-Glu inhibitor into MurD active site using Argus lab.

Note: Software: Argus Lab (www.planaria-software.com).

## **References:**

## Theory:

- 1. Lewars, E. (2003), Computational Chemistry, Kluwer academic Publisher.
- 2. Cramer, C.J.(2004), Essentials of Computational Chemistry, John Wiley & Sons.
- 3. Hinchcliffe, A. (1996), Modelling Molecular Structures, John Wiley & Sons.
- 4. Leach, A.R.(2001), Molecular Modelling, Prentice-Hall.

#### **Practical:**

- 1. Lewars, E. G. (2011), Computational Chemistry, Springer (India) Pvt. Ltd. Chapter 1 & 2.
- 2. Engel, T.; Reid, P.(2012), Physical Chemistry, Prentice-Hall. Chapter 26.

## **Teaching Learning Process:**

Conventional methods of teaching i.e. lectures, PPTs, Hands on practice of molecule centric problems with maximum characterization parameters and recently designed lead drug molecules

## **Assessment Methods:**

- Assignment based on Theoretical designing of small molecules of drug prospective
- Presentation on fundamentals of drug designing and molecular modelling
- Test
- Semester end examination

## **Keywords:**

Molecular modelling, Quantum Mechanical Method, Cartesian Coordinates, Molecular Dynamics, Force Field, Software of Computational Chemistry.

Course Code: CHEMISTRY -DSE-5
Course Title: Novel Inorganic Solids

Total Credits: 06 (Credits: Theory-04, Practical-02)

(Total Lectures: Theory- 60, Practical-60)

## **Objectives:**

Solid-state chemistry also referred as material chemistry currently has emerged with great focus on novel inorganic solids. It has found enormous applications in both industrial and research arenas and has helped to shape modern day recyclable adsorbents and catalysts. Novel inorganic-organic hybrid nanocomposites have received a lot of attention because of their abundance and cost-effective nature they can be utilized as catalysts, as a nano reactor to host reactants for synthesis and for the controlled release of biomolecules. Materials such as semiconductors, metals, composites, nanomaterials, carbon or high-tech ceramics make life easier in this era and are great sources of industrial growth and technological changes. Therefore, its exposure to the undergraduates with science backgrounds can groom them for future researches.

## **Learning Outcomes:**

## By the end of the course, the student will be able to:

- Understand the mechanism of solid-state synthesis.
- Explain about the different characterization techniques and their principle.
- Understand the concept of nanomaterials, their synthesis and properties.
- Explain the mechanism of growth of self-assembled nanostructures.
- Appreciate the existence of bioinorganic nanomaterials.
- Explain the importance of composites, conducting polymers and their applications.

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• Understand the usage of solid materials in various instruments, batteries, etc. which would help them to appreciate the real life importance of these materials

## Unit 1

**Basic introduction to solid-state chemistry:** Semiconductors, different types of semiconductors and their applications.

**Synthesis of inorganic solids:** Conventional heat and beat method, Co-precipitation method, Sol-gel method, Hydrothermal method, Chemical vapor deposition (CVD), Ion-exchange and Intercalation method.

(Lectures: 10)

## Unit 2

Characterization techniques of inorganic solids: Powder X-ray Diffraction, UV-visible spectroscopy, Scanning Electron Microscopy (SEM), Transmission Electron Microscopy (TEM), Fourier-Transform Infrared (FTIR) spectroscopy, Brunauer–Emmett–Teller (BET) surface area analyser, Dynamic Light Scattering (DLS)

(Lectures: 10)

## Unit 3

Cationic, anionic and mixed solid electrolytes and their applications. Inorganic pigments – coloured, white and black pigments.

One-dimensional metals, molecular magnets, inorganic liquid crystals.

(Lectures: 10)

#### Unit 4

**Nanomaterials:** Overview of nanostructures and nanomaterials, classification, preparation and optical properties of gold and silver metallic nanoparticles, concept of surface plasmon resonance, carbon nanotubes, inorganic nanowires, Bioinorganic nanomaterials, DNA and its nanomaterials, natural and artificial nanomaterials, self-assembled nanostructures, control of nanoarchitecture, one dimensional control.

(Lectures: 10)

## Unit 5

**Composite materials:** Introduction, limitations of conventional engineering materials, role of matrix in composites, classification, matrix materials, reinforcements, metal-matrix composites, polymer-matrix composites, fibre-reinforced composites, bio-nanocomposites, environmental effects on composites, applications of composites.

(Lectures: 10)

## Unit 6

**Speciality polymers:**Conducting polymers - Introduction, conduction mechanism, polyacetylene, polyparaphenylene, polyanilineand polypyrrole, applications of conducting polymers, ion-exchange resins and their applications.

**Ceramic & Refractory:**Introduction, classification, properties, manufacturing and applications of ceramics, refractory and superalloys as examples.

(Lectures: 10)

#### **Practical:**

## (Credits: 2, Laboratory periods: 60)

## **Chemistry Practical: Novel Inorganic Solids**

- 1. Synthesis of silver nanoparticles by chemical methods and characterization using UV-visible spectrophotometer.
- 2. Synthesis of silver nanoparticles by green approach methods and characterization using UV-visible spectrophotometer.
- 3. Preparation of polyaniline and its characterization using UV-visible spectrophotometer.
- 4. Synthesis of metal sulphide nanoparticles (MnS, CdS, ZnS, CuS, NiO) and characterization using UV-visible spectrophotometer.
- 5. Intercalation of hydrogen in tungsten trioxide and its conductivity measurement using conductometer.
- 6. Synthesis of inorganic pigments (PbCrO<sub>4</sub>, ZnCrO<sub>4</sub>, Prussian Blue, Malachite).
- 7. Synthesis of pure ZnO and Cu doped ZnO nanoparticles.
- 8. Preparation of zeolite A and removal of Mg and Ca ions from water samples quantitatively using zeolite.

#### References:

#### Theory:

- 1. West, A. R. (2014), Solid State Chemistry and Its Application, Wiley.
- 2. Smart, L. E.; Moore, E. A., (2012), **Solid State Chemistry: An Introduction** CRC Press Taylor & Francis.
- 3. Rao, C. N. R.; Gopalakrishnan, J. (1997), New Direction in Solid State Chemistry, Cambridge University Press.
- 4. Poole Jr.; Charles P.; Owens, Frank J. (2003), **Introduction to Nanotechnology**, John Wiley and Sons.

#### **Practicals:**

- 1. Orbaek, W.; McHale, M.M.; Barron, A. R.; Synthesis and Characterization of Silver Nanoparticles for An Undergraduate Laboratory, J. Chem. Educ. 2015, 92, 339–344.
- 2. MacDiarmid, G.; Chiang, J.C.; Richter, A.F.; Somasiri, N.L.D.(1987), **Polyaniline: Synthesis and Characterization of the Emeraldine Oxidation State by Elemental Analysis**, L. Alcaeer (ed.), Conducting Polymers, 105-120, D. Reidel Publishing.

- 3. Cheng, K.H.; Jacobson, A.J.; Whittingham, M.S. (1981), Hexagonal Tungsten Trioxide and Its Intercalation Chemistry, Solid State Ionics, 5, 1981, 355-358.
- 4. Ghorbani H.R.; Mehr, F.P; Pazoki, H; Rahmani, B.M.; Synthesis of ZnO Nanoparticles by Precipitation Method, Orient J Chem 2015, 31(2).

## **Teaching Learning Process:**

Blackboard, Power point presentations, Assignments, Field Trips to Industry, Different working models ICT enabled classes, Interactive sessions, Debate, recent literature using internet and research articles.

## **Assessment Methods:**

Students' evaluation will be done on the basis of regular class test, presentations and assignments as a part of internal assessment during the course as per the curriculum. End semester university examination will be held for both theory and practical. In practical, assessment will be done based on continuous evaluation, performance in the experiment on the date of examination and viva voce.

## **Keywords:**

Solid State Chemistry, Nanomaterials, Solid electrolyte, Inorganic Pigments, Self-assembled, Composite Materials, Instrumentation, Polymers.

Course Code: CHEMISTRY -DSE-6

**Course Title: Research Methodology For Chemistry** 

Total Credits: 06 (Credits: Theory-05, Tutorial-01)

(Total Lectures: Theory- 75, Tutorial-15)

## **Objectives:**

The objective of this paper is to formulate the research problems and connect the research outcomes to the society. Student should be able to assess the local resources and opportunities in public domains. It further helps in gaining the knowledge of safety and ethical handlings of chemicals in lab and households.

## **Learning Outcomes:**

## By the end of the course, the students will be able to:

- Learn how to identify research problems.
- Evaluate local resources and need for addressing the research problem
- Find out local solution.
- Know how to communicate the research findings.

## Unit 1

#### **Literature Survey**

**Print:** Sources of information: Primary, secondary, tertiary sources; Journals: Journal abbreviations, abstracts, current titles, reviews, monographs, dictionaries, text-books, current contents, Introduction to

Chemical Abstracts and Beilstein, Subject Index, Substance Index, Author Index, Formula Index, and other Indices with examples.

**Digital:** Web resources, E-journals, Journal access, TOC alerts, Hot articles, Citation index, Impact factor, H-index, E-consortium, UGC infonet, E-books, Internet discussion groups and communities, Blogs, Preprint servers, Search engines, Scirus, Google Scholar, ChemIndustry, Wiki- Databases, ChemSpider, Science Direct, SciFinder, Scopus.

Information Technology and Library Resources: The Internet and World Wide Web. Internet resources for chemistry. Finding and citing published information. Open source Lead lectures. Open source chemistry designing sources, Essentials of Problem formulation and communication with society.

(Lectures: 20)

#### Unit 2

#### Methods of Scientific Research and Writing Scientific Papers

Reporting practical and project work. Idea about public funding agencies of research, Writing literature surveys and reviews. Organizing a poster display. Giving an oral presentation. Writing scientific papers – justification for scientific contributions, bibliography, description of methods, conclusions, the need for illustration, style, publications of scientific work. Writing ethics. Avoiding plagiarism. Assessment of locally available resources.

(Lectures: 20)

#### Unit 3

## **Chemical Safety and Ethical Handling of Chemicals**

Safe working procedure and protective environment, protective apparel, emergency procedure and first aid, laboratory ventilation. Safe storage and use of hazardous chemicals, procedure for working with substances that pose hazards, flammable or explosive hazards, procedures for working with gases at pressures above or below atmospheric level. Safe storage and disposal of waste chemicals. Recovery, recycling and reuse of laboratory chemicals. Procedure for laboratory disposal of explosives. Identification, verification and segregation of laboratory waste. Disposal of chemicals in the sanitary sewer system. Incineration and transportation of hazardous chemicals.

(Lectures: 12)

#### Unit 4

#### **Data Analysis**

The Investigative Approach: Making and Recording Measurements. SI Units and their use. Scientific method and design of experiments.

Analysis and Presentation of Data: Descriptive statistics. Choosing and using statistical tests. Chemometrics. Analysis of variance (ANOVA), Correlation and regression, Curve fitting, fitting of linear equations, simple linear cases, weighted linear case, analysis of residuals, General polynomial fitting, linearizing transformations, exponential function fit, r and its abuse. Basic aspects of multiple linear regression analysis.

Biostatistics: brief introduction and data handling.

(Lectures: 13)

#### **Exposure of chemistry software**

Chemistry Students must be given exposure to applications of molecular modelling softwares e.g. Hyperchem, Schrodinger etc. Hands on experiments of docking.

(Lectures: 10)

#### **References:**

## Theory:

- 1. Dean, J.R.; Jones, A.M.; Holmes, D;, Reed, R.; Jones, A.Weyers, J. (2011), **Practical skills in chemistry**, Prentice-Hall.
- 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, Chapman Hall, London.
- 4. Levie, R. de.(2001), How to use Excel in analytical chemistry and in general scientific data analysis, Cambridge University Press.
- 5. Le, C.T.; Eberly, L.E. (2016), Introductory Biostatistics, Wiley.

#### **Additional Resources:**

- 1. Chemical safety matters IUPAC IPCS, Cambridge University Press, 1992.
- 2. OSU safety manual 1.01.

## **Teaching Learning Process**

Lecture with conventional teaching aids, presentations, invited talks on thrusting areas, group discussions, literature surveyand lab visit.

## **Assessment Methods**

- Internal assessment through assignments and class test.
- Writing review on identified research problem
- Poster presentation
- End semester university examination

## **Keywords**

Review of research papers, writing research papers, citation, and Laboratory safety.

B.Sc. Industrial Chemistry University of Delhi

Course Code: CHEMISTRY -DSE-7

**Course Title: Dissertation** 

**Total Credits: 06** 

## **Objectives:**

The Objective is to enable student to identify a problem in the field of chemistry and to carry out literature survey, design an experiment, perform experiment, analyse data and write a report.

## **Learning Outcomes:**

## By the end of the dissertation, the students will be able to;

- Do survey, study and cite published literature on a particular area of interest.
- Correlate the experimental observations with theoretical understanding.
- Interpret results, write a report and submit to the supervisor.
- Use laboratory resources judiciously.
- Work in a team under the supervision of a teacher.
- Develop scientific writing skills.

## **Content:**

- Unit 1: Identification of research problem
- Unit 2: Survey of literature
- Unit 3: Formulation of hypothesis, experimental design and methodology
- Unit 4: Analysis of data and interpretation of results
- Unit 5: Discussion and conclusion
- Unit 6: Writing a project report

## **Assessment Methods:**

The assessment will be through evaluation of the dissertation, presentation and viva voce involving external and internal examiners.

# DISCIPLINE SPECIFIC ELECTIVE COURSES (DSE) MATHOPHYSICS

## SKILL-ENHANCEMENT COURSES (SEC) CHEMISTRY

Course Code: CHEMISTRY -SEC-1
Course Title: IT Skills For Chemists

Total Credits: 04 (Credits: Theory-02, Practical-02)

(Total Lectures: Theory- 30, Practical-60)

## **Objectives:**

The objective of this course is to introduce the students to fundamental mathematical techniques and basic computer skills that will help them in solving chemistry problems. It aims to make the students understand the concept of uncertainty and error in experimental data. It acquaints the students with different software for data tabulation, calculation, graph plotting, data analysis and document preparation.

## **Learning Outcomes:**

#### By the end of the course, the students will be able to:

- Become familiar with the use of computers
- Use software for tabulating data, plotting graphs and charts, carry out statistical analysis of the data
- Solve chemistry problems and simulate graphs.
- Prepare documents that will incorporate chemical structure, chemical equations, mathematical expressions from chemistry.

#### Unit 1

## **Mathematics**

Fundamentals, mathematical functions, polynomial expressions, logarithms, the exponential function, units of a measurement, interconversion of units, constants and variables, equation of a straight line, plotting graphs.

Uncertainty in experimental techniques: Displaying uncertainties, measurements in chemistry, decimal places, significant figures, combining quantities.

Uncertainty in measurement: types of uncertainties, combining uncertainties. Statistical treatment. Mean, standard deviation, relative error. Data reduction and the propagation of errors. Graphical and numerical data reduction. Numerical curve fitting: the method of least squares (regression).

Algebraic operations on real scalar variables (e.g. manipulation of van der Waals equation in different forms). Roots of quadratic equations analytically and iteratively (e.g. pH of a weak acid). Numerical methods of finding roots (Newton-Raphson, binary –bisection, e.g. pH of a weak acid not ignoring the ionization of water, volume of a van der Waals gas, equilibrium constant expressions).

Differential calculus: The tangent line and the derivative of a function, numerical differentiation (e.g., change in pressure for small change in volume of a van der Waals gas, potentiometric titrations).

Numerical integration (Trapezoidal and Simpson's rule, e.g. entropy/enthalpy change from heat capacity data).

(Lectures: 10)

#### Unit 2

Introductory writing activities: Introduction to word processor and structure drawing (ChemSketch) software. Incorporating chemical structures, chemical equations, expressions from chemistry (e.g. Maxwell-Boltzmann distribution law, Bragg's law, van der Waals equation, etc.) into word processing documents.

(Lectures: 4)

## Unit 3

Handling numeric data: Spreadsheet software (Excel/ LibreOffice Calc), creating a spreadsheet, entering and formatting information, basic functions and formulae, creating charts, tables and graphs Incorporating tables and graphs into word processing documents. Simple calculations, plotting graphs using a spreadsheet (Planck's distribution law, radial distribution curves for hydrogenic orbitals, gas kinetic theory- Maxwell-Boltzmann distribution curves as function of temperature and molecular weight), spectral data, pressure-volume curves of van der Waals gas (van der Waals isotherms), data from phase equilibria studies. Graphical solution of equations

(Lectures: 6)

#### Unit 4

Numeric modelling: Simulation of pH metric titration curves. Excel functions LINEST and Least Squares. Numerical curve fitting, linear regression (rate constants from concentration- time data, molar extinction coefficients from absorbance data), numerical differentiation (e.g. handling data from potentiometric and pH metric titrations, pKa of weak acid), integration (e.g. entropy/enthalpy change from heat capacity data)

(Lectures: 6)

## Unit 5

Statistical analysis: Gaussian distribution and Errors in measurements and their effect on data sets. Descriptive statistics using Excel. Statistical significance testing: The t test. The F test. Presentation graphics.

(Lectures: 4)

## **Practical:**

## (Credits: 2, Laboratory periods: 60)

- 1. Potting graphs using a spreadsheet
  - i. Planck's distribution law
  - ii. Radial distribution curves for hydrogenic orbitals,

- iii. Maxwell-Boltzmann distribution curves as function of temperature and molecular weight
- iv. van der Waals isotherms
- v. Data from phase equilibria studies
- 2. Calculations using spreadsheet
  - vi. Rate constants from concentration- time data
- vii. Molar extinction coefficients from absorbance data
- viii. Numerical differentiation (e.g. handling data from potentiometric and pH metric titrations)
- ix. pKa of weak acid
- 3. Preparing a word processing document having tables, chemical structures and chemical equations

#### References:

- 1. McQuarrie, D.A. (2008), Mathematics for Physical Chemistry University Science Books.
- 2. Steiner, E.(2008), The Chemical Maths Book Oxford University Press.
- 3. Yates, P.(2007), Chemical calculations, CRC Press.
- 4. Harris, D.C. (2007), Quantitative Chemical Analysis. Freeman, Chapters 3-5.
- 5. Levie, R. de. (2001), How to use Excel in analytical chemistry and in general scientific data analysis, Cambridge Univ. Press.
- 6. Venit, S.M. (1996), **Programming in BASIC: Problem solving with structure and style**. Jaico Publishing House.

## **Teaching Learning Process:**

This course has major components of hands on exercises. The teaching learning process will require conventional teaching along with hands on exercise on computers.

#### **Assessment Methods:**

Assessment on solving chemistry related problems using spreadsheet.

Presentation on documentation preparation on any chemistry topic involving tables and graphs

Semester end practical and theory examination

## **Keywords:**

Uncertainty in measurements, roots of quadratic and polynomial equations, Newton Raphson's method, binary bisection, numerical integration, trapezoidal rule, Simpson's rule, differential calculus, least square curve fitting method, Spreadsheet, charts, tables, graphs, LINEST, t-test, F-test.

B.Sc. Industrial Chemistry University of Delhi

Course Code: CHEMISTRY -SEC-2

**Course Title: Basic Analytical Chemistry** 

Total Credits: 04 (Credits: Theory-02, Practical-02)

(Total Lectures: Theory- 30, Practical-60)

## **Objectives:**

The objective of this course is to make students aware about the importance and the concepts of chemical analysis of water and soil, using separation techniques like chromatography and instrumentation techniques like flame photometry and spectrophotometry.

## **Learning Outcomes:**

#### By the end of this course, students will be able to:

- Handle analytical data
- Determine composition and pH of soil, which can be useful in agriculture
- Do quantitative analysis of metal ions in water
- Separate mixtures using separation techniques
- Estimate macro nutrients using Flame photometry

#### Unit 1

#### Introduction

Introduction to analytical chemistry and its interdisciplinary nature, Concept of sampling. Importance of accuracy, precision and sources of error in analytical measurements. Significant figures. Presentation of experimental data and results.

(Lectures: 6)

#### Unit 2

## **Analysis of soil**

Composition of soil, concept of pH and its measurement, complexometric titrations, chelation, chelating agents, use of indicators.

(Lectures: 8)

## Unit 3

#### Analysis of water:

Definition of pure water, sources responsible for contaminating water, water sampling methods, water purification methods.

(Lectures:8)

#### Unit 4

## Chromatography

Definition and general introduction on principles of chromatography. Paper chromatography, thin layer chromatography, Column chromatography and ion-exchange chromatography.

(Lectures: 8)

## **Practical:**

## (Credits: 2, Laboratory periods: 60)

## **Chemistry Lab-Basic analytical chemistry**

- 1. Determination of pH of soil samples.
- 2. Estimation of Calcium and Magnesium ions as Calcium carbonate by complexometric titration.
- 3. Determination of pH, acidity and alkalinity of a water sample.
- 4. Determination of dissolved oxygen (DO) of a water sample.
- 5. Paper chromatographic separation of mixture of metal ion (Ni<sup>2+</sup> and Co<sup>2+</sup>).
- 6. To study the use of phenolphthalein in trap cases.
- 7. To analyze arson accelerants.
- 8. To carry out analysis of gasoline.
- 9. Estimation of macro-nutrients: Potassium, calcium and magnesium in soil samples by flame photometry.
- 10. Spectrophotometric determination of Iron in vitamin / dietary tablets.
- 11. Spectrophotometric identification and determination of caffeine and benzoic acid in soft drink.
- 12. Determination of ion exchange capacity of anion / cation exchange resin (using batch procedure if use of column is not feasible).

## **References:**

- 1. Christian, G.D. (2004), Analytical Chemistry, John Wiley & Sons.
- 2. Harris, D. C. (2007), Exploring Chemical Analysis, W.H. Freeman and Co.
- 3. Skoog, D.A.; Holler F.J.; Nieman, T.A. (2005), **Principles of Instrumental Analysis**, Thomson Asia Pvt. Ltd.
- 4. Svehla, G. (1996), Vogel's Qualitative Inorganic Analysis, Prentice Hall.
- 5. Mendham, J.; Denney, R.C.; Barnes, J.D.; Thomas, M.J.K. (2007), **Vogel's Quantitative Chemical Analysis**,6<sup>th</sup> Edition, Prentice Hall.

## **Teaching Learning Process:**

· Conventional chalk and board teaching,

- Class room interactions and group discussions
- Lab demonstrations and experiments after completion of theory part
- ICT enabled classes

#### **Assessment Methods:**

Assessment will be done on the basis of regular class test, presentations and assignments as a part of internal assessment during the course as per the curriculum. End semester university examination will be held for both theory and practical. In practical, assessment will be done based on continuous evaluation, performance in the experiment on the date of examination and viva voce.

## **Keywords:**

Analytical chemistry, Sampling, Accuracy, Precision, Significant figures, Soil analysis, Analysis of water, Chromatography, Ion exchange chromatography, Flame photometry.

Course Code: CHEMISTRY -SEC-3

**Course Title: Chemical Technology and Society** 

Total Credits: 04 (Credits: Theory-04)

(Total Lectures: Theory- 60)

## **Objectives:**

This course will help students to connect chemical technology for societal benefits. It would fulfil the gap between academia and industries.

## **Learning Outcomes:**

#### By the end of the course, the students will be able to:

- Understand the use of basic chemistry to chemical engineering
- · Learn and use various chemical technology used in industries
- Develop scientific solutions for societal needs

#### **Chemical Technology**

Basic principles of distillation, solvent extraction, solid-liquid leaching and liquid-liquid extraction, separation by absorption and adsorption. An introduction into the scope of different types of equipment needed in chemical technology, including reactors, distillation columns, extruders, pumps, mills, emulgators. Scaling up operations in chemical industry. Introduction to clean technology.

#### Society

Exploration of societal and technological issues from a chemical perspective. Chemical and scientific literacy as a means to better understand topics like air and water (and the trace materials found in them that are referred to as pollutants).

## Sources of energy

Coal, petrol and natural gas. Nuclear fusion / fission, solar, hydrogen, geothermal, tidal and hydel.

#### Properties of Polymers (Physical, thermal, Flow & Mechanical Properties)

Brief introduction to preparation, structure, properties and application of the following polymers: polyolefins, polystyrene and styrene copolymers, poly(vinyl chloride) and related polymers, poly(vinyl acetate) and related polymers, acrylic polymers, fluoro polymers, polyamides and related polymers. Phenol formaldehyde resins (Bakelite, Novolac), polyurethanes, silicone polymers, polydienes, Polycarbonates, Conducting Polymers, [polyacetylene, polyaniline, poly(p-phenylene sulphide), polypyrrole, polythiophene].

#### **Natural Polymers**

Structure, properties and applications of shellac, lignin, starch, nucleic acids and proteins.

#### Basics of drug synthesis

Application of genetic engineering

## **References:**

1. Hill, J.W.; McCreary, T.W.; Kolb, D.K. (2013), Chemistry for changing times, Pearson.

## **Teaching Learning Process:**

- Lectures using teaching aid (chalk/power point/videos)
- Group discussion
- Presentations
- Advise to students to prepare a report on technological applications
- Visit to nearby industries
- Invite people of industries for interaction with students

## **Assessment Methods:**

- · Graded assignments
- Conventional class tests
- Class seminars by students on course topics with a view to strengthening the content through width and depth
- Quizzes
- End semester university examination.

## **Keywords:**

Chemical Technology; Society; Energy; Polymer; Pollutants.

Course Code: CHEMISTRY –SEC-4
Course Title: Chemoinformatics

Total Credits: 04 (Credits: Theory-02, Practicals-

02)

(Total Lectures: Theory- 30, Practicals-60)

## **Objectives:**

The aim of the course is to introduce the students to computational drug design through structureactivity relationship, QSAR and combinatorial chemistry. The students will learn about the target analysis, virtual screening for lead discovery, structure based and ligand based design method and the use of computational techniques, library preparation and data handling.

## **Learning Outcomes:**

## By the end of the course, the students will be able to:

- Have a comprehensive understanding of drug discovery process and techniques including structure-activity relationship, quantitative structure activity relationship and the use of chemoinformatics in this, including molecular modelling and docking studies.
- Appreciate role of modern computation techniques in the drug discovery process and perform their own modelling studies.

#### Unit 1

Introduction to Chemoinformatics: History and evolution of chemoinformatics, Use of chemoinformatics, Prospects of chemoinformatics, Molecular modelling and structure elucidation.

(Lectures: 2)

## Unit 2

Representation of molecules and chemical reactions: Nomenclature, Different types of notations, SMILES coding, Matrix representations, Structure of Molfiles and Sdfiles, Libraries and toolkits, Different electronic effects, Reaction classification.

(Lectures: 2)

## Unit 3

Searching chemical structures: Full structure search, sub-structure search, basic ideas, similarity search, three dimensional search methods, basics of computation of physical and chemical data and structure descriptors, data visualization.

(Lectures: 6)

## Unit 4

Applications: Prediction of Properties of Compounds; Linear Free Energy Relations; Quantitative Structure-Property Relations; Descriptor Analysis; Model Building; Modeling Toxicity.

(Lectures: 6)

#### Unit 5

Structure-Spectra correlations; Prediction of NMR, IR and Mass spectra; Computer Assisted Structure elucidations; Computer Assisted Synthesis Design

(Lectures: 6)

## Unit 6

Introduction to drug design; Target Identification and Validation; Lead Finding and Optimization; Analysis of HTS data; Virtual Screening; Design of Combinatorial Libraries; Ligand-Based and Structure Based Drug design; Application of Chemoinformatics in Drug Design.

(Lectures: 8)

#### **Practical:**

(Credits: 2, Laboratory periods: 60)

- 1. Overview of Rational Drug Design, Ligands and Targets
- 2. In silico representation of chemical information
  - i. CIF IUCr Crystallographic Information Framework
  - ii. CML Chemical Markup Language
  - iii. SMILES -- Simplified Molecular Input Line Entry Specification
  - iv. InChi -- IUPAC International Chemical Identifier
  - v. Other representations
- 3. Chemical Databases and Data Mining
  - Cambridge Structural Database CCDC CSD
  - Crystallographic Open Database COD
  - Protein Data Bank PDB Ligand Explorer
  - Chemspider
  - Other Data Bases
- 4. Molecular Drawing and Interactive Visualization
  - ChemDraw
  - MarvinSketch
  - ORTEP
  - Chimera, RasMol, PyMol
- 5. Computer-Aided Drug Design Tools
  - Molecular Modeling Tools
  - Structural Homology Modeling Tools
  - Docking Tools and Screening Tools

- Other tools
- 6. Building a Ligand
  - · Building ab initio
  - Building from similar ligands
  - Building with a known macromolecular target
  - Building without a known macromolecular target
  - Computational assessment of activity and toxicity and drugability.

## **References:**

- 1. Leach, A. R.; Gillet, V. J. (2007), An introduction to Chemoinformatics, Springer.
- 2. Gasteiger, J.; Engel, T. (2003), Chemoinformatics: A text-book. Wiley-VCH.
- 3. Gupta, S. P. (2011), QSAR & Molecular Modeling. Anamaya Pub.
- Gasteiger, J. Handbook of cheminformatics: from data to knowledge in 4 volumes, Wiley.

#### **Additional Resources:**

1. Jürgen, B. (2004), Chemoinformatics Concepts, Methods, and Tools for Drug Discovery, Springer

## **Teaching Learning Process:**

The course aims to introduce students to different cheminformatics methods and its use in drug research through practicals. It is a rather new discipline of science. It concerns with the applications of computer to solving the chemistry problems related to drug designing and drug discovery.

The course will give emphasis on active learning in students through a combination of lectures, tutorials and practical sessions. The underlying principles will be explained in lectures and the practicals will establish the understanding of these principles through applications to drug research.

#### **Assessment Methods:**

- Formative assessment supporting student learning in Cheminformatics practicals
- Summative assessment
- Review of a case study
- Exercise based on SAR and QSAR-Report
- · Practical exam of five hours

## **Keywords:**

Cheminformatics, Virtual Chemical Library, Virtual Screening, SAR-QSAR, Drug Design lead discovery.

Course Code: CHEMISTRY –SEC-5

**Course Title: Analytical Clinical Biochemistry** 

Total Credits: 04 (Credits: Theory-02, Practical-02)

(Total Lectures: Theory- 30, Practical-60)

## **Objectives:**

The objective of this course is to deliver information about biochemically significant features of the proteins, enzymes, nucleic acids and lipids, using suitable examples. This includes classification, properties and biological importance of biomolecules. The course provides an overview of drug receptor interaction and Structure Activity Relation (SAR) studies. It will introduce the students to the concept of genetic code and concept of heredity. Key emphasis is placed on understanding the basic principles that govern the biological functions of biomolecules.

## **Learning Outcomes:**

## By the end of the course, the students will be able to:

- Understand and establish how the structure of biomolecules determines their reactivity and biological uses.
- Understand the basic principles of drug-receptor interaction and structure activity relation (SAR).
- Gain an insight into concept of heredity through biological processes like replication, transcription and translation.
- Demonstrate an understanding of the biochemistry of diseases.
- Understand the application of chemistry in biological systems.

#### Unit 1

#### Metabolism

Biological importance of carbohydrates and proteins, Introduction to metabolism (catabolism, anabolism), ATP: the universal currency of cellular energy, outline of catabolic pathways of fats, proteins and carbohydrate-glycolysis, alcoholic and lactic acid fgermentation, Krebs cycle.

(Lectures: 4)

## Unit 2

#### **Enzymes**

Nomenclature, classification, Characterisation, Mechanism of enzyme action, factors affecting enzyme action, Coenzymes and cofactors and their role in biological reactions, Specificity of enzyme action (Including stereospecificity), Enzyme inhibitors and their importance, Introduction to biocatalysis: Importance in —green chemistry and chemical industry. Drug action-receptor theory. Structure – activity relationships of drug molecules, binding role of –OH group, -NH<sub>2</sub> group, double bond and aromatic ring.

(Lectures: 8)

## Unit 3

#### Lipids

Classification. Biological importance of triglycerides and phosphoglycerides and cholesterol; Liposomes and their biological functions and underlying applications, Lipoproteins. Properties, functions and biochemical functions of steroid hormones and peptide hormones

(Lectures: 6)

#### Unit 4

#### **Nucleic Acids**

Components of nucleic acids: adenine, guanine, thymine and cytosine (structure only), other components of nucleic acids, nucleosides and nucleotides (numbering), structure of DNA (Watson-Crick model) and RNA (types of RNA), genetic code, biological roles of DNA and RNA: replication, transcription and translation.

(Lectures: 6)

#### Unit 5

#### **Biochemistry of disease**

A diagnostic approach by blood/ urine analysis, Blood: composition and functions of blood, blood coagulation. Blood collection and preservation of samples, Anaemia, Urine: Collection and preservation of samples. Formation of urine. Composition and estimation of constituents of normal and pathological urine. Regulation, estimation and interpretation of data for blood sugar, urea, creatinine, cholesterol and bilirubin.

(Lectures: 6)

## **Practical:**

(Credits: 2, Laboratory periods: 60)

Chemistry Lab: Analytical clinical biochemistry

- 1. Proteins-Qualitative tests
- 2. Lipids qualitative Tests.
- 3. Determination of the iodine number of oil.
- 4. Determination of the saponification number of oil.
- 5. Determination of acid value of fats and oils.
- 6. Determination of cholesterol using Liebermann- Burchard reaction.
- 7. Estimation of DNA by diphenylamine reaction
- 8. Determination of amount of protein using Lowry's method.
- 9. Determination of enzyme activity

## **References:**

#### Theory:

- 1. Devlin, T.M. (2010), Textbook of Biochemistry with Clinical Correlation, Wiley.
- 2. Berg, J. M.; Tymoczko, J. L.; Stryer, L. (2002), Biochemistry, W. H. Freeman.
- 3. Satyanarayana, U.; Chakrapani, U. (2017), **Fundamentals of Biochemistry**, Books and Allied (P) Ltd.
- 4. Lehninger, A.L; Nelson, D.L; Cox, M.M. (2009), Principles of Biochemistry, W. H. Freeman.

5. Finar, I. L. **Organic Chemistry** (Volume 1 & 2), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).

#### Practical:

- 1. Dean, J.R.; Jones, A.M.; Holmes, D;, Reed, R.; Jones, A.Weyers, J. (2011), **Practical skills in chemistry**, Prentice-Hall.
- Wilson, K.; Walker, J. (2000), Principles and techniques of practical biochemistry, Cambridge University Press.
- 3. Gowenlock, A.H. (1988), Varley's Practical Clinical Biochemistry, CRC Press.

## **Teaching Learning Process:**

- The teaching learning process will involve the traditional chalk and black board method.
- Certain topics like Mechanism of enzyme action, drug receptor theory, transcription and translation, SAR etc. where traditional chalk and talk method may not be able to convey the concept, are taught through audio-visual aids.
- Students are encouraged to participate actively in the classroom through regular presentations on curriculum based topics.
- As the best way to learn something is to do it yourself, practicals are planned in such a way so
  as to reinforce the topics covered in theory.

## **Assessment Methods:**

Assessmentwill be done on the basis of regular class test, presentations and assignments as a part of internal assessment during the course as per the curriculum. End semester university examination will be held for both theory and practical. In practical, assessment will be done based on continuous evaluation, performance in the experiment on the date of examination and viva voce.

## **Keywords:**

Metabolism, Enzymes, Mechanism of enzyme action and Inhibition, Structure activity relation (SAR), Drug Receptor Theory, Biocatalysis, Lipids and their biological functions, Nucleic acids and concept of heredity, Biochemistry of diseases.

Course Code: CHEMISTRY -SEC-6

**Course Title: Green Methods in Chemistry** 

Total Credits: 04 (Credits: Theory-02, Practicals-

02)

(Total Lectures: Theory- 30, Practicals-60)

## **Objectives:**

- To inspire the students about the chemistry which is good for human health and environment.
- To evaluate suitable technologies for the remediation of hazardous substances.
- To make students aware of how chemical processes can be designed, developed and run in a sustainable way.
- To acquire the knowledge of the twelve principles of green chemistry and how to apply in green synthesis.

- To make students aware about the benefits of using green chemistry.
- To have the idea of Biocatalytic Process—Conversion of Biomass into chemicals.

## **Learning Outcomes:**

#### By the end of this course, students will be able to:

- Get idea of toxicology, environmental law, energy and the environment
- Think to design and develop materials and processes that reduce the use and generation of hazardous substances in industry.
- Think of chemical methods for recovering metals from used electronics materials.
- Get ideas of innovative approaches to environmental and societal challenges.
- Know how chemicals can have an adverse/potentially damaging effect on human and vegetation.
- Critically analyse the existing traditional chemical pathways and processes and creatively think about bringing environmentally benign reformations in these protocols.
- Convert biomass into valuable chemicals through green technologies.

## Unit 1

#### Introduction

- Definition of green chemistry and how it is different from conventional chemistry and environmental chemistry.
- Need of green chemistry
- Importance of green chemistry in- daily life, Industries and solving human health problems (four examples each).
- A brief study of Green Chemistry Challenge Awards (Introduction, award categories and study about five last recent awards).

(Lectures:8)

#### Unit 2

#### Twelve Principles of Green Chemistry

The twelve principles of the Green Chemistry with their explanations

Special emphasis on the following:

- Prevention of waste / byproducts, pollution prevention hierarchy.
- Green metrics to assess greenness of a reaction: environmental impact factor, atom economy and calculation of atom economy.
- Green solvents-supercritical fluids, water as a solvent for organic reactions, ionic liquids, solvent less reactions, solvents obtained from renewable sources.
- Catalysis and green chemistry- comparison of heterogeneous and homogeneous catalysis, biocatalysis, asymmetric catalysis and photocatalysis.
- · Green energy and sustainability.
- Real-time analysis for pollution prevention.
- Prevention of chemical accidents, designing greener processes, inherent safer design, principle
  of ISD "What you don't have cannot harm you", greener alternative to Bhopal Gas Tragedy
  (safer route to carcarbaryl) and Flixiborough accident (safer route to cyclohexanol) subdivision
  of ISD, minimization, simplification, substitution, moderation and limitation.

(Lectures:14)

## Unit 3

The following Real-world Cases in green chemistry should be discussed:

Surfactants for carbon dioxide – replacing smog producing and ozone depleting solvents with CO<sub>2</sub> for precision cleaning and dry cleaning of garments.

Designing of environmentally safe marine antifoulant.

Rightfit pigment: Synthetic azo pigments to replace toxic organic and inorganic pigments.

An efficient, green synthesis of a compostable and widely applicable plastic (polylactic acid) made from corn

(Lectures:8)

## **Practical:**

(Credits: 2, Laboratory periods: 60)

## Chemistry Lab- Green methods in chemistry

Characterization by m. pt.; U.V.-Visible spectroscopy, IR spectroscopy, and any other specific method should be done (wherever applicable).

- 1. Preparation and characterization of nanoparticles of gold using tea leaves/ silver nanoparticles using plant extracts.
- 2. Preparation and characterization of biodiesel from vegetable oil preferably waste cooking oil.
- 3. Extraction of D-limonene from orange peel using liquid CO<sub>2</sub> prepared from dry ice.
- 4. Mechanochemical solvent free, solid-solid synthesis of azomethine using p-toluidine and ovanillin (various other combinations of primary amine and aldehyde can also be tried).
- 5. Solvent free, microwave assisted one pot synthesis of phthalocyanine complex of copper(II).
- 6. Designing and conducting an experiment by utilizing the products and by-products obtained in above preparations which become waste otherwise if not used. This is done by critical thinking and literature survey.

Some representative examples:

- 7. Use of nanoparticles as catalyst for a reaction.
- 8. Use of azomethine for complex formation.
- 9. Conversion of byproduct of biodiesel to a useful product.

#### References:

## Theory:

- 1. Anastas, P.T.; Warner, J.C.(1998), Green Chemistry, Theory and Practice, Oxford University Press.
- 2. Lancaster, M.(2016), Green Chemistry An Introductory Text. 2nd Edition, RSC Publishing.
- Cann ,M. C.; Umile, T.P. (2008), Real world cases in Green chemistry Vol 11, American chemical Society, Washington.
- 4. Matlack, A.S.(2001), Introduction to Green Chemistry, Marcel Dekker.
- 5. Ryan, M.A.; Tinnesand, M. (2002), **Introduction to Green Chemistry** (Ed), American Chemical Society, Washington DC.

#### **Practical:**

 Kirchoff, M.; Ryan, M.A. (2002), Greener approaches to undergraduate chemistry experiment. American Chemical Society, Washington DC.

- 2. Sharma, R.K.; Sidhwani, I.T.; Chaudhari, M.K.(2013), **Green Chemistry Experiments: A monograph,** I.K. International Publishing House Pvt Ltd. New Delhi.
- 3. Pavia, D.L.; Lamponam, G.H.; Kriz, G.S.W. B.(2006), Introduction to organic Laboratory Technique-A Microscale approach, 4<sup>th</sup> Edition, Brrooks-Cole Laboratory Series for Organic chemistry.
- **4.** Sharma R. K., Sharma, C., & Sidhwani, I.T. Solventless and one-pot synthesis of Cu(II) phthalocyanine complex: a green chemistry experiment. Journal of Chemical Education, 2010, 88(1), 86-88.
- 5. Sharma, R. K., Gulati, S., & Mehta, S. Preparation of gold nanoparticles using tea: a green chemistry experiment. Journal of Chemical Education, 2012, 89(10), 1316-1318.
- **6.** Wealth from waste: A green method to produce biodiesel from waste cooking oil and generation of useful products from waste further generated "A social Awareness Project" Indu Tucker Sidhwani, Geeta Saini, Sushmita Chowdhury, Dimple Garg, Malovika, Nidhi Garg, Delhi University Journal of Undergraduate Research and Innovation, Vol 1, Issue 1, Feb 2015. ISSN: 2395-2334.

## **Teaching Learning Process:**

- ICT enabled classes
- Power point presentations
- visit to pharmaceutical industry
- Through videos classes
- Interactive classes

#### **Assessment Methods:**

- Graded assignments
- Conventional class tests
- Class seminars by students on course topics with a view to strengthening the content through width and depth
- Quizzes
- End semester university examination.

## **Keywords:**

Green Chemistry, Twelve principles, Sustainable chemistry, Green energy, Marine antifoulant, Non toxic pigments.

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## SKILL-ENHANCEMENT COURSES (SEC) INDUSTRIALCHEMISTRY

Course Code: INDUSTRIAL CHEMISTRY –SEC-1
Course Title: Instrumental Methods of Analysis

Total Credits: 04 (Credits: Theory-02, Practical-02)

(Total Lecture: Theory-30, Practical-60)

## **Objective:**

#### The Objective of this course is to make students aware about the following concepts:

- Spectroscopic methods of analysis
- Principles of UV and Visible spectrophotometry and its applications
- Various components of UV and Visible spectrophotometry
- Single and double beam instruments
- Atomic spectroscopy types and its applications
- <sup>1</sup>H NMR instrumentation and its applications

## **Learning Outcomes:**

#### By the end of this course, students should be able to understand:

- What are the different types of spectroscopic methods of analysis.
- The instrumentation and the applications of the UV- Visible, Atomic, IR, <sup>1</sup>H NMR spectrometry

## Unit 1

An introduction to Spectroscopic Methods of Analysis

(Lectures: 03)

#### Unit 2

#### **UV- Visible Spectrophotometry:**

- A. Lambert-Beer's law
- B. Principles, Instrumentation, Single/double beam instrument
- C. Applications: Effect of solvent on  $\lambda_{max}$ , Effect of cis-trans geometrical isomerism (e.g. stillbene), calculation  $\lambda_{max}$  of different compounds (Woodward-Fieser Rule and Schott's Rule) and calculation of stoichiometric ratios of metal-ligand complex (Job's method)

(Lectures: 06)

## Unit 3 IR Spectrophotometry: A. Principle B. Instrumentation C. Applications: Identification of the functional groups and simple Organic molecules (Lectures: 05) Unit 4 **Atomic Spectroscopy:** A. Types B. Atomizer C. Atomic absorption and emission D. Applications (Lectures: 08) Unit 5 <sup>1</sup>H NMR Spectroscopy: A. Principle B. Instrumentation C. Factors affecting chemical shift (Electronegativity, Anisotropy, etc.) D. Spin-spin coupling E. Coupling constant

(Lectures: 08)

## **Practical:**

(Credits: 2, Laboratory periods: 60)

**Analytical Chemistry Lab: Instrumental Methods of Analysis** 

Applications: Deuterium exchange, effect of restricted rotation (e.g. DMF), identification

of simple organic compounds using <sup>1</sup>H NMR spectra along with IR spectral data.

- 1. Verification of Lambert-Beer's law using UV-Vis spectrophotometer for CuSO<sub>4</sub> solution.
- 2. Determination of the pK<sub>a</sub> of an indicator (phenolphthalein) using spectrophotometer.
- 3. To determine isoelectric pH of a protein.
- 4. Identification of structure of simple organic compounds using IR- spectroscopy (IR spectra should be provided).
- 5. Synthesis of acetanilide and its characterisation using <sup>1</sup>H NMR and IR spectroscopy.
- 6. Synthesis of *m*-dinitro benzene and its characterisation using <sup>1</sup>H NMR and IR spectroscopy.
- 7. Isolation of DNA from onion and its characterisation using UV spectroscopy.

#### References:

- 1. Kemp, W. (1991), Organic Spectroscopy, PalgraveMacmillan.
- Dyer, J.R.(1978), Applications of Absorption Spectroscopy of Organic Compounds, Prentice Hall.
- Banwell, C.N. (2006), Fundamentals of Molecular Spectroscopy, Tata McGraw-Hill Education.
- 4. Smith, B.C. (1998), Infrared Spectral Interpretations: A Systematic Approach, CRC Press.
- 5. Atkins, P.; Paula, J.de. (2016), Elements of Physical Chemistry, Oxford University Press.

## **Teaching Learning Process**

- 1. Conventional chalk and board teaching,
- 2. Group discussions
- 3. Lab demonstrations and experiments after completion of theory part
- **4.** Power point presentation

#### **Assessment Methods**

- · Presentations by individual student
- Class tests
- Laboratory tests
- Written assignment(s)
- End semester University theory and practical examination

## **Keywords:**

Spectroscopic Methods, IR-Spectrophotometry, Atomic Spectroscopy, <sup>1</sup>H NMR Spectroscopy

Course Code: INDUSTRIAL CHEMISTRY –SEC-2

**Course Title: Business Skills for Chemists** 

Total Credits: 04 (Credits: Theory-04)

(Total Lecture: Theory-60)

## **Objectives:**

The objective of this course is to enhance the business and entrepreneurial skills of undergraduate chemistry students and improve their employment prospects. The course will orient the students to understand the Industry linkage with chemistry, challenges and business opportunities. It will expose

the students to the concepts of intellectual property rights, patents and commercialisation of innovations.

## **Learning Outcomes:**

#### By the end of this course, students will be able to:

- 1. Learn basics skills of of business and project management.
- 2. Understand the process of product development and business planning that includes environmental compliancy.
- 3. Learn the process by which technical innovations are conceived and converted into successful business ventures.
- 4. Understand the intellectual property rights and patents which drive business viability and commercialization of innovation.
- 5. Relate to the importance of chemistry in daily life, along with the employment and business opportunities. They will effectively use the skills to contribute towards the well-being of the society and derive commercial value.

#### Unit 1

## Chemistry in industry

Current challenges and opportunities for the chemistry based industries.

Role of chemistry in India and global economies.

Chemistry based products in the market.

(Lectures: 10)

#### Unit 2

#### **Business Basics**

Key business concepts, Business plans, Market need, Project management, Routes to market, Concept of entrepreneurship

(Lectures: 12)

#### Unit 3

## **Project Management**

Different stages of a project:

- Ideation
- Bench work
- Pilot trial
- Production
- Promotion/ Marketing

(Lectures: 10)

## Unit 4

#### **Commercial Realisation and Case Studies**

- Commercialisation
- · Case study of Successful business ideas in chemistry
- · Case study of Innovations in chemistry
- Financial aspects of business with case studies

(Lectures: 10)

#### Unit 5

## **Intellectual Property Rights**

Introduction to IPR & Patents

(Lectures: 6)

#### Unit 6

#### **Environmental Hazards**

Industries involving hazardous chemicals. Importance of development of cost-effective alternative technology. Environmental ethics.

(Lectures: 12)

Students can be taken for industrial visits for practical knowledge and experience. Group of 4-5 students may be asked to prepare business plan based on some innovative ideas and submit as a project / presentation discussing its complete execution.

## **References:**

- 1. www.rsc.org
- 2. Nwaeke, L.I.(2002), Business Concepts and Perspectives, Springfield Publishers.
- 3. Silva, T. D. (2013), Essential Management Skills for Pharmacy and Business Managers, CRC Press.

## **Teaching Learning Process:**

- Class room teaching board method or power point presentations
- Class room interactions and group discussions
- Through videos and online sources
- Visit to chemical industries for real understanding of whole process

#### **Assessment Methods:**

- Written examination and class tests
- Oral presentation of project proposal along with written assignment.

## **Keywords:**

Business skills, Chemical industry, Entrepreneurship, Project management, Intellectual property rights, Environmental ethics.

Course Code: INDUSTRIALCHEMISTRY –SEC-3
Course Title: Intellectual Property Rights

Total Credits: 04 (Total Lectures: Theory-60)

## **Objectives:**

The course aims to give insights into the basics of the Intellectual Property (IP) and in its wider purview it encompasses intricacies relating to IP. This course is designed to introduce a learning platform to those who may be involved in the making and creation of various forms of IP, besides the effective management of IPR of other creators. The course may also provide cursory understanding of the overall IP ecosystem in the country.

## **Learning Outcomes:**

## At the end of this course, students will be able to:

- Learn theoretical concepts of evolution of Intellectual Property Laws, and to differentiate between the different kinds of IP.
- Know the existing legal framework relating to IP in India.
- Comprehend the value of IP and its importance in their respective domains.
- This course may motivate the students to make their career in multifaceted field of intellectual property rights.

#### Unit 1

#### Introduction

Basic concept of Intellectual Property, Rationale behind Intellectual Property, Justifications for protection of IP, IPR and Economic Development, Major International Instruments relating to the protection of IP. The World Intellectual Property Organization (WIPO), WTO and TRIPS Agreement.

(Lectures: 8)

#### Unit 2

## Copyright and Related rights

Introduction to copyright and its relevance, subject matter and conditions of protection, ownership and term of copyright, rights under copyright law, infringement of copyright and remedies, exceptions to infringement/ public rights.

(Lectures: 10)

## Unit 3

#### **Patents**

Introduction, Criteria for obtaining patents, Patentable subject matter, Non patentable inventions, Procedure for registration, Term of patent and Rights of patentee, Patent Cooperation Treaty & International registration, Basic concept of Compulsory license and Government use of patent, Infringement of patents and remedies, Software patents and importance for India, Utility model & patent, Trade secrets and know-how agreement, Traditional Knowledge and efforts of Indian Govt. for its protection.

(Lectures: 15)

#### Unit 4

#### **Trade Marks**

Meaning of mark and Trademark, Categories of Trademark: Service Mark, Certification Mark, Collective Mark, Well known Mark and Non-conventional Mark, Criteria for registrability of trademark: Distinctiveness & non- deceptiveness, A good Trade Mark & its functions, Procedure for registration and Term of protection, Grounds for refusal of trademark registration, Assignment and licensing of marks (Character merchandising), Infringement and Passing Off, Salient Features of Indian Trade Mark Act,1999.

(Lectures: 8)

#### Unit 5

#### Designs, GI and Plant Varieties Protection

Designs: Meaning of design protection, Concept of original design, Registration & Term of protection, Copyright in Designs.

Geographical Indication: Meaning of GI, Difference between GI and Trade Marks, Registration of GI, Term & implications of registration, Concept of Authorized user, Homonymous GI

Plant Variety Protection and Farmer's Right: Meaning, Criteria of protection, Procedure for registration, effect of registration and term of Protection, Benefit Sharing and Farmer's rights

(Lectures: 12)

#### Unit 6

#### **Enforcement and Protection**

Enforcement of Intellectual Property Rights: Counterfeiting and Piracy, Understanding Enforcement of IP and Enforcing IPRs, Enforcement under TRIPS Agreement, Role of Customs and Police in IPR Protection

(Lectures: 7)

## **Practical:**

No Practical as such. However, students may be asked to prepare a project on different topics of IPR and present them before the class.

## **References:**

- 1. Pandey, N.; Dhami, K. (2014), Intellectual Property Rights, PHI Learning Pvt. Ltd.
- 2. Acharya, N.K.(2001), Text Book of Intellectual Property Rights, Asia Law House.
- Ganguli, P. (2001), Intellectual Property Rights: unleashing the knowledge economy. Tata McGraw Hill.

#### **Additional Resources:**

- 1. https://www.wipo.int
- 2. Ahuja, V.K.(2017), Law Relating to Intellectual Property Rights, Lexis Nexis.
- 3. Wadehra, B.L. (2000), Law Relating to Patents, Trade Marks, Copyright, Designs & Geographical Indications. Universal law Publishing Pvt. Ltd..
- 4. Journal of Intellectual Property Rights (JIPR); NISCAIR(CSIR).

## **Teaching Learning Process:**

This course must be taught through lecture in class and by invited talks of experts. The students must visit the nearby intellectual property office or some law firm to have an idea of the way the work is being done there.

## **Assessment Methods:**

The course is designed to be completed in 60 periods. The internal assessment shall be 25% (Class Test 10%, Assignment/project presentation 10% and attendance 5%) and the semester exam at the end of semester shall be 75%.

## **Keywords:**

Intellectual Property, IP Laws, Patents, Copyright, Trademark, WIPO.

Course Code: INDUSTRIAL CHEMISTRY –SEC-4

**Course Title: Pharmaceutical Chemistry** 

Total Credits: 04 (Credits: Theory-02, Practical-02)

(Total Lectures: Theory- 30, Practical-60)

## **Objectives:**

The objective of this paper is to develop basic understanding of drugs discovery, design, development and their side effects. The course will cover synthesis of major drug classes including-analgesics, antipyretics, anti- inflammatory agents, antibacterial and antifungal agents, antiviral agents, central nervous system agents and drugs for HIV--AIDS. An overview of fermentation process and production of certain dietary supplements and certain common antibiotics will be discussed.

#### **Learning Outcomes:**

#### By the end of this course, students will be able to:

- Gain insight into retro-synthesis approach in relation to drug design and drug discovery.
- Learn synthetic pathways of major drug classes.
- Understand the fermentation process and production of ethanol, citric acids, antibiotics and some classes of vitamins.

#### Unit 1

#### Introduction

Drug discovery, design and development: Sources of drugs: biological, marine, minerals and plant tissue culture, physio-chemical aspects (optical, geometric and bioisosterism) of drug molecules and biological action, drug receptor interaction, basic retro-synthetic approach for development of drug. Cause of side effect of drugs like ibuprofen, cetirizine, thalidomide. Difference between drug and poison.

(Lectures: 7)

## Unit 2

## **Drugs and Pharmaceuticals**

Study of pharmaceutical aids like talc, diatomite, kaolin, bentomite, gelatin and natural colours

Synthesis of the representative drugs of the following classes: analgesics agents, antipyretic agents, anti-inflammatory agents (Aspirin); antibacterial and antifungal agents (Sulphonamides; Sulphanethoxazol, Sulphacetamide, Trimethoprim); antiviral agents (Acyclovir), central nervous system agents (Phenobarbital, Diazepam), Cardiovascular (Glyceryl trinitrate), antilaprosy (Dapsone), HIV-AIDS related drugs (AZT- Zidovudine).

(Lectures:15)

## Unit 3

#### **Fermentation**

Aerobic and anaerobic fermentation. Production of (i) Ethyl alcohol and citric acid, (ii) Antibiotics; Penicillin, Cephalosporin, Chloromycetin and Streptomycin, (iii) Lysine, Glutamic acid, Vitamin B2, Vitamin B12 and Vitamin C.

(Lectures: 8)

## **Practical:**

(Credits: 2, Laboratory periods: 60)

Chemistry Lab: Pharmaceutical chemistry

- 1. Preparation of aspirin and its analysis.
- 2. Preparation of paracetamol and its analysis.
- 3. Preparation of sulphacetamide of sulphonamide and its analysis.
- 4. Determination of alcohol contents in liquid drugs/galenical.
- 5. Determination of ascorbic acid in vitamin C tablets by iodometric or coulometric titrations.
- 6. Synthesis of ibuprofen.
- 7. Analysis of commercial vitamin C tablets by iodometric and coulometric titrimetry.

#### **References:**

## Theory:

- 1. Patrick, G. (2017), Introduction to Medicinal Chemistry, Oxford University Press.
- 2. Singh H.; Kapoor V.K. (1996), Medicinal and Pharmaceutical Chemistry, Vallabh Prakashan.
- Foye, W.O.; Lemke, T. L.; William, D.A. (1995), Principles of Medicinal Chemistry, B.I. Waverly Pvt. Ltd.

#### **Practical:**

- 1. Kjonaas, R.A.; Williams, P.E.; Counce, D.A.; Crawley, L.R. **Synthesis of Ibuprofen**. J. Chem. Educ., 2011, 88 (6), pp 825–828 DOI: 10.1021/ed100892p.
- Marsh, D.G.; Jacobs, D.L.; Veening, H. Analysis of commercial vitamin C tablets by iodometric and coulometric titrimetry. J. Chem. Educ., 1973, 50 (9), p 626. DOI: 10.1021/ed050p626

## **Teaching Learning Process:**

The teaching learning process will involve the traditional chalk and black board method. Certain topics like retro-synthetic approach and fermentation processes are taught through audio-visual aids. Students are encouraged to participate actively in the classroom through regular presentations on curriculum based topics.

## **Assessment Methods:**

Assessmentwill be done on the basis of regular class test, presentations and assignments as a part of internal assessment during the course as per the curriculum. End semester university examination will be held for both theory and practical. In practical, assessment will be done based on continuous evaluation, performance in the experiment on the date of examination and viva voce.

## **Keywords:**

Retro-synthesis, Drug discovery, Design and synthesis, Side effects, Fermentation.

Course Code: INDUSTRIAL CHEMISTRY —SEC-5

**Course Title: Pesticide Chemistry** 

Total Credits: 04 (Credits: Theory-02, Practical-02)

(Total Lectures: Theory- 30, Practical-60)

## **Objectives:**

Pesticide plays an important role in controlling quantity as well quality of the economic crops by protecting them from the various pests. They are used for prevention of much spoilage of stored foods and also used for prevention of certain diseases, which conserves health and has saved the lives of millions of people and domestic animals. Keeping the importance of pesticides in mind this course is aimed to introduce synthesis and application of pesticides.

## **Learning Outcomes:**

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Students will be able to learn about the basic role of pesticide in everyday life, various ingredients and their role in controlling the pest. Students can also educate the farmers/gardeners to choose the appropriate pesticides for their crop production.

#### Unit 1

**Introduction:** Classification, synthesis, structure activity relationship (SAR), mode of action, uses and adverse effects of representative pesticides in the following classes: Organochlorines (DDT, Gammaxene); Organophosphates (Malathion, Parathion); Carbamates (Carbofuran and Carbaryl); Quinones (Chloranil), Anilides (Alachlor and Butachlor).

(Lectures:12)

#### Unit 2

Botanical insecticides [No structure elucidation or synthesis is required for the following compounds:]Alkaloids(Nicotine); Pyrethrum (natural and synthetic pyrethroids); Azadirachtin; Rotenone and Limonene.

(Lectures:8)

## Unit 3

**Pesticide formulations**: Wettable powders, Surfactants, Emulsifiable concentrates, Aerosols, Dust and Granules, Controlled Release Formulations.

(Lectures:6)

#### Unit 4

New Tools in Biological Pest Control: Repellants, Chemosterilants, Antifeedants, Sex attractants.

(Lectures:4)

## **Practical:**

## (Credits: 2, Laboratory periods: 60)

- 1. To carryout market survey of potent pesticides with details as follows:
  - a) Name of pesticide b) Chemical name, class and structure of pesticide c) Type of formulation available and Manufacturer's name d) Useful information on label of packaging regarding: Toxicity, LD50 ("Lethal Dose, 50%"), Side effects and Antidotes.
- 2. To carryout market survey of potent botanical pesticides with details as follows:
  - a) Botanical name and family; b) Chemical name (active ingredient) and structure of active ingredient; c) Type of formulation available and Manufacturer's name; d) Useful information on label of packaging regarding: Toxicity, LD50 ("Lethal Dose, 50%"), Side effects and Antidotes.
- 3. Preparation of simple Organochlorine pesticides.
- 4. To calculate acidity/alkalinity in given sample of pesticide formulations as per BIS specifications.
- 5. To calculate active ingredient in given sample of pesticide formulations as per BIS specifications.
- 6. Preparation of Neem based botanical pesticides.

## **References:**

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- 1. Perry, A.S.; Yamamoto, I.; Ishaaya, I.; Perry, R.Y.(1998), Insecticides in Agriculture and Environment, Springer-Verlag Berlin Heidelberg.
- 2. Kuhr, R.J.; Derough, H.W.(1976), Carbamate Insecticides: Chemistry, Biochemistry and Toxicology, CRC Press, USA.

## **Teaching Learning Process:**

Conventional chalk and board teaching with power point presentation, you tube videos and presentations from students on relevant topics.

## **Assessment Methods:**

Internal assessment through assignments and class test. End semester written and practical examination.

## **Keywords:**

Structure Activity Relationship (SAR), Organochlorines, Organophosphates, Carbamates, Quinones, Anilides, Botanical, Alkaloids, Pyrethrum, Azadirachtin, Rotenone, Limonene, Pesticide formulations, Repellants, Chemosterilants, Antifeedants, Sex attractants, Controlled release pesticide formulation.

Course Code: INDUSTRIAL CHEMISTRY -SEC-6

**Course Title: Fuel Chemistry** 

Total Credits: 04 (Credits: Theory-02, Practical-02)

(Total Lectures: Theory- 30, Practical-60)

## **Objectives:**

The course aims to provide students with a basic scientific and technical understanding of the production, behaviour and handling of hydrocarbon fuels and lubricants, including emerging alternative & renewable fuels. This will enable them to be industry ready to contribute effectively in the field of petroleum chemistry and technology.

## **Learning Outcomes:**

- The course covers both conventional petroleum-based fuels, and alternative & renewable fuels, including gaseous fuels.
- The students will learn the chemistry that underpins petroleum fuel technology, will understand
  the refining processes used to produce fuels and lubricants and will know how differences in
  chemical composition affect properties of fuels and their usage in different applications.
- The course will also cover origin of petroleum, crude oil, composition, different refining processes employed industrially to obtain different fractions of petroleum. Further, course will cover various alternative and renewable fuels like Biofuels (Different generations), Gaseous Fuels (e.g. CNG, LNG, CBG, Hydrogen etc.).
- The course will also cover fuel product specifications, various test methods used to qualify different types of fuels as well characterization methods.
- Review of energy scenario (Global & India), Energy sources (renewable and non-renewable).
   Types of Crude Oils, Composition and Properties. Crude oil assay

#### Unit 1

Review of energy sources (renewable and non-renewable). Classification of fuels and their calorific value. Determination of calorific value by Bomb calorimeter and Junker's calorimeter.

(Lectures:4)

#### Unit 2

Coal: Analysis of coal, Proximate and ultimate Analysis, Uses of coal (fuel and nonfuel) in various industries, its composition, carbonization of coal. Coal gas, producer gas and water gas composition and uses. Fractionation of coal tar, uses of coal tar bases chemicals, requisites of a good metallurgical coke, Coal gasification (Hydrogasification and Catalytic gasification), Coal liquefaction and Solvent Refining.

(Lectures:7)

#### Unit 3

Petroleum and Petrochemical Industry: Composition of crude petroleum, Refining and different types of petroleum products and their applications.

(Lectures:4)

#### Unit 4

Fractional Distillation (Principle and process), Cracking (Thermal and catalytic cracking),

Reforming Petroleum and non-petroleum fuels (LPG, CNG, LNG, bio-gas, fuels derived from biomass), fuel from waste, synthetic fuels (gaseous and liquids), clean fuels.

(Lectures:6)

## Unit 5

Petrochemicals: Vinyl acetate, Propylene oxide, Isoprene, Butadiene, Toluene and its derivatives Xylene.

(Lectures:4)

## Unit 6

Lubricants: Classification of lubricants, lubricating oils (conducting and non-conducting) Solid and semi-solid lubricants, synthetic lubricants.

Properties of lubricants (viscosity index, cloud point, pore point and anilline Point) and their determination.

(Lectures:5)

#### **Practical:**

## (Credits: 2, Laboratory periods: 60)

- 1. Test Methods for Petroleum products
- 2. To prepare biodiesel from vegetable oil
- 3. Calorific value of a fuel
- 4. Characterization of different petroleum products using UV and IR
- 5. To determine pore point and cloud point of fuel
- 6. To determine the viscosity of biodiesel ay various temperature using biodiesel.
- 7. To determine free fatty acid content in given sample.
- 8. To determine the density of the given fuel sample.

## Reference:

Stocchi, E.(1990), Industrial Chemistry, Vol -I, Ellis Horwood Ltd. UK.

## **Teaching Learning Process:**

- Teaching Learning Process for the course is visualized as largely student-focused.
- Transaction through an intelligent mix of conventional and modern methods.
- Lectures by Industry Experts
- Visit to Industry

## **Assessment Methods:**

- Written exams-both objective and subjective questions.
- Dissertation work on a given topic Preparation of literature report followed by presentation.
- Internal Assessment.
- End semester university examination for theory and practical.

## **Keywords:**

Energy; Fuels; Petroleum; Biofuels; Synthetic Lubricants

Course Code: INDUSTRIAL CHEMISTRY -SEC-7

**Course Title: Basic Principles and Laboratory Operations** 

Total Credits: 04 (Credits: Theory-02, Practical-02)

(Total Lectures: Theory- 30, Practical-60)

## **Objectives:**

#### The Objective of this course is to make students aware about the following concepts:

- SI Units, concentration terms.
- Various analytical methods
- Types of errors in chemical analysis
- Statistical tests of data (F test, t test, Q test for bad data, the method of least squares).
- Safety with chemicals and waste.

## **Learning Outcomes:**

## At the completion of this course, students should be able to understand

- What are SI units
- Use of analytical equipments
- Types of errors in chemical analysis
- Statistical tests of data
- Safety with chemicals and waste.

#### Unit 1

#### **Basic Concepts:**

#### A. SI Units

- Definitions of the Seven Base Units (Mass, Length, Time, Temperature, Amount of
- substance, Electrical current and Luminous intensity),
- Derived units,
- · Conversion between units,
- Significant figures.

## B. Chemical concentrations

- Mole, molar mass
- Calculations in grams and moles
- Solutions and their concentrations:
- Molar concentration
- Analytical molarity
- Equilibrium molarity of a particular species
- Percent concentration
- Parts per million/billion (ppm, ppb)
- Volume ratios for dilution procedures
- p-functions.
- C. Preparing solutions: standard solutions, primary standards, secondary standards.

#### (Lectures:8)

## Unit 2

## **Introduction to Analytical Chemistry and Analytical Methods**

General steps in chemical analysis

Introduction to methods of detecting analytes

- a) Physical
- b) Electromagnetic radiations
- c) Electric charge. (Lectures: 2)

## Unit 3

## **Laboratory Operations**

Description and use of common laboratory apparatus: Volumetric flasks, burettes, Pipettes, meniscus readers, weighing bottles, different types of funnels, chromatographic columns, chromatographic jars, desiccators, drying ovens, filter crucibles, rubber policeman.

Calibration and use of volumetric glass ware.

pH meter: components of pH meter, use of pH meter, maintenance of pH meter, application of data

Laboratory notebook. (Lectures: 10)

## Unit 4

## **Errors in Chemical Analysis**

Types of errors

Accuracy and Precision, Absolute and relative uncertainty, propagation of uncertainty.

The Gaussian distribution, mean and standard de\~ation, confidence intervals.

Statistical tests of data (F test, t test, Q test for bad data, the method of least squares).

Calibration curve.

Safety with chemicals and waste.

(Lectures:10)

## **Practical:**

(Credits: 2, Laboratory periods: 60)

## Chemistry Lab: Basic principles & Laboratory Operations

1. Use and calibration of volumetric equipments (volumetric flasks, pipettes and burettes).

- 2. Preparation of standard solutions of acids and bases.
- 3. Estimation of sodium carbonate by titrating with hydrochloric acid
- 4. Preparation of standard solution of EDTA
- 5. Estimation of magnesium using EDTA
- 6. Determination of total hardness of water,
- 7. Use of pH meter: determination of pH of given dilute solutions of shampoos and soaps

#### References

- 1. Higson, S. P.J. (2003), Analytical Chemistry, Oxford University Press.
- 2. Skoog, D.A.; West, D.M. (2003), Fundamentals of Analytical Chemistry, Brooks/Cole.
- 3. Christian, G.D.(2004), Analytical Chemistry, 6th Edition, John Wiley & Sons, New York.
- 4. Fifield, F.W.; Kealey, D. (2000), Principles and Practice of Analytical Chemistry, Wiley.
- 5. Dean J. A. (1997), Analytical Chemistry Handbook, McGraw Hill.

## **Additional Resources:**

- 1. Day. R. A.; Underwood, A. L. (1991), Quantitative Analysis, Prentice Hall of India.
- 2. Gordus, A. A. (1985), Schaum's Outline of Analytical Chemistry, Tala McGraw-Hill.
- 3. Harris, D. C. (2007), Exploring Chemical Analysis, W.H. Freeman and Co.

## **Teaching Learning Process**

- Conventional chalk and board teaching,
- Visit chemical industries/ Drug industries to get information about the various instruments used in industries
- ICT enabled classes.
- Power point presentations.
- Interactive sessions
- To get recent information through the internet.

## **Assessment Methods**

- Presentations by Individual Student
- Class Tests
- Laboratory Tests
- Written assignment(s)
- End semester University Theory and Practical Examination

## **Keywords**

SI Units, Concentrations terms, Analytical methods, Laboratory operations, Types of errors, Statistical Tests of data

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