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UNIVERSITY OF DELHI

Bachelor of Science (Prog.) Analytical Chemistry

(Effective from Academic Year 2019-20)

Revised Syllabus as approved by

Academic Council

Date: 15 & 16 July 2019 No:

Executive Council

Date: 20 & 21 July 2019 No:

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

List of Contents Page No.

Preamble

The objective of anyprogramme 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 BSc (Prog.) with Analytical Chemistry offer courses in the areas of inorganic, organic, physical, materials and analytical. 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 Analytical 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 programmeB.Sc. (Prog.) with Analytical Chemistry will help students in making an informed decision regarding the goals that they wish to pursue in further education and life, at large.

B.Sc. Programme Analytical Chemistry

1. Introduction:

The Learning Outcomes-based curriculum framework is designed around the Choice-based credit system (CBCS)and is intended to suit the present day needs of the student in terms of securing their path towards higher studies or employment. The courses can be evaluated following the grading system, which is considered to be better than the conventional marks system. The uniform grading system will also enable potential employers in assessing the performance of the candidates. The Choice-based credit system (CBCS) provides an opportunity for the students to choose courses from the prescribed courses comprisingof:

1. **Core Course:** compulsory course studied by a candidate as a core requirement is termed as a Core course.
2. **Elective Course:** A course which can be chosen from a pool of courses and which may be very specific or specialized subject of study which enables an exposure to some other discipline/subject is called an Elective Course.

Discipline Specific Elective (DSE) Course: Elective courses offered by the main discipline/subject of study is referred to as Discipline Specific Elective.

Skill Enhancement Course (SEC): These courses may be chosen from a pool of courses designed to provide desired skills to an under graduate student along with the main subjects.

3. **Ability Enhancement Courses (AEC):** There are two mandatory**Ability Enhancement Compulsory Courses (AECC)** which are :

(i) Environmental Science
(ii) English

Program Duration:

The B.Sc. Programme with Analytical Chemistry is of three years 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.

Teaching-Learning Program:

The teaching-learning involves theory classes (Lectures) of one hour duration and practical classes. The curriculum will be delivered through various methods including chalk and talk, power point presentations, audio, video tools, E-learning/E-content, virtual labs, simulations, field trips/Industry visits, seminars (talks by experts), workshops, projects, models and class discussions. The assessment broadly will comprise of Internal Assessment (Continuous Evaluation) and End Semester Examination. Each theory paper carries 100 marks with 25% marks for Internal Assessment and 75% for End Semester examination. The internal Assessment will be through Class test, assignment, oral presentation, worksheets and short project. Each practical paper is of 50 marks.

2. Learning Outcome – based Curriculum Framework in B.Sc. Prog. With Analytical Chemistry

The Learning Outcomes-based Curriculum Framework (LOCF) for the B.Sc. Programme Analytical Chemistry is designed to allow for flexibility in programme design and course content development, while at the same time maintaining a basic uniformity in structure in comparison with other universities across the country. The B.Sc. Programme with Analytical Chemistry covers a wide range of courses of interdisciplinary nature. The core courses that are part of the programme are designed to build a strong Analytical Chemistry knowledge base in the student, and furthermore, acquaints the students with the applied aspects of this fascinating discipline as well. The student is thus equipped to pursue higher studies in an institution of her/his choice, and to apply the skills learnt in the programme to solve practical problems. The programme offers a wide range of elective courses to the student. These include skill enhancement courses that prepare the student for an eventual job in academia or industry.

3. Graduate Attributes in B.Sc. Prog. With Analytical Chemistry

Some of the characteristic attributes of graduate in B.Sc. Programme with Analytical Chemistry include:

Knowledge acquisition: gathers in-depth knowledge of basic and applied areas of Analytical Chemistry.

Analytical Chemistrylaboratory skills: understands methods of safe handling of various equipments, all basic analytical, qualitative and quantitative laboratory techniques.
Interdisciplinary approach: becomes aware of the role of Analytical Chemistry in interdisciplinary research as well as in daily life.

Environmental literacy: develops a basic understanding of the Analytical Chemistry principles that have environmental implications, and gains an awareness of environmental safety of chemicals that are used in the laboratories and follows protocols for their safe disposal.
Scientific logic: develops scientific logic and approaches to a problem with critical reasoning. **Independence in thought**: cultivates independent thinking and is able to integrate knowledge from other disciplines and fit that knowledge into the context of Analytical Chemistry`.

Team work: understands the importance and strengths of interacting with and working alongside people from diverse backgrounds.

Communication skills: develops effective communication skills through oral presentations of ongoing developments in the field and the compiling of information in the form of reports.

Awareness of ethical issues: Is aware of what constitutes unethical behaviour-plagiarism, fabrication and misrepresentation or manipulation of data.

Ethics: acquires an awareness of work ethics and ethical issues in scientific research as well as plagiarism policies.

Self-motivation: develops self-discipline, planning and organization skills, and time management skills.

4. Qualification descriptors for Graduates in in B.Sc. Prog. With Analytical Chemistry

The qualification description for B.Sc. Programme with Analytical Chemistry includes:

- Demonstration of a clear and exhaustive understanding of the basic concepts of Analytical Chemistry and an awareness of the emerging areas of the field.
- Enhancement of ability to read, assimilate and discuss scholarly articles and research papers of Analytical Chemistry as well as interdisciplinary areas of sciences.
- Acquisition of practical laboratory skills, enabling the accurate design of an experiment and systematic collection of experimental data.
- Ability to analyse and interpret 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 Analytical Chemistry using the concepts and knowledge acquired.
- Demonstration of the ability to work effectively and productively, independently or as part of a team.

5. Program Learning Outcomes in in B.Sc. Prog. With Analytical Chemistry

B.Sc. programme with Analytical Chemistry is designed to develop in-depth knowledge of the core concepts and principles of Analytical Chemistry. Undergraduates pursuing this programme of study go through laboratory work that specifically develops their quantitative and qualitative skills, provides opportunities for critical thinking and team work and exposes them to techniques useful for applied areas of scientific study.

- Students acquire sound theoretical knowledge and understanding of the fundamental concepts, principles and processes in Analytical Chemistry.
- Quantitative Analytical Instrumentation technique learnt during the course. The programme also provides ample training in handling basic chemical laboratory instruments and their use in analytical and biochemical determinations. Undergraduates on completion of this programme can join interdisciplinary branches like chemistry, pharmaceutical industries, material testing and biochemical labs besides standard chemical laboratories.
- Communication: Communication is a highly desirable attribute to possess. Opportunities to enhance student's ability to write methodical, logical and precise reports are inherent to the structure of the programme. Techniques that effectively communicate scientific chemical content to large audiences are acquired through oral and poster presentations and regular laboratory report writing.
- Capacity Enhancement: Modern day scientific environment requires students to possess ability to think independently as well as be able to work productively in groups. This requires some degree of balancing. The Analytical Chemistry course is

designed to take care of this important aspect of student development through effective teaching learning process.

- Portable Skills: Besides communication skills, the programme develops a range of portable or transferable skills in students that they can carry with them to their new work environment after completion of Analytical Chemistry programme. These are problem solving, numeracy and mathematical skills- error analysis, units and conversions, information retrieval skills, IT skills and organizational skills. These are valued across work environments.
- Communication Skills: The course develop effective communication skills, through oral and Poster Presentation.

6. **Structure of the Programme in B.Sc. Prog. With Analytical Chemistry**

The programme includes:

1. **Core Courses (CC)(12 Papers, 6 Credit each) 72 credits**
2. **Elective courses**

   Discipline Specific Elective (DSE) **(6 Papers, 6 Credit each) 36 Credits**

   Skill Enhancement Course (SEC) **(4 papers, 4 Credit each) 16 Credits**
3. **Ability Enhancement Compulsory Courses (AECC) (2 papers, 4 credit each) 8 Credits.**

The programme consists of

1. **Six-credit courses:** All six credit courses comprise of theory classes (four credits) and practical (two credits)
2. **Four-credit courses:** Four credit courses comprise of theory classes (two credits) and practical (two credits).
3. **Five-credit courses:** Five credit courses comprise of theory classes (five credits).
4. **One credit courses**: One credit courses comprise of tutorial classes only (one credit).

For theory classes one credit indicates a one hour lecture per week while for practical one credit indicates a two-hour session per week.

There will be **twelve Core Courses** which are to be compulsorily studied to complete the requirements for B.Sc. Programme with Analytical Chemistry. The students will study **three Core Courses each in Semester I, II, III and IV**. The Core Courses are of six credits each (four credits theory and two credits practical).

The programme offers **four Discipline-Specific Electives (DSEs) in Analytical Chemistry**, of which the student must choose any **two** in each of the Semesters V and VI. The DSEs will be of six credits each (four credits theory and two credits practical).

The programme also offers **nine Discipline-Specific Electives (DSEs) in Chemistry**, of which the student must choose any **two** in each of the Semesters V and VI. The DSEs will be of six credits each (four credits theory and two credits practical).

The programme also offers **five Discipline-Specific Electives (DSEs) in Matho-physics**, of which the student must choose **one each from maths and physics** for the Semester V and VI. The DSEs will be of six credits each (for physics four credits theory and two credits practical and for maths five credits theory and one credit tutorial).

A particular option of DSE course will be offered in Semesters V and VI semesters only if the minimum number of students opting for that course is 10. The number of students who will be allowed to opt for DSE will vary from college to college depending upon the infrastructural facilities and may vary each year.

The students will undertake one **Skill Enhancement courses (SEC) of four credits** each in semesters III, IV, V and VI which they can choose from the list of SEC courses offered by their college. The SEC courses are of four credits each (two credits theory and two credits practical).

The two compulsory **Ability Enhancement Compulsory Courses (AECC):** AE1 (Environmental Science) and AE2 (English Communication) will be of four credits each (theory only). The student has to take one each in Semester I and II.

To acquire a degree in B.Sc. Programme with Analytical Chemistry a student must study twelve Core Courses, six Discipline-Specific Electives, four Skill Enhancement Courses and two compulsory Ability Enhancement Courses. A student has to study a minimum of 132 credits to get a degree in B.Sc. Programme Analytical 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

*Number of Courses student has to study.

6.1 Semester-wise distribution of Courses and Credit distribution for B.Sc. Prog. With Analytical Chemistry

Core Courses			
Seme-ster	**Course Code**	**Course Title**	**Credits T= Theory P= Practical/Tutorial**
I	CC-AC1: CORE COURSE ANALYTICAL CHEMISTRY-1	Basic Principles and Laboratory Operations	T=4 P=2
I	CC – C1: CORE COURSE CHEMISTRY-1	Atomic Structure, Bonding, General Organic Chemistry & Aliphatic Hydrocarbons	T=4 P=2
I	PHY-I		T=4 P=2
II	CC – AC2: CORE COURSE ANALYTICAL CHEMISTRY-2	Separation Methods-1	T=4 P=2
II	CC – C2: CORE COURSE CHEMISTRY-2	Chemical Energetics, Equilibria and Functional Group Organic Chemistry-I	T=4 P=2
II	MTS-I		T=5 Tutorial=1
III	CC – AC3: CORE COURSE ANALYTICAL CHEMISTRY-3	Quantitative Methods of Analysis	T=4 P=2
III	CC – C3: CORE COURSE CHEMISTRY-3	Solutions, Phase Equilibrium, Conductance, Electrochemistry and Functional Group Organic Chemistry-II	T=4 P=2
III	MTS-II	MATHS-II	T=5 Tutorial=1
IV	CC – AC4: CORE COURSE ANALYTICAL CHEMISTRY-4	Separation Method-II	T=4 P=2
IV	CC – C4: CORE COURSE CHEMISTRY-4	Chemistry of s- and p-Block Elements, States of Matter and Chemical Kinetics	T=4 P=2
IV	PHY-II		T=4 P=2

Discipline Specific Elective Courses (DSE) refer to the list of courses in page 8			
Seme ster	**Course Code**	**Course Title**	**Credits T= Theory P= Practical**
V	Analytical Chemistry DSE		T=4, P=2
	Chemistry DSE		T=4, P=2
	Physics DSE		T=4, P=2
VI	Analytical Chemistry DSE		T=4, P=2
	Chemistry DSE		T=4, P=2
	Mathematics DSE		T=5, Tutorial=1

Skill Enhancement Courses (SEC) refer to the list of courses in page 8			
Seme Ster	**Course Code**	**Course Title**	**Credits T= Theory P= Practical**
III	SEC-1		T=4, P=2

IV	SEC-2		T=4, P=2
V	SEC-3		T=4, P=2
VI	SEC-4		T=4, P=2

Ability Enhancement Compulsory Courses (AECC)			
Seme Ster	**Course Code**	**Course Title**	**Credits T= Theory**
I/II	AEC-I	Environmental Science	T=4
I/II	AEC-II	English Communicatio	T=4

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.

Discipline Specific Elective Courses (DSE):

Analytical Chemistry DSE (Any two)

1. Analytical Biochemistry
2. Instrumental Methods of Analysis
3. Green Chemistry
4. Industrial Chemicals and Environment

Chemistry DSE (Any two)

1. Applications of Computers in Chemistry
2. Molecular Modelling and Drug Design
3. Novel Inorganic Solids
4. Polymer Chemistry
5. Research Methodology for Chemistry
6. Inorganic Materials of Industrial Importance
7. Chemistry of d-block elements, Quantum Chemistry and Spectroscopy
8. Organometallics, Bioinorganic Chemistry, Polynuclear Hydrocarbons and UV, IR Spectroscopy
9. Molecules of Life

Mathophysics DSE (One each from Maths and Physics)

Skill Enhancement Courses (SEC) (Any four)

1. Biotechnology
2. Forensic Science
3. Green Methods in Chemistry
4. Intellectual Property Rights
5. Business Skills for Chemists
6. Fuel Chemistry
7. Pesticide Chemistry
8. Chemoinformatics

7. Teaching-Learning Process

B.Sc. programme with Analytical Chemistry aims to make the student proficient in theoretical background and practical training in all aspects of Analytical chemistry. It also helps them to develop an appreciation of the importance of Analytical chemistry in different contextsthrough the transfer of knowledge in the classroom as well as in the laboratory.

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 labs, animations. An interactive mode of teaching will be used. The student will be encouraged to participate in discussions and deliver seminars on some topics. A problem-solving approach will be adopted wherever suitable.

In the laboratory the student will first learn good laboratory practices and then get hands-on training on basic Analytical Chemistry techniques and methods. The student will participate in field trips to industries that will facilitate his/her understanding of the employment.

8. Assessment Methods

The student will be assessed over the duration of the programme by many different methods. These include short objectives-type quizzes, assignments, written and oral examinations, group

discussions and presentations, problem-solving exercises, case study presentations, experimental design planning, execution of experiments, seminars, preparation of reports, and presentation of practical records. The wide range of assessment tasks aim to break the monotony of having a single assessment method.

CORE COURSE

SEMESTER 1

Course Code: CC – AC1: CORE COURSE ANALYTICAL CHEMISTRY-1
Course Title: Basic Principles and Laboratory Operations
Total Credits: 06 (Credits: Theory-04, Practical-02)
(Total Lectures: Theory- 60, Practical-60)

Objectives:

The objective of this course is to make students aware about the SI Units, concentration terms, various analytical methods, types of errors in chemical analysis, statistical tests of data and safe usage of chemicals and its waste.

Course Learning Outcomes:

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

- Understand about SI units
- Learn use of analytical equipments
- Know types of errors in chemical analysis
- Handle statistical tests of data
- Know safety with chemicals and waste.

Unit 1

Basic Concepts:

A. SI Units

- Definitions of the Seven Base Units (Mass, Length, Time, Temperature, Amount ofsubstance, 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: 15)

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: 05)

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: 20)

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 deviation, 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: 20)

Practical:

(Credits: 02, Laboratory periods: 60)

Analytical 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

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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.
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2. Gordus, A. A. (1985), **Schaum's Outline of Analytical Chemistry,** Tala McGraw-Hill.
3. Dean J. A. (1997), Analytical Chemistry Handbook, McGraw Hill.
4. 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:

- 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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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 ψ and ψ^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_l and m_s. Shapes of s, p and d atomic orbitals, nodal planes, discovery of spin, spin quantum number (s) and magnetic spin quantum number (m_s).

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

Ionic 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 solubility 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_2O, NH_3, PCl_5, SF_6, ClF_3, SF_4) 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 1st and 2nd periods (including idea of s-p mixing) and heteronuclear diatomic molecules such as CO, NO and NO^+.

(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. $KMnO_4$) 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_2 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 $KMnO_4$, ozonolysis and oxidation with hot alk. $KMnO_4$. 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 $KMnO_4$.

2. Estimation of Mohr's salt by titrating it with $KMnO_4$.

3. Estimation of water of crystallization in Mohr's salt by titrating with $KMnO_4$.

4. Estimation of Fe (II) ions by titrating it with $K_2Cr_2O_7$ using internal indicator.

5. Estimation of Cu (II) ions iodometrically using $Na_2S_2O_3$.

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.

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Theory:

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3. Mann, F.G.; Saunders, B.C.(2009),**Practical Organic Chemistry**, Pearson Education.

Additional references:

1. Douglas, B.E.; McDaniel, D.H.; Alexander, J.J. (1994). **Concepts and Models of Inorganic Chemistry**, John Wiley & Sons.
2. Eliel, E. L. (2000), **Stereochemistry of Carbon Compounds**, Tata McGraw Hill.

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 – AC2: CORE COURSE ANALYTICAL CHEMISTRY-2
Course Title: Separation Methods-1

Total Credits: 06 **(Credits: Theory-04, Practical-02)**
(Total Lectures: Theory- 60, Practical-60)

Objective:

To acquire basic knowledge of the analytical chemistry of important techniques that will provide the basis for their industrial production methods.To provide an adequate mastery of analytical methods used for the determination of commercial/domestic raw materials and finished product quality.

Course Learning Outcomes:

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

- Become familiar with fundamental concepts of partition coefficients and their role in achieving separations across different types of chromatography.
- Develop the core skills to parse existing chromatographic protocols and identify the key factors influencing a chromatography experiment.
- Understand the underlying assumptions of the most common chromatographic separation techniques and approaches to method validation.
- Understand the concept of solubility and their application in separation using distribution law.
- Learn application of dialysis and membrane for various techniques.

Unit 1

Chromatography

Classification of chromatographic methods: Principles of differential migration, description of chromatographic process, distribution coefficients, modes of chromatography, performing column chromatography.

(Lectures: 10)

Unit 2

Chromatography

Theory and practice:Introduction, the chromatography (elution time and volume) capacity factor, column efficiency and resolution, sample preparation.

(Lectures: 08)

Unit 3

Techniques of paper chromatography:

Experimental modifications, various modes of developments, nature of paper, detections of spots, retardation factors, factors that affect reproducibility of R_f values (due to paper, solvent system, sample, development procedures), selection of solvent, quantitative analysis, applications.

(Lectures: 10)

Unit 4

Thin layer chromatography:

Stationary phase, adsorbents, liquid phase support, plate preparation, mobile phase, sample application, development, saturation of chamber, detection of spot, R_f values (effect of adsorbent,solvent, solute, development process),quantitative analysis,applications.

(Lectures: 12)

Unit 5

Solvent Extraction

Distribution law, determination of distribution ratio, batch extraction, continuous extraction, discontinuous extraction, counter current extraction.

(Lectures: 10)

Unit 6

Dialysis and membrane filtration

General laboratory methods, filters-nitrocellulose, fiberglass and polycarbonates.

(Lectures: 10)

Practical:

(Credits: 2, Laboratory periods: 60)

Analytical Chemistry Lab:Separation Method-I

1.Separation and identification of monosaccharides present in the given mixture by radial paper Chromatography.
2.Separation of ortho-nitrophenol and para-nitrophenol by thin layer chromatography.
3.Separation of constituents of leaf pigments by thin layer chromatography.
4.Analysis of soil.
i.Determination of pH of soil.
ii.Determination of total soluble salts.
iii.Determination of carbonate and bicarbonate.
iv.Determination of calcium,magnesium and iron.
5.Determination of adulterant in some common food items.
i.Chicory in coffee powder.
ii.Foreign resin in asafetida.
iii.Chilli powder
iv.Turmeric powder.
v.Pulses

vi.Milk.

References:

1. Fifield,F.W.; Kealey, D. (2000), **Principles and Practice of Analytical Chemistry,** Wiley.
2. Harris, D. C. (2007),**Exploring Chemical Analysis**, W.H. Freeman and Co.
3. Harris, D. C. (2007),**Quantitative Chemical Analysis**,6th Edition, Freeman
4. Mikes, O. (2000),Laboratory Handbook of Chromatographic methods, D.Van Nostrand Company Inc.

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:

Chromatography, TLC, Solvent extraction, Dialysis, Membrane Filtration.

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

Course Title: Chemical Energetics, Equilibria and Functional 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 1º, 2º & 3º.

Preparation: starting from alcohols (1º, 2º & 3º) 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 $NaNH_2/NH_3$ (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 1º, 2º & 3º.

Preparation: Methods of preparation of 1º, 2º & 3º 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 $KMnO_4$, acidic $K_2Cr_2O_7$ and conc. HNO_3), 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_3, NH_4Cl).
4. Determination of enthalpy of hydration of copper sulphate.

Ionic equilibria:

1. 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.
2. Kapoor, K.L. (2015),**A Textbook of Physical Chemistry**,Vol 1, 6th Edition, McGraw Hill Education.
3. Kapoor, K.L.(2015), **A Textbook of Physical Chemistry**, Vol 2, 6th Edition,McGraw Hill Education.
4. B.R.Puri, L.R.Sharma, M.S.Pathania, (2017),**Principles of Physical Chemistry**, Vishal Publishing Co.
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. 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 ofPractical 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.

SEMESTER III

Course Code: CC – AC3: CORE COURSE ANALYTICAL CHEMISTRY-3

Course Title: Quantitative Methods of Analysis

Total Credits: 06 (Credits: Theory-04, Practical-02)
(Total Lectures: Theory- 60, Practical-60)

Objectives:

The objective of this course is to make students aware about the gravimetric and volumetric methods of analysis, various types of titrations, equilibria principles, the Henderson-Hasselbalch equationvarious centrifugation methods andenvironmental analysis.

Course Learning Outcomes:

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

- Various quantitative methods of analysis like
- Gravimetric Analysis
- Volumetric methods of analysis
- Various Centrifugation Methods
- Environmental Analysis

Unit 1

Gravimetric Analysis:

A. Precipitation methods

B. Volatilization methods. (The analyte or its decomposition products are volatilized atsuitable temperature. The volatile product is then collected and weighed, or, alternatively, the mass of the product is determined indirectly from the loss in mass of the sample. e.g. determination of the sodium hydrogen carbonates content of antacid tablets)

C. Properties of precipitates and precipitating reagents:

Particle size, Filterability of precipitates (factors that determine particle size, formation of precipitates and particle size),

Colloidal precipitates (coagulation of colloids, peptization of colloids, treatment of colloidal precipitates).

Crystalline precipitates (particle size and filterability).

Co- precipitation (surface adsorption, mixed-crystal formation, occlusion, and mechanical entrapment, co precipitation errors).

Precipitation from homogeneous solution (the use of the technique of homogeneous solutions to effect precipitation).

D. Drying and ignition of precipitates

E.Practical gravimetric procedures.

(Lectures: 15)

Unit 2

Volumetric Analysis

- Definitions : Titrimetry, Volumetric titrimetry, Gravimetric titrimetry, Coulometric titrimetry. The equivalence point, the end point
- Volumetric methods of analysis: Classification of volumetric methods, theory of indicators and buffers. Equilibria principles, Aqueous and non-aqueous acid-base titration. Redox titrations, Complexometric titrations, Precipitation titrations.
- Typical problems involumetric titrimetry
- Sigmoidal titration curves
- The Henderson-Hasselbalch equation.

(Lectures: 15)

Unit 3

Centrifugation Methods:

- Introduction
- Sedimentation and relative centrifugal force
- Different types of rotors.
- Density gradient
- Types of centrifugation techniques.

(Lectures: 15)

Unit 4

Introduction to Environmental Analysis:

- Sampling method
- Environmental pollution from industrial effluents and radiochemical waste.
- Introduction to water and waste analysis.

(Lectures: 15)

Practical:

(Credits: 2, Laboratory periods: 60)

Analytical Chemistry Lab : Quantitative Methods of Analysis

1. Determination of the pKa of a weak acid by potentiometric/pH titration.
2. Determination of the strength of the given ferric chloride solution by titrating it against EDTA
3. Determination of the capacity of an anionic exchange resin.
4. Homogeneous precipitation of nickel as its dimethylglyoxime.
5. Draw the absorbance of bromophenol blue using a colorimeter.
6. Verification of Beer Lambert's law.
7. Determination of the formula of the chelate formed between iron (III) and salicylic acid.

8. Determination of the formula of the chelate formed between iron (III) and Tiron.

References:

1. Willard, Merritt, Dean, Settle (2004),**Instrumental Methods of Analysis**, CBS Publishers & Distributors.
2. Skoog, D.A.; West, D.M.; Holler, F.J.; Crouch, S.R. (2014),**Fundamentals of Analytical Chemistry,**CengageLearning.
3. Harris, D.C. (2015),**Quantitative Chemical Analysis**, W.H.Freeman& Company.
4. Mikes, O. (2000), **Laboratory Handbook of Chromatographic methods**, D.Van Nostrand Company Inc.
5. Fifield,F.W.; Kealey, D. (2000), **Principles and Practice of Analytical Chemistry,** Wiley.

Additional Resources:

1. Mendham, J., Denney, R.C., Barnes, J.D.; Thomas, M.J.K. (2000); **Vogel's Quantitative Chemical Analysis**, Prentice Hall.
2. Wilson, K.; Walker, J. (2000), **Principles and Techniques of Practical Biochemistry**, Cambridge University Press.

Teaching Learning Process:

- Conventional chalk and board teaching,
- Visit chemical industries to get information about the technologies and environmental pollution from industrial effluents.
- ICT enabled classes.
- Power point presentations.
- Interactive sessions, Debate.

Assessment Methods:

- Presentations by Individual Student
- Class Tests
- Written assignment(s)
- End semester University theory and practical examination

Keywords:

Gravimetric analysis, Volumetric analysis, Centrifugation methods, Environmental analysis, Industrial effluents, Wastewater analysis.

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, $FeCl_3$-H_2O 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_2, 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 $–NH_2$ group, complexation with Cu^{2+} 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.

2. 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:

Theory:

1. Barrow, G.M. (2006), **Physical Chemistry**, 5th 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.
4. Kapoor, K.L. (2013),**A Textbook of Physical Chemistry**,Vol 3, 3rd 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).

Practical:

1. 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 ofPractical Organic Chemistry**, Pearson.
3. Mann, F.G.; Saunders, B.C. (2009),**Practical Organic Chemistry**, 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

SEMESTER IV

Course Code: CC – AC4: CORE COURSE ANALYTICAL CHEMISTRY-4
Course Title: Separation Method-II
Total Credits: 06 **(Credits: Theory-04, Practical-02)**
(Total Lectures: Theory- 60, Practical-60)

Objective:

Objective of this course is to learn the separation techniques and its application and radioisotopic techniques.

Course Learning Outcomes:

At the end of the course, student should be able to understand:

- Various types of separation techniques and their applications
- Electrophoretic techniques
- Radioisotopic techniques

Unit 1

Column Chromatography

A. General: columns, matrix materials, stationary phase, column packing, application of sample, column development and sample elution, detectors and fraction collectors, applications.

B. High performance liquid chromatography: Principle, column, matrices and stationary phases, column packing, mobile phase and pumps, application of sample, detectors, applications.

C. Adsorption chromatography: Principle, adsorbents, solvents, nature of solute, operating parameters, retention volumes and times, applications.

D. Liquid-liquid partition, chromatography: Principle, normal phase chromatography, reversed phase liquid chromatography, applications.

E. Ion-exchange chromatography: Principle, ion exchangers, ion- exchange equilibria, ion- exchange resin selectivity, column operations (column development, detection of solute bands), factors affecting retention volumes, applications.

F. Gel chromatography: Principle, types of gels, separation by gel chromatography, applications.

G. Affinity chromatography: Principle, materials, selection and attachment of ligand, practical procedure, applications.

H. Gas-liquid chromatography: Apparatus and materials, preparation and application of samples, separation conditions, detectors, applications.

(Lectures: 30)

Unit 2

Electrophoretic Techniques:

A. Principle, apparatus, support media (paper, cellulose acetate membranes, gels)

B. SDS-PAGE, native gels, gradient gels, isoelectric focusing, 2D-PAGE, continuous flow electrophoresis, detection, estimation and recovery of proteins in gels.

C. Western Blotting, Electrophoresis of Nucleic Acids, Capillary Electrophoresis.

D. Isoelectric Focusing.

(Lectures: 15)

Unit 3

Radioisotopic Techniques:

Nature of radioactivity. Detection and measurement of radioactivity, Biochemical assays (radioimmuno-assays) to detect the presence and absence of radioisotopes. Applications of radioactive isotopes to label biological molecules. Estimation of the concentration of different constituents of plasma, body fluids, urine, blood etc. Inherent advantages and restrictions of radiotracer experiments, safety aspects.

(Lectures: 15)

Practical:

(Credits: 2, Laboratory periods: 60)

Analytical Chemistry Lab: Separation Method-2

1. Determination of the residual chlorine in city water supply using colorimetry.

2. Determination of adsorption isotherm of acetic acid on activated charcoal and determination of the adsorption constant(k).

3. Determination of the capacity of an anion exchange resin.

4. Determination of the capacity of a cation exchange resin.

5. Separation of compounds using adsorption column chromatography.

6. Determination of isoelectric point of an amino acid.

7. Determination of void volume of a gel column.

References:

1. Mikes, O. (2000), Laboratory Handbook of Chromatographic methods, D. Van Nostrand Company Inc.
2. Fifield,F.W.; Kealey, D. (2000), **Principles and Practice of Analytical Chemistry,** Wiley.
3. Mendham, J.; Denney, R.C.; Barnes, J.D.; Thomas, M.J.K.; (2000), **Vogel's Quantitative Chemical Analysis**, Prentice Hall.
4. Wilson, K.; Walker, J. (2000),**Principles and Techniques of Practical Biochemistry**, Cambridge University Press.

Additional Resources:

5. Holme, D.J.; Peck, H. (1998),**Analytical Biochemistry**, Prentice Hall.
6. Freifelder, D. (1983),**Physical Biochemistry**, W.H.Freeman & Company.
7. Plummer, D.T.(2001),**Introduction to Practical Biochemistry**, McGraw-Hill.

Teaching Learning Process:

- Lectures using teaching aid (chalk/power point/videos),
- Group discussion,
- Presentations,
- Advise to students to prepare a report.

Assessment Methods:

a. Presentation by individual student
b. Class test
c. Laboratory test
d. Written assignments
e. End semester University theory and practical examinations

Keywords:

Chromatography; HPLC, Electrophoresis, Radioisotopic techniques.

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_3, N_2H_4, N_3H, NH_2OH) Oxoacids of P, S and Cl, Halides and oxohalides: PCl_3, PCl_5, $SOCl_2$ and SO_2Cl_2.

(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_2, 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_4^+, Pb^{2+}, Bi^{3+}, Cu^{2+}, Cd^{2+}, Fe^{3+}, Al^{3+}, Co^{2+}, Ni^{2+}, Mn^{2+}, Zn^{2+}, Ba^{2+}, Sr^{2+}, Ca^{2+}, K^+

Anions: CO_3^{2-}, S^{2-} , SO_3^- , NO_2^- , CH_3COO^-, Cl^-, Br^-, I^-, NO_3^-,SO_4^{2-} , PO_4^{3-} , BO_3^{3-} , $C_2O_4^{2-}$, F^-.

(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_2SO_4 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**, 3rd Edition,Wiley India.
5. Castellan, G. W.(2004),**Physical Chemistry**, Narosa.
6. Kapoor, K.L. (2015),**A Textbook of Physical Chemistry**, Vol.1, 6th Edition, McGraw Hill Education.
7. Kapoor, K.L. (2015),**A Textbook of Physical Chemistry**, Vol.5, 3rd 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.
2. 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) ANALYTICAL CHEMISTRY

Course Code:Analytical Chemistry DSE-1

Course Title: Analytical Biochemistry

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

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

Objectives:

The Objective of the courseis to learn about proteins, enzymes, nucleic acids and lipids, using suitable examples, drug receptor interaction and Structure Activity Relation (SAR) studies along genetic code and concept of heredity.

Learning Outcomes:

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

- Learn how the structure of biomolecules determines their reactivity and biological uses.
- Know basic principles of drug-receptor interaction and structure activity relationship (SAR).
- Know biochemistry of diseases.

Unit 1

Carbohydrates and Proteins:

Basic understanding of the structures and properties of carbohydrates, biological importance of carbohydrates,
Monosaccharides: Constitution and absolute configuration of glucose and fructose, epimers and anomers, mutarotation, Haworth projections and conformational structures;Structure elucidation of glucose and fructose (Fischer's proof), Interconversions of aldoses and ketoses; Killiani-Fischer synthesis and Ruff degradation;
Disaccharides – Structure elucidation of maltose, lactose and sucrose.
Polysaccharides – Elementary treatment of starch, cellulose and glycogen.

Amino Acids, Peptides and Proteins:
α-Amino Acids - Classification and characterization,. Zwitterions, pKa values, isoelectric point and electrophoresis;
Proteins: Classification, Primary, secondary and tertiary structures of proteins, test for proteins, isolation, characterization, biological importance; denaturation of proteins.

(Lectures: 16)

Unit 2

Enzymes:
Nomenclature,classification, characterization, mechanism of enzyme action, factors affecting enzyme action, co-enzymes and co-factors and their role in biological reactions, specificity of enzyme action(Including stereo-specificity), effect of pH, temperature and ionic solution, on enzyme activity,

enzyme inhibitors and their importance, phenomenon of inhibition(competitive and non competitive inhibition including allosteric inhibition). 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_2 group, double bond and aromatic ring.

(Lectures: 12)

Unit 3

Lipids:

Introduction to oils and fats; common fatty acids present in oils and fats, Hydrogenation of fats and oils,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: 06)

Unit 4

Concept of Energy in Biosystems:

Cells obtain energy by the oxidation of foodstuff (organic molecules). Introduction to Metabolism (catabolism, anabolism), ATP: the universal currency of cellular energy, ATP hydrolysis and free energy change. Agents for transfer of electrons in biological redox systems: NAD+, FAD. Outline of catabolic pathways of Fats, Proteins and Carbohydrate-Glycolysis, Alcoholic and Lactic acid Fermentation, Krebs Cycle.Caloric value of food, standard caloric content of food types.

(Lectures: 08)

Unit 5

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.Introduction to gene therapy.

(Lectures: 08)

Unit 6

Biochemistry of disease:

A diagnostic approach by blood/ urine analysis. **Blood:** Composition and functions of blood, blood coagulation. Blood collection and preservation of samples. Anemia,**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: 10)

Practical:

(Credits: 2, Laboratory periods: 60)

Analytical Chemistry Lab: Analytical Biochemistry

1. Carbohydrate- qualitative and quantitative.
2. Proteins-qualitative tests
3. Lipids – qualitative Tests.
4. Determination of the iodine number of oil.
5. Determination of the saponification number of oil.

6. Determination of acid value of fats and oils.
7. Determination of cholesterol using Liebermann- Burchard reaction.
8. Estimation of DNA by diphenylamine reaction
9. Isolation and characterization of DNA from Onion/cauliflower.
10. Determination of amount of protein using Lowry's method/ Biuret method.
11. Determination of enzyme activity.

References

1. Devlin, T. M. (2010),**Textbook of Biochemistry with Clinical Correlations**, John Wiley & Sons.
2. Berg, J.M., Tymoczko, J.L.; Stryer, L. (2010),**Loose-leaf Version for Biochemistry**, W.H.Freeman.
3. Lehninger, A.L., Nelson, D.L.;Cox, M. (2004),**Principle of Biochemistry**,W.H.Freeman.
4. Morrison, R. N.; Boyd, R. N. **Organic Chemistry**, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
5. Finar, I. L. **Organic Chemistry** (Volume 1& 2), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).

Additional Resources:

1. Swahney, S.K.; Singh, R. (2001), **Introductory Practical Biochemistry**, Narosa Publishing House.
2. Cooper,T.G. (2011),**The Tools of Biochemistry**, Wiley India Pvt Ltd.
3. Wilson, K.; Walker, J. (2000), **Principles and Techniques of Practical Biochemistry**, Cambridge University 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.

AssessmentMethods

Students evaluation is done on the basis of regular class test and assignments during the course as per the curriculum.

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:Analytical Chemistry DSE-2
Course Title: Instrumental Methods of Analysis
Total Credits: 06 (Credits: Theory-04, Practical-02)
(Total Lectures: Theory- 60, 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
- ^{1}H NMR instrumentation and its applications

Course 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, ^{1}H NMR spectrometry

Unit 1

An introduction to spectroscopic methods of analysis

(Lectures: 06)

Unit 2

UV- Visible Spectrophotometry:

A. Lambert-Beer's law

B. Principles, Instrumentation, Single/double beam instrument

C. Applications: Effect of solvent on λ_{max} , Effect of cis-trans geometrical isomerism (e.g. stillbene), calculation λ_{max} of different compounds (Woodward-Fieser Rule and Schott's Rule) and calculation of stoichiometric ratios of metal-ligand complex (Job's method)

(Lectures: 15)

Unit 3

IR Spectrophotometry:

A. Principle

B. Instrumentation

C. Applications: Identification of the functional groups and simple organic molecules

(Lectures: 09)

Unit 4

Atomic Spectroscopy:

A. Types

B. Atomizer

C. Atomic absorption and emission

D. Applications **(Lectures: 15)**

Unit 5

^{1}H NMR Spectroscopy:

A. Principle

B. Instrumentation

C. Factors affecting chemical shift (Electronegativity, Anisotropy, etc.)

D. Spin-spin coupling

E. Coupling constant

Applications: Deuterium exchange, effect of restricted rotation (e.g. DMF), identification of simple organic compounds using ^{1}H NMR spectra along with IR spectral data.

(Lectures: 15)

Practical:

(Credits: 2, Laboratory periods: 60)

Analytical Chemistry Lab: Instrumental Methods of Analysis

1. Verification of Lambert-Beer's law using UV-Vis spectrophotometer for $CuSO_4$ solution.

2. Determination of the pK_a 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 ^{1}H NMR and IR spectroscopy.
6. Synthesis of *m*-dinitro benzene and its characterisation using ^{1}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.
2. Dyer, J.R.(1978),**Applications of Absorption Spectroscopy of Organic Compounds**, Prentice Hall.
3. 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.

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, ^{1}H NMR Spectroscopy

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Course Code: Analytical Chemistry DSE-3
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

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_2 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 (C^2S^3); 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_2 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.
3. 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**,4th 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_2S 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, Twelveprinciples 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, Co-crystal controlled solid state synthesis, Sustainable development, Presidential green chemistry awards.

Course Code: Analytical Chemistry–DSE-4
Course Title: Industrial Chemicals and Environment
Total Credits: 06 (Credits: Theory-04, Practical-02)
(Total Lectures: Theory- 60, Practical-60)

Objectives:

The objective of this course is to make students aware about the concepts of different gases and their industrial production, uses, storage and hazards. Manufacturing, applications, analysis and hazards of the Inorganic Chemicals, Preparation of Ultra-Pure metals for semiconducting technology, Air and Water pollution, control measures for Air and Water Pollutants, Catalyst and Biocatalyst, Energy and Environment.

Learning Outcomes:

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

- The different toxic gases and their toxicity hazards
- Safe design systems for large scale production of industrial gases.
- Manufacturing processes, handling and storage of inorganic chemicals.
- Hazardous effects of the inorganic chemicals on human beings and vegetation.
- The requirement of ultra-pure metals for the semiconducting technologies
- Composition of air, various air pollutants, effects and control measures of air pollutants.
- Different sources of water, water quality parameters, impacts of water pollution, water treatment.
- Different industrial effluents and their treatment methods.
- Different sources of energy.
- Generation of nuclear waste and its disposal.
- Use of biocatalyst in chemical industries.

Unit 1:

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, and sulphur dioxide. **(Lectures: 6)**

Unit 2:

Inorganic Chemicals: Manufacture, applications, analysis and hazards in handling the following chemicals: hydrochloric acid, nitric acid, sulphuric acid, caustic soda, borax, bleaching powder, sodium thiosulphate, hydrogen peroxide, potassium dichromate and potassium permanganate

(Lectures: 10)

Unit 3:

Industrial Metallurgy: Preparation of ultrapure metals for semiconductor technology.

(Lectures: 4)

Unit 4:

Environment and its segments:

Ecosystems. Biogeochemical cycles of carbon, nitrogen and sulphur.

Air Pollution: Major regions of atmosphere,chemical and photochemical reactions in atmosphere.

Air pollutants: types, sources, particle size and chemical nature; Photochemical smog: its constituents and photochemistry. Major sources of air pollution, Pollution by SO_2, CO_2, CO, NO_x, H_2S and other foul smelling gases, methods of estimation of CO, NO_x, SO_x and control procedures, Effects of air pollution on living organisms and vegetation

Greenhouse effect and Global warming, Environmental effects of ozone, Ozone depletion by oxides of nitrogen, chlorofluorocarbons and halogens, Air pollution control, Settling Chambers, Venturi Scrubbers, Cyclones, Electrostatic Precipitators (ESPs).

(Lectures:15)

Unit 5:

Water Pollution:

Hydrological cycle, water resources, aquatic ecosystems, Sources and nature of water pollutants, Techniques for measuring water pollution, Impacts of water pollution on hydrological cycle and ecosystems. Water purification methods. Effluent treatment plants (primary, secondary and tertiary treatment). Industrial effluents from the following industries and their treatment: electroplating, textile, tannery, dairy, petroleum and petrochemicals, agro fertilizer.

Sludge disposal. Industrial waste management, incineration of waste.

Water treatment and purification (reverse osmosis, electro dialysis, ion exchange).

Water quality parameters for wastewater, industrial water and domestic water.

(Lectures:15)

Unit 6:

Energy & Environment: Sources of energy: Coal, petrol and natural gas. Nuclear fusion / fission, solar, hydrogen, geothermal, tidal and hydel.

Nuclear Pollution: Disposal of nuclear waste, nuclear disaster and its management.

Biocatalysis: Introduction to biocatalysis: Importance in green chemistry and chemical industry.

(Lectures: 10)

Practical:

(Credits: 2, Laboratory periods: 60)

Chemistry Lab: Industrial Chemicals & Environment

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.

5. Measurement of chloride, sulphate and salinity of water samples by simple titration method ($AgNO_3$ and potassium chromate).

6. Estimation of total alkalinity of water samples (CO_3^{2-}, HCO_3^-) using double titration method.

7. Measurement of dissolved CO_2

8. Determination of hexavalent Chromium Cr(VI) concentration in tannery wastes/waste water sample using UV-Vis spectrophotometry technique.

9. Preparation of borax/ boric acid

References:

Theory

1. Manahan, S.E. (2017),**Environmental Chemistry**, CRC Press
2. Buchel, K.H.; Moretto, H.H.; Woditsch, P.(2003),**Industrial Inorganic Chemistry**, Wiley-VCH.
3. De, A.K.(2012), **Environmental Chemistry,** New Age International Pvt., Ltd.
4. Khopkar, S.M**.**(2010), **Environmental Pollution Analysis**, New Age International Publisher.

Practical

1. Vowles, P.D.; Connell, D.W. (1980),**Experiments in Environmental Chemistry: A Laboratory Manual**, Vol.4, Pergamon Series in Environmental Science.
2. Gopalan, R.; Anand, A.; Sugumar R.W. (2008),**A Laboratory Manual for Environmental Chemistry**, I. K. International.

Teaching Learning Process:

- Conventional chalk and board teaching,
- Visit to chemical industries to get information about the technologies, methods to check pollutants and its treatment.
- ICT enabled classes.
- Power point presentations.
- Interactive sessions.
- To get recent information through the internet.

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:

Air pollution,Biocatalysis, Environment,Green chemistry, Industrial gases, Inorganic chemicals, Metals, Ultrapure metals,Sources of energy,Water pollution.

DISCIPLINE SPECIFIC ELECTIVE COURSES (DSE) CHEMISTRY

Course Code: Chemistry DSE-1

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:

1. 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:

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-2

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.

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_2O, H_2S, H_2Se using PM3.

10. Compare the HAH bond angles for the second row hydrides (BeH_2, CH_4, NH_3, H_2O) 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 ºC, 100 ºC, 108 ºC, 82 ºC, respectively).

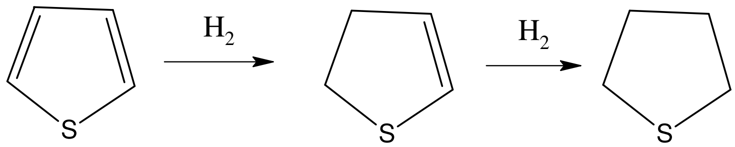
12. Compute the resonance energy of benzene by comparison of its enthalpy of hydrogenation with that of cyclohexene.

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-3

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:

1. Understand the mechanism of solid-state synthesis.
2. Explain about the different characterization techniques and their principle.
3. Understand the concept of nanomaterials, their synthesis and properties.
4. Explain the mechanism of growth of self-assembled nanostructures.
5. Appreciate the existence of bioinorganic nanomaterials.
6. Explain the importance of composites, conducting polymers and their applications.
7. 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 ($PbCrO_4$, $ZnCrO_4$, 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-4

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, Poly-functional 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

1. 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 Gravimetry-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:

1. Allcock, H.R.; ; Lampe, F. W.; Mark, J. E. (2003),**Contemporary Polymer Chemistry**, Prentice-Hall.
2. Fried, J.R. (2003), **Polymer Science and Technology**, Prentice-Hall.
3. 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: Chemistry DSE-5
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.

Course Code: Chemistry DSE-6
Course Title: Inorganic Materials of Industrial Importance
Total Credits: 06 (Credits: Theory-04, Practical-02)
(Total Lectures: Theory- 60, Practical-60)

Objectives:

The course introduces learners to the diverse roles of inorganic materials in the industry. It gives an insight into how these raw materials are converted into products used in day to day life. Students learn about silicates, fertilizers, surface coatings, batteries, engineering materials for mechanical construction as well as the emerging area of nano-sized materials. The course helps develop the interest of students in the frontier areas of inorganic and material chemistry.

Learning Outcomes:

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

- Learn the composition and applications of the different kinds of glass.
- Understand glazing of ceramics and the factors affecting their porosity.
- Give the composition of cement and discuss the mechanism of setting of cement.
- Explain the suitability of fertilizers for different kinds of crops and soil.
- Explain the process of formulation of paints and the basic principle behind the protection offered by the surface coatings.
- Explain the principle, working and applications of different batteries.
- List and explain the properties of engineering materials for mechanical construction used in day to day life.
- Explain the synthesis and properties of nano-dimensional materials, various semiconductor and superconductor oxides.

Unit 1

Silicate Industries

Glass: Glassy state and its properties, classification (silicate and non-silicate glasses). Manufacture and processing of glass. Composition and properties of the following types of glasses: Soda lime glass, lead glass, armoured glass, different types of safety glass, borosilicate glass, fluorosilicate glass, coloured glass, photosensitive glass, photochromic glass, glass wool and optical fibre.

Ceramics: Brief introduction to types of ceramics. glazing of ceramics.

Cement: Manufacture of Portland cement and the setting process, Different types of cements: quick setting cements, eco-friendly cement (slag cement), pozzolana cement.

(Lectures: 10)

Unit 2

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: 10)

Unit 3

Surface Coatings:

Brief introduction to and classification of surface coatings, paints and pigments: formulation, composition and related properties, pigment volume concentration (PVC)and critical pigment volume concentration (CPVC), fillers, thinners, enamels and emulsifying agents. Special paints: heat retardant, fire retardant, eco-friendly paints, plastic paints, water and oil paints. Preliminary methods for surface preparation, metallic coatings (electrolytic and electroless with reference to chrome plating and nickel plating), metal spraying and anodizing.

Contemporary surface coating methods like physical vapor deposition, chemical vapor deposition, galvanising, carburizing, sherardising, boriding, nitriding and cementation.

(Lectures: 18)

Unit 4

Batteries:

Primary and secondary batteries, characteristics of an Ideal Battery, principle, working, applications and comparison of the following batteries: Pb- acid battery, Li-metal batteries, Li-ion batteries, Li-polymer batteries, solid state electrolyte batteries, fuel cells, solar cells and polymer cells.

(Lectures: 8)

Unit 5

Engineering materials for mechanical construction:

Composition, mechanical and fabricating characteristics and applications of various types of cast irons, plain carbon and alloy steels, copper, aluminum and their alloys like duralumin, brasses and bronzes cutting tool materials, superalloys, thermoplastics, thermosets and composite materials.

(Lectures: 8)

Unit 6

Nano dimensional materials

Introduction to zero, one and two-dimensional nanomaterial: Synthesis, properties and applications of fullerenes, carbon nanotubes, carbon fibres, semiconducting and superconducting oxides.

(Lectures: 6)

Practical:

(Credits: 2, Laboratory periods: 60)

Chemistry Lab: Inorganic materials of industrial importance

1. Detection of constituents of Ammonium Sulphate fertilizer (Ammonium and Sulphate ions) by qualitative analysis and determine its free acidity.

2. Detection of constituents of CAN fertilizer (Calcium, Ammonium and Nitrate ions) fertilizer and estimation of Calcium content.

3. Detection of constituents of Superphosphate fertilizer (Calcium and Phosphate ions) and estimation of phosphoric acid content.

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

5. Analysis of (Cu, Ni) in alloy or synthetic samples (Multiple methods involving Complexometry, Gravimetry and Spectrophotometry).

6. Analysis of (Cu, Zn) in alloy or synthetic samples (Multiple methods involving Iodometry, Complexometry and Potentiometry).

7. Synthesis of pure ZnO and Cu doped ZnO nanoparticles.

8. Synthesis of silver nanoparticles by green and chemical approach methods and its characterization using UV-visible spectrophotometer.

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. 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.
4. Kent, J. A. (ed**)** (1997),**Riegel's Handbook of Industrial Chemistry**, CBS Publishers, New Delhi.
5. Poole Jr.; Charles P.; Owens, Frank J.(2003), **Introduction to Nanotechnology**, John Wiley and Sons.

Practical:

1. Svehla, G.(1996),**Vogel's Qualitative Inorganic Analysis**, Prentice Hall.
2. Banewicz, J. J.; Kenner, C.T. **Determination of Calcium and Magnesium in Limestones and Dolomites**, Anal. Chem., 1952, 24 (7), 1186–1187.
3. Ghorbani, H. R.; Mehr, F.P.; Pazoki, H.; Rahmani B. M. **Synthesis of ZnO Nanoparticles by Precipitation Method.** Orient J Chem 2015;31(2).
4. 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.

Additional Resources:

1. Kingery, W. D.; Bowen H. K.; Uhlmann, D. R. (1976),**Introduction to Ceramics**, Wiley Publishers, New Delhi.
2. Gopalan, R. Venkappayya, D.; Nagarajan, S. (2004),**Engineering Chemistry**, Vikas Publications.

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:

Assessment will be done based on 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:

Silicates, Ceramics, Cement, Fertilizers, Surface Coatings, Batteries, Engineering materials for mechanical construction, Nano dimensional materials.

Course Code: Chemistry DSE-7

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:

1. Understand chemistry of d and f block elements, Latimer diagrams, properties of coordination compounds and VBT and CFT for bonding in coordination compounds
2. Understand basic principles of quantum mechanics: operators, eigen values, averages, probability distributions.
3. Understand and use basic concepts of microwave, IR and UV-VIS spectroscopy for interpretation of spectra.
4. 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 Δ. 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

- 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.
- Estimation of (i) Mg^{2+} or (ii) Zn^{2+} by complexometric titrations using EDTA.
- Estimation of total hardness of a given sample of water by complexometric titration.
- Determination of the composition of the Fe^{3+} - salicylic acid complex / Fe^{2+} - phenanthroline complex in solution by Job's method.

Section B: Physical Chemistry

UV/Visible spectroscopy

- Study the 200-500 nm absorbance spectra of $KMnO_4$ and $K_2Cr_2O_7$ (in 0.1 M H_2SO_4) and determine the λ_{max} values. Calculate the energies of the two transitions in different units (J molecule^{-1}, kJ mol^{-1}, cm^{-1}, eV).
- Study the pH-dependence of the UV-Vis spectrum (200-500 nm) of $K_2Cr_2O_7$
- 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 $CuSO_4/KMnO_4/K_2Cr_2O_7/CoSO_4$ in a solution of unknown concentration

Chemical Kinetics; Study the kinetics of the following reactions.

1. Initial rate method: Iodide-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.
5. Kapoor, K.L. (2015),**A Textbook of Physical Chemistry**, Vol.5, 3rd Edition, McGraw Hill Education.
6. Kapoor, K.L. (2015),**A Textbook of Physical Chemistry**, Vol.4, 5th 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.
3. 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.
2. Petrucci, R. H.(1989),**General Chemistry: Principles and Applications**, Macmillan Publishing Co.

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-8

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^{2+} and Cd^{2+} 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.

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. π-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^+, K^+ and Mg^{2+} ions: Na/K pump; Role of Mg^{2+} ions in energy production and chlorophyll. Brief introduction to oxygen transport and storage (haemoglobin-myoglobin system). Brief introduction about toxicity of metal ions ($Hg^{2+}$and Cd^{2+}).

(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, λ_{max} & ε_{max}, chromophores & auxochromes, bathochromic & hypsochromic shifts. Application of Woodward rules for calculation of λ_{max} for the following systems: conjugated dienes - alicyclic, homoannular and heteroannular; α,β-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_f value in each case:

(Fe^{3+}, Al^{3+} and Cr^{3+}) or (Ni^{2+}, Co^{2+}, Mn^{2+} 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, $MgCl_2$ and $LiCl_3$.

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.
3. 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 Edition, 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**, 3rd Edition, John Wiley.
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.

Course Code: Chemistry DSE-9
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_2 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 ofPractical Organic Chemistry**, Pearson.
2. **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.

SKILL ENHANCEMENT COURSES (SEC) CHEMISTRY

Course Code: Chemistry SEC-1
Course Title: Biotechnology
Total Credits: 04 **(Total Lectures: Theory- 60)**

Objectives:

The objective of this course is to have a firm foundation of the fundamentals and applications of biotechnology.

Learning Outcomes:

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

- Develop an understanding of the different aspects of biotechnology.
- Discuss the significance of recombinant DNA technology and its application in recent times.
- Understand the concept of enzyme activities and their use in industries and clinics.
- Comprehend the use of microbes in industries for mass production.
- Develop concepts of transgenic plant development and crop improvement.
- Understand the aspects of animal biotechnology and ethics associated with it.

This would help the students to develop interactions/linkages with the industry and venture into Science entrepreneurship.

Unit I Scope of Biotechnology
Definition and Multidisciplinary Applications of biotechnology, Basic Introduction of Cell, DNA, RNA and Proteins.**(Lectures: 8)**

Unit II Recombinant DNA Technology
Introduction to genes and their role in cell, Techniques in rDNA technology: Vector selection, rDNA Creation, Transfering rDNA to host, Checking the expression in host, PCR. Application of rDNA Technology.
(Lectures: 12)
Unit III Enzyme Technology:
Introduction to Enzymes, Catalysis, Inhibition and Enzyme Kinetics: Competitive, Non-Competitive, Uncompetitive. Industrial and Clinical uses of Enzymes.
(Lectures: 8)

Unit IV Industrial Biotechnology
Different types of fermentation processes, Downstream Processes, Microbial production of Amino Acids, organic solvents, Antibiotics, Beverages, Vitamins. Single cell protein.
(Lectures: 10)

Unit V Plant and Animal Biotechnology

Plant tissue culture and somatic cell variations, their applications in crop improvement, plant transformation-vectors and methods, transgenic plants with useful agronomic traits and products, Animal cell culture and media, primary culture and cell line, cell viability and cell toxicity, organ culture and tissue engineering, gene manipulation and transgenic animals, gene therapy, Bio-ethics.
(Lectures:14)

Unit VI Computational Biology
Nuceolide and protein sequence databases, Gene and Protein annotations, protein structural databases and visualisation, introduction to DNA sequenceing, protein sequencing and insilico drug development. **(Lectures:8)**

Suggested Readings:

1. Gupta, P.K. (2003),**Biotechnology and Genomics**, Rastogi publishers.
2. Dubey, R.C. (2014),**A textbook of Biotechnology**,S.Chand.
3. Chaudhuri, K. (2012), **Recombinant DNA Technology,** The Energy and Resources Institute, TERI.
4. Chawla, H.S. (2014), **Introduction to plant biotechnology**, 3rdEdition, Oxibh.
5. Rastogi, P. (2013), **Bioinformatics: Methods and Applications: Genomics, Proteomics and Drug Discovery**, Prentice Hall.

Teaching learning process:

- Conventional chalk and board teaching,
- Class interactions and discussions
- Powerpoint presentation on essential topics
- Massive online open coursewares

Assessment methods:

- Presentations by individual student/ group of three students
- Class tests, MCQs at periodic intervals.
- Written assignment(s)
- End semester University theory and practical examination

Keywords

Biotechnology, Cell, DNA, RNA, Proteins, Genes, rDNA technology, Vectors, Host, PCR, Enzymes, Catalysis, Inhibition, Enzyme Kinetics, Competitive, Non-Competitive, Uncompetitive, Fermentation, Downstream Processes, Amino Acids, Antibiotics, Beverages, Vitamins, Single cell protein, Tissue culture, Somatic cell variations, Crop improvement, Plant transformation-vectors, Transgenic plants, Cell culture, Media, Primary culture, Cell line, Cell viability , Cell toxicity, Organ culture, Tissue engineering, Transgenic animals, Gene therapy, Bio-ethics, Nuceolide and protein Sequence databases, Annotation, Protein structural databases, Visualisation, DNA sequencing, Protein sequencing, Insilico drug development.

Course Code: Chemistry SEC-2

Course Title: Forensic Science

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

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

Objectives:

Forensic Science pertains to analysis and examination of physical evidence recovered from a crime scene to legal proceedings. Examination of fingerprints, toxic substances detection of blood and biological fluids, as well as examination of skeletal material, hair fiber etc. is performed to provide scientific opinion for legal purposes. This course introduces application of chemistry in forensic science.

Learning Outcomes:

At the end of this course student would be able to:

- Get exposure on the use of forensic science for crime investigation.
- Know the application of chemical analysis in forensic science
- Know about drug abuse and its impact on our society
- Learn how drug related crime can be controlled.

Unit 1

Fundamentals: Definition, History, Development and Scope of Forensic Science, Divisions of Forensic Science and Laboratory set up., Fingerprint Identification – history & development, biological basis of fingerprint, pattern types, scene of crime prints, methods of processing latent/fingerprints, ridge characteristics, comparison of fingerprints for establishing complete identity., Question Documents – definition, handwriting, characteristics, natural variation, comparison and forgery; Forensic Photography – techniques and importance.Tool Marks – their identification and importance in forensic science; Trace Evidence – definition, identification and their importance in forensic science.

(Lectures:12)

Unit 2

Forensic Chemistry - Introduction, Conventional methods of Chemical analysis, Presumptive tests (colour and spot); Drugs of Abuse; Forensic Toxicology – Introduction and classification; Introduction and general methods of chemical analysis for alcohol; Classification of poisons. arson, explosives and gun powder analysis, study of hair and fibers.

(Lectures: 6)

Unit 3

Forensic Serology: Identification and detection of biological fluids (blood, semen, saliva and urine) and their medical importance..narco analysis, brain fingerprinting, and DNA fingerprinting.

(Lectures:6)

Unit 4

Instrumentation: Basic Principles, Theory and Application of Spectroscopy (U.V., I.R., AES, AAS and Mass) and its forensic applications. Electrophoresis (Immuno- and Iso-electrofocussing) theory, principle and techniques, X-Ray (Hard and Soft) techniques and their forensic applications, SEM, and chromatography.

(Lectures:6)

Practical:

(Credits:2, Laboratory periods:60)

Analytical chemistry Lab- Forensic Science

1. Synthesis of nitrocellulose.
2. To perform thin layer chromatography on alkaloids
3. Practical demonstration of procedure of taking fingerprints
   (a) Identification of pattern types
   (b) Developing latent fingerprints
4. Analysis and identification of drugs using UV and IR
   (a) Barbiturates
   (b) Marijuana
5. Disguised and forged question document examination.
6. Spot test for blood identification
7. To perform reinsch test for heavy metals

References:

1. Saferstein, R.,Crimanilistics, Prentice Hall (2004).
2. Sharma, B., R. Forensic science in criminal investigation and trials CLA, Allahabad (2013).

Course Code: Chemistry SEC-3
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:08)**

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, *so*lvent less reactions, solvents obtained from renewable sources.
- Catalysis and green chemistry- comparison of heterogeneous and homogeneous catalysis, bio-catalysis, 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_2 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).

- Preparation and characterization of nanoparticles of gold using tea leaves/ silver nanoparticles using plant extracts.
- Preparation and characterization of biodiesel from vegetable oil preferably waste cooking oil.
- Extraction of D-limonene from orange peel using liquid CO_2 prepared from dry ice.
- Mechanochemical solvent free, solid-solid synthesis of azomethine using p-toluidine and o-vanillin (various other combinations of primary amine and aldehyde can also be tried).
- Solvent free, microwave assisted one pot synthesis of phthalocyanine complex of copper(II).
- 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.
- Use of azomethine for complex formation.
- 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.
3. 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:

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**,4th 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.

Course Code: Chemistry SEC-4
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.
3. 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: Chemistry SEC-5
Course Title: Business Skills for Chemists
Total Credits: 04 **(Total Lectures: 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: Chemistry SEC-6
Course Title: Fuel Chemistry
Total Credits: 04 (Credits: Theory-02, Practicals-02)
(Total Lectures: Theory- 30, Practicals-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 and aniline 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: Chemistry SEC-7
Course Title: Pesticide Chemistry
Total Credits: 04 (Credits: Theory-02, Practicals-02)
(Total Lectures: Theory- 30, Practicals-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:

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, LD_{50} ("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, LD_{50} ("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:

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: Chemistry SEC-8
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 structure-activity 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.
4. 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.

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